New Nonlinear FETI-DP Methods Based on a Partial Nonlinear Elimination of Variables

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1 Introduction

We introduce two new nonlinear FETI-DP (Finite Element Tearing and Interconnecting - Dual-Primal) methods based on a partial nonlinear elimination and provide a comparison to Newton-Krylov-FETI-DP, Nonlinear-FETI-DP-1, and -2 methods [3, 4]. In contrast to classical Newton-Krylov-FETI-DP methods, where a geometrical decomposition after linearization is performed, in nonlinear FETI-DP methods, the nonlinear problem is decomposed before linearization. The approaches help to localize work and thus are well suited for modern computer architectures. Recently, an inexact nonlinear FETI-DP implementation using PETSc and BoomerAMG has scaled, for nonlinear hyperelasticity, to the largest supercomputers currently available, i.e., to more than half a million MPI ranks [6] on the JUQUEEN supercomputer (Julich Supercomputing Centre), more than half a million cores [6] on the Mira supercomputer (Argonne National Laboratory), and later [5] the complete Mira ($786K$ cores). To the best of our knowledge, this is the largest range of parallel scalability reported for any domain decomposition method. Here, we now describe new variants of nonlinear FETI-DP methods.

2 Nonlinear FETI-DP Methods

In all nonlinear FETI-DP methods, a geometrical decomposition of the computational domain Ω into nonoverlapping subdomains $\Omega_i, i = 1, ..., N$ is

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performed before linearizing the nonlinear problem. In the more traditional Newton-Krylov-FETI-DP approach a discrete nonlinear problem $A(u) = 0$ associated with Ω is linearized first. Let $K_i(u_i) = f_i,\ i = 1, ..., N$, be the local finite element problem on subdomain Ω_i and let W_i be the associated finite element space; see [4], for a detailed definition. We define the nonlinear, discrete block operator $K(u)$ and the corresponding vectors u and f by

$$K(u) := \begin{pmatrix} K_1(u_1) \\ \vdots \\ K_N(u_N) \end{pmatrix}, \ u := \begin{pmatrix} u_1 \\ \vdots \\ u_N \end{pmatrix}, \text{ and } f := \begin{pmatrix} f_1 \\ \vdots \\ f_N \end{pmatrix}. \tag{1}$$

As in linear FETI-DP, we decompose the degrees of freedom into variables interior to subdomains (I), dual interface variables (Δ), and primal variables (Π), e.g., on vertices. Using the standard partial assembly operator R_Π^T, [1, 7] we define the nonlinear, partially assembled operator $\widetilde{K}(\tilde{u}) := R_\Pi^T K(R_\Pi \tilde{u})$ and the right hand side $\tilde{f} := R_\Pi^T f$. We define the usual space of partially continuous discrete functions by $\widetilde{W} \subset W := W_1 \times \cdots \times W_N$. Using the standard FETI-DP jump operator B, we can formulate the nonlinear FETI-DP master system, first introduced in [3]

$$\begin{aligned} \widetilde{K}(\tilde{u}) + B^T\lambda - \tilde{f} &= 0 \\ B\tilde{u} \qquad\qquad &= 0. \end{aligned} \tag{2}$$

In [4], two approaches have been suggested to solve the nonlinear system (2): linearize first (Nonlinear-FETI-DP-1 or NL-1) and eliminate first (Nonlinear-FETI-DP-2 or NL-2). The first variant is based on a Newton linearization of the saddle point system and a solution of the resulting linear system. The second variant is based on a nonlinear elimination of the variable $\tilde{u}$ in (2) before linearization. While in NL-1 nonlinear problems in $\widetilde{W}$ are solved as an initial guess, in NL-2 the solution of nonlinear problems in $\widetilde{W}$ is included into each Newton step, often resulting into faster convergence. In both methods the quality of the coarse space directly influences the Newton convergence. Thus, for problems where a good coarse space is known, NL-2 is often the best choice. However, if a good coarse space is not available, current nonlinear FETI-DP methods might fail to converge without spending effort in globalization. Here, we introduce new nonlinear FETI-DP methods based on a *partial* nonlinear elimination. In these methods, all primal variables are linearized before elimination, which also allows the definition of inexact FETI-DP variants; see also [6, 7]. In the new methods, the choice of primal variables has a weaker influence on the Newton convergence and local nonlinear problems are also computationally cheaper.

