A Newton-Krylov-FETI-DP Method with an Adaptive Coarse Space Applied to Elastoplasticity

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1 Introduction

We consider a Newton-Krylov-FETI-DP algorithm to solve problems in elastoplasticity. First, the material model and its discretization will be described. The model contains a Prandtl-Reuss flow rule and a von Mises flow function. We restrict ourselves to the case of perfect elastoplasticity; thus, there is no hardening. For more information on elastoplasticity; see, e.g., Carstensen and Klose [2002], Han and Reddy [2013], Simo and Hughes [1998]. In this material model we will have local nonlinearities introduced by plastic material behavior in activated zones of the domain. For the finite element discretization we follow the framework given in Carstensen and Klose [2002]. Second, we will briefly present the linearization and the FETI-DP method which is used to solve the linearized problems. For more details on the FETI-DP algorithm, see, e.g., Klawonn et al. [2002, 2008], Farhat et al. [2001], Toselli and Widlund [2005]. The convergence of the Newton-Krylov-FETI-DP method using a standard coarse space with vertices and edge averages can deteriorate when the plastically activated zone intersects the interface introduced by the domain decomposition. In this case, we use an adaptive coarse space which successfully decreases the number of cg iterations and the condition numbers of the preconditioned linearized systems. Only a small amount of adaptive constraints is needed if the plastically activated zone is restricted to a small part of the domain. Additional constraints are needed mainly in the final time and Newton steps. The additional constraints for the coarse space are chosen by a strategy proposed in Mandel and Sousedík [2007] for linear elliptic problems. In contrast to their implementation, here,

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the additional constraints will be implemented using a deflation approach; see Klawonn and Rheinbach [2012].

2 Elastoplastic Material Model and Discretization

The material model is derived from the quasi-static equation of equilibrium

$$\operatorname{div} \sigma(x,t) = f(x,t);$$

see, e.g., Carstensen and Klose [2002], Simo and Hughes [1998], Han and Reddy [2013]. Let d be the dimension of the domain. Multiplying the equation with $v \in H^1_D(\Omega)^d := \{v \in H^1(\Omega)^d : v = 0 \text{ on } \Gamma_D\}$ and application of the Gauss theorem yields the weak formulation: Find $u \in H^1(\Omega)^d$ which satisfies $u = w$ on Γ_D, such that for all $v \in H^1_D(\Omega)^d$:

$$\int_\Omega \sigma(u) : \epsilon(v) dx = \int_\Omega f \cdot v dx + \int_{\Gamma_N} g \cdot v ds. \tag{1}$$

By discretization in time using the implicit Euler method we obtain:
Find $u_n \in H^1(\Omega)^d$ with $u_n = w$ on Γ_D, such that $\forall v \in H^1_D(\Omega)^d$

$$\int_\Omega \sigma_n : \varepsilon(v)\, dx = \int_\Omega f_n\, v\, dx + \int_{\Gamma_N} g_n \cdot v\, ds,$$

where σ_n is dependent on the displacement u_n. This dependency is determined by the von Mises flow function and the chosen type of hardening. In this article we consider perfect elastoplastic material behavior and hardening effects are absent. In this case the von Mises flow function is given by $\Phi(\sigma) = |\text{dev}(\sigma)| - \sigma_y$, where σ_y is the yield point and $\text{dev}\,(\sigma) = \sigma - \frac{1}{d}\text{tr}\,(\sigma)\text{I}_{d\times d}$. The tension tensor in the n-th timestep is then linear elastic if $\Phi(\sigma_n) \leq 0$ and plastic otherwise. In the first case we have

$$\sigma_n = (\lambda + \mu)\text{tr}(\varepsilon(u_n - u_{n-1}) + \mathbb{C}^{-1}\sigma_{n-1}) + 2\mu\text{dev}(\varepsilon(u_n - u_{n-1}) + \mathbb{C}^{-1}\sigma_{n-1})$$

with the Lamé constants λ, μ and the fourth order elasticity tensor $\mathbb{C}$. In the second case the tension tensor in the n-th timestep reads

$$\begin{aligned}\sigma_n = &(\lambda + \mu)\text{tr}(\varepsilon(u_n - u_{n-1}) + \mathbb{C}^{-1}\sigma_{n-1}) \\ &+ \sigma_y \frac{\text{dev}(\varepsilon(u_n - u_{n-1}) + \mathbb{C}^{-1}\sigma_{n-1})}{|\text{dev}(\varepsilon(u_n - u_{n-1}) + \mathbb{C}^{-1}\sigma_{n-1})|}.\end{aligned}$$

Note that in the first case, we have a linear relationship between the tension and the displacement, while in the second case, we have a nonlinearity introduced by normalizing the deviatoric term. For a more detailed description how to obtain the time discrete tension tensor explicitly for different types of hardening, see Carstensen and Klose [2002].

