# A Nonlinear FETI-DP Method with an Inexact Coarse Problem

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**Abstract** A new nonlinear version of the well-known FETI-DP method (Finite Element Tearing and Interconnecting Dual-Primal) is introduced. In this method, the nonlinear problem is decomposed before linearization. Nonlinear approaches to domain decomposition can be viewed as a strategy to localize computational work for the efficient use with future extreme-scale supercomputers. As opposed to known nonlinear FETI-DP algorithms, in the new method the coarse solver can be replaced by a preconditioner, i.e., the coarse solve can be inexact. It is expected that the new method can show a superior parallel scalability if the number of subdomains is large. If the coarse solver is exact and the method is applied to linear problems then the method is equivalent to the standard FETI-DP method. Numerical results for up to 32768 cores are presented using cycles of an algebraic multigrid for the coarse problem of the new method.

**Key words:** Domain Decomposition, FETI-DP, Nonlinear

## 1 Introduction

We present a new nonoverlapping, nonlinear domain decomposition method with an inexact solution of the coarse problem. The method can be seen as an inexact reduced version of a recent nonlinear FETI-DP method [27].

In this method, the nonlinear problem is decomposed before linearization. This is opposed to standard Newton-Krylov-Domain-Decomposition methods

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where the decomposition is performed after linearization. Nonlinear FETI-DP methods were introduced in [26, 27] as nonlinear versions of the well known family of FETI-DP domain decomposition methods.

In domain decomposition methods of the FETI-DP [17, 16, 31, 32, 29, 33] and BDDC type [13, 9, 35, 34, 36] the coarse spaces are constructed from partial assembly of the finite elements. This has facilitated the extension of the scalability of these methods, see, e.g., [44, 37, 28, 30, 43, 41]. Inexact FETI-DP methods were introduced in [28] and their parallel scalability has been demonstrated in [31, 40].

Nonlinear approaches to domain decomposition are not new but have attracted recent interest as a strategy to localize computational work. Reduction of communication and synchronization is expected to be crucial to obtain good performance on future supercomputers.

The nonlinear, overlapping ASPIN (Additive Schwarz Preconditioned Inexact Newton) approach was introduced in Cai and Keyes [6]. See also [6, 25, 7, 24] and Groß and Krause [22, 21]. Nonlinear domain decomposition as a coupling method has been used, e.g., in fluid-structure interaction; see Deparis et al. [12, 11], Deparis [10], or Fernandez et al. [18]; it has also been used for the coupling of multiphase flow, see, e.g., Ganis et al. [20, 19]. Nonlinear FETI-1 methods were introduced in Pebrel at al. [39], nonlinear Neumann-Neumann methods, as a scalable solver approach, in Bordeu et al. [4]. Nonlinear Schwarz methods as a solver, i.e., not as a preconditioner, have already been considered much earlier, see, e.g., [14, 5]. The solution of local nonlinear problems can also be embedded into standard methods and has been denoted nonlinear localization; see Cresta et al. [8].

## 2 Nonlinear FETI-DP formulation

Let $\Omega_i, i = 1, \dots, N$, be a decomposition of the domain $\Omega \subset \mathbb{R}^d,\ d = 2, 3$, into nonoverlapping subdomains. Each subdomain is a union of finite elements. We denote the associated local finite element spaces by $W_i$ and the product space by $W = W_1 \times \dots \times W_N$. We consider the minimization of a nonlinear energy $J : V^h \to \mathbb{R}$,

$$J(u) = \textstyle\sum_{i=1}^{N} J_i(u_i), \tag{1}$$

where the $J_i : W_i \to \mathbb{R}$, $i = 1, \dots, N$ are local energy functionals on the subdomains $\Omega_i$. For standard problems, such as nonlinear elasticity, discretized by finite elements the global energy can be written as a sum of the local nonlinear energies on the nonoverlapping subdomains; for details, see [27].

Let $\varphi_{i,j}$, $i = 1, \dots, N$, $j = 1, \dots, N_i$ the nodal finite element basis functions for the local finite element space $W_i$. We write $J_i'(u_i)(\varphi_{i,j})$ in the form

$$J_i'(u_i)(\varphi_{i,j}) = (K_i(u_i) - f_i)_j$$

where $K_i(u_i)$ depends on $u_i$ and $f_i$ is independent of $u_i$.