3 Nonlinear FETI-DP Based on Partial Elimination

Derivation of the Method We partition $\tilde{u} := (\tilde{u}_E^T, \tilde{u}_L^T)^T$ and $\tilde{f} := (\tilde{f}_E^T, \tilde{f}_L^T)^T$ into a set of variables $E \subseteq B := [I\ \Delta]$, and the remaining variables $L := (B \setminus E) \cup \Pi$. The variables $\tilde{u}_E$ will be eliminated from the nonlinear saddle point system (2) while the variables $\tilde{u}_L$ will be linearized. Accordingly, we partition

$$\widetilde{K}(\tilde{u}) = (\widetilde{K}_E(\tilde{u}_E, \tilde{u}_L)^T, \widetilde{K}_L(\tilde{u}_E, \tilde{u}_L)^T)^T, \text{ and}$$

$$D\widetilde{K}(\tilde{u}) = \begin{bmatrix} D_{\tilde{u}_E}\widetilde{K}_E(\tilde{u}_E, \tilde{u}_L) & D_{\tilde{u}_L}\widetilde{K}_E(\tilde{u}_E, \tilde{u}_L) \\ D_{\tilde{u}_E}\widetilde{K}_L(\tilde{u}_E, \tilde{u}_L) & D_{\tilde{u}_L}\widetilde{K}_L(\tilde{u}_E, \tilde{u}_L) \end{bmatrix} =: \begin{bmatrix} D\widetilde{K}_{EE} & D\widetilde{K}_{EL} \\ D\widetilde{K}_{LE} & D\widetilde{K}_{LL} \end{bmatrix}. \quad (3)$$

We can reformulate the nonlinear FETI-DP saddle point system (2) as

$$\begin{aligned} \widetilde{K}_E(\tilde{u}_E, \tilde{u}_L) + B_E^T\lambda - \tilde{f}_E &= 0 \\ \widetilde{K}_L(\tilde{u}_E, \tilde{u}_L) + B_L^T\lambda - \tilde{f}_L &= 0 \\ B_E\tilde{u}_E + B_L\tilde{u}_L &= 0, \end{aligned} \quad (4)$$

with $B = [B_E\ B_L]$. We perform a (local) nonlinear elimination of $\tilde{u}_E$. To construct our new nonlinear FETI-DP methods, we first derive a nonlinear Schur complement in $(\tilde{u}_L, \lambda)$. Let $(\tilde{u}_E^*, \tilde{u}_L^*, \lambda^*)$ be a solution of (4). We assume there is an implicit function h with the following property in a neighborhood of $(\tilde{u}_E^*, \tilde{u}_L^*, \lambda^*)$:

$$\widetilde{K}_E(h(\tilde{u}_L^*, \lambda^*), \tilde{u}_L^*) + B_E^T\lambda^* - \tilde{f}_E = 0. \quad (5)$$

Here, we consider the first equation from (4). The derivative of the implicit function is

$$Dh(\tilde{u}_L, \lambda) = (D_{\tilde{u}_L}h(\tilde{u}_L, \lambda), D_\lambda h(\tilde{u}_L, \lambda)), \quad (6)$$

$$\text{where } D_{\tilde{u}_L}h(\tilde{u}_L, \lambda) = -(D_{\tilde{u}_E}\widetilde{K}_E(h(\tilde{u}_L, \lambda), \tilde{u}_L))^{-1} D_{\tilde{u}_L}\widetilde{K}_E(h(\tilde{u}_L, \lambda), \tilde{u}_L) \quad (7)$$

$$\text{and } D_\lambda h(\tilde{u}_L, \lambda) = -(D_{\tilde{u}_E}\widetilde{K}_E(h(\tilde{u}_L, \lambda), \tilde{u}_L))^{-1} B_E^T. \quad (8)$$

