Abstract. Arterial walls in the healthy physiological regime are characterized by nearly incompressible, anisotropic, hyperelastic material behavior. Polyconvex material functions representing such materials typically incorporate a penalty function to account for the incompressibility. Unfortunately, the penalty will affect the conditioning of the stiffness matrices. For high penalty parameters the performance of iterative solvers will degrade and when using direct solvers the quality of the solutions will deteriorate. In this paper, an augmented Lagrange approach is used to cope with the almost incompressibility condition. Here, the penalty parameter can be chosen much smaller and as a consequence the arising linear systems of equations have better properties. An improved convergence is then observed for the FETI-DP domain decomposition method which is used as an iterative solver.

1. Introduction. In this paper, we analyze the expansion of arterial walls using a FETI-DP domain decomposition within a quasi-static process. Arterial walls are biological soft tissues and therefore almost incompressible. Their behavior is anisotropic as a consequence of embedded collagen fibers. Major blood vessels are composed of distinct tissue layers, i.e., the intima (tunica intima), the media (tunica media), and the adventitia (tunica adventitia). We assume that the influence of the intima on the mechanical properties is negligible.

In Brands et al. [2] we have compared several material models describing the mechanical behavior of arterial walls in order to study the mechanical response and the influence on the nonlinear iteration as well as on the FETI-DP domain decomposition method which we use to solve the linearized systems of equations. It was found that for all material models considered here, the material parameters, which include the parameters to adjust the almost incompressibility, have a substantial influence on the convergence of the iterative solution method. It is of course well known already in the context of linear elasticity that almost incompressibility can have a major impact on iterative solvers.

Here, we will take a different approach as opposed to [2]. We consider a single material model and investigate different ways to incorporate the almost incompressibility constraint. Partial results have already been reported in a proceedings article [3]. In the classical approach, a penalty enforcing the geometric constraint that the determinant of the deformation gradient \( F \) is close to 1, \( \det(F) \approx 1 \), is added to the free energy, using a weight \( \varepsilon_1 \) which is referred to as the penalty parameter. Only for \( \varepsilon_1 \) approaching infinity, the constraint is fulfilled exactly. Unfortunately, using high penalty parameters results in ill-conditioned linearized systems which affect the performance of iterative solvers such that the convergence rate degrades significantly. For direct solvers, the computed solutions may become meaningless.

Alternatively, if the augmented Lagrange approach, see Simo and Taylor [4] as well as Fortin and
Fig. 1.1. Layered finite element model of an arterial segment discretized using 10-noded tetrahedra; Image from [1]. The outer layers show the geometry of the reconstructed media, intima, and plaque (from left to right).

Fortin [5], is taken for the almost incompressibility constraint, in addition to the penalty term, a Lagrange multiplier $\mu_T$ is introduced on each finite element $T$ and $\mu_T (\det(F) - 1)$ is added element-wise to the energy $\psi$.

The Lagrange multiplier will be computed iteratively by an Uzawa-like iteration

$$\mu_{T,k+1} = \mu_{T,k} + \xi_k (\det(F) - 1), \quad (1.1)$$

where in our computations in Section 7 the sequence $\xi_k$ will be chosen as a constant $\xi_k = \xi$.

We formally collect all local multipliers $\mu_{T,k}$ in a vector $\mu_k = (\mu_{T,k})_T$. The iteration for $\mu_k$ may be nested with the Newton iteration, see Figure 6.2 in Section 6, or may be carried out simultaneously, see Figure 6.3 in Section 6. In the nested approach (NAL), for each value of $\mu_k$, a nonlinear system is solved using the Newton iteration until convergence. In the simultaneous approach (SAL), the value of $\mu_k$ is changed according to (1.1) after each single Newton step. It is thus performed embedded in or simultaneously with the Newton iteration. Note that due to the $F$-approach, see Section 4, the element-wise constraint $\det(F) = 1$ is enforced only in a mean sense to avoid locking effects, i.e., we will enforce $\theta = 1$, for the element-wise scalar-valued variable $\theta$, instead of $\det(F) = 1$, see Section 4.

There exist domain decomposition solvers that are robust in the almost incompressible linear elasticity setting, see Klawonn et al. [6], Li and Widlund [7], Rheinbach [8], Dohrmann and Lehoucq [9], and others. But for recent nonoverlapping algorithms such as FETI-DP and BDDC (Balancing Domain Decomposition by Constraints) methods the coarse spaces becomes quite large, especially in 3D. New coarse unknowns have to be introduced for every edge and face of each subdomain. There has been some progress in reducing the size of the coarse space using a hybrid FETI-DP method [10] in 2D. In [10], a single additional coarse unknown for each subdomain is sufficient.

Nevertheless, in this paper, we use a FETI-DP method with a coarse space for compressible elasticity. In Brands et al. [2], we have seen that this will result in an acceptable performance even in the nonlinear almost incompressible setting. In nonlinear almost incompressible elasticity, before convergence, the the violation of the incompressibility constraint will show local variations. Such a situation does not directly correspond to a linear elastic model with a single global Poisson ratio $\nu$ for the complete computational domain but rather to a varying incompressibility within the domain. Note that recent results for linear elasticity with varying Poisson ratio $\nu$ show that all FETI-DP and BDDC methods are robust with respect to localized almost incompressibility as long as the distance of the incompressible inclusions to the subdomain boundaries are bounded from below by a constant, see Gippert et al. [11, 12].

