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Alexander Heinlein, Axel Klawonn, and Oliver Rheinbach

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Fakultät für Mathematik und Informatik

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09599 FREIBERG

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Parallel Overlapping Schwarz with an Energy-Minimizing Coarse Space

Alexander Heinlein[1], Axel Klawonn[1], and Oliver Rheinbach[2]

1 Introduction and Description of the Method

The GDSW preconditioner is a two-level overlapping Schwarz preconditioner introduced in Dohrmann et al. [2008a] with a proven condition number bound for the general case of John domains for scalar elliptic and linear elasticity model problems. It is algebraic in the sense that it can be constructed from the assembled system matrix. However, compared to FETI-DP (see Toselli and Widlund [2005]) or BDDC methods, in GDSW the standard coarse space is relatively large, especially in three dimensions. In Dohrmann and Widlund [2010], a related hybrid preconditioner with a reduced coarse problem for three-dimensional elasticity was introduced. Here, the degrees of freedom (d.o.f.) corresponding to the faces are modified.

The GDSW preconditioner is a two-level additive overlapping Schwarz preconditioner with exact local solvers; cf. Toselli and Widlund [2005]. It can be written as

$$M_{\mathrm{GDSW}}^{-1} = \Phi \left(\Phi^T A \Phi\right)^{-1} \Phi^T + \sum_{i=1}^{N} R_i^T \tilde{A}_i^{-1} R_i, \tag{1}$$

cf. Dohrmann et al. [2008b]. The matrix Φ is the essential ingredient of the GDSW preconditioner. It is composed of coarse space functions which are discrete harmonic extensions from the interface to the interior degrees of freedom of nonoverlapping subdomains. The values on the interface are restrictions of the nullspaces of the operator to the interface.

[1]Mathematisches Institut, Universität zu Köln, Weyertal 86-90, 50931 Köln, Germany. e-mail: {alexander.heinlein,axel.klawonn}@uni-koeln.de

[2] Institut für Numerische Mathematik und Optimierung, Fakultät für Mathematik und Informatik, Technische Universität Bergakademie Freiberg, Akademiestr. 6, 09596 Freiberg, Germany. e-mail: oliver.rheinbach@math.tu-freiberg.de

For $\Omega \subset \mathbb{R}^2$ being decomposed into John domains, the condition number of the GDSW preconditioner is bounded by

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

cf. Dohrmann et al. [2008a,b]. Here, H is the size of a subdomain, h is the size of a finite element, and δ is the overlap.

Implementation Our parallel implementation of the GDSW preconditioner is based on Trilinos version 12.0; cf. Heroux et al. [2005]. For the mesh partitioning, we use ParMETIS by Karypis et al. [2011], the problems corresponding to the first level are solved using UMFPACK by Davis and Duff [1997] (version 5.3.0), and the coarse level is solved using Mumps by Amestoy et al. [2001] (version 4.10.0) in parallel mode. For the finite element implementation, we use the library LifeV; see Formaggia et al. [2002-2004] (version 3.8.8).

On the JUQUEEN BG/Q supercomputer at JSC Jülich, we use the clang compiler 4.7.2 and the Engineering and Scientific Subroutine Library 5.1 (ESSL) for the compilation of Trilinos and the GDSW preconditioner implementation. On the Cray XT6m at the University of Duisburg-Essen, we use the Intel compiler 11.1 and the Cray Scientific Library (libsci) 10.4.4.

2 Model Problems

For the tests of our GDSW implementation, we consider model problems in two and three dimensions. The domain Ω is the unit square $[0,1]^2$ or cube $[0,1]^3$. The domain is decomposed either in a structured way, i.e., into squares, or in an unstructured way, using the ParMETIS mesh partitioner.

Laplacian in 2D The first model problem is: find $u \in H^1(\Omega)$

$$\begin{aligned} -\Delta u &= 1 \qquad \text{in } \Omega, \\ u &= 0 \qquad \text{on } \partial\Omega. \end{aligned} \tag{3}$$

Linear Elasticity in 2D The second model problem is: find $u \in (H^1(\Omega))^2$;

$$\begin{aligned} \operatorname{div}\boldsymbol{\sigma} &= f \qquad \text{in } \Omega, \\ \mathbf{u} &= 0 \qquad \text{on } \partial\Omega_D \end{aligned} \tag{4}$$

with the right hand side $f = [0.1, 0]^T$, and the Lamé parameters $\lambda = 1/2.6$ and $\mu = 0.3/0.52$. In addition, $\partial\Omega_D = \partial\Omega \cap \{x = 0\}$.