Inserting the implicit function into equations two and three from (4) we can define a nonlinear Schur complement by

$$S_L(\tilde{u}_L, \lambda) := \begin{bmatrix} \widetilde{K}_L(h(\tilde{u}_L, \lambda), \tilde{u}_L) + B_L^T\lambda - \tilde{f}_L \\ B_E h(\tilde{u}_L, \lambda) + B_L\tilde{u}_L \end{bmatrix}. \quad (9)$$

We finally solve the nonlinear problem $S_L(\tilde{u}_L^*, \lambda^*) = 0$ with Newton's method and obtain the iteration

$$\begin{pmatrix} \tilde{u}_L^{(k+1)} \\ \lambda^{(k+1)} \end{pmatrix} = \begin{pmatrix} \tilde{u}_L^{(k)} \\ \lambda^{(k)} \end{pmatrix} - (DS_L(\tilde{u}_L^{(k)}, \lambda^{(k)}))^{-1} S_L(\tilde{u}_L^{(k)}, \lambda^{(k)}). \quad (10)$$

Using (7) and (8), the short hand notation introduced in (3), and, for simplicity, omitting the variables and indices, we obtain

$$DS_L(\tilde{u}_L, \lambda) = \begin{bmatrix} D\widetilde{K}_{LL} - D\widetilde{K}_{LE} D\widetilde{K}_{EE}^{-1} D\widetilde{K}_{EL} & -D\widetilde{K}_{LE} D\widetilde{K}_{EE}^{-1} B_E^T + B_L^T \\ -B_E D\widetilde{K}_{EE}^{-1} D\widetilde{K}_{EL} + B_L & -B_E D\widetilde{K}_{EE}^{-1} B_E^T \end{bmatrix}. \tag{11}$$

It is easy to verify that the derivative of the nonlinear Schur complement in (11) is equal to the Schur complement of the derivative of the nonlinear saddle point system in (4). Therefore, we can use any FETI-DP type method and solve a linear system equivalent to the linear system in (10). In order to assemble and solve (10) we need to compute $h(\tilde{u}_\Pi^{(k)}, \lambda^{(k)})$ first. We consider local nonlinear problems in each global Newton step, arising from the first equation in (4)

$$\widetilde{K}_E(h(\tilde{u}_L^{(k)}, \lambda^{(k)}), \tilde{u}_L^{(k)}) + B_E \lambda^{(k)} - \tilde{f}_E = 0. \tag{12}$$

Since $\tilde{u}_L^{(k)}$ and $\lambda^{(k)}$ are given as results of the k-th step of the global Newton iteration (10), we can simply perform a local Newton iteration to find $\tilde{u}_E^{(k)} = h(\tilde{u}_L^{(k)}, \lambda^{(k)})$. The local iteration writes

$$\tilde{u}_E^{(l+1)} = \tilde{u}_E^{(l)} - (D\widetilde{K}(\tilde{u}_E^{(l)}, \tilde{u}_L^{(k)}))_{EE}^{-1} \, (\widetilde{K}_E(\tilde{u}_E^{(l)}, \tilde{u}_L^{(k)}) + B_E \lambda^{(k)} - \tilde{f}_E). \tag{13}$$

Let us finally remark that, since $E \cap \Pi = \emptyset$, $D\widetilde{K}(\tilde{u}_E^{(l)}, \tilde{u}_L^{(k)}))_{EE}$ is block diagonal and thus all computations in (13) are local to the subdomains.

Two Different Variants We suggest two different choices of E. First, we define $E := B = [I \; \Delta]$ as the set of interior and dual variables. Consequently, we have $L = \Pi$, $B_E = B_B$, and $B_L = 0$. This defines the Nonlinear-FETI-DP-3 (NL-3) method, where local nonlinear problems in u_B are solved in each global Newton step; see Fig. 1. In this method, the coarse space can slightly influence the convergence of Newton's method, since primal constraints on edges, or faces in three dimensions, influence the variables u_B. As a second choice, we use $E := I$ and thus we have $L = \Delta \cup \Pi =: \Gamma$, $B_E = 0$, and $B_L = B_\Gamma$. This leads to the Nonlinear-FETI-DP-4 (NL-4) method, where local nonlinear problems in u_I are solved in each global Newton step; see Fig. 2. In this method, the coarse space cannot influence Newton's method, since the local problems are independent of the variables on the interface.

