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Alexander Heinlein, Oliver Rheinbach, Friederike Röver, Stefan Sandfeld, Dominik Steinberger

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Applying the FROSch Overlapping Schwarz Preconditioner for Dislocation Mechanics in Deal.II

Alexander Heinlein[2,3], **Oliver Rheinbach**[1,], **Friederike Röver**[1,], **Stefan Sandfeld**[1,], and **Dominik Steinberger**[1,]

[1] Fakultät für Mathematik und Informatik, Technische Universität Bergakademie Freiberg, Akademiestr. 6, 09599 Freiberg
[2] Department of Mathematics and Computer Science, University of Cologne, Weyertal 86-90, 50931 Cologne
[3] Center for Data and Simulation Science, University of Cologne, Germany, URL: http://www.cds.uni-koeln.de

Parallel computational results for problems in dislocation mechanics are presented using the deal.II adaptive finite element software and the Fast and Robust Overlapping Schwarz Preconditioner (FROSch).

1 Mechanical Model

We consider a linear elastic problem

$$\operatorname{div}\sigma = 0, \sigma = \sigma^T, \sigma = C : \varepsilon^{\text{el}},$$

describing a dislocation microstructure, where u is the unknown displacement and $\varepsilon^{\text{el}} = \frac{1}{2}\left(\nabla u + (\nabla u)^T\right)$. Here, σ is the stress tensor, ε^{el} the elastic strain tensor, and C the stiffness tensor. Dislocations are one-dimensional defects in crystalline materials. A dislocation is the boundary of a planar area where a displacement of the crystal planes by the so-called Burgers vector $\vec{b}$ has occurred. Within the linear elastic model, dislocations can be modeled using an eigenstrain approach [7,8] by expressing the total strain as a sum $\varepsilon^{\text{tot}} = \varepsilon^{\text{el}} + \varepsilon^{\text{eig}}$, where ε^{eig} is the eigenstrain contribution due to the dislocation microstructure. The area enclosed by a dislocation, described by a perpendicular vector $\vec{A}$, is discretized, and the eigenstrain contributions of each point are regularized using the non-singular formulation proposed by Cai et al. [4], using $\mathrm{d}\varepsilon^{\text{eig}} = \frac{1}{2}(\vec{b}\otimes \mathrm{d}\vec{A} + \mathrm{d}\vec{A}\otimes\vec{b})$, similarly to the work [12]; see also [13, 14] for details.

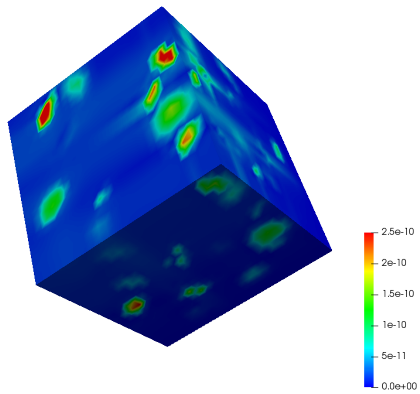

Fig. 1: Displacement u for the model problem described in Section 1 with multiple dislocation in the microstructure.

2 The GDSW Preconditioner

The GDSW (Generalized Dryja–Smith–Widlund) preconditioner is a two-level overlapping Schwarz preconditioner [5, 6, 15]; it is based on a decomposition of the computational domain into overlapping subdomains and can be written in the form

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

where $K_i := R_i K R_i^T$ and R_i is the restriction to the ith overlapping subdomain. The rows of Φ correspond to the coarse basis functions. For linear elliptic problems, the condition number is bounded by $\kappa(M_{\text{GDSW}}^{-1}K) \le C\left(1+\frac{H}{\delta}\right)\left(1+\log\left(\frac{H}{h}\right)\right)^2$, where h is the size of a finite element, H the size of a nonoverlapping subdomain and δ the size over the overlap [5, 6]. An advantage of the GDSW preconditioner is that it can be constructed in an algebraic fashion from the assembled stiffness matrix. An implementation of the GDSW preconditioner has been included in the Trilinos package ShyLU as the Fast and Robust Overlapping Schwarz framework (FROSch) [9, 10]. For the model problem described above, we interfaced the preconditioner to the deal.II software library [2]. Deal.II provides wrapper classes to Trilinos based on the linear algebra package Epetra.

3 Numerical Results

To evaluate the strong scalability of the GDSW and the the more recent RGDSW preconditioner [11] for the model problem decribed above, we performed experiments on High Performance Compute Cluster at the TU Bergakademie Freiberg; the RGDSW preconditioner is a variant of the GDSW preconditioner, where the dimension of the coarse matrix K_0 is significantly reduced. Sparse linear systems arising from the preconditioner were solved using the sparse direct solver *KLU* provided by the Trilinos package Amesos [1]. All tests were performed using Q1 finite elements and an initial structured decomposition into subdomains. The decomposition was performed by p4est [3]. For the GDSW preconditioner, we always choose an overlap of one layer of elements. As a Krylov solver, we apply the GMRES implementation from the Trilinos package Belos with a relative stopping criterion $\|r^k\|/\|r^0\| \leq 10^{-6}$, where r_0 and r^k are the initial residual and the residual in the kth iteration, respectively. *Solver Time* denotes the time to solution consisting of the time to build the preconditioner (*Setup Time*) and the time spent in the Krylov iteration (*Krylov Time*); the *Setup Time* also includes the matrix factorizations. Our results, starting with 32 768 cells and performing one cycle of adaptive refinement, are presented in Table 1. The GDSW and RGDSW preconditioners scale well when scaling from 8 to 64 cores; however, given the smaller coarse space, RGDSW outperforms GDSW for the larger problem.

		GDSW					RGDSW				
Refinement cycle	# Cores	# D.o.f.	Iter	Setup Time	Krylov Time	Solver Time	# D.o.f.	Iter	Setup Time	Krylov Time	Solver Time
0	8	107 811	75	90.03 s	8.55 s	**98.58 s**	107 811	120	83.86 s	15.83 s	**99.69 s**
	16	107 811	112	19.14 s	5.92 s	**25.06 s**	107 811	143	17.96 s	8.56 s	**26.52 s**
	32	107 811	93	5.64 s	2.72 s	**8.36 s**	107 811	120	4.10 s	3.90 s	**8.00 s**
	64	107 811	69	2.85 s	1.41 s	**4.26 s**	107 811	92	1.88 s	1.74 s	**3.62 s**
1	8	364 410	119	651.48 s	53.60 s	**705.08 s**	364 410	151	107.89 s	90.42 s	**198.31 s**
	16	363 942	134	141.38 s	27.00 s	**168.38 s**	363 942	170	53.56 s	44.22 s	**97.78 s**
	32	363 480	120	45.98 s	12.48 s	**58.46 s**	363 480	153	37.14 s	14.66 s	**51.80 s**
	64	363 165	115	34.99 s	9.83 s	**44.82 s**	363 165	137	14.48 s	7.60 s	**22.08 s**

Table 1: Strong scaling tests for the model problem described in Section 1 using the GDSW and RGDSW preconditioner.

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