18^{th} International Conference on the Application of Computer
Science and Mathematics in Architecture and Civil Engineering
K. Gürlebeck and C. Könke (eds.)
Weimar, Germany, 07–09 July 2009

SPARSE APPROXIMATE COMPUTATION OF SADDLE-POINT PROBLEMS ARISING FROM FETI-DP DISCRETIZATION

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Keywords: Domain decomposition, Saddle Point, FETI-DP, preconditioners, heterogeneous elasticity problems.

Abstract. *The numerical simulation of microstructure models in 3D requires, due to enormous d.o.f., significant resources of memory as well as parallel computational power. Compared to homogeneous materials, the material hetrogeneity on microscale induced by different material phases demand for adequate computational methods for discretization and solution process of the resulting highly nonlinear problem. To enable an efficient/scalable solution process of the linearized equation systems the heterogeneous FE problem will be described by a FETI-DP (Finite Element Tearing and Interconnecting - Dual Primal) discretization. The fundamental FETI-DP equation can be solved by a number of different approaches. In our approach the FETI-DP problem will be reformulated as Saddle Point system, by eliminating the primal and Lagrangian variables. For the reduced Saddle Point system, only defined by interior and dual variables, special Uzawa algorithms can be adapted for iteratively solving the FETI-DP saddle-point equation system (FETI-DP SPE). A conjugate gradient version of the Uzawa algorithm will be shown as well as some numerical tests regarding to FETI-DP discretization of small examples using the presented solution technique. Furthermore the inversion of the interior-dual Schur complement operator can be approximated using different techniques building an adequate preconditioning matrix and therewith leading to substantial gains in computing time efficiency.*

1 MOTIVATION

Modern digital material approaches, such as multiscale and molecular dynamic simulations, allow to study detailed response of complex, heterogeneous elastic and physical nonlinear material behaviour on various scales. These approaches require enormous hardware resources with respect to computing power and main memory, due to large number of degrees of freedom in the discretized models. For the numerical part the algorithms to be implemented should then be executed in the best way of efficiency and computation time. Actually the modern FETI-DP algorithm based on non-overlapping domain decomposition techniques [1] provide a scalable approach solving large and distributed FE systems. In this paper a modified and robust computation procedure based on reformulated FETI-DP Saddle Point system will be presented. Thereby the solution of the basic FETI-DP equation systems is done by using approximated Jacobi-preconditioners. This approach avoids large numerical efforts of inverting domain stiffness matrices associated with the dual variables.

This paper will present in section 2 the basic dual-primal FETI [2] method. In section 3 the reformulation to a saddle-point equation system (SPE) will be shown as well as approximation techniques for the inversion of the saddle point matrix using special Jacobi-preconditioners. Section 4 continues with two versions of the algorithmic implementation of the FETI-DP SPE, showing a possible adaption of the conjugate gradient (CG) method for the iterative computation of the reformulated FETI-DP saddle-point approximation.

2 FETI-DP DISCRETIZATION METHODS

Iterative domain decomposition methods for non-overlapped partitionings like the FETI-DP method are more efficient as classical Schur complement methods regarding to computational efficiency. For any dual-primal FETI (Finite Element Tearing and Interconnecting, [3]) decomposition the d.o.f. of the resulting domain boundaries are described as primal and dual variables, indicated by index Π and Δ, respectively. All other domain interior d.o.f. are denoted as interior variables. After summarizing the dual and interior variables denoted by index B the unknown nodal vector has three components:

- the displacement vector with interior and dual variables $\mathbf{u}_B$
- the displacement vector with primal variables $\widetilde{\mathbf{u}}_\Pi$
- and the vector of Lagrangian multipliers λ

2.1 Fundamental equation of FETI-DP discretization methods

The fundamental equation for the FETI-DP discretization is given as:

$$\begin{bmatrix} K_{BB} & \widetilde{K}_{\Pi B}^T & B^T \\ \widetilde{K}_{\Pi B} & \widetilde{K}_{\Pi\Pi} & \mathit{0} \\ B & \mathit{0} & \mathit{0} \end{bmatrix} \begin{Bmatrix} \mathbf{u}_B \\ \widetilde{\mathbf{u}}_\Pi \\ \lambda \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_B \\ \widetilde{\mathbf{f}}_\Pi \\ \mathbf{0} \end{Bmatrix} \tag{1}$$

which has been sorted with regard to variables $\mathbf{u}_B$, $\widetilde{\mathbf{u}}_\Pi$, λ. The global FETI-DP matrix in the equation above has the following components described as:

- K_{BB} as block-diagonal matrix resulting from global interior and dual d.o.f.
- $\widetilde{K}_{\Pi\Pi}$ as assembled block-diagonal matrix resulting from primal d.o.f.
- B as jump operator connecting dual d.o.f. of different domains