3 Linearization

We need to linearize the nonlinear discrete problem in every time step. For this we will represent the problem as a root finding problem. We define the p-th component of the vector field F by

$$F_p(u_n) = \int_{\Omega} \sigma_n : \varepsilon(\varphi_p)\, dx - \int_{\Omega} f_n \cdot \varphi_p\, dx - \int_{\Gamma_N} g_n \cdot \varphi_p\, ds.$$

Then the nonlinear problem reads: Solve $F(u_n) = 0$. The Newton update in the $(k+1)$-th Newton step is $u_n^{k+1} = u_n^k + \Delta u_n^{k+1}$ with Δu_n^{k+1} defined by

$$DF(u_n^k)\Delta u_n^{k+1} = -F(u_n^k),$$

where the tangential stiffness matrix DF is given by $(DF(u_n^k))_{pq} = \frac{\partial F_p(u_n^k)}{\partial u_{n,q}^k}$. In our numerical examples we iterate in each timestep until the residual satisfies $||F(u_n^k)||_2 \leq 10^{-10} + 10^{-6}||F(u_n^0)||_2$, where $u_n^0 := 0$; for the stopping criterion, see, e.g. [Carstensen and Klose, 2002, p. 171, l. 34 of the source code], [Kelley, 1995, p. 73, (5.4)]. To guarantee the convergence we will use the Armijo rule, see, e.g., Kelley [1995], as a line search algorithm. In each Newton iteration we will first set $\tau = 1$ as an initial step length and then assemble local stiffness matrices $K^{(i)} = DF(u_n^{k,(i)})$ and right-hand sides $f^{(i)} = F(u_n^{k,(i)})$, $i = 1, \ldots, N$. Then we will solve the linearized system

$$DF(u_n^k)\Delta u_n^{k+1} = -F(u_n^k)$$

with FETI-DP as described in the following section. Our trial update is given by $u_{n,\tau}^{k+1} = u_n^k + \tau \Delta u_n^{k+1}$. We test if the Armijo condition

$$||F(u_{n,\tau}^{k+1})||_2 < (1 - 10^{-4} \cdot \tau)||F(u_n^k)||_2$$

is satisfied. In this case we update $u_n^{k+1,(i)} \leftarrow u_{n,\tau}^{k+1,(i)}$. Otherwise we halve the step length $\tau \leftarrow \tau/2$.

4 FETI-DP and Deflation

We will now briefly describe the FETI-DP algorithm. For more details on FETI-DP, see, e.g., Klawonn et al. [2008, 2002], Toselli and Widlund [2005].

Let the primal variables, for example, vertices or edge averages in subdomain Ω_i be denoted by $u_\Pi^{(i)}$ and the remaining variables be denoted by $u_B^{(i)}$, and the corresponding stiffness matrices and right-hand sides be sorted accordingly. Then, we have for the local stiffness matrices $K^{(i)}$ and local load vectors $f^{(i)}$

$$K^{(i)} = \begin{bmatrix} K_{BB}^{(i)} & K_{\Pi B}^{(i)T} \\ K_{\Pi B}^{(i)} & K_{\Pi\Pi}^{(i)} \end{bmatrix} \quad \text{and} \quad f^{(i)} = \begin{bmatrix} f_B^{(i)} \\ f_\Pi^{(i)} \end{bmatrix},$$

respectively. We denote by $K_{BB} = \operatorname{diag}_{i=1}^N K_{BB}^{(i)}$, $K_{\Pi\Pi} = \operatorname{diag}_{i=1}^N K_{\Pi\Pi}^{(i)}$, and $K_{\Pi B} = [K_{\Pi B}^{(1)}, \ldots, K_{\Pi B}^{(N)}]$. We introduce the following notation