2. Continuum Mechanical Foundations. In the reference configuration, the computational domain, i.e., the body of interest, is indicated by $B \subset \mathbb{R}^3$, parametrized in $X$ and the current configuration by $S \subset \mathbb{R}^3$, parametrized in $x$. The non-linear function $\varphi_t : B \rightarrow S$ maps the points $X \in B$ onto points $x \in S$ at the time $t \in \mathbb{R}$. Here, the deformation gradient $F$ and the right Cauchy-Green tensor $C$ are
defined by
\[ F = \text{Grad} \varphi \quad \text{and} \quad C = F^T F \] (2.1)

with the Jacobian \( J(X) := \det F(X) > 0 \). We consider hyperelastic materials, where the existence of a strain energy function \( \psi \) is postulated and defined per unit reference volume. We focus on energy functions in the form \( \psi = \hat{\psi}(C, M^{(1)}, M^{(2)}) \), where the last two tensorial arguments \( M^{(a)} := A^{(a)} \otimes A^{(a)} | a = 1, 2 \) are the so-called structural tensors. These arguments characterize the anisotropy of the material, where the unit directions \( A^{(1)} \) and \( A^{(2)} \) are approximations of the collagen fiber bundle orientations in the artery. The formulation of anisotropic constitutive functions based on the concept of structural tensors was first introduced in an attractive way by Boehler [13]. An overview of the theory of representations of tensor functions can be found in the excellent review Zheng [14].

For the construction of specific constitutive equations we need the invariants of the deformation tensor and the additional structural tensors. The principle invariants of \( C \) are
\[ I_1 := \text{tr} (C), \quad I_2 := \text{tr} [\text{Cof} C], \quad I_3 := \det(C), \] (2.2)

where \( \text{Cof}(C) = \det(C)C^{-T} \).

For the modeling of the mechanical behavior of the arterial wall we assume that the response can be approximated by two superimposed transversely isotropic models. This is based on the fact that only weak interactions between the two fiber directions are observed; for further arguments, see Holzapfel et al. [15]. Therefore, the additional (mixed) invariants of interest are
\[ J_4^{(a)} := \text{tr} [CM^{(a)}], \quad J_5^{(a)} := \text{tr} [C^2 M^{(a)}] \quad \text{for} \quad a = 1, 2 , \] (2.3)

see, e.g., [16] and the references therein. The set of differential equations for the underlying boundary value problem is governed by the local form of the balance of linear momentum for the quasi-static case
\[ \text{Div}(P) + \bar{f}_0 = 0 \] with \( P = FS \), (2.4)

here, \( P \) characterizes the 1st Piola-Kirchhoff stress tensor. The 2nd Piola-Kirchhoff stress tensor is computed by \( S = 2 \partial_C \psi \) and \( \bar{f}_0 \) is the body force vector.

3. Free Energy Functions for Soft Biological Tissue. Many biological tissues, such as arteries, are fiber enforced materials composed of an almost incompressible matrix substance with embedded collagen fibers. The arrangement of the fibers in arterial walls is characterized by two preferred directions helically wound along the artery. The material behavior of the collagen fiber bundles is represented by the superposition of two transversely isotropic models; see Holzapfel et al. [15]. Thus, the strain energies are given by
\[ \psi = \psi^{\text{iso}}(C) + \psi^{\text{ti}}(C, M^{(1)}) + \psi^{\text{ti}}(C, M^{(2)}) . \] (3.1)

There exist different possibilities to model the mechanical response of soft biological tissue; see, e.g., [17, 15]. We are interested in polyconvex energy functions. For the construction of anisotropic, polyconvex functions to ensure the existence of minimizers, see, e.g., [18]. Here, we use the model due to [15], which was denoted model \( \psi_B \) in [2],
\[ \psi = c_1 \left( I_1 I_3^{-1/3} - 3 \right) + \sum_{a=1}^2 \frac{k_1}{2k_2} \left\{ \exp \left( k_2 \left( J_4^{(a)} I_3^{-1/3} - 1 \right)^2 \right) - 1 \right\} \]
\[ + \varepsilon_1 (I_3^{\varepsilon_2} + I_3^{-\varepsilon_2} - 2)^{\alpha} . \] (3.2)
FIG. 3.1. Comparison of the penalty function $\psi_p(I_3) = \varepsilon_1(I_3^{\varepsilon_2} + I_3^{-\varepsilon_2} - 2)$ for the two sets of parameters for the media; see Table 3.1.

<table>
<thead>
<tr>
<th>Model</th>
<th>Layer</th>
<th>$\varepsilon_1$ [kPa]</th>
<th>$\varepsilon_1$</th>
<th>$\varepsilon_2$</th>
<th>$\alpha$</th>
<th>$k_1$ [kPa]</th>
<th>$k_2$ [-]</th>
<th>$\beta_f$ [-]</th>
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<td>7.17459</td>
<td>70.0</td>
<td>8.5</td>
<td>1</td>
<td>3.6865e-3</td>
<td>51.1512</td>
<td>3.6865e-3</td>
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<tr>
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<td>med.</td>
<td>9.22575</td>
<td>360.0</td>
<td>9.0</td>
<td>1</td>
<td>192.857</td>
<td>2626.84</td>
<td>43.9</td>
</tr>
<tr>
<td>$\psi$ Augmented</td>
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<td>7.17459</td>
<td>10.0</td>
<td>4.0</td>
<td>1</td>
<td>3.6865e-3</td>
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<td>1</td>
<td>192.857</td>
<td>2626.84</td>
<td>43.9</td>
</tr>
</tbody>
</table>

Table 3.1

The parameter fit is performed under the assumption of incompressibility $(\det(F) = 1)$. The penalty parameters $\varepsilon_1$ and $\varepsilon_2$ are not fitted but chosen a posteriori such that a good fit is still obtained; see Figure 3.2. The parameter $\beta_f$ is the angle between the fibers and the circumferential direction.

