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TU Bergakademie Freiberg

Fakultät für Mathematik und Informatik

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A Highly Scalable Implementation of Inexact Nonlinear FETI-DP without Sparse Direct Solvers

Axel Klawonn[1], Martin Lanser[1], and Oliver Rheinbach[2]

[1] Mathematisches Institut, Universität zu Köln, Weyertal 86-90, 50931 Köln, Germany. E-mail:{axel.klawonn,martin.lanser}@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

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Abstract. A variant of a nonlinear FETI-DP domain decomposition method is considered. It is combined with a parallel algebraic multigrid method (BoomerAMG) in a way which completely removes sparse direct solvers from the algorithm. Scalability to 524 288 MPI ranks is shown for linear elasticity and nonlinear hyperelasticity using more than half of the JUQUEEN supercomputer (JSC, Jülich).

1 Introduction

Classically, nonlinear partial differential equations are solved using a Newton-Krylov approach in which the discretized nonlinear problem is first linearized and then solved by a (possibly globalized) Newton method. In each Newton step, the linear system is then solved iteratively using a Krylov subspace method combined with a scalable preconditioner, e.g., from domain decomposition. In [13,14], nonlinear FETI-DP domain decomposition approaches were proposed where the order of the geometrical decomposition and the linearization is interchanged.

Nonlinear domain decomposition as a scalable solution method includes the Additive Schwarz Preconditioned Inexact Newton method [6] (see also [12,7,11,8]) and its recent multiplicative version [20]. Moreover, nonlinear FETI-1 methods [21] and nonlinear Neumann-Neumann methods as a solver [5] are nonlinear domain decomposition methods related to ours.

Versions of nonlinear FETI-DP domain decomposition methods scale to the largest supercomputers currently available, i.e., they have scaled to 524 288 cores [16] and later to the complete Mira supercomputer, i.e., 786 432 cores [15] and 63 billion displacement unknowns in nonlinear hyperelasticity. This is the currently largest range of parallel scalabilty reported for any domain decomposition method. Similarly, but for linear problems, BDDC methods have scaled to 458 752 cores [1]. Algebraic Multigrid (AMG) methods for elasticity have also recently scaled to the same range, i.e., 262 144 cores [2].

In this paper, we consider a new variant of nonlinear FETI-DP domain decomposition methods; see [19]. It is combined with an algebraic multigrid (AMG) method, completely removing sparse direct solvers from the algorithm.

2 Inexact Nonlinear FETI-DP

The inexact nonlinear FETI-DP approach, first introduced in [19], is a combination of inexact FETI-DP, described in [18], and Nonlinear-FETI-DP-1, introduced in [14]. In this section, we provide a brief description of the method. Our approach is based on the solution of the nonlinear FETI-DP saddle point system

$$\begin{aligned} \widetilde{K}(\tilde{u}) + B^T\lambda - \tilde{f} &= 0 \\ B\tilde{u} \qquad\qquad &= 0 \end{aligned} \tag{1}$$

using Newton's method, which leads to linearized systems of the form

$$\begin{bmatrix} D\widetilde{K}(\tilde{u}) & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} \delta\tilde{u} \\ \delta\lambda \end{bmatrix} = \begin{bmatrix} \widetilde{K}(\tilde{u}) + B^T\lambda - \tilde{f} \\ B\tilde{u} \end{bmatrix}; \tag{2}$$

see also [14] for a detailed description of nonlinear FETI-DP methods.

As in classical linear FETI-DP methods, we assume a nonoverlapping domain decomposition of the computational domain. The resulting interface variables are split into primal (Π) and dual variables (Δ). Variables in the interior part of the subdomains are denoted by I, and we define the index set $B := [I\ \Delta]$. The block matrix $D\widetilde{K}(\tilde{u})$ is partially assembled in the primal variables Π, while the remaining part of $D\widetilde{K}(\tilde{u})$ typically is block diagonal. Each diagonal block is associated to one of the FETI-DP subdomains. The operator B is a classical jump operator, well known from any FETI-DP literature. Following the notation in [18], we define

$$\mathcal{A} := \begin{bmatrix} D\widetilde{K}(\tilde{u}) & B^T \\ B & 0 \end{bmatrix}, \quad \mathcal{F} := \begin{bmatrix} \widetilde{K}(\tilde{u}) + B^T\lambda - \tilde{f} \\ B\tilde{u} \end{bmatrix}, \quad \text{and} \quad x := \begin{bmatrix} \delta\tilde{u} \\ \delta\lambda \end{bmatrix}.$$