4 Numerical Results

As a first model problem, we consider a scaled p-Laplace equation

$$-\mathrm{div}(\alpha |\nabla u|^2 \nabla u - \beta \nabla u) = 1 \;\text{ in } \Omega, \qquad u = 0 \;\text{ on } \partial\Omega, \tag{14}$$

Init: $(u_B^{(0)}, \tilde{u}_\Pi^{(0)}) = \tilde{u}^{(0)} \in \widetilde{W}$, $\lambda^{(0)} = 0$
for $k = 0, ..., convergence$

    for $l = 0, ..., convergence$
        build: $\widetilde{K}(\tilde{u}^{(l)})$ and $D\widetilde{K}(\tilde{u}^{(l)})$
        solve: $(D\tilde{K}(\tilde{u}^{(l)}))_{BB}\delta u_B^{(l)} = K_B(\tilde{u}^{(l)}) + B_B^T\lambda^{(k)} - f_B$ //local problems
        compute steplength $\alpha^{(l)}$
        update: $\tilde{u}^{(l+1)} := \tilde{u}^{(l)} - \alpha^{(l)} \left(\delta u_B^{(l)T}, 0\right)^T$ //update only on B
    end
    $\tilde{u}^{(k)} := \tilde{u}^{(l+1)}$
    build: $\tilde{K}(\tilde{u}^{(k)})$ and $D\tilde{K}(\tilde{u}^{(k)})$
    solve: $DS_\Pi(\tilde{u}_\Pi^{(k)}, \lambda^{(k)}) \begin{pmatrix} \delta\tilde{u}_\Pi^{(k)} \\ \delta\lambda^{(k)} \end{pmatrix} = \begin{pmatrix} \widetilde{K}_\Pi(\tilde{u}^{(k)}) - \tilde{f}_\Pi \\ B_B u_B^{(k)} \end{pmatrix}$ //solve equivalent FETI-DP system
    compute steplength $\alpha^{(k)}$
    update: $\lambda^{(k+1)} := \lambda^{(k)} - \alpha^{(k)}\delta\lambda^{(k)}$
    update: $\tilde{u}_\Pi^{(k+1)} := \tilde{u}_\Pi^{(k)} - \alpha^{(k)}\delta\tilde{u}_\Pi^{(k)}$
    $\tilde{u}^{(0)} := \left(u_B^{(l+1)T}, \tilde{u}_\Pi^{(k+1)T}\right)^T$
    $\lambda^{(0)} := \lambda^{(k+1)}$

end

Fig. 1 Pseudocode of Nonlinear-FETI-DP-3.

Init: $(u_I^{(0)}, \tilde{u}_\Gamma^{(0)}) = \tilde{u}^{(0)} \in \widetilde{W}$, $\lambda^{(0)} = 0$
for $k = 0, ..., convergence$

    for $l = 0, ..., convergence$
        build: $\widetilde{K}(\tilde{u}^{(l)})$ and $D\widetilde{K}(\tilde{u}^{(l)})$
        solve: $(D\tilde{K}(\tilde{u}^{(l)}))_{II}\delta u_I^{(l)} = K_I(\tilde{u}^{(l)}) - f_I$ //local problems
        compute steplength $\alpha^{(l)}$
        update: $\tilde{u}^{(l+1)} := \tilde{u}^{(l)} - \alpha^{(l)} \left(\delta u_I^{(l)T}, 0\right)^T$ //update only on I
    end
    $\tilde{u}^{(k)} := \tilde{u}^{(l+1)}$
    build: $\tilde{K}(\tilde{u}^{(k)})$ and $D\tilde{K}(\tilde{u}^{(k)})$
    solve: $DS_\Gamma(\tilde{u}_\Gamma^{(k)}, \lambda^{(k)}) \begin{pmatrix} \delta\tilde{u}_\Gamma^{(k)} \\ \delta\lambda^{(k)} \end{pmatrix} = \begin{pmatrix} \widetilde{K}_\Gamma(\tilde{u}^{(k)}) + B_\Gamma^T\lambda^{(k)} - \tilde{f}_\Gamma \\ B_\Gamma u_\Gamma^{(k)} \end{pmatrix}$ //solve equivalent FETI-DP system
    compute steplength $\alpha^{(k)}$
    update: $\lambda^{(k+1)} := \lambda^{(k)} - \alpha^{(k)}\delta\lambda^{(k)}$
    update: $\tilde{u}_\Gamma^{(k+1)} := \tilde{u}_\Gamma^{(k)} - \alpha^{(k)}\delta\tilde{u}_\Gamma^{(k)}$
    $\tilde{u}^{(0)} := \left(u_I^{(l+1)T}, \tilde{u}_\Gamma^{(k+1)T}\right)^T$
    $\lambda^{(0)} := \lambda^{(k+1)}$