Here $\langle b \rangle$ denotes the Macauley brackets defined by $\langle b \rangle = \frac{1}{2} (|b| + b)$, with $b \in \mathbb{R}$. The penalty term $\psi_P = \varepsilon_1(I_3^{\varepsilon_2} + I_3^{-\varepsilon_2} - 2)^\alpha$ with the penalty parameters $\varepsilon_1$ and $\varepsilon_2$, models the incompressibility by penalizing deviations from the constraint $1 = I_3 = \det C = (\det(F))^2$; see also Figure 3.1.

The 4th-order elasticity tensor can be computed from $\psi$ using

$$C = 4 \frac{\partial^2 \psi}{\partial C \partial C} = 4 \frac{\partial}{\partial C} \left( \sum_i \frac{\partial \psi}{\partial L_i} \frac{\partial L_i}{\partial C} \right) = 4 \sum_i \left( \frac{\partial^2 \psi}{\partial C \partial \partial} \frac{\partial L_i}{\partial C} + \frac{\partial \psi}{\partial L_i} \frac{\partial^2 L_i}{\partial C \partial C} \right),$$

with the invariants $\{L_i|1,7\} = \{I_1, I_2, I_3, J^{(1)}_4, J^{(2)}_4, J^{(1)}_5, J^{(2)}_5\}$. One of the contributions to the stiffness matrix stemming from the penalty term $\psi_P$ is therefore

$$\frac{\partial \psi_P}{\partial I_3} = \varepsilon_1 \alpha (I_3^{\varepsilon_2} + I_3^{-\varepsilon_2} - 2)^{\alpha-1} \varepsilon_2 (I_3^{\varepsilon_2-1} - I_3^{-\varepsilon_2-1})$$  \hspace{1cm} (3.3)$$

and

$$\frac{\partial^2 \psi_P}{\partial^2 I_3} = \varepsilon_1 \alpha(\alpha - 1) (I_3^{\varepsilon_2} + I_3^{-\varepsilon_2} - 2)^{\alpha-2} \left( \varepsilon_2 (I_3^{\varepsilon_2-1} - I_3^{-\varepsilon_2-1}) \right)^2$$

$$+ \varepsilon_1 \alpha (I_3^{\varepsilon_2} + I_3^{-\varepsilon_2} - 2)^{\alpha-1} \varepsilon_2 \left( (\varepsilon_2 - 1) I_3^{\varepsilon_2-2} + (\varepsilon_2 + 1) I_3^{-\varepsilon_2-2} \right).$$  \hspace{1cm} (3.4)$$

We can see that the influence of this term grows linearly with $\varepsilon_1$ and exponentially with $\varepsilon_2$. The condition number of the stiffness matrix may deteriorate accordingly.
We consider an abdominal aorta and adjust our function to this biological material. We assume that the mechanical influence of the intima in atherosclerotic arteries is negligible. In the healthy part of the artery it is therefore neglected and in the diseased part it is considered as part of the plaque. In order to find the parameters for our model, we adjust the stresses from the material models to the experimental stresses in Holzapfel [19], where separated layers of an abdominal aorta were studied in uniaxial tension tests. We have chosen to use a different adjustment strategy than in our earlier publication [2]. Here, the fit of the parameters is performed under the assumption that the material is incompressible. We therefore have to enforce the incompressibility constraint separately, i.e., when using a penalty approach we have to chose sufficiently large penalty parameters, see Table 3.1. In the augmented Lagrange approach, a sufficiently accurate stopping criterion has to be chosen for the augmented Lagrange loop, i.e., we have to chose a sufficiently small $TOL$, see Figure 6.2 and 6.3. The results of the parameter adjustment for the material models are summarized in Table 3.1. The plaque is modelled, as in [2], as an isotropic Mooney–Rivlin material,

$$
\psi_{\text{Mooney–Rivlin}} = \beta_1 I_1 + \eta_1 I_2 + \delta_1 I_3 - \delta_2 \ln I_3,
$$

where $\beta_1 = 80.0 \text{ kPa}$, $\eta_1 = 250.0 \text{ kPa}$ and $\delta_1 = 2000.0 \text{ kPa}$. To obtain a stress-free state in the reference configuration the parameter $\delta_2$ has to satisfy $\delta_2 = \beta_1 + 2\eta_1 + \delta_1$.

![Data fits while assuming incompressibility. For the resulting parameters, see Table 3.1.](image)

4. The Three-Field Method. In order to treat the quasi-incompressible material, we relax the point-wise incompressibility constraint and only penalize volumetric changes in a mean sense on every 10-noded tetrahedral finite element. This is accomplished, as in [2], by applying a three-field formulation, known as the $\bar{F}$-approach; see, e.g., Simo [20, Section 45].

Let $J = \det(F)$, then we can introduce $\bar{F}$ as

$$
F = J^{1/3} \bar{F}, \quad \bar{F} := J^{-1/3} F.
$$

From this definition, we clearly have $\det(\bar{F}) = 1$. We then introduce a new, element-wise scalar variable $\theta$, such that $\theta = J$ will be satisfied on every finite element in a mean sense, and define

$$
\bar{F} := \theta^{1/3} \bar{F}, \quad \bar{C} := \bar{F}^T \bar{F}
$$

with $\bar{F} = \bar{F}(\varphi, \theta)$, $\bar{C} = \bar{C}(\varphi, \theta)$. We consider the following three-field Lagrangian using the multiplier $\pi$

$$
L(\varphi, \theta, \pi) = \int_B \psi(\bar{C}(\varphi, \theta)) + \pi(J(\varphi) - \theta) dx - V_{\text{ext}}(\varphi),
$$

where $V_{\text{ext}}(\varphi)$ is the potential energy of external forces; for more details, see Simo [20, Section 45]. We then choose a $P_2 - P_0 - P_0$ mixed finite element discretization for $\varphi, \theta$, and $\pi$, i.e., piecewise quadratic
elements for the deformation field \( \varphi \) and piecewise constant elements for the scalar fields \( \theta \) and \( \pi \). Static condensation of \( \theta \) and \( \pi \), which can be performed locally on each finite element, leads to a reduced problem that we will then solve by a Newton iteration. In the case of the augmented Lagrange methods our functional is

\[
L(\varphi, \theta, \pi, \mu) = \int_B \psi(\bar{C}(\varphi, \theta)) + \pi(J(\varphi) - \theta) dx - V_{ext}(\varphi) + \int_B \mu(\theta - 1) dx.
\]

which is discretized by a \( P_2 - P_0 - P_0 - P_0 \)-approach. Again \( \theta \) and \( \pi \) are statically condensed. The Lagrange multiplier field \( \mu \) is found using an Uzawa-like iteration; see Figures 6.2 and 6.3.