The final classical FE equation system can be formulated using the above notation. The local stiffness matrices, load vector and vector of unknown variables follow then as:

$$K^{(i)} = \begin{bmatrix} K_{II}^{(i)} & K_{\Delta I}^{(i)T} & K_{\Pi I}^{(i)T} \\ K_{\Delta I}^{(i)} & K_{\Delta\Delta}^{(i)} & K_{\Pi\Delta}^{(i)T} \\ K_{\Pi I}^{(i)} & K_{\Pi\Delta}^{(i)} & K_{\Pi\Pi}^{(i)} \end{bmatrix} \; ; \quad \mathbf{u}^{(i)} = \begin{Bmatrix} \mathbf{u}_I^{(i)} \\ \mathbf{u}_\Delta^{(i)} \\ \mathbf{u}_\Pi^{(i)} \end{Bmatrix} ; \quad \mathbf{f}^{(i)} = \begin{Bmatrix} \mathbf{f}_I^{(i)} \\ \mathbf{f}_\Delta^{(i)} \\ \mathbf{f}_\Pi^{(i)} \end{Bmatrix} \tag{2}$$

with I as interior, Δ as dual and Π as primal indices. Summarizing interior and dual variables denoted by index B the vectors results in:

$$\mathbf{u}_B^{(i)} = \begin{bmatrix} \mathbf{u}_I^{(i)} & \mathbf{u}_\Delta^{(i)} \end{bmatrix}^T ; \qquad \mathbf{f}_B^{(i)} = \begin{bmatrix} \mathbf{f}_I^{(i)} & \mathbf{f}_\Delta^{(i)} \end{bmatrix}^T$$

For the stiffness matrices (local/domain based and assembled) without primal d.o.f. it follows:

$$K_{BB}^{(i)} = \begin{bmatrix} K_{II}^{(i)} & K_{\Delta I}^{(i)T} \\ K_{\Delta I}^{(i)} & K_{\Delta\Delta}^{(i)} \end{bmatrix} \; ; \quad \text{assembled: } K_{BB} = \mathrm{diag}_{i=1}^{N}(K_{BB}^{(i)})$$

The elimination of the interior, dual and primal d.o.f. leads to:

$$\begin{bmatrix} K_{BB} & \widetilde{K}_{\Pi B}^T & B^T \\ 0 & \widetilde{S}_{\Pi\Pi} & -\widetilde{S}_{\alpha\Pi}^T \\ 0 & 0 & -F \end{bmatrix} \begin{bmatrix} \mathbf{u}_B \\ \widetilde{\mathbf{u}}_\Pi \\ \lambda \end{bmatrix} = \begin{bmatrix} \mathbf{f}_B \\ \widetilde{\mathbf{f}}_\Pi - \widetilde{K}_{\Pi B} K_{BB}^{-1} \mathbf{f_B} \\ -\mathbf{d} \end{bmatrix} \tag{3}$$

with

$$\widetilde{S}_{\Pi\Pi} = \widetilde{K}_{\Pi\Pi} - \widetilde{K}_{\Pi B}^T K_{BB}^{-1} \widetilde{K}_{\Pi B} \tag{4}$$

as Schur complement operator of $\widetilde{K}$

$$F = B K_{BB}^{-1} B^T + B K_{BB}^{-1} \widetilde{K}_{\Pi B}^T \widetilde{S}_{\Pi\Pi}^{-1} \widetilde{K}_{\Pi B} K_{BB}^{-1} B^T \tag{5}$$

$$\mathbf{d} = B K_{BB}^{-1} \mathbf{f}_B - B K_{BB}^{-1} \widetilde{K}_{\Pi B}^T \widetilde{S}_{\Pi\Pi}^{-1} \Big(\widetilde{\mathbf{f}}_\Pi - \widetilde{K}_{\Pi B} K_{BB}^{-1} \mathbf{f}_B \Big) \tag{6}$$

The final reduced equation system is given as:

$$F\lambda = \mathbf{d} \tag{7}$$

In most cases F will not be explicitly generated and a (preconditioned) conjugate gradient method is used for the iterative computation of the particular equation systems. In the following section it will be shown how to solve the saddle-point equation system obtained from the above described FETI-DP discretization. Thereby a conjugate gradient version of an Uzawa [4] iteration scheme will be modified for solving the resulting FETI-DP SPE.

