Improving the Convergence of Schwarz Methods for Helmholtz Equation

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1 Introduction

Various domain decomposition methods have been proposed for the Helmholtz equation, with the Optimized Schwarz Method (OSM) being one of them (see e.g. [7] 9 for a review of various domain decomposition methods, and [3] for the details of 10 OSM). In this paper, we focus on OSM, which is based on the idea of using approx-11 imated half-space Dirichlet-to-Neumann (DtN) maps to improve the convergence of 12 the Schwarz methods; current version of the OSM is based on polynomial approx-13 imation of the half-space DtN map. See [8] for a review of various approaches to 14 approximating the half-space DtN map (more commonly referred to as Absorbing 15 Boundary Conditions (ABCs)).

There are two approximations in the OSM that affect its convergence rate – the 17 first being the approximation of the rest of the domain as unbounded and the second 18 being the approximation of the half-space stiffness (square-root operator) as a poly-19 nomial. In contrast with the polynomial approximation used in OSM, we utilize the 20 method of Perfectly Matched Discrete Layers (PMDL), which has close links to the 21 well-known Perfectly Matched Layers (PML) (see [1]) and the rational approximation of the square-root operator. The resulting PMDL-Schwarz method is shown to 23 converge faster than the second-order OSM. The rest of the paper contains a brief 24 review of OSM and PMDL concepts, followed by an outline of the new PMDL-25 Schwarz method and illustration of its effectiveness with the help of convergence 26 factor analysis and a numerical example. 27

Model Problem. We consider the governing equation,

$$-\frac{\partial^2 \hat{u}}{\partial x^2} - \frac{\partial^2 \hat{u}}{\partial y^2} - \omega^2 \hat{u} = \hat{f}, \quad (x, y) \in (-\infty, \infty) \times [0, L],$$
(1a)

$$\hat{u}(\cdot,0) = \hat{u}(\cdot,L) = 0. \tag{1b}$$

Applying Fourier Sine transform along the *y* direction, the above equation reduces ²⁹ to a 1-D form: ³⁰

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$$-\frac{\partial^2 u}{\partial x^2} - k^2 u = f, \quad x \in (-\infty, \infty),$$
(2)

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where $k = \sqrt{\omega^2 - k_y^2}$, k_y is the wavenumber along y and u, f are the Fourier sym- 31 bols corresponding to \hat{u} , \hat{f} respectively. For simplicity, we shall use the above 1-D 32 equation to discuss the main ideas in this paper, but note that the proposed method is 33 applicable to more complex equations and geometries. Also, since the focus of this 34 paper is to improve the treatment of the transmission condition at an interface, it is 35 sufficient to consider the case of two subdomains. Thus the domain is decomposed 36 into two subdomains: $\Omega_1 \equiv (-\infty, 0)$ and $\Omega_2 \equiv (0, \infty)$, with the interface at x = 0. 37

2 Optimized Schwarz Methods

Optimized Schwarz Method is a domain decomposition method that is a variant of ³⁹ the Schwarz Alternating Method (see e.g. [7]). In the Schwarz Alternating Method, ⁴⁰ the displacement and traction continuity across the artificial interface are enforced by ⁴¹ applying a mixed boundary condition of the form $\mathscr{B}(\cdot) \equiv \partial(\cdot)/\partial \mathbf{n} + \Lambda(\cdot)$ where **n** is ⁴² the normal vector at the interface and the operator Λ is a parameter of the method. ⁴³ The Schwarz iteration scheme for solving (2) is given by: ⁴⁴

$$-\frac{\partial^2 u_1^{j+1}}{\partial x^2} - k^2 u_1^{j+1} = f_1, \quad x \in \Omega_1, \quad -\frac{\partial^2 u_2^{j+1}}{\partial x^2} - k^2 u_2^{j+1} = f_2, \quad x \in \Omega_2, \quad (3a)$$

$$\mathscr{B}_{1}u_{1}^{j+1} = \mathscr{B}_{1}u_{2}^{j}, \quad x = 0, \qquad \qquad \mathscr{B}_{2}u_{2}^{j+1} = \mathscr{B}_{2}u_{1}^{j+1}, \quad x = 0, \qquad (3b)$$

$$\mathscr{B}_{1}(\cdot) \equiv \frac{\partial(\cdot)}{\partial \mathbf{n}_{1}} + \Lambda_{1}(\cdot), \qquad \qquad \mathscr{B}_{2}(\cdot) \equiv \frac{\partial(\cdot)}{\partial \mathbf{n}_{2}} + \Lambda_{2}(\cdot), \qquad (3c)$$

where the operators $\Lambda_{1,2}$ are the parameters of the iteration that determine the convergence rate. The problem now reduces to choosing the parameters that lead to 46 optimal convergence of the iteration scheme. The parameters are commonly chosen 47 to be scalars but they can be operators that are optimized for convergence [3]. The 48 dependence of the convergence on the choice of parameters is better understood by 49 looking at the convergence factor ρ , which is defined as 50

$$\hat{e}_i^{j+1} = \rho \left| \hat{e}_i^{j} \right|, \tag{4}$$

where $\hat{e}_i^j = |u - u_i^j|$ is the error in the solution in subdomain *i* at iteration *j*. Thus, 51 after one cycle of iteration, the error in solution reduces by ρ and the iterative scheme 52 converges to a solution as long as $\rho < 1$. 53