Let us define the nonlinear, discrete block operator $K(u)$ and the corresponding block vectors $u$ and $f$, i.e.,

$$K(u) := \begin{pmatrix} K_1(u_1) \\ \vdots \\ K_N(u_N) \end{pmatrix}, \quad f := \begin{pmatrix} f_1 \\ \vdots \\ f_N \end{pmatrix}, \quad \text{and} \quad u := \begin{pmatrix} u_1 \\ \vdots \\ u_N \end{pmatrix}. \tag{2}$$

We then define the nonlinear, partially assembled operator $\widetilde{K}(\tilde{u}) := R_{\Pi}^T K(R_{\Pi}\tilde{u})$,and the corresponding partially assembled right hand side $\tilde{f} := R_{\Pi}^T f$. Here we use the FETI-DP partial assembly operator $R_{\Pi}^T$ that is also used to define the coarse problem of standard (linear) FETI-DP methods; see, e.g., [29, 42] for the notation. Let $B$ be the standard FETI-DP jump operator, we can then introduce the nonlinear FETI-DP master system [26, 27]

$$\begin{aligned} &\widetilde{K}(\tilde{u}) + B^T\lambda - \tilde{f} = 0 \\ &B\tilde{u} \qquad\qquad\quad\;\; = 0. \end{aligned} \tag{3}$$

The nonlinear FETI-DP methods Nonlinear-FETI-DP-1 (NL-1) and Nonlinear-FETI-DP-2 (NL-2), see [26, 27], are also based on the master system (3).

We assume that, as a result of a sufficient number of primal constraints, the operator $\widetilde{K}$ is continuously differentiable and locally invertible. We use Newton's method applied to (3) to obtain fast local convergence and a line search as globalization strategy.

## 3 An Inexact Reduced Nonlinear FETI-DP Method

Newton's method applied to (3) results in the linearized system

$$\begin{bmatrix} D\widetilde{K}(\tilde{u}) & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} \Delta\tilde{u} \\ \Delta\lambda \end{bmatrix} = \begin{bmatrix} \widetilde{K}(\tilde{u}) + B^T\lambda - \tilde{f} \\ B\tilde{u} \end{bmatrix}. \tag{4}$$

Following the standard FETI-DP approach, we partition $\Delta\tilde{u}$ into the primal variables $\Delta\tilde{u}_{\Pi}$ and the dual variables $\Delta\tilde{u}_B$, i.e., $\Delta\tilde{u}^T = \begin{bmatrix} \Delta u_B^T & \Delta\tilde{u}_{\Pi}^T \end{bmatrix}$. We then obtain from (4) the system

$$\begin{bmatrix} (D\widetilde{K}(\tilde{u}))_{BB} & (D\widetilde{K}(\tilde{u}))_{\Pi B}^T & B_B^T \\ (D\widetilde{K}(\tilde{u}))_{\Pi B} & (D\widetilde{K}(\tilde{u}))_{\Pi\Pi} & 0 \\ B_B & 0 & 0 \end{bmatrix} \begin{bmatrix} \Delta u_B \\ \Delta\tilde{u}_{\Pi} \\ \Delta\lambda \end{bmatrix} = \begin{bmatrix} (\widetilde{K}(\tilde{u}))_B + B_B^T\lambda - f_B \\ (\widetilde{K}(\tilde{u}))_{\Pi} - \tilde{f}_{\Pi} \\ B_B u_B \end{bmatrix}. \tag{5}$$

Assuming enough primal constraints such that $(D\widetilde{K}(\tilde{u}))_{BB}$ is invertible, we then eliminate of $u_B$ and obtain a reduced system

