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A Three-Level Extension of the GDSW Overlapping Schwarz Preconditioner in Three Dimensions

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1 The Standard GDSW Preconditioner

The GDSW (Generalized Dryja–Smith–Widlund) preconditioner is a two-level overlapping Schwarz domain decomposition preconditioner [23] with exact local solvers [5, 4]. The GDSW preconditioner can be written in the form

$$M_{\text{GDSW}}^{-1} = \underbrace{\Phi K_0^{-1} \Phi^T}_{\text{Coarse Level}} + \underbrace{\sum_{i=1}^{N} R_i^T K_i^{-1} R_i}_{\text{First Level}}, \tag{1}$$

where $K_0 = \Phi^T K \Phi$ is the coarse matrix and the $K_i = R_i K R_i^T$, $i = 1, ..., N$, correspond to the local overlapping subdomain problems. By $V_1, \ldots, V_N$, we denote the local subspaces corresponding to the overlapping subdomains, and V^0 denotes the corresponding coarse space. The restriction operators on the subdomain level are defined as $R_i : V^h(\Omega) \to V_i := V^h(\Omega_i')$ for $i = 1, \ldots, N$. The columns of the matrix Φ correspond to the coarse basis function which are chosen to to be discrete harmonic extension from the interface of the nonoverlapping decomposition to the interior degrees of freedom. The interface values are restrictions of the elements of the null space of the operator to the edges, vertices, and faces. For linear elliptic problems, the condition number of the Schwarz operator is bounded by

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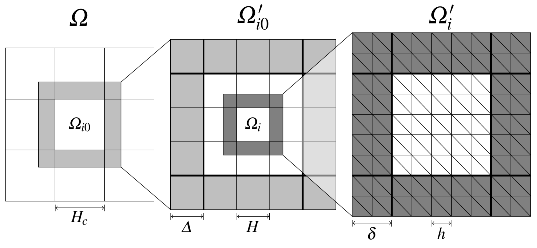


Fig. 1 Structured decomposition of an exemplary two-dimensional computational domain Ω into nonoverlapping subregions Ω_{i0} (left), a zoom into one overlapping subregion Ω'_{i0} consisting of subdomains Ω_i (middle), and a zoom into one overlapping subdomain Ω'_i (right). Each level of zoom corresponds to one level of the preconditioner; image taken from [13].

$$\kappa(M_{\text{GDSW}}^{-1}K) \leq C\left(1+\frac{H}{\delta}\right)\left(1+\log\left(\frac{H}{h}\right)\right)^2, \tag{2}$$

where h is the size of a finite element, H the size of a nonoverlapping subdomain, and δ the width of the overlap; see [4, 5, 6]. An important advantage of the GDSW preconditioner is that it can be constructed in an algebraic fashion from the fully assembled matrix K and without the need of an additional coarse triangulation. This will also facilitate the construction of the three-level GDSW preconditioner presented in the following section.

2 The Three-Level GDSW Preconditioner

If a direct solver is used for the solution of the coarse problem in (1), this can become a bottleneck for a large number of subdomains; cf. [11, 9]. As a remedy, in this paper, we apply the GDSW preconditioner recursively to the coarse problem, resulting in a three-level extension of the GDSW preconditioner; see [13] for the corresponding algorithm in two dimensions. Our three-level GDSW method is related to the three-level BDDC method [24]. A further recursive application of the preconditioner, resulting in a multilevel extension similar to multi-level BDDC methods [18, 2, 16], multilevel Schwarz methods [17, 21], or multigrid methods [8], is algorithmically straightforward but out of the scope of this paper. The scalability of the two-level method can also be improved by reducing the size of the GDSW coarse space; cf. [14, 7]. Here, instead of using coarse basis functions corresponding to subdomain edges, vertices, and, faces, new basis functions are constructed, e.g., corresponding only to the vertices. In this paper, we will construct three-level GDSW methods using standard as well as reduced dimension coarse spaces.

To define the three-level GDSW preconditioner, we decompose the domain Ω into nonoverlapping subregions Ω_{i0} of diameter H_c; see [24] and Figure 1 for a graphical representation of the decomposition Ω in two dimensions. Each subregion is decomposed into nonoverlapping subdomains of diameter H. Extending each subregion Ω_{i0} to Ω'_{i0} by recursively adding layers of subdomains, an overlapping decomposition into subregions is obtained. The overlap on subregion level is denoted by Δ; the overlap on the subdomain level is denoted by δ, consistent with the notation of the two-level method; see Figure 1.

