



Technical Report Series Center for Data and Simulation Science

Axel Klawonn, Martin Lanser, Matthias Uran

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Technical Report ID: CDS-2021-03

Available at <https://kups.ub.uni-koeln.de/id/eprint/37735>

Submitted on March 29, 2021

Adaptive Nonlinear Elimination in Nonlinear FETI-DP Methods

Axel Klawonn, Martin Lanser, and Matthias Uran

1 Introduction

In recent years, we have formulated a unified framework that covers all nonlinear FETI-DP as well as nonlinear BDDC methods; see [3]. Both belong to the class of non-overlapping domain decomposition methods and can be used for the solution of discrete nonlinear problems of the form $A(\bar{u}) = 0$. For example, such systems arise from the discretization of nonlinear partial differential equations. In contrast to the traditional Newton-Krylov-DD approach (see [3]), where we first linearize the problem and then decompose it into subdomains, the order of operations is turned around in nonlinear domain decomposition methods. A nonlinear elimination of a subset of finite element unknowns before linearization allows us to interpret nonlinear FETI-DP methods as nonlinear right-preconditioned Krylov methods; see [3]. Although the unified framework covers arbitrary choices of elimination sets, only a few different types of elimination sets have been considered so far. All of them are based on the classification in interior, dual, and primal variables, which is a natural thing to do in FETI-DP methods but obviously not problem-dependent. In order to design a nonlinear FETI-DP method that fits optimally to an arbitrary problem, it is necessary to use problem-dependent or adaptive elimination sets. In this article, we describe, how to use the residual of the nonlinear FETI-DP saddle point system to choose the elimination set. First studies were performed under our guidance as part of a master thesis [6] and can also be found in [7]. The idea of using the residual to determine an elimination set is adapted from Cai and Gong in [1], where they have introduced the idea in the context of inexact Newton methods.

Axel Klawonn^{1,2}, Martin Lanser^{1,2}, Matthias Uran^{1,2}

¹Department of Mathematics and Computer Science, Division of Mathematics, University of Cologne, Weyertal 86-90, 50931 Cologne, Germany, e-mail: axel.klawonn@uni-koeln.de, martin.lanser@uni-koeln.de, m.uran@uni-koeln.de, url: <https://www.numerik.uni-koeln.de>

²Center for Data and Simulation Science, University of Cologne, Germany, url: <https://www.cds.uni-koeln.de>

2 Nonlinear FETI-DP

Before we describe the process of determining problem-dependent elimination sets, let us first recall the most relevant ideas of nonlinear domain decomposition methods and of the unified framework of nonlinear FETI-DP methods to introduce a suitable notation. For a detailed description, we also refer to [2, 3] and the references therein.

Throughout this paper, we assume that we have a computational domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, which is divided into N non-overlapping subdomains Ω_i , i.e., $\Omega = \bigcup_{i=1}^N \Omega_i$. Each subdomain is the union of finite elements and the associated finite element spaces are denoted by $W^{(i)}$. We denote the product space of all finite element spaces as $W = W^{(1)} \times \dots \times W^{(N)}$. In FETI-DP methods, we partition all variables into interior (I), dual (Δ), and primal (Π) variables, where only continuity in the primal variables is prescribed and continuity in the dual variables is enforced by Lagrange multipliers λ iteratively. Therefore, we further introduce a subspace $\tilde{W} \subset W$ of all finite element functions from W that are continuous in the primal variables. A simple choice of primal variables are subdomain vertices. For completeness, we also introduce the subspace $\widehat{W} \subset W$, which contains all finite element functions that are continuous across the complete interface and it holds $\widehat{W} \subset \tilde{W} \subset W$.

As it was shown in [2], finding the solution of the fully assembled finite element problem is equivalent to solving the nonlinear FETI-DP saddle point system

$$A(\tilde{u}, \lambda) = \begin{bmatrix} \tilde{K}(\tilde{u}) + B^T \lambda - \tilde{f} \\ B\tilde{u} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \tilde{u}, \tilde{f}, \tilde{K}(\tilde{u}) \in \tilde{W}. \quad (1)$$

This system is the basis for all nonlinear FETI-DP methods. Here, the linear constraints $B\tilde{u} = 0$ together with Lagrange multipliers $\lambda \in V := \text{range}(B)$ enforce continuity in all dual variables.