For the Schwarz method in (3), the convergence factor can be shown to be (see 54 for e.g. [3]) 55

$$\rho = \left| \left(\frac{\Lambda_1 - \mathscr{K}_2}{\Lambda_1 + \mathscr{K}_1} \right) \left(\frac{\Lambda_2 - \mathscr{K}_1}{\Lambda_2 + \mathscr{K}_2} \right) \right|,\tag{5}$$

where \mathcal{K}_1 and \mathcal{K}_2 are the DtN maps of the subdomains Ω_1 and Ω_2 respectively. ⁵⁶ It is clear from (5) that the iterative scheme does not converge (because $\rho = 1$) for ⁵⁷

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a pure Neumann ($\Lambda_i = 0$) or Dirichlet ($\Lambda_i = \infty$) interface condition. Also, if $\Lambda_1 = 58$ \mathscr{K}_2 or $\Lambda_2 = \mathscr{K}_1$, then $\rho = 0$ and the Schwarz iterative scheme converges in two 59 iterations, i.e., the parameters are optimal. However, DtN maps are known only for 60 special cases and even then are usually non-local operators that are expensive to 61 compute accurately. Thus we look for local approximations to these DtN maps that 62 are accurate and computationally efficient. 63

Optimized Schwarz Methods [3] essentially approximate the DtN map of the subdomains by polynomial approximations of the DtN map of an unbounded domain, 65 e.g. the second-order OSM makes the approximation 66

$$\mathscr{K}_{1} = -i\sqrt{\omega^{2} - k_{y}^{2}} \approx p + q k_{y}^{2}, \qquad (6)$$

where p, q are parameters that are found by minimizing the convergence factor over 67 the entire range of allowed vertical wavenumbers k_y . Note that there are other variants 68 of OSM based on zeroth-order approximation; in this paper, we focus on the best 69 available OSM, namely the second-order OSM. 70

3 A Schwarz Method with Improved Convergence

It appears to us that OSM uses polynomial approximation for reasons of implementability. A better approximation would be to use higher order rational approximations, which have been investigated extensively in the context of Absorbing 74 Boundary Conditions (ABCs); it is now possible to implement these resulting ABCs 75 and can also be used in the context of Schwarz methods. In this paper, we propose 76 the use of a rational approximation in a recent ABC called Perfectly Matched Discrete Layers (formerly known as Continued Fraction ABCs – see [4]) instead of the 78 polynomial approximation in (6). 79

The rational approximation corresponding to PMDL is given by:

$$\mathscr{K}_1 = -\mathrm{i}\,\sqrt{\omega^2 - k_y^2} \approx \mathscr{S}_n^{pmdl}\,,\tag{7}$$

where

$$\begin{aligned} \mathscr{S}_{n}^{pmdl} &= p_{n} - \frac{q_{n}^{2}}{p_{n+1} + \frac{q_{n-1}^{2}}{p_{n-1} + \left(p_{n-2} - \frac{q_{n-2}^{2}}{p_{n-2} + (\dots)}\right)}, \end{aligned}$$
(8)
$$\begin{aligned} p_{i} &= \frac{1}{4L_{i}} \left(4 - k^{2}L_{i}^{2}\right) \\ q_{i} &= \frac{1}{4L_{i}} \left(-4 - k^{2}L_{i}^{2}\right) \end{aligned}$$
 $i = 1 \dots n.$ (9)

where L_i are the parameters that determine the accuracy of the approximation. 82

The error in the approximation (7) is typically analyzed through the so-called ⁸³ reflection coefficient, which has been shown to be (for details, see [4]) ⁸⁴

$$R = \prod_{i=1}^{n} \left| \frac{\mathscr{K}_1 - p_i}{\mathscr{K}_1 + p_i} \right|^2.$$
(10)

If R = 0, then the approximation is exact, and the deviation from zero indicates magnitude of error in the approximation; smaller the value of R, better the approximation. So from (10) and (9), it is clear that the accuracy of proposed approximation hinges on the choice of L_i .