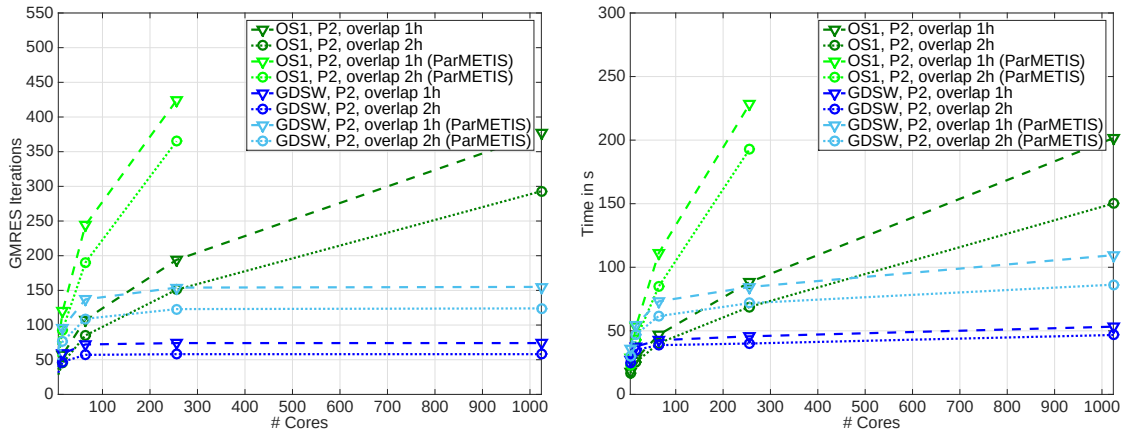

Fig. 1 Weak scaling for the Laplacian model problem in 2D, cf. (3), using P2 finite elements: number of iterations (left), runtimes (right). For the structured and the unstructured decomposition (ParMETIS), we have approximately 40 000 d.o.f. per subdomain.

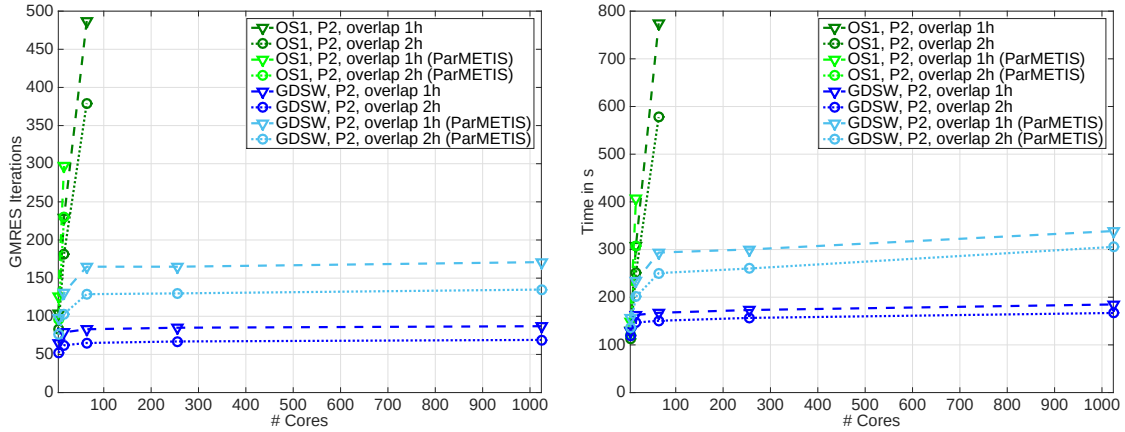

Fig. 2 Weak scaling for the linear elastic model problem in 2D, cf. (4), using P2 finite elements: number of iterations (left), runtimes (right). For the structured and the unstructured decomposition (ParMETIS), we have approximately 80 000 d.o.f. per subdomain.