$$\begin{bmatrix} \widetilde{S}_{\Pi\Pi} & -(D\widetilde{K}(\tilde{u}))_{\Pi B}(D\widetilde{K}(\tilde{u}))_{BB}^{-1}B_B^T \\ -B_B(D\widetilde{K}(\tilde{u}))_{BB}^{-1}(D\widetilde{K}(\tilde{u}))_{\Pi B}^T & -B_B(D\widetilde{K}(\tilde{u}))_{BB}^{-1}B_B^T \end{bmatrix} \begin{bmatrix} \Delta\tilde{u}_\Pi \\ \Delta\lambda \end{bmatrix}$$
$$= \begin{bmatrix} (\widetilde{K}(\tilde{u}))_\Pi - \tilde{f}_\Pi - (D\widetilde{K}(\tilde{u})_{\Pi B}(D\widetilde{K}(\tilde{u}))_{BB}^{-1}\big((\widetilde{K}(\tilde{u}))_B + B_B^T\lambda - f_B\big) \\ B_B u_B - B_B(D\widetilde{K}(\tilde{u}))_{BB}^{-1}\big((\widetilde{K}(\tilde{u}))_B + B_B^T\lambda - f_B\big) \end{bmatrix} \tag{6}$$

which we write as $\mathcal{A}_r x_r = \mathcal{F}_r$ using the same notation as in [28] for linear problems. The Schur complement

$$\widetilde{S}_{\Pi\Pi} = (D\widetilde{K}(\tilde{u}))_{\Pi\Pi} - (D\widetilde{K}(\tilde{u}))_{\Pi B}(D\widetilde{K}(\tilde{u}))_{BB}^{-1}(D\widetilde{K}(\tilde{u}))_{\Pi B}^T \tag{7}$$

is the coarse problem of the FETI-DP method. In this paper, we will apply a preconditioned Krylov method to the block system (6), using the block-triangular preconditioner

$$\widehat{\mathcal{B}}_r^{-1} = \begin{bmatrix} \widehat{S}_{\Pi\Pi}^{-1} & 0 \\ -M^{-1}B_B(D\widetilde{K}(\tilde{u})_{BB}^{-1}(D\widetilde{K}(\tilde{u}))_{\Pi B}^T\widehat{S}_{\Pi\Pi}^{-1} & -M^{-1} \end{bmatrix} \tag{8}$$

cf. [28, 31], where the irFETI-DP method (inexact reduced FETI-DP) for linear problems was introduced.

Here, $M^{-1}$ is one of the standard FETI-DP preconditioners. In this paper, we always use the Dirichlet preconditioner [42]. Moreover, $\widehat{S}_{\Pi\Pi}^{-1}$ is assumed to be a good preconditioner for the coarse problem $\widetilde{S}_{\Pi\Pi}$. Since the preconditioner (8) is unsymmetric we have to use a Krylov space method suitable for unsymmetric systems. In this paper we will use GMRES. The use of conjugate gradients requires a symmetric reformulation.

In this nonlinear FETI-DP method the continuity of the solution is, in general, not reached until convergence of the Newton method. This is different from FETI-DP methods applied after Newton linearization where each Newton iterate is continuous. This method is thus not identical to a standard Newton-Krylov FETI-DP approach.

Note that the elimination of $\tilde{u}_\Pi$ from (6) leads to the Nonlinear-FETI-DP-1 (NL1) method $F_{NL1}\Delta\lambda = d$, introduced in [26, 27]. But this requires an exact solver for $\widetilde{S}_{\Pi\Pi}$.

## 4 Initial Values for the Nonlinear FETI-DP Method

The convergence of Newton-type methods depends on a good initial value. We are interested to find a suitable initial value $\tilde{u}^{(0)}$ for the Newton iteration presented in Section 3. This initial value has to be continuous in all primal variables $\tilde{u}_\Pi^{(0)}$ but may be discontinuous in the dual variables $u_B^{(0)}$. Of course, it should provide a good local approximation of the problem. We can obtain such an initial value $\tilde{u}^{(0)}$ from solving the nonlinear problem

$$\widetilde{K}(\tilde{u}^{(0)}) = \tilde{f} - B^T \lambda^{(0)} \tag{9}$$

by some Newton type iteration for some given initial value $\lambda^{(0)}$. In this paper we set $\lambda^{(0)} = 0$. The solution of (9) requires the solution of local nonlinear subdomain problems which are only coupled in the primal unknowns. This step thus requires only communication in the primal variables and is otherwise completely parallel. It may be seen as a nonlinear localization step.