In general, L_i are chosen to be complex or imaginary to better approximate the ⁸⁹ DtN map for propagating wave modes and are chosen to be real when evanescent ⁹⁰ modes are important. While the parameters L_i can be optimized using the concepts ⁹¹ discussed in [5], in this paper we choose L_i based on the OSM parameters (see ⁹² Sect. 4). ⁹³

Implementation of PMDL. While the rational form of the PMDL approximation in (8) is useful for analysis, the following matrix form proves to be useful for 95 implementation: 96

$$\begin{bmatrix} \mathscr{S}_{n}^{pmdl} u_{b} \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \begin{bmatrix} p_{1} & q_{1} & 0 & \cdots & 0 \\ q_{1} & p_{1} + p_{2} & q_{2} & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & q_{n-1} & p_{n-1} + p_{n} & q_{n} \\ 0 & \cdots & 0 & q_{n} & p_{n} \end{bmatrix} \begin{bmatrix} u_{b} \\ u_{a,1} \\ u_{a,2} \\ \vdots \\ u_{a,n-1} \end{bmatrix}, \quad (11)$$

where p_i, q_i are given by (9) and $u_{a,i}$ are auxiliary variables that are introduced to 97 facilitate the implementation and have no direct physical relevance to the problem. 98 The equivalence between (8) and (11) can be easily seen by eliminating the auxil-99 iary dof $u_{a,i}$ from (11) to recover (8). The matrix form of PMDL enables an easy 100 implementation of the rational approximation as a simple tri-diagonal matrix. 101

PMDL, a link between Rational ABCs and Perfectly Matched Layers. While102the matrix form of the PMDL approximation in (11) is based on the rational approx-103imation in (8), it is intimately linked to impedance-preserving discretization of PML104proposed in [4]. Unlike PML, the impedance is preserved even after discretization105and thus the approximation is named perfectly matched discrete layers, PMDL. This106link is substantial in that it provides a way to derive and easily implement PMDL approximations for more complex cases such as corners [4] and anisotropic elasticity108[6].109

The ease of implementation of PMDL is in fact the impetus behind proposed 110 method. As implied by (10), the accuracy of approximation can be easily increased 111 by adding auxiliary variables, which is equivalent to adding lines of nodes parallel 112 to the interface. As will be shown in Sect. 4, addition of just one auxiliary variable, 113 which has minimal increase in computational cost per iteration, significantly reduces 114 the convergence factor and the number of iterations needed. 115

(12)

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Implementation of the PMDL-Schwarz method. The proposed 116 PMDL-Schwarz method is essentially the Schwarz Alternating method with the 117 operator Λ_1 chosen to be the DtN map obtained using PMDL, i.e., $\Lambda_1 = \mathcal{S}_n^{pmdl}$ 118 where \mathcal{S}_n^{pmdl} is given by (11). Thus the interface condition in (3) for Ω_1 can be 119 written as 120

$$\frac{\partial}{\partial \mathbf{n_1}}(u_1^{j+1} - u_2^j) + \mathscr{S}_n^{pmdl}(u_1^{j+1} - u_2^j) = 0.$$

Substituting (11) in (12), we get the PMDL-Schwarz formulation as

$$\begin{bmatrix} \frac{\partial u_{1}^{j+1}}{\partial \mathbf{n}_{1}} \\ 0 \\ \vdots \\ 0 \end{bmatrix} + \begin{bmatrix} p_{1} & q_{1} & 0 & \cdots & 0 \\ q_{1} & p_{1} + p_{2} & q_{2} & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & q_{n-1} & p_{n-1} + p_{n} & q_{n} \\ 0 & \cdots & 0 & q_{n} & p_{n} \end{bmatrix} \begin{bmatrix} u_{1}^{j+1} \\ u_{a,1} \\ u_{a,2} \\ \vdots \\ u_{a,n-1} \end{bmatrix} = \begin{bmatrix} -\frac{\partial u_{2}^{j}}{\partial \mathbf{n}_{2}} + p_{1} u_{2}^{j} \\ q_{1} u_{2}^{j} \\ 0 \\ \vdots \\ 0 \end{bmatrix} .$$

$$(13)$$

Note that the formulation of the interface condition for Ω_2 can be derived in an 122 identical manner and hence is not repeated here. 123

4 Comparison Between OSM and PMDL-Schwarz Methods 124

In this section, we compare the performance of OSM and PMDL-Schwarz method 125 both theoretically (using convergence factors) and in a numerical simulation involving multiple domains and closed boundaries. 127

Convergence Factors: Consider the stiffness approximation of the second-order 128 OSM (see [3]), 129

$$\mathscr{S}_{osm} = \frac{ab - \omega^2}{a + b} + \frac{1}{a + b}k_y^2. \tag{14}$$