5. FETI-DP Method. Domain decomposition methods are divide-et-impera algorithms where an approximate inverse is constructed from solving small problems on subdomains and a small global problem. Here, we use as a nonoverlapping domain decomposition method, see Figure 7.2, a member of the well known family of FETI-DP methods; see [21, 22, 23, 24, 25, 26, 27] and the references therein. Domain decomposition methods are naturally parallel algorithms, for a FETI-DP method parallel scalability has been demonstrated for more than 65,000 processors cores [28].

Our approach is a classical Newton-Krylov-FETI-DP approach, i.e., we linearize first and then use the FETI-DP domain decomposition method to solve the linearized systems. The augmented Lagrange approach may be then characterized as a augmented-Lagrange-Newton-Krylov-FETI-DP method.

FETI methods have been used to solve large structural mechanics problems on massively parallel machines; see [29, 30, 26, 28]. An introduction to domain decomposition methods is given in the books [31, 32, 33]. Finite Element Tearing and Interconnecting (FETI) domain decomposition methods were first introduced by Farhat and Roux [34]. The more recent FETI-DP methods were first introduced in Farhat et al. [21, 22] and further developed, e.g., in [23, 24, 25, 26].

In FETI-DP methods the computational domain \( \mathcal{B} \) is partitioned into nonoverlapping subdomains \( \mathcal{B}_i \) where one or several subdomains are assigned to each processor; see Figure 7.2. Each subdomain \( \mathcal{B}_i \) has a typical diameter \( H \) and its boundary is denoted by \( \partial \mathcal{B}_i \). Moreover, \( \mathcal{B}_i, i = 1, \ldots, N \), is the union of finite elements with matching finite element nodes on the boundaries of neighboring subdomains across the interface \( \Gamma := \bigcup_{i \neq j} \partial \mathcal{B}_i \cap \partial \mathcal{B}_j \). We use a graph partitioner [35] to define the decomposition of the body into subdomains. Note that in our present algorithm the definition of the subdomains is a completely algebraic process and does not need access to geometric data. We make use of the weak form of the balance of linear momentum on each subdomain which is, neglecting body forces, given by

\[
G = \int_{\mathcal{B}_i} \delta \bar{F} : P(\bar{F}) \, dV - \int_{\partial \mathcal{B}_{i,\sigma}} \delta \bar{u} \cdot t \, dA, \tag{5.1}
\]

with the traction vector \( t = P N \) acting on the Neumann boundary \( \partial \mathcal{B}_{i,\sigma} \), the outward unit normal \( N \) on \( \partial \mathcal{B}_{i,\sigma} \), the virtual displacement field \( \delta \bar{u} \), and the virtual deformation gradient \( \delta \bar{F} \).

For each subdomain \( \mathcal{B}_i \), we assemble the local stiffness matrices \( K^{(i)} \) and load vectors \( f^{(i)} \), \( i = 1, \ldots, N \). We can write the linearized subdomain problems as

\[
K^{(i)}(\Delta D^{(i)}) = f^{(i)}, \tag{5.2}
\]

where \( \Delta D^{(i)} \) denotes the local displacement increment on subdomain \( \mathcal{B}_i \) in the current Newton step, see Section 7.

These local problems will in general not have a unique solution as they may lack essential Dirichlet boundary conditions. This is particularly the case for all interior subdomains, i.e., subdomains \( \mathcal{B}_i \) where \( \partial \mathcal{B}_i \cap \partial \mathcal{B} = \emptyset \).

Let us define the interface by \( \Gamma = \bigcup_{i=1}^N \partial \mathcal{B}_i \setminus \partial \mathcal{B} \). If we view the \( N \) local problems in (5.2) as \( N \) independent problems then the solutions will be discontinuous across the interface \( \Gamma \).
Writing the subdomain matrices and right hand sides block form, we obtain

\[
K = \begin{bmatrix}
K^{(1)} & \cdots & K^{(N)} \\
\vdots & \ddots & \vdots \\
K^{(N)} & \cdots & K^{(1)}
\end{bmatrix}, \quad \Delta D = \begin{bmatrix}
\Delta D^{(1)} \\
\vdots \\
\Delta D^{(N)}
\end{bmatrix}, \quad f = \begin{bmatrix}
f^{(1)} \\
\vdots \\
f^{(N)}
\end{bmatrix}.
\]

The discrete problem can be formulated as minimization problem continuity constraint \( Bu = 0 \) on the interface \( \Gamma \). The matrices \( B = [B^{(1)}, \ldots, B^{(N)}] \) have entries from \( 0, 1, -1 \). We introduce Lagrange multipliers \( \lambda \) to enforce the continuity along the subdomain interface \( \Gamma \) and obtain the problem:

Find \( (\Delta D, \lambda) \), such that

\[
\begin{cases}
K(\Delta D) + B^T\lambda = f \\
B(\Delta D) = 0
\end{cases}
\]

This problem can be solved by eliminating the displacement variables \( \Delta D \) and solving the resulting Schur complement system by a Krylov subspace method. In this paper we use GMRES as our Krylov subspace method. Note that the iteration is performed only on the interface, which significantly reduces the memory requirements for the GMRES method.