We apply a Krylov method, e.g., GMRES, to the preconditioned system

$$\mathcal{B}_L^{-1}\mathcal{A}x = \mathcal{B}_L^{-1}\mathcal{F} \tag{3}$$

in order to solve the linearized system in each Newton step. The block triangular preconditioner $\mathcal{B}_L$ is defined by

$$\mathcal{B}_L := \begin{bmatrix} \widehat{K}^{-1} & 0 \\ M^{-1}B\widehat{K}^{-1} & M^{-1} \end{bmatrix},$$

where $\widehat{K}^{-1}$ is a sufficiently good preconditioner for $D\widetilde{K}(\tilde{u})$, and M^{-1} is one of the standard FETI-DP preconditioners. Throughout this paper, the

```
Init: ũ^(0) ∈ W̃
for k = 0, ..., convergence
    build: K̃(ũ^(k)), DK̃(ũ^(k)), and M^{-1}
    iterative Krylov solve for x = [δũ^{(k)T}, δλ^(k)] using left
    preconditioner B_L^{-1} := B_L^{-1}(K̂^{-1}, M^{-1}):
        𝒜x = ℱ        // (see eq. (3))
    update:
    ũ^(k+1) := ũ^(k) − δũ^(k)
    λ^(k+1) := λ^(k) − δλ^(k)
end
```

Fig. 1. Pseudocode of the **Inexact-Nonlinear-FETI-DP**. The application of $\widehat{K}^{-1}$ consists of cycles of a parallel AMG method.

application of $\widehat{K}^{-1}$ consists of one V-cycle of a parallel AMG method applied to the complete system $D\widetilde{K}(\tilde{u})$. We investigate two different choices for the preconditioner M^{-1}. First, we use the standard Dirichlet preconditioner

$$M^{-1} := M^{-1}_{\mathrm{FETI_D}} := \sum_{i=1}^{N} B^{(i)}_{\Delta,D}\, S^{(i)}_{\Delta\Delta}\, B^{(i)T}_{\Delta,D},$$

which is a weighted sum of Schur complements $S^{(i)}_{\Delta\Delta} := DK^{(i)}_{\Delta\Delta} - DK^{(i)}_{\Delta I}\,(DK^{(i)}_{II})^{-1}\,DK^{(i)T}_{\Delta I}$ on the dual part of the interface. Here, the matrices $DK^{(i)}_{II}$, $DK^{(i)}_{\Delta\Delta}$, and $DK^{(i)}_{\Delta I}$ correspond to blocks of the tangential matrix $D\widetilde{K}(\tilde{u})$ and are local to the i-th subdomain.

Second, to completely remove sparse direct solvers from the method, we can replace an application of $\left(DK^{(i)}_{II}\right)^{-1}$ by some cycles of a local AMG method. We denote this modified Dirichlet preconditioner by $M^{-1}_{\mathrm{FETI_{D/AMG}}}$. Let us note that this approach does not guarantee spectral equivalence to the (exact) Dirichlet preconditioner unless the interior system is solved accurately enough. Nevertheless, this modified preconditioner often leads to appropriate results; see also [17]. Finally, the complete algorithm is presented in Fig. 1.

We have implemented the Inexact-Nonlinear-FETI-DP method in PETSc 3.6.2 [4] using C/C++ and MPI. We decided to implement the matrix $D\widetilde{K}(\tilde{u})$ and the jump operator B as MPI parallel sparse matrices of the type *MPIAIJ*, which is provided by PETSc. All rows of $D\widetilde{K}(\tilde{u})$ corresponding to the interior and interface nodes of the i-th subdomain are distributed to the same MPI rank, i.e., the local subdomain block $\left[\, DK^{(i)}_{BB}(\tilde{u})\; D\widetilde{K}^{(i)}_{B\Pi}(\tilde{u}) \,\right]$ is assigned to one MPI rank. The rows corresponding to the globally assembled FETI-DP coarse space are distributed equally to all MPI ranks, and thus we do not obtain the typical block structure

$$D\widetilde{K}(\tilde{u}) := \begin{bmatrix} DK_{BB}(\tilde{u}) & D\widetilde{K}^T_{\Pi B}(\tilde{u}) \\ D\widetilde{K}_{\Pi B}(\tilde{u}) & D\widetilde{K}_{\Pi\Pi}(\tilde{u}) \end{bmatrix}$$