$$\begin{bmatrix} K_{BB} & \tilde{K}_{\Pi B}^T \\ \tilde{K}_{\Pi B} & \tilde{K}_{\Pi\Pi} \end{bmatrix} = \begin{bmatrix} I_B & 0 \\ 0 & R_\Pi^T \end{bmatrix} \begin{bmatrix} K_{BB} & K_{\Pi B}^T \\ K_{\Pi B} & K_{\Pi\Pi} \end{bmatrix} \begin{bmatrix} I_B & 0 \\ 0 & R_\Pi \end{bmatrix},$$

where R_Π^T is the partial assembly operator in the primal variables. We define a jump operator B_B consisting of entries $0, 1$, and -1, which enforces continuity in the remaining unknowns by $B_B u_B = 0$. Then the FETI-DP system reads $F\lambda = d$, with

$$\begin{aligned} F &= B_B K_{BB}^{-1} B_B^T + B_B K_{BB}^{-1} \widetilde{K}_{\Pi B}^T \widetilde{S}_{\Pi\Pi}^{-1} \widetilde{K}_{\Pi B} K_{BB}^{-1} B_B^T, \\ d &= B_B K_{BB}^{-1} f_B - B_B K_{BB}^{-1} \widetilde{K}_{\Pi B}^T \widetilde{S}_{\Pi\Pi}^{-1} \left(\tilde{f} - \widetilde{K}_{\Pi B} K_{BB}^{-1} f_B \right), \end{aligned}$$

where $\widetilde{S}_{\Pi\Pi} = \widetilde{K}_{\Pi\Pi} - \widetilde{K}_{\Pi B} K_{BB}^{-1} \widetilde{K}_{\Pi B}^T$. We further partition the remaining variables $u_B^{(i)} = [u_I^{(i)T} \, u_\Delta^{(i)T}]^T$ into dual variables on the interface $u_\Delta^{(i)}$ and inner variables $u_I^{(i)}$ and the stiffness matrices and right-hand sides accordingly. Define $K_{\Delta\Delta} = \operatorname{diag}_{i=1}^N K_{\Delta\Delta}^{(i)}$, $K_{II} = \operatorname{diag}_{i=1}^N K_{II}^{(i)}$, and $K_{\Delta I} = [K_{\Delta I}^{(1)} \ldots K_{\Delta I}^{(N)}]$. The FETI-DP algorithm is the preconditioned conjugate gradient algorithm applied to $F\lambda = d$ with the Dirichlet preconditioner

$$M^{-1} = B_{B,D} \, [0 \quad I_\Delta]^T \left(K_{\Delta\Delta} - K_{\Delta I} K_{II}^{-1} K_{\Delta I}^T \right) [0 \quad I_\Delta] \, B_{B,D}^T.$$

An additional coarse level in the FETI-DP method can be introduced by a deflation approach; see, e.g., Klawonn and Rheinbach [2012] for more details. We will aggregate constraints as columns in a matrix U. The constraint $U^T B u = 0$ will be enforced by introducing projections $P = U(U^T F U)^{-1} U^T F$ and $Q = I - P$. Then the projected system $Q^T F \lambda = Q^T d$ will be solved iteratively, while $P^T F \lambda = P^T d$ will be solved directly. We can also solve the original system with the balancing preconditioner $M_{BP}^{-1} = Q M^{-1} Q^T + P F^{-1}$ where M^{-1} is the classical Dirichlet preconditioner instead; see, e.g., Klawonn and Rheinbach [2012].

5 Adaptive Coarse Space

The presentation in this section follows the ideas proposed in Mandel and Sousedík [2007] for linear elliptic problems. We will start our Newton-Krylov-FETI-DP algorithm with an initial coarse space consisting of vertex constraints as primal variables enforced by subassembly. It is well known that the condition number satisfies $\kappa(M^{-1}F) \leq \omega := \sup_{w\in\widetilde{W}} \frac{|P_D w|_S^2}{|w|_S^2}$, where $P_D := B_{B,D}^T B_B$; see, e.g., Klawonn et al. [2002], Toselli and Widlund [2005]. Consider a local edge between the subdomains Ω_i and Ω_j and define $S_{E_{ij}} := \operatorname{diag}(S^{(i)}, S^{(j)})$. Let $B_{E_{ij}}$ be a local version of the Matrix B defined as the matrix with the rows of $[B^{(i)} \quad B^{(j)}]$, which consist of a 1 and a -1 and are zero elsewhere. Let $\widetilde{W}_{E_{ij}}$ be the subspace of functions in $W^{(i)} \times W^{(j)}$ which are continuous in vertices which both subdomains have in common and define