In FETI-DP methods some continuity constraints on primal displacement variables \( \Delta \tilde{D}_\Pi \) are enforced throughout iterations. The local subdomain problems are invertible if a sufficient number of primal constraints are chosen. These primal constraints also constitute a coarse problem for the method making it numerically scalable.

After incorporating the primal constraints we obtain the saddle point system

\[
\begin{bmatrix}
\tilde{K} & B^T \\
B & 0
\end{bmatrix}
\begin{bmatrix}
\Delta \tilde{D} \\
\lambda
\end{bmatrix} =
\begin{bmatrix}
\tilde{f} \\
0
\end{bmatrix},
\]

where the matrix \( \tilde{K} \) and right hand side \( \tilde{f} \) are partially coupled in the primal variables,

\[
\tilde{K} = \begin{bmatrix}
K^{(1)}_{BB} & \cdots & K^{(1)}_{\Pi B} \\
\vdots & \ddots & \vdots \\
K^{(N)}_{BB} & \cdots & K^{(N)}_{\Pi B}
\end{bmatrix}, \quad \tilde{f} = \begin{bmatrix}
f^{(1)}_{B} \\
\vdots \\
f^{(N)}_{B}
\end{bmatrix}.
\]

Choosing a sufficient number of primal variables the matrix \( \tilde{K} \) becomes positive definite. We can now reduce the system of equations to an equation in \( \lambda \). It remains to solve

\[
F_{feti} \lambda = d,
\]

where \( F_{feti} = B\tilde{K}^{-1}B^T \).

To precondition \( F_{feti} \), we use the classical Dirichlet preconditioner

\[
M^{-1} := B_D R_D^T S R_D B_D^T,
\]

where \( S \) is the Schur complement obtained by eliminating the interior variables in every subdomain, i.e.,

\[
S = \begin{bmatrix}
S^{(1)} & \cdots & S^{(N)}
\end{bmatrix}.
\]
Here, \( R_F \) is a restriction matrix, consisting of zeros and ones, that, when applied to a vector \( \Delta \tilde{D} \), removes the interior variables from \( \Delta \tilde{D} \). The matrices \( B_P \) are scaled variants of the jump operator \( B \) where, in the simplest case, the contribution from and to each interface node is scaled by the inverse of the multiplicity of the node. We define the multiplicity of a node as the number of subdomains it belongs to. For heterogeneous problems a more elaborate scaling, using an appropriate scaling factor, defined by the coefficients \( \rho_i \), is necessary; see, e.g., [23, p. 1532, Formula (4.3)] and [36, p. 1403, Formula (6)].

6. Algorithms. In our nonlinear scheme we solve a sequence of linear problems obtained from Newton’s method, see, e.g., Figure 6.1. This is also referred to as (pseudo) time stepping or load stepping. To obtain a fair comparison between the different approaches, we have chosen a well-known automatic time stepping strategy. We increase \( \Delta t \) when the number of Newton iterations is smaller than a certain threshold and decrease \( \Delta t \) if it is larger than a given threshold.

The simultaneous augmented Lagrange (SAL) approach, where the iteration for the Lagrange multiplier is performed simultaneously with the Newton correction, can be viewed as an inexact Newton-like method. Thus, a quadratic convergence rate cannot be expected. Here, we have to chose the bounds for the auto time stepping more generously. For all approaches the maximal time step size was bounded from above by a certain value. In Figures 6.1, 6.2, and 6.3, we describe the algorithms in detail.

7. Application and Numerical Results. In this section we report on simulations using the finite element model of an arterial segment with an embedded plaque, see Figure 7.1, obtained from IVUS ultra sound data; see [37, 1]. The discretization uses 10-noded tetrahedral elements which results in 1.3M degrees of freedom for the displacement. A significant portion of the unknowns is located inside the plaque component. We have 300K tetrahedra generating 300K unknowns for the Lagrange multiplier \( \mu \) in the augmented Lagrange method. A pressure of up to 33.33 kPa (≈ 250 mmHg) is applied to the interior of the arterial segment.

For the computations we apply our simulation environment consisting of the Finite Element Program FEAP of R. L. Taylor, University of California, and our parallel implementation of the Finite Element Tearing and Interconnecting - Dual Primal method (FETI-DP) to simulate our 3D problems. The computations were performed on an AMD Opteron compute server with 16 cores at 2.5 Ghz. For our parallel solver we use MPI, PETSc [38, 39, 40], UMFPACK [41] and the ACML.

The residual norm of the Newton step is computed as the Euclidean norm of the right hand side vector. The stopping criterion for the Newton method is either the reduction of the absolute residual norm to a value less than \( 10^{-5} \) or an absolute residual norm of less than \( 10^{-4} \) for three consecutive Newton steps.

The size of the incremental load steps (pseudo time) is controlled by the automatic time stepping scheme; see Section 6. For the penalty approach we increase \( \Delta t \) when the number of Newton iterations is smaller than 6 and decrease \( \Delta t \) when it is larger than 9. This choice produced the best results. In the nested augmented Lagrange approach (NAL), for the auto time stepping, we only consider the first Newton iteration within each augmented Lagrange iteration since this is the critical step. The later Newton steps typically converge faster compared to the first step. In the simultaneous augmented Lagrange (SAL) approach the bounds for the auto time stepping are chosen much larger, i.e., as 18 and 36, see the discussion in Section 6. In all cases the maximal time step size was bounded from above by \( \Delta t_{\text{max}} = 0.4 \).