3 SOLVING THE FETI-DP SADDLE-POINT PROBLEM

The basic formulation for FETI-DP dicretizations of chapter 2 can be reformulated as Saddle Point equation system (SPE) by simply eliminating the primal variables. The basic notation of the FETI-DP Saddle Point system is given by

$$\begin{bmatrix} K_{BB} & B^T \\ & \\ B & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u}_B \\ \\ \lambda \end{bmatrix} = \begin{bmatrix} \mathbf{f}_{B,mod} \\ \\ 0 \end{bmatrix} \tag{8}$$

with $\mathbf{f}_{B,mod} = \mathbf{f}_B - \widetilde{K}^T_{\Pi B} \widetilde{\mathbf{u}}_\Pi$. The second row of the basic equation system (5) can be written as

$$\widetilde{K}_{\Pi\Pi}\, \widetilde{\mathbf{u}}_\Pi = \widetilde{\mathbf{f}}_\Pi - \widetilde{K}_{\Pi B}\, \mathbf{u}_B \tag{9}$$

The main feature of Saddle Point equation systems results in comfortable solution approach which allows iterative solver techniques for eq. (8) without knowing the exact inversion of K_{BB} and without loosing the optimal scaling properties of the FETI-DP algorithm. One additional advantage occurs with the resulting right hand side, where all terms according to the Langragian multipliers λ are zero, which reduces the original inverting problem to block K_{BB} if $\mathbf{u}_B$ should be iterativly solved. With the first row of eq. (8) it follows:

$$K_{BB}\, \mathbf{u}_B = \mathbf{f}_B - \widetilde{K}^T_{\Pi B}\, \widetilde{\mathbf{u}}_\Pi - B^T \lambda \tag{10}$$

Introducing eq. (9) this equation changes to:

$$K_{BB}\, \mathbf{u}_B = \mathbf{f}_B - \widetilde{K}^T_{\Pi B} \widetilde{K}^{-1}_{\Pi\Pi} \left(\widetilde{\mathbf{f}}_\Pi - \widetilde{K}_{\Pi B} \mathbf{u}_B \right) - B^T \lambda \tag{11}$$

with the definition of $\widetilde{\mathbf{f}}_{B,S}$ and introduction of the interior-dual Schur complement operator $\widetilde{S}_{BB}$ as follows

$$\widetilde{\mathbf{f}}_{B,S} = \widetilde{K}^T_{\Pi B} \widetilde{K}^{-1}_{\Pi\Pi} \widetilde{\mathbf{f}}_\Pi \quad ; \qquad \widetilde{S}_{BB} = K_{BB} - \widetilde{K}^T_{\Pi B} \widetilde{K}^{-1}_{\Pi\Pi} \widetilde{K}_{\Pi B} \tag{12}$$

the final notation leads to:

$$K_{BB}\, \mathbf{u}_B = \mathbf{f}_B - \widetilde{\mathbf{f}}_{B,S} + \left(K_{BB} - \widetilde{S}_{BB} \right) \mathbf{u}_B - B^T \lambda \tag{13}$$

The reduced and inverted FETI-DP SPE becames then to:

$$\mathbf{u}_B = \widetilde{S}^{-1}_{BB} \left(\mathbf{f}_B - \widetilde{\mathbf{f}}_{B,S} - B^T \lambda \right) = \widetilde{S}^{-1}_{BB} \left(\widetilde{\mathbf{g}}_{B,S} - B^T \lambda \right) \tag{14}$$

The modified FETI-DP SPE follows with

$$\begin{bmatrix} \widetilde{S}_{BB} & B^T \\ & \\ B & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u}_B \\ \\ \lambda \end{bmatrix} = \begin{bmatrix} \widetilde{\mathbf{g}}_{B,S} \\ \\ 0 \end{bmatrix} \tag{15}$$

Taking the condition $B\mathbf{u}_B = 0$ and replacing $\mathbf{u}_B$ with the first row of eq. (15) results in

$$B \widetilde{S}^{-1}_{BB} B^T \lambda = B \widetilde{S}^{-1}_{BB} \widetilde{\mathbf{g}}_{B,S} \tag{16}$$

With

$$\widetilde{Q}_{BB} = B\widetilde{S}_{BB}^{-1}B^T \quad and \quad \widetilde{\mathbf{c}}_{B,S} = B\widetilde{S}_{BB}^{-1}\widetilde{\mathbf{g}}_{B,S} \tag{17}$$

the gradient of the quadratic function

$$F(\lambda) = \frac{1}{2}\lambda^T\widetilde{Q}_{BB}\lambda - \widetilde{\mathbf{c}}_{B,S}^T\lambda \tag{18}$$

results in

$$-\nabla F(\lambda^{(k)}) = \widetilde{\mathbf{c}}_{B,S} - \widetilde{Q}_{BB}\lambda = B\widetilde{S}_{BB}^{-1}\widetilde{\mathbf{g}}_{B,S} - B\widetilde{S}_{BB}^{-1}B^T\lambda^{(k)} = B\mathbf{u}_B^{(k)} \tag{19}$$

which corresponds to the basic functional of the conjugate gradient method. Backsubstitution into eq. (19) yields:

$$-\nabla F(\lambda^{(k)}) = B\left[K_{BB} - \widetilde{K}_{\Pi B}^T\widetilde{K}_{\Pi\Pi}^{-1}\widetilde{K}_{\Pi B}\right]\left(\mathbf{f}_B - \widetilde{K}_{\Pi B}^T\widetilde{K}_{\Pi\Pi}^{-1}\widetilde{\mathbf{f}}_\Pi\right) \tag{20}$$

$$-\left[B\left[K_{BB} - \widetilde{K}_{\Pi B}^T\widetilde{K}_{\Pi\Pi}^{-1}\widetilde{K}_{\Pi B}\right]B^T\right]\lambda^{(k)} = B\mathbf{u}_B^{(k)} \tag{21}$$