end

Fig. 2 Pseudocode of Nonlinear-FETI-DP-4.

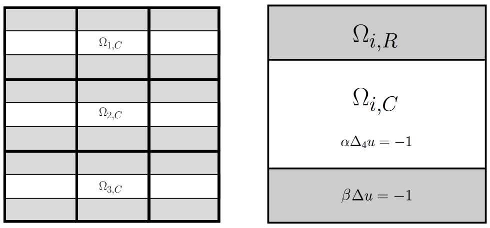

Fig. 3 Left: Example for a decomposition of Ω in $N = 9$ subdomains, intersected by 3 channels $\Omega_{i,C}, i = 1, 2, 3$. We define $\Omega_C = \bigcup_i \Omega_{i,C}$. Right: Subdomain Ω_i with channel $\Omega_{i,C}$ of width $\frac{H}{2}$, where H is the size of a subdomain.

Table 1 p-Laplace problem; channels of p-Laplace ($p = 4$) with high coefficient $1e6$ in standard linear Laplacian matrix. **N**: number of subdomains; **Krylov It.**: sum of CG iterations over all Newton steps; **local solves**:number of local factorizations on subdomains; **coarse solves**: number of FETI-DP coarse problem factorizations. Best results are marked in **bold face** and red color.

N	Solver	# Krylov It.	# local solves	# coarse solves	Min. cond.	Max. cond.
64	NK-FETI-DP	864	19	19	95.9	31 265.6
	Nonlinear-FETI-DP-1	537	26	26	39.5	151.5
	Nonlinear-FETI-DP-2	225	34	34	39.6	95.9
	Nonlinear-FETI-DP-3	264	36	6	30.4	95.9
	Nonlinear-FETI-DP-4	1343	56	17	95.8	32 520.7
256	NK-FETI-DP	2341	19	19	158.1	59 730.5
	Nonlinear-FETI-DP-1	1128	26	26	60.5	255.2
	Nonlinear-FETI-DP-2	**481**	**34**	34	60.6	158.4
	Nonlinear-FETI-DP-3	529	38	**6**	39.6	158.9
	Nonlinear-FETI-DP-4	2766	54	18	158.0	60 415.5

where $\alpha, \beta : \Omega \to \mathbb{R}$ are coefficient functions given by

$$\alpha(x) = \begin{cases} 10^6 & \text{if } x \in \Omega_C \\ 0 & \text{elsewhere} \end{cases} \qquad \beta(x) = \begin{cases} 0 & \text{if } x \in \Omega_C \\ 1 & \text{elsewhere;} \end{cases} \tag{15}$$

see Fig. 3 for a definition of Ω_C.

In Table 1, we present results for the p-Laplace problem (14). Here, NL-4 and Newton-Krylov-FETI-DP both require many Krylov iterations. The local nonlinear problems on the interior part of the subdomains solved in NL-4 cannot resolve the strongly global nonlinearity of the channels. Comparable good results in terms of Krylov space iterations are obtained using NL-2 and NL-3. The new NL-3 method additionally reduces the number of FETI-DP coarse solves drastically and thus is potentially faster in a parallel setup. In contrast to NL-2, where in each global Newton step nonlinear problems in $\widetilde{W}$ including the FETI-DP coarse problem have to be solved, in NL-3 and NL-4 the coarse solves are only necessary in the global Newton iteration.