The parameter \( \xi_k = \xi \) is chosen by hand from trial and error using a small finite element model (SAL, TOL=10^{-2}; \( \xi = 5.0 \times 10^2 \); SAL, TOL=10^{-3}; \( \xi = 1.0 \times 10^3 \); NAL: \( \xi = 5.0 \times 10^2 \)). In this sense, our results are not sharp but rather give an upper bound on the performance of the augmented Lagrange approaches.

For the FETI-DP domain decomposition method, we use a decomposition into 224 subdomains; see Figure 7.2. The continuity constraint in the FETI-DP method generates 400K unknowns for the Lagrange multiplier \( \lambda \), see (5.4) and Figure 7.2. The FETI-DP Krylov iteration is stopped when the absolute residual is reduced to \( 5 \times 10^{-9} \).
The total cost of the computation can roughly be estimated by multiplying the number of global Newton steps by the corresponding average number of (inner) FETI-DP iterations, see Tables 7.1, 7.2, 7.4, and 7.3. In Table 7.5 the data is collected in compact form for comparison.

<table>
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<tr>
<th>t</th>
<th>Newton steps</th>
<th>∅ FETI-DP its</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.010</td>
<td>9</td>
<td>172.2</td>
</tr>
<tr>
<td>0.020</td>
<td>5</td>
<td>173.0</td>
</tr>
<tr>
<td>0.036</td>
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<td>175.8</td>
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<td>5</td>
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</tr>
<tr>
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<td>189.3</td>
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<td>0.141</td>
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<td>187.0</td>
</tr>
<tr>
<td>0.204</td>
<td>6</td>
<td>201.8</td>
</tr>
<tr>
<td>0.267</td>
<td>5</td>
<td>195.6</td>
</tr>
<tr>
<td>0.367</td>
<td>7</td>
<td>208.0</td>
</tr>
<tr>
<td>0.467</td>
<td>7</td>
<td>204.1</td>
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<tr>
<td>0.567</td>
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<td>207.4</td>
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<td>0.725</td>
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<td>217.8</td>
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<td>0.884</td>
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<td>242.0</td>
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<tr>
<td>1.386</td>
<td>6</td>
<td>253.8</td>
</tr>
<tr>
<td>1.637</td>
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<td>266.3</td>
</tr>
<tr>
<td>1.889</td>
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<td>279.4</td>
</tr>
<tr>
<td>2.287</td>
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<td>301.0</td>
</tr>
<tr>
<td>2.500</td>
<td>6</td>
<td>312.5</td>
</tr>
</tbody>
</table>

Σ 112 Total ∅ 220.8

Table 7.1

Newton iteration for the penalty formulation (P). Pseudo-time t, number of Newton steps, average number of Krylov iterations per Newton step. TOL=10\(^{-2}\). Simulation until 33.33 kPa (250 mmHg = Pseudotime 2.5).

Our results show that the use of the augmented Lagrange method can significantly improve the properties of the linearized systems occurring in the nonlinear solution scheme, i.e., the FETI-DP iterative method converges in a lower number of iterations. The convergence of the nonlinear scheme is also improved, i.e., in our nonlinear scheme larger pseudo time steps ∆t can be chosen. Of course, an additional iteration process for the Lagrange multiplier is introduced.

The comparison of Tables 7.1 and 7.2 show that in case of the simultaneous augmented Lagrange approach the additional cost for the augmented Lagrange iteration is more than amortized by the faster convergence of the nonlinear scheme and the linear iterative solver. The nested augmented Lagrange approach has a considerably higher cost; see Table 7.3.

Clearly, the linear systems resulting from the augmented Lagrange approaches are better conditioned. We should note here that ill-conditioning not only influences the convergence of iterative solvers but it also affects direct solvers, i.e., the quality of the solution will deteriorate.

Moreover, in the augmented Lagrange approaches the volumetric change is exactly controlled during the iteration process, i.e., we have satisfied element-wise the condition |det(F) - 1| ≤ 10\(^{-2}\) in Tables 7.2 and 7.3. In the penalty approach the volumetric change produced by the chosen penalty parameters is only known a posteriori. In our example in Table 7.1 the solution using the penalty approach only satisfies |det(F) - 1| ≤ 0.02084; see Table 7.5. In the augmented Lagrange approach, for a slightly higher cost, we can also enforce |det(F) - 1| ≤ 10\(^{-3}\) by setting TOL=10\(^{-3}\); cf. Table 7.4 and 7.5.
### Simultaneous AL, TOL=10^{-2}

<table>
<thead>
<tr>
<th>t</th>
<th>Newton/AL steps</th>
<th>∅ FETI-DP its</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.010</td>
<td>9</td>
<td>99.3</td>
</tr>
<tr>
<td>0.026</td>
<td>4</td>
<td>100.5</td>
</tr>
<tr>
<td>0.051</td>
<td>5</td>
<td>101.4</td>
</tr>
<tr>
<td>0.091</td>
<td>5</td>
<td>102.4</td>
</tr>
<tr>
<td>0.154</td>
<td>6</td>
<td>104.2</td>
</tr>
<tr>
<td>0.254</td>
<td>7</td>
<td>105.3</td>
</tr>
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<td>0.412</td>
<td>9</td>
<td>109.1</td>
</tr>
<tr>
<td>0.664</td>
<td>13</td>
<td>118.8</td>
</tr>
<tr>
<td>1.062</td>
<td>14</td>
<td>138.2</td>
</tr>
<tr>
<td>1.462</td>
<td>17</td>
<td>158.8</td>
</tr>
<tr>
<td>1.862</td>
<td>18</td>
<td>179.7</td>
</tr>
<tr>
<td>2.261</td>
<td>18</td>
<td>202.5</td>
</tr>
<tr>
<td>2.500</td>
<td>16</td>
<td>215.9</td>
</tr>
<tr>
<td>Σ</td>
<td>141</td>
<td>Total ∅ 150.2</td>
</tr>
</tbody>
</table>

**Table 7.2**

Simultaneous augmented Lagrange (SAL) iteration. Pseudo-time \( t \), number of Newton/AL steps, average number of Krylov iterations per Newton/AL step. TOL=10^{-2}, \( ξ = 5.0 \times 10^2 \). Simulation until 33.33 kPa (250 mmHg = Pseudotime 2.5).