3 Numerical Results

We first show parallel scalability results in two and three dimensions. Finally, we show an application of the preconditioner within a block preconditioner in monolithic fluid-structure interaction.

The model problems are discretized using piecewise quadratic (P2) finite elements. Our default Krylov method is GMRES and will be used also for the symmetric positive definite model problems. Our stopping criterion is the relative criterion $\left\|r^{(k)}\right\|_2 / \left\|r^{(0)}\right\|_2 \leq 10^{-7}$ with $r^{(0)}$ and $r^{(k)}$ being the initial and the k-th residual, respectively. In our experiments, each subdomain is assigned to one processor core.

Weak Scalability in 2D We use five different meshes with $H/h = 100$ and an increasing number of subdomains; see Tables 1 and 2. The results of weak scaling tests from 4 to 1 024 processor cores for both model problems

# Subdomains	4	16	64	256	1024
Total problem, P2 finite elements	160 801	641 601	2 563 201	10 246 401	40 972 801
Avg. first level, P2, overlap 1h	41 207.5	41 612.6	41 815.7	41 917.3	41 968.1
Avg. first level, P2, overlap 2h	42 020	42 837.8	43 248.7	43 454.7	43 557.8
Coarse level	5	33	161	705	2 945
Avg. first level, P2, overlap 1h (ParMETIS)	41 581.5	41 841.9	42 101.8	42 225.7	42 263.1
Avg. first level, P2, overlap 2h (ParMETIS)	42 686.5	43 243.7	43 752.9	43 999.4	44 077.9
Coarse level (ParMETIS)	3	45	241	1 129	4 822

Table 1 Number of degrees of freedom of the total mesh, coarse and local space dimensions of the GDSW preconditioner for the weak scaling tests in Fig. 1.

# Subdomains	4	16	64	256	1024
Total problem, P2	321 602	1 286 408	5 126 402	20 492 802	81 945 602
Avg. first level, P2, overlap 1h	82 415	83 225.2	83 631.3	83 834.6	83 936.3
Avg. first level, P2, overlap 2h	84 040	85 675.5	86 497.4	86 909.3	87 115.6
Coarse level	14	90	434	1 890	7 874
Coarse level, no rotations	10	66	322	1 410	5 890
Avg. first level, P2, overlap 1h (ParMETIS)	83 163	83 683.9	84 203.6	84 451.3	84 526.2
Avg. first level, P2, overlap 2h (ParMETIS)	85 373	86 487.4	87 505.8	87 998.7	88 155.9
Coarse level (ParMETIS)	9	120	633	2 950	12 567
Coarse level, no rotations (ParMETIS)	6	90	482	2 258	9 644

Table 2 Number of degrees of freedom of the total mesh, coarse and local space dimensions of the GDSW preconditioner for the weak scaling tests in Fig. 2 and Fig. 3.

and an overlap $\delta = 1h$ or $\delta = 2h$ are presented in Fig. 1 and 2. The GDSW preconditioner is numerically and parallel scalable, i.e., the number of iterations is bounded, both, for structured and unstructured decompositions, and the time to solution grows only slowly. The one-level preconditioner (OS1) does not scale numerically, and the number of iterations grows very fast. Indeed, for the unstructured decomposition, no convergence is obtained for OS1 within 500 iterations for more than 256 subdomains for the scalar problem and for more that 16 subdomains for elasticity. This is, of course, also due to the comparably small overlap. As a result of the better constant in (2), for the GDSW preconditioner, we observe better convergence for structured decompositions. Note that for the case of four subdomains the overlapping subdomains are significantly smaller.

A detailed analysis of different phases of the method is presented for linear elasticity in 2D in Fig. 3. We consider the standard full GDSW coarse space and the GDSW coarse space without rotations, i.e., the rotations are omitted from the coarse space. This latter case is not covered by the bound (2), but the results indicate numerical and parallel scalability.

Strong Scalability in 2D Results for strong parallel scaling tests are shown in Fig. 4 for linear elasticity in 2D. We observe very good strong scalability for structured and unstructured domain decompositions. Note that the number of d.o.f. per subdomain decreases when increasing the number of processor cores, and, to a certain extend, we thus benefit from an increasing speed of the local sparse direct solvers.