As introduced in [3, 4], we use a nonlinear right-preconditioner $M(\tilde{u}, \lambda)$ that is nonlinear in \tilde{u} and linear in λ ; see [3, 4] for some desirable properties of M . Instead of $A(\tilde{u}, \lambda) = 0$, we now solve $A(M(\tilde{u}, \lambda)) = 0$ with a Newton-Krylov method.

Following [3], the application of a nonlinear right-preconditioner can be interpreted as (partial) nonlinear elimination process (see also [5]), where different choices of M lead to different elimination sets. With this interpretation, it is obvious to divide the overall set of variables into two different subsets E and L , where E contains all variables that should be nonlinearly eliminated by the preconditioner M , and L contains the remaining variables in which will be linearized.

After an appropriate rearrangement, we can represent all quantities in eq. (1) according to the variable split into the subsets E and L . For example, we obtain $\tilde{f} = [\tilde{f}_E^T \ \tilde{f}_L^T]^T$ and $B = [B_E \ B_L]$. Thus, we can write the nonlinear saddle point system (eq. (1)) as

$$A(\tilde{u}_E, \tilde{u}_L, \lambda) = \begin{bmatrix} \tilde{K}_E(\tilde{u}_E, \tilde{u}_L) + B_E^T \lambda - \tilde{f}_E \\ \tilde{K}_L(\tilde{u}_E, \tilde{u}_L) + B_L^T \lambda - \tilde{f}_L \\ B_E \tilde{u}_E + B_L \tilde{u}_L \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

With the application of the nonlinear right-preconditioner, we now aim to eliminate all variables \tilde{u}_E , which correspond to the subset E . Thus, our preconditioner is implicitly defined by solving the nonlinear equation

$$\tilde{K}_E(M_{\tilde{u}_E}(\tilde{u}_L, \lambda), \tilde{u}_L) + B_E^T \lambda - \tilde{f}_E = 0, \quad (2)$$

where we have $M(\tilde{u}_E, \tilde{u}_L, \lambda) := (M_{\tilde{u}_E}(\tilde{u}_L, \lambda), \tilde{u}_L, \lambda)$, since, by construction, M is linear in \tilde{u}_L and λ . After we have computed the nonlinear preconditioner M by solving eq. (2) with Newton's method, we obtain the nonlinear Schur complement system

$$S_L(\tilde{u}_L, \lambda) := \begin{bmatrix} \tilde{K}_L(M_{\tilde{u}_E}(\tilde{u}_L, \lambda), \tilde{u}_L) + B_L^T \lambda - \tilde{f}_L \\ B_E M_{\tilde{u}_E}(\tilde{u}_L, \lambda) + B_L \tilde{u}_L \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

This can be solved with the traditional Newton-Krylov-FETI-DP approach ([2]); see [3]. Putting it all together, in each of these (outer) Newton iterations, M has to be recomputed, resulting in two nested Newton loops.

3 A Problem-Dependent Choice of the Elimination Set

In [3], we have considered four different variants of Nonlinear-FETI-DP which are denoted as NL- i , $i = 1, \dots, 4$. In all these methods, the elimination set is chosen a priori with respect to the sets I , Δ , and Π . We have $E_{\text{NL-1}} = \emptyset$, $E_{\text{NL-2}} = [I \ \Delta \ \Pi]$, $E_{\text{NL-3}} = [I \ \Delta]$, and $E_{\text{NL-4}} = [I]$. In our earlier experiments, these methods often improved the nonlinear convergence behavior compared to the traditional Newton-Krylov-FETI-DP approach; see [3]. Furthermore, NL-3 and NL-4 show a high potential in reducing the computing time for large problems since the nonlinear elimination can be carried out completely independently for each subdomain without the need for communication and synchronization. For further information, we refer to [3] and the references therein.

However, we have also considered a model problem in [3] for which the performance of NL-4 is worse than the traditional NK-FETI-DP approach. This demonstrates that the choice of a good elimination set is essential for the performance of nonlinear FETI-DP methods. At the same time, it also suggests that there are problems for which the other NL-FETI-DP variants might perform poorly. Accordingly, we should incorporate information about the problem into the choice of the elimination set in order to construct a nonlinear FETI-DP method that is tailored to the specific problem in the best possible way.