# MPI ranks	D.o.f.	M^{-1}	Newton It.	It.	Time to Solution	Eff.	Time Assembly eq. (2)	Time Setup $\hat{K}^{-1}$	Time Setup M^{-1}	Time GMRES
32	1 644 162	$M^{-1}_{\mathrm{FETI_D}}$	1	23	46.3s	100.0%	5.7s	8.6s	10.2s	20.1s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	1	27	51.4s	100.0%	5.7s	8.7s	2.9s	32.6s
128	6 565 122	$M^{-1}_{\mathrm{FETI_D}}$	1	20	45.2s	102.4%	5.8s	8.8s	11.4s	17.7s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	1	25	49.5s	103.8%	5.8s	8.8s	2.9s	30.4s
512	26 237 442	$M^{-1}_{\mathrm{FETI_D}}$	1	18	45.3s	102.2%	5.9s	8.8s	11.5s	17.5s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	1	23	49.5s	103.8%	5.9s	8.9s	2.9s	30.3s
2 048	104 903 682	$M^{-1}_{\mathrm{FETI_D}}$	1	15	41.4s	111.8%	5.8s	8.9s	11.6s	13.5s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	1	22	46.0s	111.7%	5.8s	8.9s	3.0s	26.9s
8 192	419 522 562	$M^{-1}_{\mathrm{FETI_D}}$	1	14	40.9s	113.2%	5.9s	9.1s	11.4s	12.7s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	1	20	44.1s	116.6%	5.9s	9.1s	3.0s	24.5s
32 768	1 677 905 922	$M^{-1}_{\mathrm{FETI_D}}$	1	12	39.9s	116.0%	6.2s	9.3s	11.7s	11.0s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	1	20	44.9s	114.5%	6.2s	9.3s	3.0s	24.6s
131 072	6 711 255 042	$M^{-1}_{\mathrm{FETI_D}}$	1	13	42.2s	109.7%	6.7s	9.9s	11.4s	11.9s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	1	20	46.5s	110.5%	6.7s	9.8s	3.0s	24.6s
524 288	26 844 282 882	$M^{-1}_{\mathrm{FETI_D}}$	1	14	50.5s	91.7%	9.2s	11.1s	11.4s	13.2s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	1	22	56.9s	90.3%	9.3s	11.1s	3.3s	27.8s

Table 1. Linear 2D beam; one V-cycle of BoomerAMG with nodal HMIS coarsening and GM interpolation is used in all cases; **It.** denotes the number of GMRES iterations; the baseline of the parallel efficiency **Eff.** is the time to solution on 32 MPI ranks (1 node).

in our implementation. We always try to distribute a primal variable to one of the MPI ranks handling a neighboring subdomain. This strategy should reduce communication. The rows of B^T are distributed equivalently.
As preconditioner for $D\widetilde{K}(\tilde{u})$, we always use one V-cycle of BoomerAMG [9]. In some of our numerical tests, we also use the global matrix (GM) approach introduced in [3] and used in [2], which guarantees the exact interpolation of chosen smooth error vectors, e.g., rigid body modes (rotations and translations). This can improve the quality of AMG as preconditioner for elasticity problems. If using the GM interpolation, we have to provide the rotations on the finite element space $\widetilde{W}$, i.e., the rotation of the coarse space and the subdomain nodes. We also present an algorithmic description of Inexact-Nonlinear-FETI-DP in form of a pseudocode in Fig. 1.

3 Model Problems and Numerical Results

We consider three different elasticity problems. First, we investigate a compressible linear elasticity problem

$$-2\mu \operatorname{div}(\varepsilon(u)) - \lambda \operatorname{grad}(\operatorname{div}(u)) = f$$

with $\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}, \mu = \frac{E}{2(1+\nu)}$. We choose $E = 210$ and $\nu = 0.3$, consider a rectangular domain $\Omega := [0\,,\,8] \times [0\,,\,1]$ and a homogeneous Dirichlet boundary condition in all nodes $(x, y) \in \Omega$ with $x = 0$. A constant volume force