### Nested AL, TOL=10^{-2}

<table>
<thead>
<tr>
<th>t</th>
<th>Newton steps</th>
<th>∅ FETI-DP its</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.010</td>
<td>10</td>
<td>99.2</td>
</tr>
<tr>
<td>0.020</td>
<td>5</td>
<td>99.8</td>
</tr>
<tr>
<td>0.036</td>
<td>6</td>
<td>101.2</td>
</tr>
<tr>
<td>0.061</td>
<td>6</td>
<td>102.2</td>
</tr>
<tr>
<td>0.101</td>
<td>10</td>
<td>103.1</td>
</tr>
<tr>
<td>0.164</td>
<td>18</td>
<td>104.0</td>
</tr>
<tr>
<td>0.227</td>
<td>18</td>
<td>104.1</td>
</tr>
<tr>
<td>0.327</td>
<td>23</td>
<td>106.0</td>
</tr>
<tr>
<td>0.427</td>
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<tr>
<td>0.585</td>
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<td>115.4</td>
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<tr>
<td>0.744</td>
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<tr>
<td>0.902</td>
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<td>130.7</td>
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<tr>
<td>1.061</td>
<td>40</td>
<td>138.9</td>
</tr>
<tr>
<td>1.312</td>
<td>45</td>
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<td>163.7</td>
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<tr>
<td>1.815</td>
<td>49</td>
<td>182.5</td>
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<tr>
<td>2.066</td>
<td>57</td>
<td>191.4</td>
</tr>
<tr>
<td>2.317</td>
<td>65</td>
<td>206.2</td>
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<tr>
<td>2.500</td>
<td>57</td>
<td>216.6</td>
</tr>
<tr>
<td>Σ</td>
<td>618</td>
<td>Total ∅ 154.0</td>
</tr>
</tbody>
</table>

**Table 7.3**

Nested augmented Lagrange (NAL) iteration. Pseudo-time \( t \), number of Newton steps, average number of Krylov iterations per Newton/AL step. TOL=10^{-2}, \( ξ = 5.0 \times 10^6 \). Simulation until 33.33 kPa (250 mmHg = Pseudotime 2.5).
Simultaneous AL, TOL=$10^{-3}$

<table>
<thead>
<tr>
<th>$t$</th>
<th>Newton/AL steps</th>
<th>∅ FETI-DP its</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.010</td>
<td>9</td>
<td>99.3</td>
</tr>
<tr>
<td>0.026</td>
<td>6</td>
<td>100.3</td>
</tr>
<tr>
<td>0.051</td>
<td>8</td>
<td>101.3</td>
</tr>
<tr>
<td>0.091</td>
<td>10</td>
<td>102.2</td>
</tr>
<tr>
<td>0.154</td>
<td>15</td>
<td>103.0</td>
</tr>
<tr>
<td>0.254</td>
<td>13</td>
<td>104.2</td>
</tr>
<tr>
<td>0.412</td>
<td>15</td>
<td>108.9</td>
</tr>
<tr>
<td>0.664</td>
<td>18</td>
<td>119.8</td>
</tr>
<tr>
<td>1.062</td>
<td>37</td>
<td>143.5</td>
</tr>
<tr>
<td>1.462</td>
<td>38</td>
<td>164.6</td>
</tr>
<tr>
<td>1.862</td>
<td>37</td>
<td>188.1</td>
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<tr>
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<td>212.3</td>
</tr>
<tr>
<td>2.500</td>
<td>35</td>
<td>233.1</td>
</tr>
</tbody>
</table>

Σ 284 Total ∅ 161.4

Table 7.4

Simultaneous augmented Lagrange (SAL) iteration. Pseudo-time $t$, number of Newton/AL steps, average number of Krylov iterations per Newton/AL step. TOL=$10^{-3}$, $\xi = 1.0 \times 10^3$. Simulation until 33.33 kPa (250 mmHg = Pseudotime 2.5).

<table>
<thead>
<tr>
<th>Penalty</th>
<th>Load steps</th>
<th>Global Newton</th>
<th>∅ FETI-DP it</th>
<th>min($\text{det}(F)$)</th>
<th>max($\text{det}(F)$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>19</td>
<td>112</td>
<td>220.8</td>
<td>0.99265</td>
<td>1.02084</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(min = 170, max = 316)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

TOL=$10^{-2}$

| Simult. AL (SAL) | 13   | 141  | 150.2 | 0.99006 | 1.00997 |
|                 |      |      | (min = 98, max = 217) |                       |                      |

| Nested AL (NAL) | 19   | 618  | 154.0 | 0.99039 | 1.00997 |
|                 |      |      | (min = 98, max = 427) |                       |                      |

TOL=$10^{-3}$

| Simult. AL (SAL) | 13   | 248  | 161.4 | 0.99990 | 1.00099 |
|                 |      |      | (min = 98, max = 368) |                       |                      |

Table 7.5

Comparison of the Methods. We can estimate the total cost roughly by multiplying the number of global Newton iterations by the average number of FETI-DP iterations.

In the results in Tables 7.2, 7.3, and 7.4, we see that the number of Newton/AL-iterations increases during the simulation. This may be due to the fact that in the beginning of the simulation only a very small number of finite elements violate the element-wise condition $|\text{det}(F) - 1| \leq 10^{-2}$ and the number of such elements increases during the simulation.