In this paper, we introduce a Nonlinear-FETI-DP method with problem-dependent or adaptive elimination sets, which are determined with respect to the residual of the nonlinear saddle point system eq. (1). This strategy is inspired by an article by Gong and Cai [1], where a similar approach was presented in the context of a nonlinear elimination preconditioned inexact Newton method. The underlying idea is that the elimination set contains all variables corresponding to large absolute values in the

nonlinear residual. First studies for the use in nonlinear FETI-DP methods are also presented in [6, 7].

Let us first specify the residual that we consider. As usual, we are interested in finding the solution (u^*, λ^*) of $A(u^*, \lambda^*) = 0$ with $(u^*, \lambda^*) = M(\tilde{u}, \lambda)$. Especially, we are interested in the first component u^* , since the Lagrange multipliers are only introduced to guarantee continuity of the final solution across the interface. Therefore, we do not consider the complete residual of the nonlinear saddle point system but only the part belonging to the variable \tilde{u} . Let us assume that we have finished the k -th outer iteration, i.e., we have computed $\lambda^{(k)} = \lambda^{(k-1)} - \delta\lambda^{(k-1)}$ and $\tilde{u}^{(k)} = g^{(k-1)} - \delta\tilde{u}^{(k-1)}$, where $g^{(k-1)} := \left[M_{\tilde{u}_E} \left(\tilde{u}_L^{(k-1)}, \lambda^{(k-1)} \right), \tilde{u}_L^{(k-1)} \right]$ is the vector after eliminating \tilde{u}_E and $\delta\lambda^{(k-1)}, \delta\tilde{u}^{(k-1)}$ are the corresponding Newton updates. Thus, $g^{(k-1)}$ includes the solution of the inner Newton method in the k -th outer loop. Then, the elimination set for iteration $k + 1$ is build with respect to the residual

$$A \left(\tilde{u}^{(k)}, \lambda^{(k)} \right) \Big|_{\tilde{u}} = \tilde{K} \left(\tilde{u}^{(k)} \right) + B^T \lambda^{(k)} - \tilde{f};$$

cf. the first line of eq. (1). As the tilde indicates, all quantities are only assembled in the primal variables and might have different values in a physical point belonging to more than one subdomain. To obtain a single value for each global degree of freedom, we make use of the dual assembly operator $R_\Delta^T : \tilde{W} \rightarrow \tilde{W}$ which yields the residual

$$\bar{r}^{(k)} := R_\Delta^T \cdot A \left(\tilde{u}^{(k)}, \lambda^{(k)} \right) \Big|_{\tilde{u}}.$$

From $R_\Delta^T B^T \lambda^{(k)} = 0$, we obtain

$$\bar{r}^{(k)} = R_\Delta^T \tilde{K} \left(\tilde{u}^{(k)} \right) - R_\Delta^T \tilde{f} = R_\Delta^T R_\Pi^T K \left(R_\Pi \tilde{u}^{(k)} \right) - R_\Delta^T R_\Pi^T f,$$

where $R_\Pi^T : W \rightarrow \tilde{W}$ is the assembly operator in the primal variables; see, e.g. [2]. From the last line of [3, Eq. 17], we obtain

$$B g^{(k-1)} - B_E \delta\tilde{u}_E^{(k-1)} - B_L \delta\tilde{u}_L^{(k-1)} = B \left(g^{(k-1)} - \delta\tilde{u}^{(k-1)} \right) = 0,$$

which automatically implies that $\tilde{u}^{(k)}$ is continuous across the interface. Thus, the residual is identical to the fully assembled residual $R_\Delta^T R_\Pi^T K \left(R_\Pi R_\Delta \tilde{u}^{(k)} \right) - R_\Delta^T R_\Pi^T f = R^T K \left(R \tilde{u}^{(k)} \right) - R^T f$ as long as we use a step length equal to 1 in the outer Newton iteration, which we assume throughout this article for simplicity.