# MPI ranks	D.o.f.	M^{-1}	Newton It.	It.	Time to Solution	Eff.	Time Assembly eq. (2)	Time Setup $\hat{K}^{-1}$	Time Setup M^{-1}	Time GMRES
32	643 602	$M^{-1}_{\mathrm{FETI_D}}$	4	66	53.4s	100.0%	5.7s	14.3s	11.7s	21.0s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	4	70	56.7s	100.0%	5.7s	14.2s	4.4s	31.5s
128	2 567 202	$M^{-1}_{\mathrm{FETI_D}}$	4	65	55.1s	96.9%	5.8s	14.8s	12.6s	21.0s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	4	72	58.8s	96.4%	6.0s	14.8s	4.4s	32.7s
512	10 254 402	$M^{-1}_{\mathrm{FETI_D}}$	4	57	55.2s	96.7%	6.0s	17.0s	12.6s	18.7s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	4	66	58.5s	96.9%	6.1s	17.0s	4.4s	30.2s
2 048	40 988 802	$M^{-1}_{\mathrm{FETI_D}}$	4	52	54.5s	98.0%	6.1s	17.6s	12.7s	17.2s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	4	64	58.6s	96.8%	6.1s	17.6s	4.4s	29.4s
8 192	163 897 602	$M^{-1}_{\mathrm{FETI_D}}$	4	52	55.9s	95.5%	6.4s	18.2s	12.7s	17.7s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	4	64	59.5s	95.3%	6.4s	18.2s	4.5s	29.5s
32 768	655 475 202	$M^{-1}_{\mathrm{FETI_D}}$	4	52	57.6s	92.7%	6.7s	19.2s	12.7s	17.7s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	4	70	64.6s	87.8%	6.7s	19.2s	4.5s	32.8s
131 072	2 621 670 402	$M^{-1}_{\mathrm{FETI_D}}$	4	44	60.4s	88.4%	8.6s	21.8s	12.8s	15.0s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	4	61	65.7s	86.3%	8.5s	21.6s	4.7s	28.5s
524 288	10 486 220 802	$M^{-1}_{\mathrm{FETI_D}}$	4	47	86.6s	61.7%	17.6s	28.6s	14.0s	17.1s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	4	66	94.0s	60.3%	17.8s	28.6s	5.7s	32.5s

Table 2. Nonlinear 2D beam; one V-cycle of BoomerAMG with nodal HMIS coarsening and GM interpolation is used in all cases; **It.** denotes the number of GMRES iterations; the baseline of the parallel efficiency **Eff.** is the time to solution on 32 MPI ranks (1 node); all values are summed values over the 4 Newton steps.

in y-direction is applied to the complete **linear 2D beam**; see Table 1 for some weak scalability results. As a second model problem, we consider the same domain, boundary condition, material parameters, and volume force, but choose a nonlinear Neo-Hooke material. The strain energy density function of the Neo-Hooke material W [22,10] is given by

$$W(u) = (\mu/2)\big(\mathrm{tr}(\mathbf{F}^T\mathbf{F}) - 3\big) - \mu \ln(J) + (\lambda/2)\ln^2(J)$$

with the deformation gradient $\mathbf{F}(x) := \nabla\boldsymbol{\varphi}(\mathbf{x})$. Here, $\boldsymbol{\varphi}(\mathbf{x}) = \mathbf{x}+\mathbf{u}(\mathbf{x})$ denotes the deformation and $\mathbf{u}(\mathbf{x})$ the displacement of $\mathbf{x}$. We present weak scalability tests for the **nonlinear 2D beam** in Table 2. Our third model problem is strongly heterogeneous. We consider a rectangular domain $[0\,,\,2] \times [0\,,\,1]$ and apply the deformation $\mathbf{F} = \begin{bmatrix} 1.1 & 0 \\ 0 & 1 \end{bmatrix}$ in each boundary node. Again, a Neo-Hooke material with $E = 210$ and $\nu = 0.3$ is used, but we consider one slightly off-centered circular inclusion of stiff material ($E = 210\,000$ and $\nu = 0.3$) in each FETI-DP subdomain. The weak scalability results for the **heterogeneous nonlinear problem** are presented in Table 3. Let us remark that we always use a single square FETI-DP subdomain per MPI rank and consider all vertices to be primal. We choose a discretization with piecewise quadratic triangular finite elements in all our experiments. All computations are performed on JUQUEEN BlueGene/Q at Forschungszentrum Jülich using 32 MPI ranks per node. We always choose HMIS coarsening and ext+i