Substituting $\Lambda_1 = \Lambda_2 = \mathscr{S}_{osm}$ in (5), we get the convergence factor of OSM to be 130

$$\rho_{osm} = \left| \frac{ab + k_y^2 - \omega^2 + i(a+b)\sqrt{\omega^2 - k_y^2}}{ab + k_y^2 - \omega^2 - i(a+b)\sqrt{\omega^2 - k_y^2}} \right|^2$$

To compare, we use a two-layer PMDL-Schwarz method with $L_1 = 2/a$, and 131 $L_2 = 2/b$, where a, b are the OSM parameters in (14). The stiffness approximation 132 of the two-layer PMDL-Schwarz method is then given by 133

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$$\begin{aligned} \mathscr{S}_{n}^{pmdl} &= p_{2} - \frac{q_{2}^{2}}{p_{2} + p_{1}}, \\ p_{2} &= \frac{1}{L_{2}} - \frac{(\omega^{2} - k_{y}^{2})L_{2}}{4}, \quad q_{2} = -\frac{1}{L_{2}} - \frac{(\omega^{2} - k_{y}^{2})L_{2}}{4} \\ p_{1} &= \frac{1}{L_{1}} - \frac{(\omega^{2} - k_{y}^{2})L_{1}}{4}. \end{aligned}$$

Substituting $\Lambda_1 = \Lambda_2 = \mathscr{S}_n^{pmdl}$ in (5), we get the convergence factor of PMDL 134 Schwarz that can be simplified to 135

$$\rho_{pmdl} = \left(\left| \frac{ab + k_y^2 - \omega^2 + i(a+b)\sqrt{\omega^2 - k_y^2}}{ab + k_y^2 - \omega^2 - i(a+b)\sqrt{\omega^2 - k_y^2}} \right|^2 \right)^2.$$

Clearly $\rho_{pmdl} = \rho_{osm}^2$, and so the parameters of PMDL-Schwarz are chosen such 136 that its convergence factor is the square of that of OSM and the method performs 137 uniformly better over the entire range of wavenumbers k_{y} . 138

It is easy to numerically verify the above result for the model problem (1a), with 139 the domain Ω decomposed into two semi-infinite layers. We take a = 20.741 i and 140 b = 47.071 to be the OSM parameters as these were shown in [3] to be optimal 141 over the allowed wavenumber range $k_v \in [\pi, 60\pi]$. Figure 1a compares the conver- 142 gence factors of OSM and PMDL-Schwarz method (with $L_1 = 2/a$ and $L_2 = 2/b$) 143 and shows clearly that the proposed method performs better over the entire range of 144 wavenumbers for a slightly increased computational cost (there is only one auxiliary 145 variable introduced, which is similar to one line of nodes in 2-D).



Fig. 1. Comparison between OSM (dotted line) and PMDL-Schwarz method (solid line). (a) Convergence Factor. (b) Convergence of Solution

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Numerical Example: In this example, Eq. (1a) is solved on a square domain 147 $(\Omega \equiv [0,1] \times [0,1])$ with $\omega = 10\pi$ and a point source f = 1/2 is applied at (0,0.5). 148 Homogeneous Neumann boundary condition is applied on the left (x = 0), Dirichlet 149 condition at the top (y = 1) and bottom (y = 0), and an ABC on the right (x = 1). 150 The computational domain is discretized using 60 bilinear finite elements along each 151 direction. The domain is decomposed into nine subdomains with three subdomains 152 along each dimension. The convergence plot is shown in Fig. 1b. As expected, the 153 PMDL-Schwarz method converges twice as fast as the conventional OSM. 154

5 Discussion

We proposed a Schwarz method for Helmholtz equation based on the concepts of 156 perfectly matched discrete layers (PMDL), a recently developed absorbing boundary 157 condition that is related to the higher order rational approximations and the Per- 158 fectly Matched Layers. By examining the convergence factor and with the help of a 159 numerical example, PMDL-Schwarz method is shown to converge faster than exist- 160 ing Optimized Schwarz Methods. Although not treated in this paper, it is important 161 to mention that the PMDL is not just limited to the Helmholtz equation, but also 162 to more complicated vector equations such as the elastic and electromagnetic wave 163 equations. Thus, it is expected that the PMDL-Schwarz method would provide ac- 164 celerated convergence in frequency domain computations in these contexts. Further- 165 more, as Waveform Relaxation Method in time domain share similar ideas with OSM 166 (see e.g. [2]), PMDL ideas can also be used to improve the convergence of existing 167 waveform relaxation methods. These extensions are subjects of ongoing research. 168

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