Next, we describe the process how to assign variables to the elimination set used for the outer iteration $k + 1$. Similar to [7], we introduce the following notation. We assume that we have n finite element nodes with l degrees of freedom each and introduce the two index sets $\mathcal{N} := \{1, \dots, n\}$ and $\mathcal{D} := \{1, \dots, m\}$, where the overall number of degrees of freedom belonging to \tilde{u} or $\bar{r}^{(k)}$ computes as $m = n \cdot l$. Since we have l degrees of freedom for each finite element node, the residual vector $\bar{r}^{(k)}$

decomposes into n subvectors $\bar{r}_{(i)}^{(k)} \in \mathbb{R}^l, i \in \mathcal{N}$, where the entries $\bar{r}_{(i)_j}^{(k)}, j = 1, \dots, l$, belong to the corresponding degrees of freedom of finite element node i . Analogously to [1], the idea is to assign those degrees of freedom to the elimination set $E^{(k+1)}$ which correspond to a finite element node i with at least one degree of freedom with a high absolute residual value, i.e., $\|\bar{r}_{(i)}^{(k)}\|_\infty \geq \rho_{\text{res}} \cdot \|\bar{r}^{(k)}\|_\infty$, where $\rho_{\text{res}} \in (0, 1]$ is a tolerance specified by the user. Let us note that thus all degrees of freedom belonging to the same physical node are either all assigned to $E^{(k+1)}$ or not. Hence, the size of the elimination set increases with a decreasing tolerance. Consequently, the index set of degrees of freedom that belong to the elimination set writes

$$E^{(k+1)} := \left\{ i_1, \dots, i_l \in \mathcal{D} \mid i \in \mathcal{N}, \|\bar{r}_{(i)}^{(k)}\|_\infty \geq \rho_{\text{res}} \cdot \|\bar{r}^{(k)}\|_\infty \right\}.$$

For the final elimination set $E^{(k+1)}$, we introduce a $\delta_{\text{res}} \in \mathbb{R}$ and extend the index set $\mathcal{D}_E^{(k+1)}$ with the indices of degrees of freedom belonging to finite element nodes with a distance of at most δ_{res} to any finite element node whose degrees of freedom have been assigned to $\mathcal{D}_E^{(k+1)}$; see c) and d) in fig. 1. Denoting the coordinates of finite element node i with v_i , the final elimination set writes

$$E^{(k+1)} := \mathcal{D}_E^{(k+1)} \cup \left\{ i_1, \dots, i_l \in \mathcal{D} \mid \begin{array}{l} i \in \mathcal{N}, \|\bar{r}_{(i)}^{(k)}\|_\infty < \rho_{\text{res}} \cdot \|\bar{r}^{(k)}\|_\infty, \\ \exists s \in \mathcal{N}, \|\bar{r}_{(s)}^{(k)}\|_\infty \geq \rho_{\text{res}} \cdot \|\bar{r}^{(k)}\|_\infty : \text{dist}(v_i, v_s) \leq \delta_{\text{res}} \end{array} \right\}.$$

Following [1], this δ_{res} is introduced to avoid sharp jumps in the residual function. With this strategy, we are able to construct a new elimination set $E^{(k)}$ in each outer Newton iteration. However, if the problem at hand is completely unknown and the initial value is somehow random, it might be disadvantageous to choose an elimination set based on the initial residual. In such cases, we recommend to choose $E^{(1)} = \emptyset$ in the first iteration before switching to the elimination strategy.

4 Numerical Results

In this section, we present numerical results for a first problem-dependent nonlinear FETI-DP variant. Since the elimination set is build with respect to the nonlinear residual, we refer to this method as Nonlinear-FETI-DP-Res method or, shorter, NL-Res. Within this section, we discuss different variants of NL-Res specified by different choices of ρ_{res} and δ_{res} . Moreover, for a single $(\rho_{\text{res}}, \delta_{\text{res}})$ pair, we compare the numerical results to those of NL- $i, i = 1, \dots, 4$. We do not compare to the traditional NK-FETI-DP approach since the NL-1 method without the computation of an initial value (see [3, 2]) is closely related to it. To distinguish between different variants of NL-Res in our tables and figures, we introduce the notation NL-R($\rho_{\text{res}}, \eta_{\text{res}}$), with $\eta_{\text{res}} \cdot h = \delta_{\text{res}}$ and h is the diameter of a finite element.