The convergence is ensured if

$$\rho(B\widetilde{S}_{BB}^{-1}B^T) < \frac{2}{\alpha} \tag{22}$$

is fullfilled - with α as fixed step size and ρ as spectral radius. Before presenting the algorithmic implementation the next section describes different methods to create a usefull preconditioning matrix M_{BB}^{-1} either approximating the inversion of the interior-dual Schur complement operator or used as implicit preconditioning matrix solving iteratively the Schur problem with the conjugate gradient method.

3.1 Various techniques in building the left-side preconditioner M^{-1}

In this section three different preconditioners will be defined for performing the element based test examples as well as numerical results as of chapter 4. The following notation for M^{-1} will be used during the next chapters:

- M_J^{-1} as the classical Jacobi preconditioning technique
- M_D^{-1} defined from the main diagonal of M_J^{-1}
- M_{triD}^{-1} as approximate tri-diagonal matrix of K_{BB}^{-1}

Of course more versions are possible but their investigation should not be the task of this paper. In matrix notation the first preconditioner is defined as:

$$M^{-1} = \begin{bmatrix} M_{BB}^{-1} & {M_{\lambda B}^{T}}^{-1} \\ \\ M_{\lambda B}^{-1} & M_{\lambda\lambda}^{-1} \end{bmatrix} = \begin{bmatrix} G & B^T \\ \\ B & 0 \end{bmatrix}^{-1} = \begin{bmatrix} \alpha E & B^T \\ \\ B & 0 \end{bmatrix}^{-1} \tag{23}$$

with B as the FETI-DP jump operator, G as an original or approximated version of K_{BB} and E as the identity matrix. Since the block M_{22}, the most important characteristic of Saddle

Point equations, is equal to zero a simple inversion of M is directly given with only sparse matrix-matrix operations and thereby very low numerical effort if B is known:

$$M^{-1} = \begin{bmatrix} \frac{1}{\alpha}\big(E - B^T\big(BB^T\big)^{-1}B\big) & B^T\big(BB^T\big)^{-1} \\ \big(BB^T\big)^{-1}B & -\alpha\big(BB^T\big)^{-1} \end{bmatrix} \tag{24}$$

The introduction of the scaling factor α means the approximation of the main diagonal of G as well as K_{BB} as scaled identity matrix αE. Considering the original main diagonal of K_{BB} as matrix C leads to the Jacobi preconditioner M_J^{-1}:

$$M_J^{-1} = \begin{bmatrix} C^{-1}\big(E - B^T\big(\beta E\big)^{-1}B\big) & B^T\big(\beta E\big)^{-1} \\ \big(\beta E\big)^{-1}B & -C\big(\beta E\big)^{-1} \end{bmatrix} \tag{25}$$

In most of the investigated examples the product of the FETI-DP jump operators results in a scaled identity matrix βE seen in the equation above. For the reduced SPE it is only necessary to construct M_{BB}^{-1} as M_J^{-1}:

$$M_J^{-1} = M_{BB}^{-1} = C^{-1}\big(E - B^T\big(\beta E\big)^{-1}B\big) \tag{26}$$

The second version M_D^{-1} takes only the main diagonal of M_J^{-1} into account:

$$M_D^{-1} = \text{ diag}[M_J^{-1}] \tag{27}$$

Further M_{triD}^{-1} is an approximate inversion of K_{BB} using the main diagonal and additionally one neighboring diagonal from above and below of the main diagonal as written as:

$$M_{triD}^{-1} = \text{ tridiag}[x_i, z_i, y_i] \sim \Big[\text{tridiag}[K_{BB}]\Big]^{-1} \tag{28}$$