Linearization of (9) results in

$$\begin{bmatrix} (D\widetilde{K}(\tilde{u}))_{BB} & (D\widetilde{K}(\tilde{u}))_{\Pi B}^T \\ (D\widetilde{K}(\tilde{u}))_{\Pi B} & (D\widetilde{K}(\tilde{u}))_{\Pi\Pi} \end{bmatrix} \begin{bmatrix} u_B \\ \tilde{u}_\Pi \end{bmatrix} = \begin{bmatrix} (\widetilde{K}(\tilde{u}))_B + B_B^T \lambda - f_B \\ (D\widetilde{K}(\tilde{u}))_\Pi - \tilde{f}_\Pi \end{bmatrix}.$$

A block elimination of $u_B$ yields the symmetric system

$$\widetilde{S}_{\Pi\Pi} \tilde{u} = \tilde{d}_\Pi \tag{10}$$

where $\widetilde{S}_{\Pi\Pi}$ is defined as in (7). We solve (10) by a Krylov method using the preconditioner $\widehat{S}_{\Pi\Pi}^{-1}$; see (8).

| N (=Cores) | Solver | Krylov-It. | Factor. | max. cond. | max. It. | Krylov-Time | Runtime |
|---|---|---|---|---|---|---|---|
| 16 | Newton-Krylov FETI-DP | 11 | 1 | 7.3 | 11 | .74s | **5.3s** |
| | Newton-Krylov irFETI-DP | 11 | 1 | 7.3 | 11 | .91s | **5.5s** |
| | irNonlinear-FETI-DP-1 | 11 | 1 | 7.3 | 11 | .92s | **5.4s** |
| 64 | Newton-Krylov FETI-DP | 22 | 1 | 8.1 | 22 | 1.5s | **6.3s** |
| | Newton-Krylov irFETI-DP | 22 | 1 | 8.0 | 22 | 2.0s | **6.7s** |
| | irNonlinear-FETI-DP-1 | 21 | 1 | 8.2 | 21 | 2.1s | **6.9s** |
| 256 | Newton-Krylov FETI-DP | 32 | 1 | 8.3 | 32 | 2.3s | **7.4s** |
| | Newton-Krylov irFETI-DP | 30 | 1 | 8.1 | 30 | 3.2s | **8.3s** |
| | irNonlinear-FETI-DP-1 | 30 | 1 | 8.3 | 30 | 4.7s | **9.9s** |
| 1024 | Newton-Krylov FETI-DP | 32 | 1 | 8.4 | 32 | 2.5s | **8.8s** |
| | Newton-Krylov irFETI-DP | 30 | 1 | 8.3 | 30 | 4.2s | **10.8s** |
| | irNonlinear-FETI-DP-1 | 28 | 1 | 8.4 | 28 | 4.3s | **11.0s** |

**Table 1** Sanity check (irNonlinear-FETI-DP-1); Cray XT6: $H/h = 256$, standard linear Laplace, Alg. A.

## 5 Numerical Results

In this section, we compare the standard Newton-Krylov approach, using either the standard FETI-DP method or the irFETI-DP [28, 31] method as

| | NK-irFETI-DP | | | irNL-FETI-DP-1 | | |
|---|---|---|---|---|---|---|
| N (Cores) | Runtime | Krylov-It. | Krylov-Time | Runtime | Krylov-It. | Krylov-Time |
| 64 (1) | 92.3s | 92 | 23.6s | 90.5s | 19 | 5.5s |
| 256 (4) | 126.5s | 88 | 31.4s | 107.0s | 20 | 7.2s |
| 1024 (16) | 91.2s | 68 | 27.9s | 97.4s | 20 | 8.2s |
| 4096 (64) | 111.8s | 67 | 30.2s | 100.9s | 20 | 9.1s |
| 16 384 (256) | 113.7s | 67 | 28.5s | 102.5s | 20 | 8.5s |
| 65 536 (1024) | 130.9s | 65 | 32.0s | 110.5s | 20 | 9.9s |

**Table 2** Comparison a standard Newton-Krylov irFETI-DP approach with the nonlinear method; Cray XT6: $H/h = 80$, $\Delta + 4\Delta_p$, $p = 4$, Alg. A.