The results shown in this section have all been computed using our sequential MATLAB implementation. If we exceed 80 inner Newton iterations within a single elimination process or if more than 40 outer Newton iterations are required, the sim-

ulation is terminated and considered as diverged. Inner and outer Newton iterations reach convergence if $\|\tilde{K}_E(M_{\tilde{u}_E}(\tilde{u}_L, \lambda), \tilde{u}_L) + B_E^T \lambda - \tilde{f}_E\|_{L_2} \leq 1e-12$ (see eq. (2)) and $\|A(\tilde{u}, \lambda)\|_{L_2} \leq 1e-12$, respectively. Here, we consider two-dimensional scalar model problems of the form

$$\begin{aligned} -\alpha \Delta_4 u - \beta \Delta_2 u &= 1 \text{ in } \Omega, \\ u &= 0 \text{ on } \partial\Omega, \end{aligned}$$

where $\alpha, \beta : \Omega \rightarrow \mathbb{R}$ and $\Delta_p u$ is the p -Laplace operator with $p = 2, 4$. For model problems from nonlinear elasticity (2D) with and without contact, we refer to [6, 7].

As a computational domain Ω , we always consider the unit square and a decomposition into equally sized square subdomains of diameter H . Each subdomain is discretized by equally sized piecewise linear finite elements (P1) of diameter h . As primal variables, we exclusively use subdomain vertices which is the most simple choice. Analogously to [4], we have to measure the parallel potential of our non-

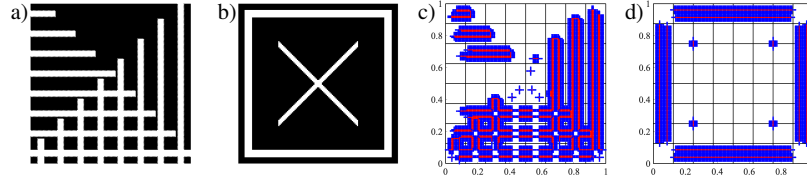


Fig. 1 a) and b): Different types of coefficient distributions. We have $\alpha = 1, \beta = 0$ in the white areas and $\alpha = 0, \beta = 1$ in the remaining (black) part. All channels as well as the cross have a width of $H/3$. c) and d): First elimination sets for NL-Res(0.1,3) for coefficients presented in a) and b). Red points belong to $\mathcal{D}_E^{(1)}$ and blue points are added due to a distance along main axes not larger than $3h$ to a red point; see section 3.

linear FETI-DP methods by considering different metrics and indicators due to our sequential MATLAB implementation. However, we have to look at slightly different indicators compared to [4], since the structure of the elimination set of NL-Res is flexible and not known a priori.

As before, we measure the need for global communication by counting the number of Krylov iterations, which are denoted as “# Krylov Its.“. In addition to that, we also count inner (“# Inner Its.“) and outer (“# Outer Its.“) Newton iterations. Note that each outer Newton iteration requires a factorization of the FETI-DP coarse problem, which is also true for each iteration in the elimination process of NL-2. In contrast to this, in NL-3 and NL-4 no coarse components are eliminated and thus a coarse factorization is only necessary in the outer loop. This property offers a higher potential for parallelization and we therefore precisely distinguished in [3] between the number of necessary coarse and local factorizations to measure the performance of the different nonlinear FETI-DP methods. In NL-Res, the elimination set is chosen problem-dependent and can contain arbitrary parts of the coarse problem and arbitrary parts of the local subdomains. Simply counting local and coarse factorizations is thus

not sufficient anymore. Here, to measure the cost of the inner Newton iteration, we introduce the average size of the elimination set as an additional indicator, which allows us to evaluate the efficiency of our nonlinear FETI-DP variants. A single iteration of the elimination process is expected to be cheaper for a small elimination set. Accordingly, the most efficient nonlinear FETI-DP method has minimal inner and outer iteration numbers and, at the same time, the smallest average size of the elimination set.