The three-level GDSW preconditioner then is defined as

$$M_{3GDSW}^{-1} = \underbrace{\Phi\Big(\overbrace{\Phi_0 K_{00}^{-1}\Phi_0^T}^{\text{Third Level}} + \overbrace{\sum_{i=1}^{N_0} R_{i0}^T K_{i0}^{-1} R_{i0}}^{\text{Second Level}}\Big)\Phi^T}_{\text{Coarse Levels}} + \underbrace{\sum_{j=1}^{N} R_j^T K_j^{-1} R_j}_{\text{First Level}}, \tag{3}$$

where $K_{00} = \Phi_0^T K_0 \Phi_0$ and $K_{i0} = R_{i0} K_0 R_{i0}^T$. On the subregion level, we define the restriction operators to the overlapping subregions Ω'_{i0} as $R_{i0} : V^0 \to V_i^0 := V^0(\Omega'_{i0})$ for $i = 1, ..., N_0$. The respective coarse space is denoted as V_{00} and spanned by the coarse basis functions Φ_0.

3 Implementation and Software Libraries

The parallel three-level GDSW implementation discussed in this paper is based on [9, 11, 12] and uses the Trilinos Epetra linear algebra package. A recent Xpetra version (FROSch - Fast and Robust Overlapping Schwarz framework [10]) is now part of the Trilinos [15] package ShyLU [19].

To test our three-level GDSW implementation, we consider the Poisson problem on the unit cube $[0,1]^3$ with homogenous Dirichlet boundary conditions on $\partial\Omega$. We use structured domain decompositions into subregions and subdomains; see Figure 1 for a representation of the two-dimensional case. Our model problem is discretized using piecewise linear finite elements. As a default Krylov method, we apply the GMRES method provided by the Trilinos package Belos [3]. Trilinos version 12.11 (Dev) is used; cf. [15].

All numerical experiments were carried out on the JUQUEEN supercomputer at JSC Julich. We use the IBM XL C/C++ compiler for Blue Gene V.12.1, and Trilinos is linked to the ESSL.

To solve the overlapping subdomain and subregion problems and the coarse problem, we always use MUMPS 4.10.0 [1] in symmetric, sequential mode, and interfaced through the Trilinos package Amesos [20]. For our experiments, we always have a one-to-one correspondence of subdomains and processor cores. We use the relative stopping criterion $\|r^k\|_2/\|r^0\|_2 \leq 10^{-6}$. Moreover, we assume that we have a fast and scalable method to identify interface degrees of freedom. This cost is therefore neglected in this paper.

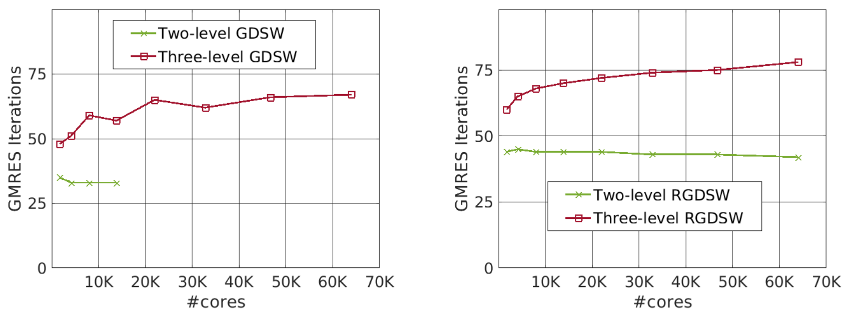


Fig. 2 Weak numerical scalability of the two- and three-level GDSW (left) and the RGDSW (right) preconditioner. All methods are numerically scalable; see Table 1 for the corresponding data.

3.1 Weak Parallel Scalability of the Three-Level GDSW Preconditioner

In this section, we focus on the weak scalability of our preconditioners. For the numerical scalability of the three-level GDSW preconditioner in two dimensions, more detailed numerical results can be found in [13]. We also compare results for the two and three-level methods using the standard coarse space (denoted by GDSW) and the reduced dimension coarse space (denoted by RGDSW). In particular, we use *Option 1*, which is the completely algebraic variant of the RGDSW coarse space; cf. [7] or [14], respectively.

The number of Krylov iterations is presented in Figure 2 and Table 1. Note that the standard two-level GDSW method fails for more than 13 824 cores since the coarse problem could not be factored any more due to memory limits. All other methods show numerical scalability for up to 64 000 cores. This includes the two-level RDSW method, which is a remarkable result since RGDSW coarse space is smaller (see also Table 2) but the coarse matrix K_0 is, however, more dense; cf. also [14].

Our results show, that the numerical scalability of both two-level methods is slightly better; cf. Figure 2 and Table 1. Moreover, the number of iterations is higher by almost a factor of two for both three-level methods; this is, however, not surprising since the direct coarse solver is replaced by a (two-level) preconditioner.