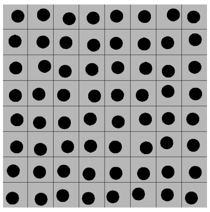
a solver, and the new nonlinear domain decomposition approach, i.e., the irNonlinear-FETI-DP-1 approach. We have implemented the algorithm pre-

| Inexact-Reduced-Nonlinear-FETI-DP (irNL-FETI-DP-1) | | | |
|---|---|---|---|
| N (=Cores) | Step | Time | Krylov-It. |
| 16 | Newton Init 1: | 5.2s | 0 |
| | Newton Init 2: | 5.2s | 0 |
| | Newton Init 3: | 5.2s | 0 |
| | Newton Init 4: | 5.2s | 0 |
| | Newton Full 1: | 7.3s | 9 |
| 64 | Newton Init 1: | 5.3s | 0 |
| | Newton Init 2: | 5.2s | 0 |
| | Newton Init 3: | 5.2s | 0 |
| | Newton Init 4: | 5.2s | 0 |
| | Newton Full 1: | 8.2s | 17 |
| 256 | Newton Init 1: | 5.4s | 0 |
| | Newton Init 2: | 5.4s | 0 |
| | Newton Init 3: | 5.4s | 0 |
| | Newton Init 4: | 5.4s | 0 |
| | Newton Full 1: | 9.5s | 21 |
| 1 024 | Newton Init 1: | 5.8s | 0 |
| | Newton Init 2: | 5.9s | 0 |
| | Newton Init 3: | 5.8s | 0 |
| | Newton Init 4: | 5.9s | 0 |
| | Newton Full 1: | 10.4s | 20 |
| 4 096 | Newton Init 1: | 7.6s | 0 |
| | Newton Init 2: | 7.5s | 0 |
| | Newton Init 3: | 7.5s | 0 |
| | Newton Init 4: | 7.5s | 0 |
| | Newton Full 1: | 13.1s | 20 |

**Table 3** irNonlinear-FETI-DP-1 on the MIRA Supercomputer (BG/P) Argonne National Laboratory; $\Delta + 4\Delta_p$, $p = 4$, $H/h = 128$. Alg. A.; joint work with **B. Smith and S. Balay (Argonne National Laboratory)**; uses only 4 out of 16 BG/Q cores. “Newton Init” refers to a Newton step for solving (9) whereas “Newton Full” refers to a Newton step for solving (3). A single full Newton step is sufficient for this problem after four steps to compute the initial value.

| Inexact-Reduced-Nonlinear-FETI-DP (irNL-FETI-DP-1) | | | | | | |
|---|---|---|---|---|---|---|
| **Nx x Ny = N (=Cores)** | **d.o.f.** | **Krylov-It.** | **Newton steps Init / Full** | **Krylov-Time** | **Runtime** | **eff.** |
| 32 | 9 443 329 | 26 | 8 / 1 | 4.19s | 112.5s | 100% |
| 128 | 37 761 025 | 31 | 8 / 1 | 5.07s | 117.8s | 96% |
| 512 | 151 019 521 | 33 | 8 / 1 | 5.49s | 119.1s | 95% |
| 2 048 | 604 028 929 | 33 | 8 / 1 | 5.65s | 119.1s | 95% |
| 8 192 | 2 416 017 409 | 34 | 8 / 1 | 6.01s | 127.9s | 88% |
| 32 768 | 9 663 873 025 | 34 | 8 / 1 | 9.13s | 151.4s | 74% |

**Table 4** irNonlinear-FETI-DP-1 on the SuperMUC supercomputer at Leibniz-Rechenzentrum in Munich; $\Delta + 4\Delta_p, p = 4, Hx/hx = 768, Hy/hy = 384$; the algorithm uses all 16 cores of the node; "Newton Init" refers to a Newton step for solving (9) whereas "Newton Full" refers to a Newton step for solving (3).



| irNL-FETI-DP-1 for Hyperelasticity | | | |
|---|---|---|---|
| **Cores** | **Problem Size** | **Total Time** | **Total Effic.** |
| 64 | 4M | 127s | 100% |
| 256 | 16M | 139s | 91% |
| 1024 | 67M | 128s | 99% |
| 4096 | 268M | 142s | 89% |

**Table 5** irNonlinear-FETI-DP-1 on the SuperMUC supercomputer at Leibniz-Rechenzentrum (LRZ) in Munich; Neo-Hooke material; $E = 210\,000$ in off-centered circular inclusions in the subdomains and $E = 210$ in the surrounding matrix material; Poisson ratio $\nu = 0.3$;a fixed displacement of 1% in x-direction is prescribed on the boundary.