The construction of each row i with three entries x_i, z_i, y_i of M_{triD}^{-1} results from solving a 3 by 3 linear equation system which can be done by the scheme:

$$\begin{bmatrix} c_{i-1}^2 + a_{i-1}^2 + b_{i-1}^2 & c_i a_{i-1} + a_i b_{i-1} & c_{i+1} b_{i-1} \\ c_i a_{i-1} + a_i b_{i-1} & c_i^2 + a_i^2 + b_i^2 & c_{i+1} a_i + a_{i+1} b_i \\ c_{i+1} b_{i-1} & c_{i+1} a_i + a_{i+1} b_i & c_{i+1}^2 + a_{i+1}^2 + b_{i+1}^2 \end{bmatrix} \begin{bmatrix} x_i \\ z_i \\ y_i \end{bmatrix} = \begin{bmatrix} b_{i-1} \\ a_i \\ c_{i+1} \end{bmatrix}$$

with $c_0 = c_1 = a_0 = b_0 = b_n = b_{n+1} = a_{i+1} = c_{n+1} = 0.$

Further K_{BB} must be symmetric definite positiv and /irreduced/ diagonal dominant for sucessfull solving the 3 by 3 equation systems which is the case for most of the FE discretization of elasticity problems. It should be mentioned that this technique will lead to bad results related to convergence behaviour as well as accuracy of the resulting vector of nodal unknowns according to the referenced literature [5]. To enable the evalutation of the approximation qualitity for the different preconditioners the Frobenius norm is used:

$$\parallel B \parallel_F^2 = \sum_i^n \sum_j^n b_{ij}^2 \tag{29}$$

The approximation error results in

$$\epsilon_F = \lim \frac{\parallel E - M_{BB}^{-1} K_{BB} \parallel_F}{\parallel K_{BB} \parallel_F} \tag{30}$$

which finally reproduces an equivalent error in the nodal solution vector $\mathbf{u} = [\mathbf{u}_I \mathbf{u}_\Delta \mathbf{u}_\Pi]^T$ of the FETI-DP discretization.

3.2 Scalable version of M^{-1}

For the scalable version we have to differ between threaded and host-involved executions. Through the structure of the jump operator B it is possible to define a scaled version of B and of the (Jacobi-) preconditioner M^{-1} for each domain j which means creating $B^{(j)}$ and $M^{(j)^{-1}}$. This allows to compute domain-wise all vectors at each step of the following algorithms and taking advantage from a full MPI parallelization approach. For instance the scalable version of the Jacobi-preconditioning matrix $M_J^{(j)^{-1}}$ under consideration of N domains will be described in the following.

Taking the main diagonal of the interior-dual stiffness matrix K_{BB} as C leads to

$$C^{-1} = \text{diag}_{j=1}^N \big(C^{(j)^{-1}} \big) \quad \text{Jacobi: } C^{(j)^{-1}} = \Big[\text{diag} \big(K_{BB}^{(j)} \big) \Big]^{-1} \tag{31}$$

and with the inversion of the product of the jump operators per domain, which results in a scaled identity matrix

$$\big[BB^T \big]^{-1} = \text{diag}_{j=1}^N \big(\frac{1}{\beta_j} E^{(j)} \big) \tag{32}$$

as well as for

$$B^T \big[BB^T \big]^{-1} B = \text{diag}_{j=1}^N \big(\frac{1}{\beta_j} \Lambda^{(j)} \big); \quad \Lambda^{(j)} = \begin{bmatrix} E_{\Delta\Delta} & -E_{\text{I}\Delta}^T \\ -E_{\text{I}\Delta} & E_{\text{II}} \end{bmatrix}^{(j)} \tag{33}$$

$M^{(j)^{-1}}$ per domain can be given with

$$M_{\{BB\}}^{(j)^{-1}} = C^{(j)^{-1}} \big(E - \frac{1}{\beta_j} \Lambda^{(j)} \big) \tag{34}$$

which results finally in a diagonal matrix $M_{\{BB\}}^{-1}$

$$M_{\{BB\}}^{-1} = \text{diag}_{j=1}^N \left(M_{\{BB\}}^{(j)^{-1}} \right) \tag{35}$$

For the full scalable computational step it follows:

$$\mathbf{u}_B = M_{BB}^{(j)^{-1}} \left(\mathbf{f}_B^{(j)} - \widetilde{\mathbf{f}}_{B,S}^{(j)} - B^{T(j)} \lambda \right) = M_{BB}^{(j)^{-1}} \left(\widetilde{\mathbf{g}}_{B,S}^{(j)} - B^{T(j)} \lambda \right) \tag{36}$$

In the next sections a modified (conjugate gradient-)version of the Uzawa algorithm for the computation of the FETI-DP saddle-point problem and some numerical tests will be presented.

4 ALGORITHMIC IMPLEMENTATION AND NUMERICAL TESTS

4.1 Sequential versions of Uzawa and Uzawa-CG

The following sequential algorithm are describing the iterative solution process of the FETI-DP saddle-point equation. Therefore the Uzawa iteration scheme for saddle-point problems was adapted and modified. The first version, seen below in algorithm 4.1, is the standard Uzawa algorithm solving the FETI-DP SPE. After obtaining the solution of the dual-interior d.o.f. and of the vector of the Langragian multipliers an update step at the end of the iteration computes the vector of primal nodal unknowns. A second (conjugate gradient) Uzawa version includes additionally the preconditioned CG method for iterative computation of the (interior-dual) Schur complement problem $\widetilde{S}_{BB}\ \mathbf{h} = \mathbf{p}$.