Let us now consider the computing times, which are more favorable for the three-level methods; see Figure 3 and Table 1. By *Solver Time*, we denote the time to solution, which is the sum of the time for the setup of the preconditioner, denoted *Setup Time*, and the time for the Krylov iteration, which we denote *Krylov Time*. The *Setup Time* includes the factorizations of the matrices on the different levels using the MUMPS sparse direct solver.

For the standard GDSW coarse space, the three-level method is faster than the two-level methods for 4 096 cores and more; see Figure 2 and Table 1. The two-level

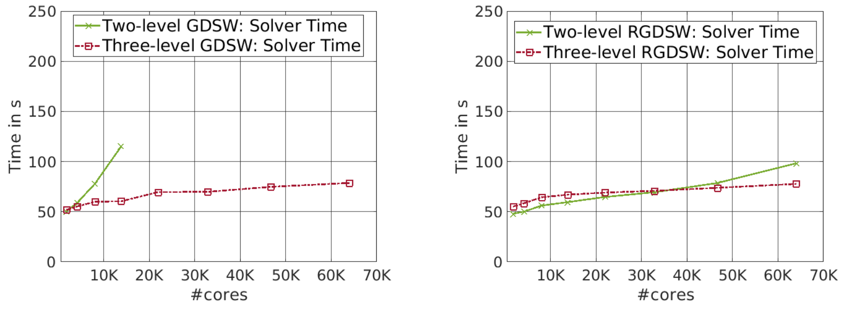


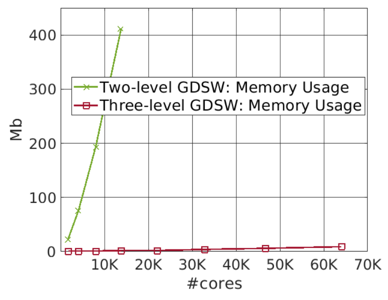
Fig. 3 Weak parallel scalability of the two- and three-level methods using the standard (left) and the reduced coarse space (right); see Table 1 for the data.

#Sub-	Two-level GDSW				Three-level GDSW				Two-level RGDSW				Three-level RGDSW			
domains	Iter	Solver	Setup	Krylov	Iter	Solver	Setup	Krylov	Iter	Solver	Setup	Krylov	Iter	Solver	Setup	Krylov
= #cores		Time	Time	Time		Time	Time	Time		Time	Time	Time		Time	Time	Time
1 728	35	50.2 s	30.9 s	19.4 s	48	51.8 s	28.3 s	23.4 s	44	**47.9 s**	26.9 s	21.1 s	60	55.2 s	26.2 s	28.9 s
4 096	33	58.7 s	35.5 s	23.2 s	51	55.1 s	30.1 s	25.0 s	45	**50.0 s**	27.6 s	22.4 s	65	58.3 s	26.7 s	31.6 s
8 000	33	77.7 s	46.3 s	31.4 s	59	60.0 s	30.2 s	29.8 s	44	**56.1 s**	32.3 s	23.8 s	68	64.4 s	30.8 s	33.7 s
13 824	33	115.2 s	69.1 s	46.0 s	57	60.4 s	31.3 s	29.1 s	44	**59.6 s**	33.3 s	26.3 s	70	67.0 s	31.9 s	35.1 s
21 952	—	—	—	—	65	69.5 s	35.0 s	34.6 s	44	**64.7 s**	34.6s	30.1 s	72	69.0 s	32.1 s	36.9 s
32 768	—	—	—	—	62	69.8 s	36.2 s	33.6 s	43	**69.4 s**	35.2 s	34.2 s	74	70.8 s	32.6 s	38.2 s
46 656	—	—	—	—	66	74.8 s	37.1 s	37.6 s	43	78.6 s	37.2 s	41.4 s	75	**73.8 s**	33.7 s	40.2 s
64 000	—	—	—	—	67	78.7 s	38.5 s	40.2 s	42	98.3 s	50.2 s	48.1 s	78	**77.7 s**	34.8 s	42.9 s

Table 1 By *Iter*, we denote number of Krylov iterations. The *Solver Time* is the sum of the *Setup Time* and *Krylov Time*. We have $H/h = 30$, $H/\delta = 15$, $H_c/H = 4$, and $H_c/\Delta = 4$. Also see Figure 2 and Figure 3. The fastest *Solver Time* is printed in bold.