First studies regarding the NL-Res approach have been carried out for the p -Laplace problem in [6, 7]. For relatively simple distributions of nonlinearity, parameters ρ_{res} and δ_{res} have been found in [7] such that the NL-Res variant yields quite similar iteration numbers compared to the best NL-FETI-DP- i method, $i = 2, 3, 4$, but using a significantly smaller average size of the elimination set E for each outer Newton iteration. Additionally, for most tested pairs of ρ_{res} and δ_{res} the NL-Res method was at least robust and converged in an acceptable number of iterations. However, in preliminary considerations of more complex distributions of nonlinearity, we already observed a significant influence of the choice of parameters on the convergence behavior of NL-Res, which complicates the right choice. The focus of this article is to discuss this observation in detail. Therefore, we consider two very complex distributions of nonlinearity; see a) and b) in fig. 1. For both problems, we obtain similar results; see table 1 as well as fig. 2. It turns out that NL-4 is the best variant of the more traditional nonlinear FETI-DP methods. Compared to NL-1 without the computation of an initial value, the number of outer Newton iterations is reduced by a factor of 2 to 3 for the largest problem sizes for both model problems.

Table 1 Simulation results of different variants of the NL-Res approach as well as the NL-1 method without computation of an initial value and the best nonlinear FETI-DP method with a constant non-empty elimination set which is NL-4 in this case. For the distribution of the coefficients; see fig. 1 a). Computational domain $\Omega = [0, 1]^2$ decomposed into 8×8 square subdomains discretized with P1 elements; $H/h = 16$.

	NL-1 no Init.	NL-4	NL-R (0.8,0)	NL-R (0.8,3)	NL-R (0.8,5)	NL-R (0.5,0)	NL-R (0.5,3)	NL-R (0.5,5)	NL-R (0.1,0)	NL-R (0.1,3)	NL-R (0.1,5)	NL-R (0.01,0)	NL-R (0.01,3)	NL-R (0.01,5)
Inner Its.	-	37	55	62	61	56	68	72	122	no	71	63	no	37
Outer Its.	15	8	14	13	13	13	13	12	18	conv.	11	12	conv.	6
Krylov Its.	307	155	287	270	267	268	256	240	355		220	207		112
Avg. Size E [%]	0.00	89.44	0.04	0.33	0.51	0.17	1.41	2.10	1.48		9.46	9.43		23.75

The performance of the various NL-Res methods can be summarized as follows: if the combination of ρ_{res} and δ_{res} leads to extremely small elimination sets, the performance of NL-Res is quite similar to that of NL-1 without the computation of an initial value. However, with the right choice of parameters, we also find variants of NL-Res that give iteration numbers at least as good as NL-4. In that case NL-Res is superior due to the much smaller average size of E . Let us remark that NL-Res(0.01,5) seems to be a good choice for both problems. However, as already mentioned, finding the right parameters is difficult. This is demonstrated by the results presented in table 1, where a small change in δ_{res} turns the best NL-Res methods (NL-Res(0.01,5) and NL-Res(0.1,5)) into non-convergent variants

(NL-Res(0.01,3) and NL-Res(0.1,3)). This hints that the elimination set cannot be chosen completely arbitrarily and especially the optimal selection of parameters has to be further analyzed; this is ongoing research. To summarize, choosing the

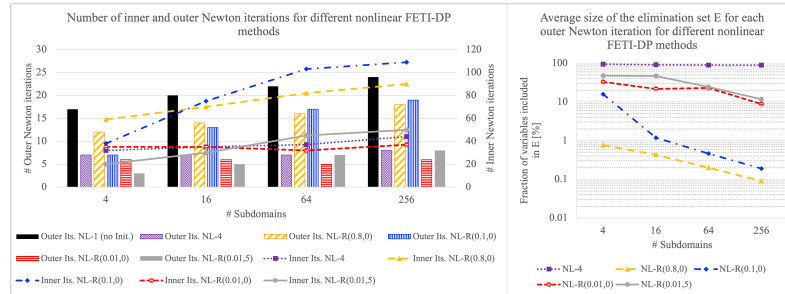


Fig. 2 Simulation results of different nonlinear FETI-DP methods including different variants of NL-Res with problem-dependent choices of the elimination set for the p-Laplace equation with a coefficient distribution as presented in fig. 1 b); square subdomains; P1 finite elements; $H/h = 16$.

right parameters is crucial for the performance of NL-Res methods, but with the right parameters, NL-Res yields similar iteration numbers compared to the best of the more traditional NL-FETI-DP- i methods, $i = 2, 3, 4$. The advantage is a variable elimination set, which is formed depending on the problem. This results in a significantly smaller average size of the elimination set and thus less computational effort in the inner loops.

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