Algorithm 4.1: Uzawa algorithm with exact iteration steps for FETI-DP SPE.

```
Require: $\widetilde{S}_{BB}$ is invertable.
Choose $\lambda^{(0)}$ and $\mathbf{u}_B^{(1)} = \widetilde{S}_{BB}^{-1}\left(\mathbf{f}_B - \widetilde{\mathbf{f}}_{B,S} - B^T\lambda^{(0)}\right)$ ; factorize $\widetilde{K}_{\Pi\Pi}$
with $\widetilde{\mathbf{f}}_{B,S} = \widetilde{K}_{\Pi B}^T\widetilde{K}_{\Pi\Pi}^{-1}\widetilde{\mathbf{f}}_\Pi$ and $\widetilde{S}_{BB}^{-1} = \left(K_{BB} - \widetilde{K}_{\Pi B}^T\widetilde{K}_{\Pi\Pi}^{-1}\widetilde{K}_{\Pi B}\right)^{-1}$
for $k = 1, 2, ...$ do
    $\mathbf{q}^{(k)} = -B\mathbf{u}_B^{(k)}$
    $\mathbf{p}^{(k)} = B^T\mathbf{q}^{(k)}$
    $\mathbf{h}^{(k)} = \widetilde{S}_{BB}^{-1}\mathbf{p}^{(k)}$
    $\alpha^{(k)} = \frac{\mathbf{q}^{(k)^T}\mathbf{q}^{(k)}}{\mathbf{p}^{(k)^T}\mathbf{h}^{(k)}}$
    $\lambda^{(k)} = \lambda^{(k-1)} - \alpha^{(k)}\mathbf{q}^{(k)}$
    $\mathbf{u}_B^{(k+1)} = \mathbf{u}_B^{(k)} + \alpha^{(k)}\mathbf{h}^{(k)}$
end for
Update $\widetilde{\mathbf{u}}_\Pi^{(k+1)} = \widetilde{K}_{\Pi\Pi}^{-1}\left(\widetilde{\mathbf{f}}_\Pi - \widetilde{K}_{\Pi B}\mathbf{u}_B^{(k+1)}\right)$
```

With the introduction of three additional vectors the conjugate gradient version of the standard Uzawa algorithm can be obtained. Furthermore a preconditioned conjugate gradient method is implicit introduced for iteratively solving the Schur complement problem and therefore avoiding the (direct) factorization of $\widetilde{S}_{BB}$. The algorithm is shown below (algorithm 4.2).