Weak Scalability for Linear Elasticity in 3D We present results of weak scalability runs for a linear elastic model problem in 3D from 8 to 4 096 cores.

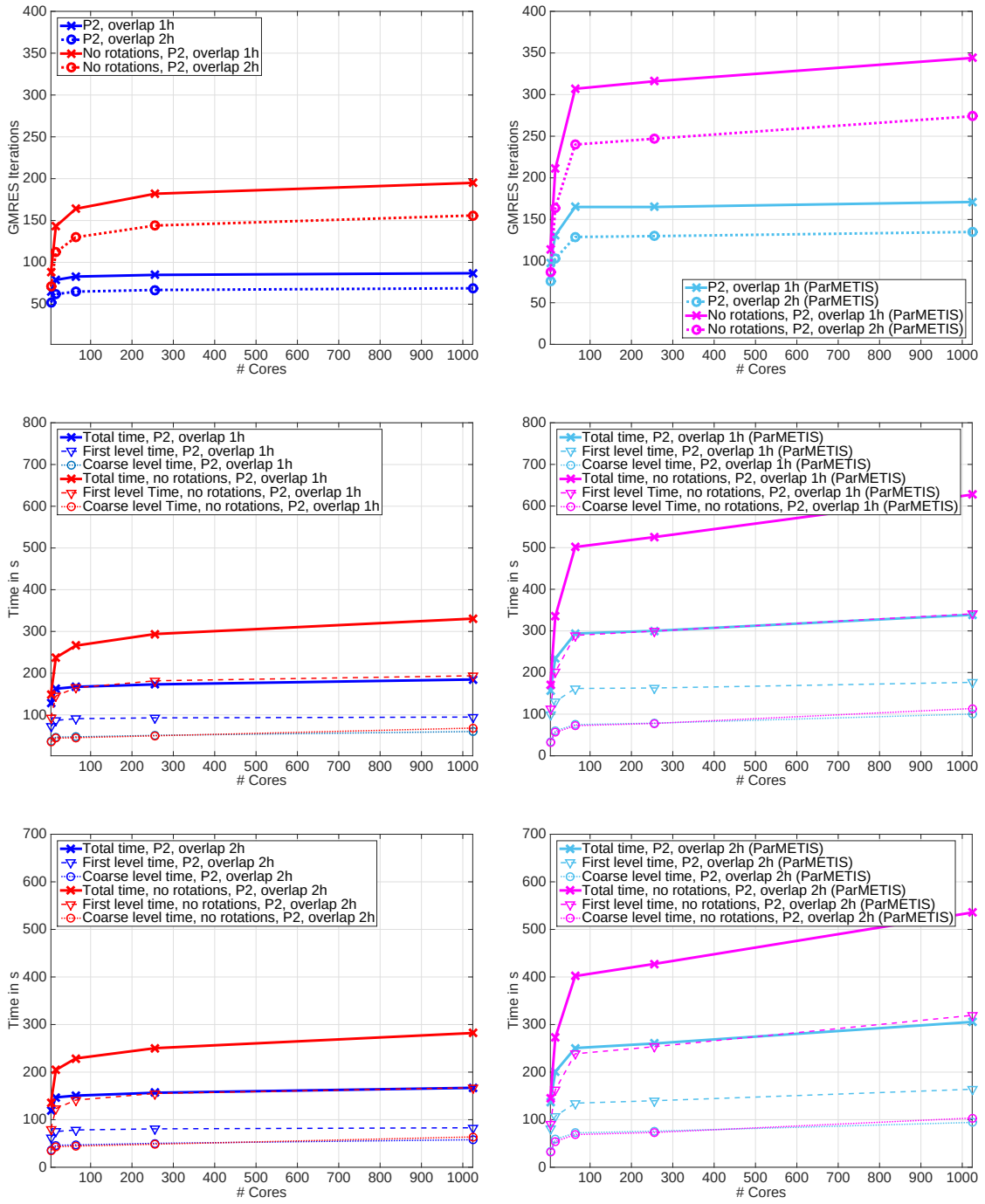

Fig. 3 Weak parallel scalability using the GDSW preconditioner for the model problem of linear elasticity in 2D, cf. (4): structured (left) and unstructured decomposition (right); number of iterations (top), timings for overlap $\delta = 1h$ (middle), and timings for overlap $\delta = 2h$ (bottom). For the structured and the unstructured decomposition (ParMETIS) we use a subdomain size of roughly 40 000 degrees of freedom.