$$\omega_{E_{ij}} := \sup_{w_{E_{ij}} \in \widetilde{W}_{E_{ij}}} \frac{|P_{D,E_{ij}} w_{E_{ij}}|^2_{S_{E_{ij}}}}{|w_{E_{ij}}|^2_{S_{E_{ij}}}}$$

as the local *condition number estimator*, where $P_{D,E_{ij}} = B^T_{D,E_{ij}} B_{E_{ij}}$ and $B_{D,E_{ij}}$ is a scaled version of $B_{E_{ij}}$. Define $\widetilde{\omega} := \max_{E_{ij}\subset\Gamma} \omega_{E_{ij}}$ as the maximum $\omega_{E_{ij}}$ of all edges on the interface. Then $\widetilde{\omega}$ is expected to be a good estimator of the bound ω of the condition number $\kappa(M^{-1}F)$. We choose a prescribed tolerance TOL ≥ 1 for the condition number. With local orthogonal projections $\Pi_{E_{ij}}$ from $W^{(i)} \times W^{(j)}$ onto $\widetilde{W}_{E_{ij}}$ and $\overline{\Pi}$ onto $\operatorname{range}(\Pi_{E_{ij}} S_{E_{ij}} \Pi_{E_{ij}})$ we solve the following local generalized eigenvalue problem on each edge

$$\begin{aligned}&\overline{\Pi}\Pi_{E_{ij}} P^T_{D,E_{ij}} S_{E_{ij}} P_{D,E_{ij}} \Pi_{E_{ij}} \overline{\Pi} w_{E_{ij}} \\ &= \mu_{E_{ij}} \left(\overline{\Pi}\left(\Pi_{E_{ij}} S_{E_{ij}} \Pi_{E_{ij}} + \sigma(I - \Pi_{E_{ij}})\right)\overline{\Pi} + \sigma(I - \overline{\Pi})\right) w_{E_{ij}},\end{aligned}$$

where $\sigma > 0$ is a shift parameter here chosen as $\max_i (S_{E_{ij}})_{ii}$; see also Mandel and Sousedík [2007]. We are only interested in eigenvectors to eigenvalues which exceed the tolerance TOL. Let the eigenvalues $\mu_{E_{ij},l},\ l = 1, .., n$ be sorted in a decreasing order. For each eigenvector $w_{E_{ij},l}$ to an eigenvalue $\mu_{E_{ij},l} \geq$ TOL, $l = 1, \ldots, k$ we set $\overline{u}_{E_{ij},l} = B_{D,E_{ij}} S_{E_{ij}} P_{D,E_{ij}} w_{E_{ij},l}$. Let $u_{E_{ij},l}$ be vectors representing functions in the Lagrange multiplier space that coincide with $\overline{u}_{E_{ij},l}$ on the edge E_{ij} and that are zero elsewhere. For each edge we collect the $u_{E_{ij},l}$ as colums of a matrix U and apply the modified Gram-Schmidt algorithm to detect and remove linearly dependent constraints.

6 Numerical Examples

In the following we will present numerical examples. Consider a square domain $\Omega = (0,1)^2$ with zero Dirichlet boundary conditions imposed on the lower edge $\{(x,y) \in \partial\Omega | y = 0\}$ which is exposed to a surface force $g(x,y,t) = (150t, 0)^T$ if $x \in \{(x,y) \in \partial\Omega | y = 1\}$ and $g(x,y,t) = 0$ elsewhere. The material has a Young modulus of $E = 206900$, a Poisson ratio of $\nu = 0.29$ and $\sigma_y = 200$. We compute the solution in the time interval $T = [0, 0.45]$ in nine time steps of step length $\Delta t = 0.05$. The space is discretized with P2 finite elements in all our examples. In the first set of numerical experiments we

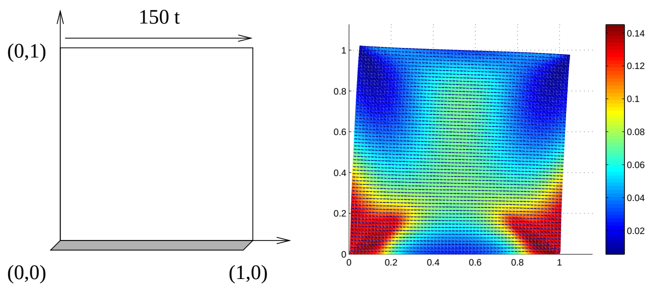

Fig. 1 Unit square with zero Dirichlet boundary conditions at the lower edge $y = 0$ exposed to a surface force $g(t) = (150t, 0)^T$ at the upper edge $y = 1$ (left). Displacement magnified by factor 20 and shear energy density in the last timestep (right). Material parameters $E = 206900$, $\nu = 0.29$ and $\sigma_y = 200$.