Algorithm 4.2: CG version of Uzawa algorithm for FETI-DP SPE with implicit PCG computation of $\widetilde{S}_{BB}\mathbf{h}^{(k)} = \mathbf{p}^{(k)}$.

```
Require: $\widetilde{S}_{BB}$ is invertable.
  1.   Choose $\lambda^{(0)}$ and $\mathbf{u}_B^{(1)} = \widetilde{S}_{BB}^{-1}\left(\mathbf{f}_B - \widetilde{\mathbf{f}}_{B,S} - B^T\lambda^{(0)}\right)$ ; factorize $\widetilde{K}_{\Pi\Pi}$
       with $\widetilde{\mathbf{f}}_{B,S} = \widetilde{K}_{\Pi B}^T\widetilde{K}_{\Pi\Pi}^{-1}\widetilde{\mathbf{f}}_\Pi$ and $\widetilde{S}_{BB} = \left(K_{BB} - \widetilde{K}_{\Pi B}^T\widetilde{K}_{\Pi\Pi}^{-1}\widetilde{K}_{\Pi B}\right)$ and
       build preconditioner $M$
  2.   Set $\mathbf{d}^{(1)} = -\mathbf{q}^{(1)} = B\mathbf{u}_B^{(1)}$
  3.   for $k = 1, 2, ...$ do
  4.   $\mathbf{p}^{(k)} = B^T\mathbf{d}^{(k)}$
  5.   $\mathbf{h}^{(k)} = \widetilde{S}_{BB}^{-1}\mathbf{p}^{(k)}$ as
     5.01   Choose $\mathbf{h}_0^{(k)}$ and $\widetilde{\mathbf{r}}_0 = \mathbf{p}^{(k)} - \widetilde{S}_{BB}\mathbf{h}_0^{(k)}$
     5.02   $\widetilde{\mathbf{h}}_0 = M\widetilde{\mathbf{r}}_0$
     5.03   $\widetilde{\mathbf{d}}_0 = \widetilde{\mathbf{h}}_0$
     5.04   for $j = 1, 2, ...$ do
     5.05   $\widetilde{\alpha}_j = \frac{\widetilde{\mathbf{r}}_j^T\widetilde{\mathbf{h}}_j}{\widetilde{\mathbf{d}}_j^T\widetilde{S}_{BB}\widetilde{\mathbf{d}}_j}$
     5.05   $\mathbf{h}_{j+1}^{(k)} = \mathbf{h}_j^{(k)} + \widetilde{\alpha}_j\widetilde{\mathbf{d}}_j$
     5.06   $\widetilde{\mathbf{r}}_{j+1} = \widetilde{\mathbf{r}}_j - \widetilde{\alpha}_j\widetilde{S}_{BB}\widetilde{\mathbf{d}}_j$
     5.07   $\widetilde{\mathbf{h}}_{j+1} = M\widetilde{\mathbf{r}}_{j+1}$
     5.08   $\widetilde{\beta}_j = \frac{\widetilde{\mathbf{r}}_{j+1}^T\widetilde{\mathbf{h}}_{j+1}}{\widetilde{\mathbf{r}}_j^T\widetilde{\mathbf{h}}_j}$
     5.09   $\widetilde{\mathbf{d}}_{j+1} = \widetilde{\mathbf{h}}_{j+1} + \beta_j\widetilde{\mathbf{d}}_j$
     5.10   end for (implicit PCG)
  6.   $\alpha^{(k)} = \frac{\mathbf{q}^{(k)T}\mathbf{q}^{(k)}}{\mathbf{p}^{(k)T}\mathbf{h}^{(k)}}$
  7.   $\lambda^{(k)} = \lambda^{(k-1)} + \alpha^{(k)}\mathbf{d}^{(k)}$
  8.   $\mathbf{u}_B^{(k+1)} = \mathbf{u}_B^{(k)} - \alpha^{(k)}\mathbf{h}^{(k)}$
  9.   $\mathbf{q}^{(k+1)} = -B\mathbf{u}_B^{(k+1)}$
 10.   $\beta^{(k)} = \frac{\mathbf{q}^{(k+1)T}\mathbf{q}^{(k+1)}}{\mathbf{q}^{(k)T}\mathbf{q}^{(k)}}$
 11.   $\mathbf{d}^{(k+1)} = -\mathbf{q}^{(k+1)} + \beta^{(k)}\mathbf{d}^{(k)}$
 12.   end for (Uzawa-CG)
 13.   Update $\widetilde{\mathbf{u}}_\Pi^{(k+1)} = \widetilde{K}_{\Pi\Pi}^{-1}\left(\widetilde{\mathbf{f}}_\Pi - \widetilde{K}_{\Pi B}\mathbf{u}_B^{(k+1)}\right)$
```

4.2 Numerical convergence tests

The first test examples in 2D with 2 elements, each for one domain, uses the (FETI-DP) Saddle Point discretization solving the six nodal unknowns with the sequential version of a conventional iterative Dirichlet-Neumann relaxation algorithm. Fig. 4.1 indicates primal d.o.f. at the node marked with a black circle. The dual d.o.f. are in the node marked with the white rectangle. The computation is based on linear elastic material and plane stress state.

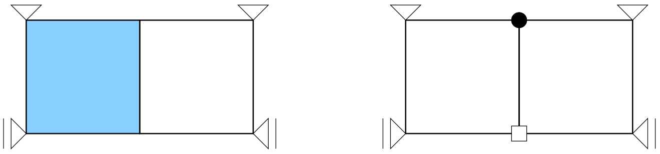

Fig. 4.1: Example (1) with 1 element per domain (left) and the resulting FETI-DP discretization (right).

This test should show the slow convergence behaviour as well as the dependency on the choice of the relaxation parameter as disadvantages of this kind of (D-N) iteration schemes. Three different types of preconditioners are considered (see section 3.2) during the convergence analysis. The relaxation parameter ω was varied between 0.8-2.0 and the obtained accuracy was taken from the 10th iteration step as illustrated in fig. 4.2. The optimal value of ω was 1.55.

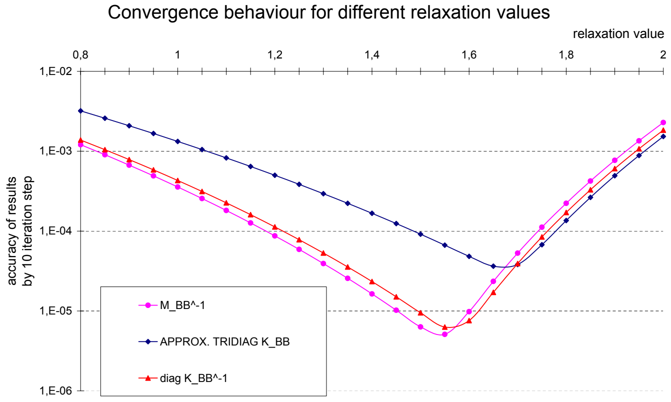

Fig. 4.2: Convergence behaviour regarding to different relaxation values and preconditioning techniques.