We consider a structured decomposition of a cube and use the full GDSW coarse space in 3D. In Fig. 5, we present the number of iterations and the timings using P2 elements using an overlap δ of one or two elements. The number of iterations seems to be bounded by a constant number, whereas the solution times increases, i.e., the cost of the (parallel) sparse direct solver used for the coarse problem is noticeable in 3D.

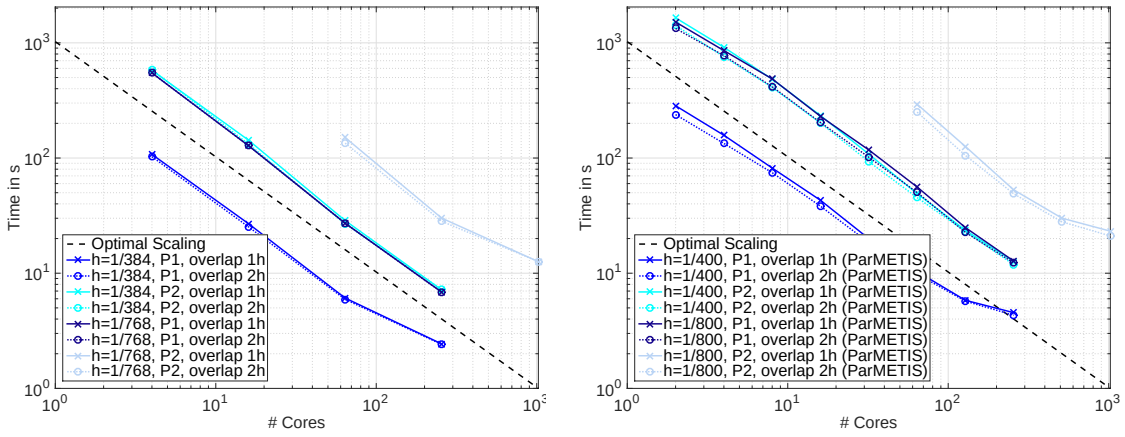

Fig. 4 Strong parallel scalability using the GDSW preconditioner for the model problem of linear elasticity in 2D, cf. (4): structured decomposition (left), ParMETIS decomposition (right).

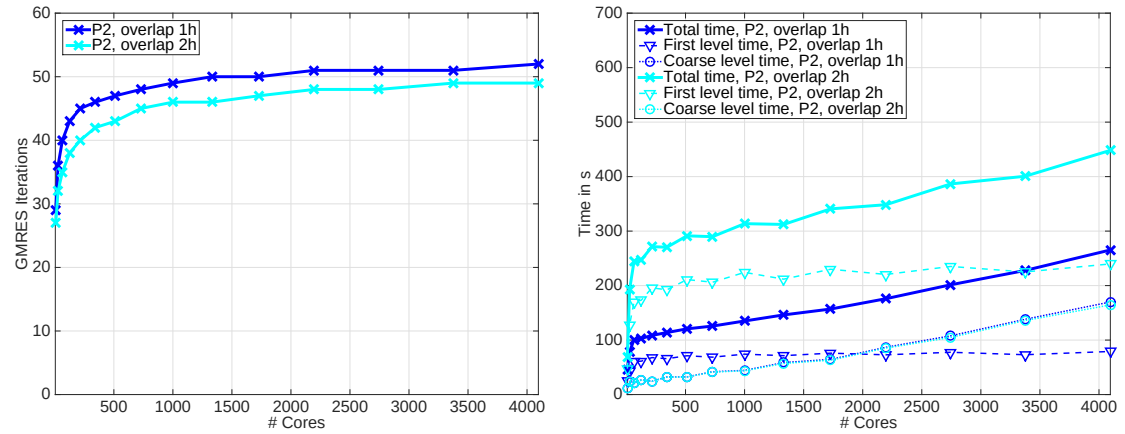

Fig. 5 Weak parallel scalability using the GDSW preconditioner for the problem of linear elasticity in 3D: number of iterations (left), timings (right). We use a subdomain size of $H/h = 6$ and P2 finite elements.