The results in Tables 7.1, 7.2, 7.3, and 7.4 also show an increase of the FETI-DP iterations during the simulation. We believe that this may in part be due to an increasing influence of the incompressibility constraint during the simulation but also results from the exponential stiffening behavior of the fibers. In [42], we have observed that the anisotropies introduced to the material wall models by the terms modeling...
the fibers can have a visible impact on the convergence of the nonlinear iteration scheme as well as the convergence of the iterative linear solver. Ideas described in [28] may improve the convergence of domain decomposition solvers for such anisotropic problems.

For completeness we also report on the parallel scalability of the FETI-DP method obtained for a single linearized system on a Cray XT6m. We use the arterial wall modell depicted in Figure 7.1 with 1.3M degrees of freedom. Here, the model was decomposed into 112 subdomains which was more suitable for the Cray supercomputer as opposed to the Opteron compute server used for the other computations.

<table>
<thead>
<tr>
<th>Cores</th>
<th>It.</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>99</td>
<td>400s</td>
</tr>
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<td>14</td>
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<td>231s</td>
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<td>99</td>
<td>79s</td>
</tr>
<tr>
<td>56</td>
<td>99</td>
<td>47s</td>
</tr>
<tr>
<td>112</td>
<td>99</td>
<td>34s</td>
</tr>
</tbody>
</table>

Table 7.6

Strong scalability benchmark on the Cray XT6m at Universität Duisburg-Essen: Parallel FETI-DP solver applied to a single linear problem from the nonlinear simulation of an arterial wall structure with 1.3M displacement variables. Decomposition into 112 subdomains. In this benchmark, the iteration was stopped when the residual was reduced by a factor of 1e07.

Acknowledgements: The work of the authors was financially supported by the Deutsche Forschungsgemeinschaft (DFG) under research grants KL 2094/2 and SCHR 570/7. We also acknowledge the scientific support by Prof. Dr. med. R. Erbel, Dr. med. D. Böse (both Universitätsklinikum Essen). We acknowledge the use of the Cray XT6m supercomputer at Universität Duisburg-Essen.

REFERENCES


Balay, S., Buschelman, K., Eijkhout, V., Gropp, W.D., Kaushik, D., Knepley, M.G., McInnes, L.C., Smith, B.F. and


Nonlinear Iteration (Penalty)

Set $k = 0$ and $t_0 = \Delta t_0$;

Apply partial load $t_k \cdot f_{\text{load}}$ if full load not yet reached;

Use Newton iteration to solve the nonlinear problem.

Solve linearized problem by the FETI-DP method using GMRES;

Apply Newton correction;

Adapt load step size $\Delta t_{k+1}$, i.e.,

$\Delta t_{k+1} = 10^{1/5} \Delta t_k$, $\Delta t_{k+1} = 10^{-1/5} \Delta t_k$, or $\Delta t_{k+1} = \Delta t_k$;

Set $t_{k+1} = t_k + \Delta t_{k+1}$;

**Fig. 6.1. Using the penalty approach for the incompressibility.**

Nonlinear Iteration (Nested Augmented Lagrange)

Set $k = 0$ and $t_0 = \Delta t_0$;

Apply partial load $t_k \cdot f_{\text{load}}$ if full load not yet reached;

Set Lagrange multiplier $\mu_0 = 0$;

Do

Use Newton iteration to solve the nonlinear problem for fixed multiplier $\mu_k$;

Solve linearized problem by the FETI-DP method using GMRES;

Apply Newton correction;

Update Lagrange parameter for all elements $T$ that violate the condition $|\theta_T - 1| \geq \text{TOL}$, i.e., $\mu_{T,k+1} = \mu_{T,k} + \xi_k (\theta_T - 1)$;

While elements $T$ with $|\theta_T - 1| \geq \text{TOL}$ exist;

Adapt load step size $\Delta t_{k+1}$, i.e., $\Delta t_{k+1} = 10^{1/5} \Delta t_k$, $\Delta t_{k+1} = 10^{-1/5} \Delta t_k$, or $\Delta t_{k+1} = \Delta t_k$;

Set $t_{k+1} = t_k + \Delta t_{k+1}$;

**Fig. 6.2. Nested augmented Lagrange (NAL) for the incompressibility [4, 5].**
Nonlinear Iteration (Simultaneous Augmented Lagrange)

Set $k = 0$ and $t_0 = \Delta t_0$;

Apply partial load $t_k \cdot f_{\text{load}}$ if full load not yet reached;

Set Lagrange multiplier $\mu_0 = 0$;

While Newton iteration has not converged and while elements $T$ with $|\theta_T - 1| \geq \text{TOL}$ exist: Solve nonlinear problem with simultaneous Newton iteration and iteration for $\mu$;

Solve linearized problem by the FETI-DP method using GMRES;

Apply Newton correction and update Lagrange parameter for all elements $T$ that violate the condition $|\theta_T - 1| \geq \text{TOL}$, i.e.,

$\mu_{T,k+1} = \mu_{T,k} + \xi_k (\theta_T - 1)$;

Adapt load step size $\Delta t_{k+1}$, i.e.,

$\Delta t_{k+1} = 10^{1/5} \Delta t_k$, $\Delta t_{k+1} = 10^{-1/5} \Delta t_k$, or $\Delta t_{k+1} = \Delta t_k$.

Set $t_{k+1} = t_k + \Delta t_{k+1}$;

Fig. 6.3. Simultaneous augmented Lagrange (SAL) for the incompressibility [4, 5].

Fig. 7.1. Cut through the atherosclerotic arterial segment with the embedded plaque; geometry obtained from IVUS data, see Figure 1.1 and [1]. The finite element model has 1.3M displacement unknowns and 300K unknowns for the Lagrange multiplier $\mu$ in the augmented Lagrange method.

Fig. 7.2. Exploded view of the nonoverlapping domain decomposition of the arterial segment into 224 nonoverlapping subdomains.