# MPI ranks	D.o.f.	M^{-1}	Newton It.	It.	Time to Solution	Eff.	Time Assembly eq. (2)	Time Setup $\hat{K}^{-1}$	Time Setup M^{-1}	Time GMRES
32	642 402	$M^{-1}_{\mathrm{FETI_D}}$	4	90	45.6s	100%	5.7s	3.6s	11.7s	23.7s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	4	98	52.2s	100%	5.8s	3.6s	3.7s	38.2s
128	2 564 802	$M^{-1}_{\mathrm{FETI_D}}$	4	110	52.3s	87.2%	6.0s	3.6s	12.3s	29.4s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	4	105	55.6s	93.9%	6.0s	3.6s	3.7s	41.3s
512	10 249 602	$M^{-1}_{\mathrm{FETI_D}}$	4	120	55.8s	81.7%	6.0s	3.8s	12.6s	32.6s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	4	111	58.6s	89.1%	6.0s	3.8s	3.7s	44.1s
2 048	40 979 202	$M^{-1}_{\mathrm{FETI_D}}$	4	129	58.7s	77.7%	6.0s	3.9s	12.6s	35.1s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	4	117	61.6s	84.7%	6.2s	4.0s	3.8s	46.7s
8 192	163 878 402	$M^{-1}_{\mathrm{FETI_D}}$	4	147	64.2s	71.0%	6.2s	4.2s	12.7s	40.2s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	4	132	68.1s	76.7%	6.4s	4.2s	3.8s	52.6s
32 768	655 436 802	$M^{-1}_{\mathrm{FETI_D}}$	4	156	68.1s	67.0%	6.5s	4.6s	12.7s	43.0s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	4	135	70.5s	74.0%	6.9s	4.6s	3.8s	54.1s
131 072	2 621 593 602	$M^{-1}_{\mathrm{FETI_D}}$	4	180	79.7s	57.2%	8.5s	5.6s	12.8s	50.2s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	4	159	85.0s	61.4%	8.6s	5.5s	4.0s	64.6s
524 288	10 486 220 802	$M^{-1}_{\mathrm{FETI_D}}$	4	189	104.7s	43.6%	17.5s	7.8s	14.0s	56.1s
		$M^{-1}_{\mathrm{FETI_{D/AMG}}}$	4	177	114.7s	45.5%	17.4s	8.0s	5.0s	75.0s

Table 3. Heterogeneous Neo-Hooke problem; one V-cycle of BoomerAMG with nodal HMIS coarsening is used in all cases; **It.** denotes the number of GMRES iterations; the baseline of the parallel efficiency **Eff.** is the time to solution on 32 MPI ranks (1 node); all values are summed values over the 4 Newton steps.

interpolations from BoomerAMG. The GM approach is used additionally in the 2D beam computations and hybrid AMG (nodal coarsening and unknown based interpolation) for the heterogeneous Neo-Hooke problem. The choice of the AMG components is motivated by our experience gained in [2]. We use UMFPACK for $M^{-1}_{\mathrm{FETI_D}}$.

The total runtime of Inexact-Nonlinear-FETI-DP basically splits into four different phases: the assembly of all parts of the saddle point system in (2) (including the assembly of the rigid body modes for the GM approach), the setup of the Dirichlet preconditioner M^{-1}, the BoomerAMG setup time to create $\hat{K}^{-1}$, and finally the iterative solution using preconditioned GMRES. Runtimes for these four phases are presented in all tables. Since the setup of M^{-1} always scales nearly perfectly, we will only discuss the remaining timings. Let us remark that the setup of $M^{-1}_{\mathrm{FETI_{D/AMG}}}$ is up to four times faster than the setup of $M^{-1}_{\mathrm{FETI_D}}$, since direct factorizations are avoided. In contrast, since an application of an AMG V-cycle is more expensive than a forward-backward solve in UMFPACK, one preconditioned GMRES iteration using $M^{-1}_{\mathrm{FETI_D}}$ is cheaper.

For the linear elastic beam (Table 1), we obtain weak scalability with more than 90% parallel efficiency. Here, we benefit from a decreasing number of GMRES iterations, which compensates some inefficiencies in the assembly of the saddle point system and the BoomerAMG setup. The direct solverfree $M^{-1}_{\mathrm{FETI}_{\mathrm{D/AMG}}}$ also convinces in runtime, and numerical as well as parallel scalability for this model problem. Similar observations can be made for the nonlinear beam (Table 2). In this case, scalability is less optimal caused by a more expensive AMG setup. However, obtaining a parallel efficiency of more than 60% scaling from 32 to 524 288 MPI ranks is still remarkable, especially, since the total problem sizes are smaller. For the heterogeneous material (Table 3), the parallel scalability suffers from a certain loss in numerical scalability. Note that the number of heterogeneities increases with the number of ranks. Let us summarize that Inexact-Nonlinear-FETI-DP showed to be robust for different homogeneous and heterogeneous elasticity problems. Also the variant without any sparse direct solvers performed well. All components of the method showed sufficient scalability.

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