Application in Fluid-Structure Interaction (FSI) We consider time-dependent monolithic FSI as in Balzani et al. [2015] but using a fully implicit scheme as in Deparis et al. [2015], Heinlein et al. [2015]. We apply a monolithic Dirichlet-Neumann preconditioner applying the GDSW preconditioner for the structural block; see Balzani et al. [2015], Heinlein et al. [2015] and the references therein. We use a pressure wave inflow condition for a tube using Mesh #1 from Heinlein et al. [2015]. We consider a Neo-Hookean material for the tube; as opposed to Heinlein et al. [2015], we here use a fixed time step of 0.0005s and show the runtimes during the simulation.

In Fig. 6, the runtimes of ten time steps using 128 cores of the Cray XT6m at the University of Duisburg-Essen are shown. We compare IFPACK, a one-level algebraic overlapping Schwarz preconditioner from Trilinos, our geometric one-level Schwarz preconditioner (OS1), the GDSW preconditioner without rotations (GDSW-nr), and the standard GDSW preconditioner for

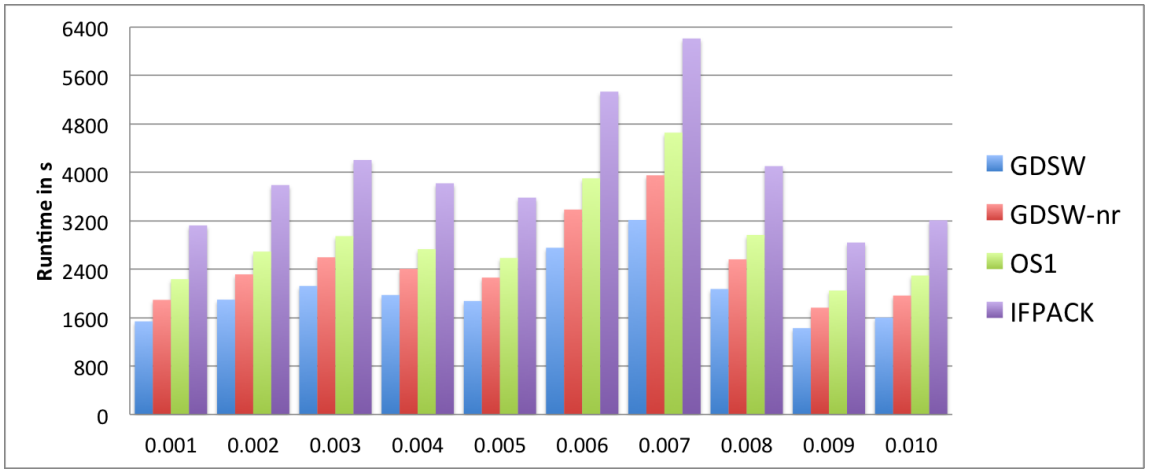

Fig. 6 Runtimes for the monolithic FSI simulation. For clarity, the runtimes of two subsequent time steps of size $\Delta t = 0.0005$s are combined. The monolithic system has approximately 1.2 million d.o.f. We use a Neo-Hookean material. "OS1" is the one-level Schwarz preconditioner, "GDSW-nr" is the GDSW preconditioner without rotations, and "GDSW" is the GDSW preconditioner with full coarse space.

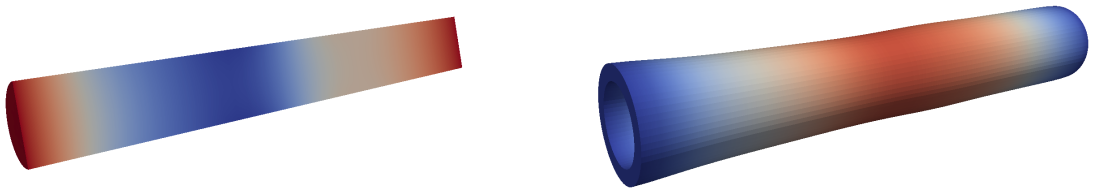

Fig. 7 Pressure and deformation at time $t = 0.007$s. The deformation is magnified by a factor of 10.

the structural block. We see that, although the computing times vary over the simulation time, the combination of the geometric overlap and a sufficiently large coarse space consistently reduces the runtime of the fully coupled monolithic FSI simulation by a factor of approximately two compared to the baseline given by IFPACK. Fig. 7 shows the pressure and the deformation at time $t = 0.007$s where we have the largest computation time per timestep, cf. Fig. 6.