Our second model problem is a nonlinear hyperelasticity problem. We consider a Neo-Hooke material ($\nu = 0.3$) with a soft matrix material ($E =$

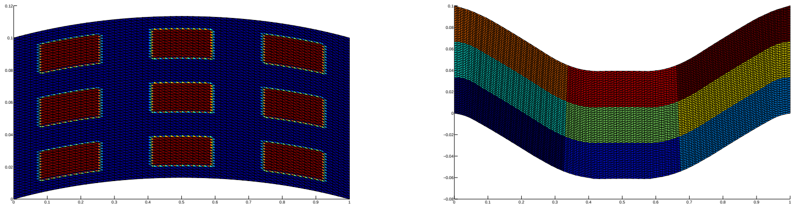

Fig. 4 Left: Initial value (reference configuration) and two different materials with $\nu = 0.3$ everywhere, $E_1 = 210\,000$ in the red inclusions, and $E_2 = 210$ in the blue matrix material. Right: Solution when a volume force $f_v = [0, -10]^T$ is applied.

Table 2 Heterogeneous Neo-Hooke problem; see Fig. 4. Using GMRES as Krylov solver and primal vertex constraints; **d.o.f.**: problem size; **N**: number of subdomains; **Krylov It.**: sum of GMRES iterations over all Newton steps; **local solves**: number of local factorizations on subdomains; **coarse solves**: number of FETI-DP coarse problem factorizations. Best results are marked in **bold face** and red color.

d.o.f.	N	Solver	#Krylov-It.	# local solves	# coarse solves
51 842	64	NK-FETI-DP	595	10	10
		NL-FETI-DP-4	356	12	6
206 082	256	NK-FETI-DP	939	**10**	10
		NL-FETI-DP-4	**491**	12	**6**

210) and stiff inclusions ($E = 210\,000$); see Fig. 4 (left) for the geometry. The strain energy density function W [2] is given by $W(u) = \frac{\mu}{2}\left(\mathrm{tr}(F^TF) - 3\right) - \mu \ln\left(\det(F)\right) + \frac{\lambda}{2}\ln^2\left(\det(F)\right)$ with the Lamé constants $\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}$, $\mu = \frac{E}{2(1+\nu)}$ and the deformation gradient $F(x) := \nabla\varphi(x)$. Here, $\varphi(x) = x + u(x)$ denotes the deformation and $u(x)$ the displacement of x. The energy functional of which stationary points are computed, is given by

$$J(u) = \int_{\Omega} W(u) - V(u)dx - \int_{\Gamma} G(u)ds,$$

where $V(u)$ and $G(u)$ are functionals related to the volume and traction forces. The nonlinear elasticity problem is discretized with piecewise linear finite elements. In Table 2 we present the results for our Neo-Hooke model problem described in Fig. 4. We only considered continuity in vertices as primal constraints, which is not an optimal coarse space for highly heterogeneous elasticity problems. This leads to divergence of NL-1 and NL-2 when using no further globalization strategy. Since the coarse space does not influence the convergence behavior of Newton-Krylov-FETI-DP and NL-4, both methods converge. Due to the local nonlinear problems solved in NL-4, the number of GMRES iterations is reduced up to 47% compared to Newton-Krylov-FETI-DP. Also the number of necessary coarse solves is reduced in NL-4. Of coarse, in the nonlinear variant, the local work is increased slightly.

5 Conclusion

We have presented new nonlinear FETI-DP variants based on a partial nonlinear elimination of interior and interface variables. These methods can remove the influence of the coarse space to the Newton convergence and can be superior if a good coarse space is not available. We have seen that the new methods can reduce the number of FETI-DP coarse solves drastically.

Acknowledgement This work was supported by the German Research Foundation (DFG) through the Priority Programme 1648 "Software for Exascale Computing" (**SPPEXA**) under KL 2094/4-1, KL 2094/4-2, RH 122/2-1 and RH 122/3-2.

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