The next example discretized by 6 elements with 2 elements per domains is partitioned in a way that all domains are sequantially coupled and each boundary is only connecting 2 domains. Again the primal nodes are denoted with black circles and the dual nodes with white rectangles, respectively. The partitioning is illustrated in fig. 4.3, upper left, the FETI-DP discretization is shown at the bottom left and on the right the duplication of the dual nodes are shown. For this example the algorithm 4.2 was used for computation of the unknowns of $\mathbf{u}_B$ and λ of the FETI-DP saddle-point problem.

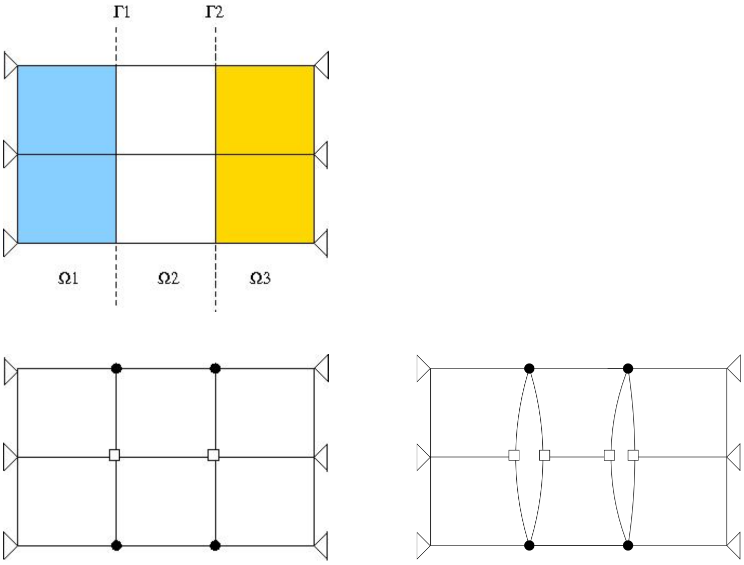

Fig. 4.3: Example (2) with FETI-DP discretization for 3 domains with 2 elements per domain: upper left - partitioning in 3 domains; bottom left - FETI-DP discretization; bottom right - duplication of the dual nodes.

The results regarding to necessary iteration steps (if TOL $\leq$ 1e-06) and the reached accuracy can be seen in the table below:

algorithm	iteration	accuracy	$\|\|\mathbf{r}_{k+1}\|\|_{\text{iPCG}}$	note
D-N	>10	1.0e-06	–	-
Uzawa	9	3.4e-07	–	-
Uzawa-CG	4	0.0e+00	–	-
Uzawa-CG iPCG (1)	4	1.0e-06	1.6e-04	with implicit PCG
Uzawa-CG iPCG (2)	4	4.6e-10	2.5e-07	with implicit PCG
Uzawa-CG iPCG (3)	4	0.0e+00	6.4e-19	with implicit PCG

The table shows the better convergence behaviour using the CG version of the Uzawa algorithm compared to the standard Uzawa iteration procedure for the computation of the resulting FETI-DP saddle-point equation system. For large discretized problems the Uzawa-CG with an implicit preconditioned conjugate gradient method for iteratively solving the Schur complement problem will lead to additional time savings.

5 OUTLOOK

Our approach results in substantial computational time savings due to avoiding the inversion of the domain stiffness matrices with direct solvers as well as keeping the scalable properties of the resulting preconditioners and FETI-DP jump operators. As a result a sequential and scalable algorithm based on the FETI-DP Saddle Point system can be obtained. First numerical results of the implemented Uzawa algorithms for FETI-DP SPE applied on multi-domain decomposition of heterogeneous elasticity problems in 3D will be presented in the conference (Fig. 5.1).

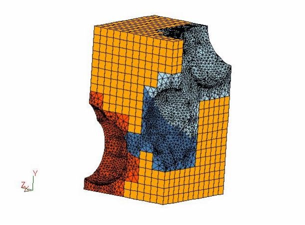

Fig. 5.1: Hybrid partitioned mesh of an artificial heterogeneous specimen.

In future research work these solution methods will be adapted for simulation of physical nonlinear problems, such as (nonlocal) damage effects in microstructure material models, leading towards new possibilities of numerical simulations for multiphase materials in 3D microscale. Furthermore the model will be adapted for the hybrid FE discretization and mechanical damage analysis of CT based image data of real multiphase samplings.

ACKNOWLEDGEMENT

These research is supported by the German Research Foundation (DFG), which is gratefully acknowledged by the authors.

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