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References

Patrick R. Amestoy, Iain S. Duff, Jean-Yves L'Excellent, and Jacko Koster. A fully asynchronous multifrontal solver using distributed dynamic scheduling. SIAM J. Matrix Anal. Appl., 23(1):15–41, January 2001.

Daniel Balzani, Simone Deparis, Simon Fausten, Davide Forti, Alexander Heinlein, Axel Klawonn, Alfio Quarteroni, Oliver Rheinbach, and Jörg Schröder. Numerical modeling of fluid-structure interaction in arteries with anisotropic polyconvex hyperelastic and anisotropic viscoelastic material models at finite strains. International Journal for Numerical Methods in Biomedical Engineering, 2015. ISSN 2040-7947. doi: 10.1002/cnm.2756. URL `http://dx.doi.org/10.1002/cnm.2756`. http://dx.doi.org/10.1002/cnm.2756.

Timothy A. Davis and Iain S. Duff. An unsymmetric-pattern multifrontal method for sparse lu factorization. SIAM J. Matrix Anal. Appl., 18(1): 140–158, January 1997.

Simone Deparis, Davide Forti, Gwenol Grandperrin, and Alfio Quarteroni. FaCSI : A block parallel preconditioner for fluid-structure interaction in hemodynamics. Technical Report 13, 2015.

Clark R. Dohrmann and Olof B. Widlund. Hybrid domain decomposition algorithms for compressible and almost incompressible elasticity. Internat. J. Numer. Meth. Engng, 82(2):157–183, 2010.

Clark R. Dohrmann, Axel Klawonn, and Olof B. Widlund. Domain decomposition for less regular subdomains: overlapping Schwarz in two dimensions. SIAM J. Numer. Anal., 46(4):2153–2168, 2008a. ISSN 0036-1429.

Clark R. Dohrmann, Axel Klawonn, and Olof B. Widlund. A family of energy minimizing coarse spaces for overlapping Schwarz preconditioners. In Domain decomposition methods in science and engineering XVII, volume 60 of Lect. Notes Comput. Sci. Eng., pages 247–254. Springer, Berlin, 2008b.

L. Formaggia, M. Fernandez, A. Gauthier, J.F. Gerbeau, C. Prud'homme, and A. Veneziani. The LifeV Project. Web, 2002-2004. URL `http://www.lifev.org`.

Alexander Heinlein, Axel Klawonn, and Oliver Rheinbach. Parallel two-level overlapping Schwarz methods in fluid-structure interaction. 2015. Accepted to Springer Lect. Notes Sci. Comput.; Proceedings of ENUMATH 2015; TUBAF Preprint 15/2015: `http://tu-freiberg.de/fakult1/forschung/preprints`.

Michael A Heroux, Roscoe A Bartlett, Vicki E Howle, Robert J Hoekstra, Jonathan J Hu, Tamara G Kolda, Richard B Lehoucq, Kevin R Long, Roger P Pawlowski, Eric T Phipps, Andrew G Salinger, Heidi K Thornquist, Ray S Tuminaro, James M Willenbring, Alan Williams, and Kendall S Stanley. An overview of the Trilinos project. ACM Trans. Math. Softw., 31(3):397–423, 2005.

George Karypis, Kirk Schloegel, and Vipin Kumar. ParMETIS - Parallel graph partitioning and sparse matrix ordering. Version 3.2. Technical report, University of Minnesota, Department of Computer Science and Engineering, April 2011.

Andrea Toselli and Olof Widlund. Domain decomposition methods—algorithms and theory, volume 34 of Springer Series in Computational Mathematics. Springer-Verlag, Berlin, 2005. ISBN 3-540-20696-5.