$n = H/h$	$N = 1/H$	max. cond	max. CG-It.	Newton its per timestep
20	2	**4.06**	**13**	1/1/1/4/4/6/7/9/11
30	2	**4.53**	**14**	1/1/3/5/5/7/8/10/11
40	2	**4.87**	**14**	1/1/3/4/5/7/9/13/13

Table 1 FETI-DP maximal condition numbers and iteration counts in Newton's scheme with a coarse space consisting of vertices and edge averages. We use P2 finite elements in all our examples.

consider a classical coarse space with only vertex and edge average constraints using different partitions into elements and subdomains. There are no problems with the classical coarse space if the plastically activated zone does not intersect the interface; see Table 1 for a decomposition in 2×2 subdomains. In this case each linearized system can be analyzed as in Gippert et al. [2012] using a slab technique. However if the plastically activated zone intersects the interface, the condition numbers and iteration counts increase considerably; see Table 2 for the results with a decomposition in 15×15 subdomains.

$n = H/h$	$N = 1/H$	max. cond	max. CG-It.
4	15	**900837**	**371**
6	15	$> \mathbf{10^6}$	$> \mathbf{1000}$
8	15	$> \mathbf{10^6}$	$> \mathbf{1000}$

Table 2 Problems with the Classical Coarse Space. FETI-DP maximal condition numbers and iteration counts.

For the results with the adaptive coarse space described in Section 5, see

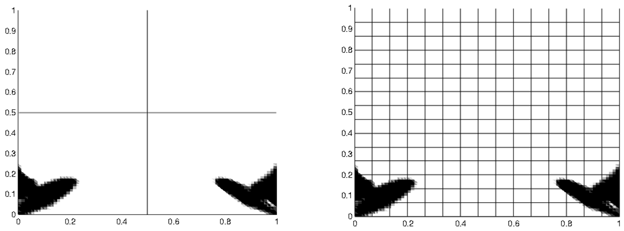

Fig. 2 Plastically activated zone in the last timestep. Decomposition into 2×2 subdomains. The plastically activated zones stay completely inside of subdomains (left). Decomposition into 15×15 subdomains. The plastically activated zones intersect the interface (right).

Table 3. The eigenpairs were computed using the MATLAB built-in function 'eig'. The complexity thus is cubic with respect to the length of the subdomain edges. For constant H/h the length of the subdomain edges is constant. Moreover, the global number of subdomain edges, and thus also the number of eigenvalue problems, grows linearly with the number of subdomains. The solution of the eigenvalue problems can, of course, be performed in parallel. The condition numbers and iteration counts decrease for the cost of a few more primal constraints in the last time steps. The tolerance is currently determined heuristically; see Table 3.

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$n = H/h$	$N = 1/H$	TOL	max cond	max it	constraints/ timestep	global dofs	constraints/ global dofs
4	15	6.0	**5.84**	**25** (25 elasticity)	0/0/0/0/0/0/19/46/121	8316	1.5%
6	15	7.0	**7.06**	**28** (27 elasticity)	0/0/0/0/0/0/29/71/180	11676	1.5%
8	15	8.0	**8.01**	**30** (29 elasticity)	0/0/0/0/0/0/35/81/225	15036	1.5%
4	15	5.9	**5.84**	**25** (25 elasticity)	0/0/0/0/0/0/19/46/123	8316	1.5%
6	15	7.1	**7.06**	**28** (27 elasticity)	0/0/0/0/0/0/29/71/179	11676	1.5%

Table 3 For each subdomain in each space direction, there are n finite elements and in each space direction there are N subdomains. TOL denotes the prescribed tolerance for the condition number, max cond the maximal condition number in the Newton iterations, max it the maximal number of preconditioned conjugate gradient iterations, and constraints/timestep the amount of constraints in each timestep. The tolerances TOL were chosen from considering the condition numbers of corresponding linear elastic problems. The number in brackets in the 'max it' column refers to the iteration counts of these corresponding elasticity problems. We can also use the condition number of the first few time steps, where the material still behaves elastically, as a reference. It can be seen that the results are not very sensitive to small changes in the tolerance.

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