#Subdomains = #Cores	Size of K_0	Factorization Time	Forward-Backward	Memory Usage	Size of K_{00}	Factorization Time	Forward-Backward	Memory Usage
	Two-level GDSW				Three-level GDSW			
1 728	10 439	1.28 s	2.08 s	23 Mb	98	<0.01 s	0.03 s	1 Mb
4 096	25 695	4.43 s	5.17 s	76 Mb	279	0.01 s	0.09 s	1 Mb
8 000	51 319	11.25 s	11.31 s	193 Mb	604	0.02 s	0.21 s	1 Mb
13 824	89 999	29.58 s	20.46 s	412 Mb	1 115	0.04 s	0.35 s	2 Mb
21 952		—	—	—	1 854	0.09 s	0.68 s	2 Mb
32 768		—	—	—	2 863	0.15 s	0.99 s	4 Mb
46 656		—	—	—	4 184	0.25 s	1.55 s	6 Mb
64 000		—	—	—	5 589	0.40 s	2.28 s	9 Mb
	Two-level RGDSW				Three-level RGDSW			
1 728	1 331	0.06 s	0.3 s	3 Mb	8	<0.01 s	0.01 s	1 Mb
4 096	3 375	0.25 s	0.87 s	8 Mb	27	<0.01 s	0.02 s	1 Mb
8 000	6 859	0.74 s	1.73 s	20 Mb	64	<0.01 s	0.03 s	1 Mb
13 824	12 167	1.81 s	3.02 s	37 Mb	125	<0.01 s	0.05 s	1 Mb
21 952	19 683	3.66 s	5.31 s	71 Mb	216	<0.01 s	0.08 s	1 Mb
32 768	29 791	6.15 s	8.25 s	122 Mb	343	0.01 s	0.13 s	1 Mb
46 656	42 875	10.39 s	12.53 s	198 Mb	512	0.02 s	0.19 s	1 Mb
64 000	59 319	16.80 s	16.96 s	313 Mb	729	0.03 s	0.27 s	2 Mb

Table 2 Costs for solving the problem on the coarsest level, i.e., using K_0 in the standard two-level GDSW and RGDSW preconditioner and using K_{00} in the three-level GDSW and RGDSW preconditioner. Here, *Factorization Time* is the time Amesos reports for the MUMPS sparse direct solver for the sum of symbolic and numerical factorization of K_0 and K_{00}, respectively; *Forward-Backward* is the sum of all times spent in forward-backward substitutions during the Krylov iteration; *Memory Usage* is the estimated amount of memory allocated by MUMPS during the factorization. See Table 1 for the corresponding *Solver Time*, *Setup Time* and *Krylov Time*. Also see Figures 5, 4.



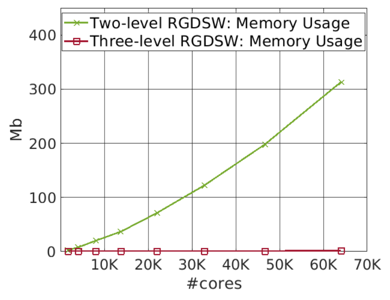
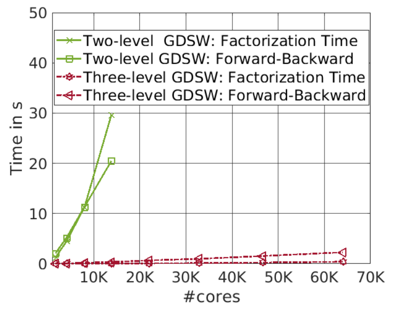


Fig. 4 Memory usage of the MUMPS direct solver for the factorization of the coarse matrix K_0 and K_{00} for the two-level and three-level GDSW method using the standard (left) and reduced coarse space (right); see Table 2 for the corresponding data.

RGDSW method is consistently the fastest method from 1 728 to to 32 768 cores. However, for 46 656 and 64 000 cores, the three-level method is faster.

For the largest problem with 1.72 billion degrees of freedom, the *Solver Time* for three-level RGDSW precondtioner (77.7s *Solver Time*) more than 20% faster than two-level RGDSW preconditioner (98.3s *Solver Time*) and also slightly faster than the three-level GDSW preconditioner (78.7s *Solver Time*). However, considering the size of K_0, we expect the two-level RGDSW to fail beyond 100 000 cores while both three-level methods will continue to scale; also cf. the memory usage for the factorazation of K_{00} in Figure 4 and Table 2.



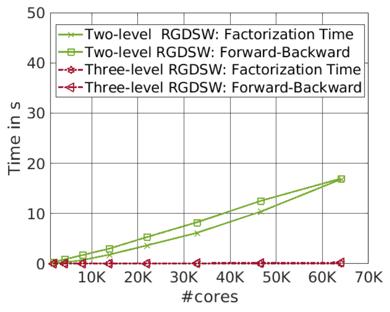


Fig. 5 Computing time for solving the problem on the coarsest level, i.e., using K_0 in the standard two-level method preconditioner ans using K_{00} for the three-level GDSW preconditioner using the standard coarse space (left) and respectively the reduced coarse space (right). See Table 2 for the corresponding data.

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