sented here using PETSc [2, 1, 3]. For all inexact algorithms, the preconditioner $\widehat{S}_{\Pi\Pi}$ for the coarse problem $\widetilde{S}_{\Pi\Pi}$ is formed by applying one iteration of BoomerAMG [23]. BoomerAMG is part of the Hypre library [15]. In all experiments we have used GMRES as a Krylov method. The Newton method is always combined with a line search using the strong Wolfe conditions; see [38]. For a minimization problem $\min_{x\in\mathbb{R}^n} J(x)$ and a descent direction $\Delta x$ the strong Wolfe conditions read $J(x + t\,\Delta x) \leq J(x) + c_1 t\,\nabla^T J(x)\,\Delta x$ and $|\nabla^T J(x + t\,\Delta x)\,\Delta x| \leq c_2 |\nabla^T J(x)\,\Delta x|$ with constants $0 < c_1 < c_2 < 1$, and where $t$ is the step length.

First, we apply all algorithms to a standard linear diffusion problem, see Table 1, as a sanity check. For this linear problem, the initialization phase, see Section 4, is omitted as it is not necessary. The test runs on 16 to 1 024 cores of a Cray XT6 show almost identical numerical and parallel performance of the different algorithms and implementations. This is expected since, for a linear problem, the Newton-Krylov-irFETI-DP method and the irNonlinear-FETI-DP-1 method are equivalent. We do see some increase in the total runtime, mainly due to an increase in the Krylov iteration time. This increase is due to an inefficient parallel distribution of the coarse problem. A redistribution would be necessary on this architecture but was not performed here. In Table 2, we then perform a weak scaling test for a nonlinear problem on the Cray XT6 at Universität Duisburg-Essen using up to 1024 cores. We have considered a nonlinear diffusion problem $\Delta u + 4\Delta_p u = f$ for $p = 4$, where $\Delta$ is the standard Laplacian and $\Delta_p$ is the p-Laplacian. The step length is chosen according to a Wolfe rule. We have considered subdomains of quite small size, i.e., $H/h = 80$, but up to 65536 subdomains.

We can see that the new method is competetive and significantly reduces the number of Krylov iterations. As a result, the inexact reduced Nonlinear-FETI-DP-1 (irNL-1) method is slightly faster.

We then have performed a weak scalability test using 16 to 4096 processor cores of the MIRA supercomputer at the Argonne National Laboratory, see Table 3. We can see that, for this problem, up to four Newton steps are performed in the initialization phase, i.e., to solve (9). No Krylov iteration is necessary in this phase. A single Newton iteration, using between 9 and 21 Krylov iterations, is sufficient to solve the nonlinear problem (3) to the desired relative tolerance of 1e-9. The parallel efficiency drops to 56% from 16 to 4096 processor cores. This was an unexpected result on the BG/Q architecture. Indeed, a performance bug in a parallel norm computation that limited scalability was identified as a result of these experiments.

After eliminating the performance bug we finally have performed a similar weak scalability test using 32 to 32768 processor cores of the SuperMUC supercomputer at the Leibniz-Rechenzentrum in Munich. The results are presented in Table 4. To solve this problem eight Newton steps are performed in the initialization phase and then a single full Newton step is sufficient to reach a tolerance of 1e-10. Overall, the algorithm needs only between 26 and 34 Krylov iterations. The parallel scalability seems satisfactory and we reach an efficiency of 74% using 32768 cores compared to the baseline of 32 cores. Let us remark, that a non negligable amount of time is spent in the MPI initialization called by PETSc in the first Newton step and we expect to obtain even better results in the future.

Finally, in Table 5, we report on weak scalability for a problem of nonlinear hyperelasticity on the SuperMUC supercomputer.

## 6 Summary

The new nonlinear FETI-DP method combines the approaches from [27] and [28] and thus can be denoted inexact reduced Nonlinear-FETI-DP-1 (irNL1). An important building block of this method is the solution of nonlinear problems on the subdomains. Algorithmically, the same building blocks as standard FETI-DP methods are used. If exact solvers are used as building blocks the new method shows the same performance as the Nonlinear-FETI-DP-1 method [27]. If an efficient preconditioner is used for the coarse problem then the scalability can be extended substantially.

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