

A Fast Solver for Finite Deformation Contact Problems

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February 21, 2006

Abstract

We present a new solver for large-scale two-body contact problems in nonlinear elasticity. It is based on an SQP-trust-region approach. This guarantees global convergence to a first-order critical point of the energy functional. The linearized contact conditions are discretized using mortar elements. A special basis transformation known from linear contact problems allows to use a monotone multigrid solver for the inner quadratic programs. They can thus be solved with multigrid complexity. Our algorithm does not contain any regularization or penalization parameters, and can be used for all hyperelastic material models.

1 Introduction

Contact problems are a frequently occurring phenomenon in computational mechanics. Many real-life problems can only be modelled taking into account the possible contact between different objects. This usually comes at the price of a highly increased mathematical complexity. While many problems in continuum mechanics are smooth and, in simple cases, even linear, mechanical contact introduces a discontinuity into the formalism. Consequently, the numerical solution of such problems is considerably more difficult. This is especially the case when the problems at hand are very large.

Because of the importance in applications, various techniques for contact problems have been presented in the literature. When the deformations are assumed to be small, the problem reduces to a linear one with linear inequality constraints. Different approaches for those problems include active-set methods [6] or domain decomposition techniques [13]. Wohlmuth and Krause [14] used mortar methods to discretize the contact conditions. This guarantees optimal discretization errors. They then solved the resulting systems using a monotone multigrid solver.

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When large deformations are considered, many of those techniques cannot be used anymore. The equations governing the behaviour of materials undergoing large deformations are nonlinear even in the absence of contact. Furthermore, the sets of admissible deformation become nonconvex. A standard way to overcome these difficulties is to regularize the contact conditions and solve the resulting equations with variants of Newton's method. The reader may consult the book by Laursen [10] for an in-depth discussion of those algorithms.

In this article we look at contact problems from an optimization perspective. Nearly all elastic material models used today are *hyperelastic* models, which means that there is an energy functional J whose critical points are solutions of the elasticity problem. When finite deformations are to be modelled, this functional is usually nonconvex, but smooth. The nonpenetration condition adds nonconvex inequality constraints to the problem.

SQP-trust-region methods have emerged in the literature as a standard way to handle such optimization problems [3]. However, their efficiency crucially depends on the availability of a fast solver for the quadratic problems occurring in each iteration of a trust-region solver. It is the aim of this article to show how the special structure of a multi-body contact problem can be exploited to make those inner quadratic problems (QPs) amenable to a multigrid solver, thus increasing the overall efficiency.

We will proceed as follows: In Section 2, we will formally pose the finite deformation contact problem. Section 3 contains the presentation of our new solver. After a brief introduction to SQP and trust-region methods we explain how the contact conditions are linearized and discretized using mortar elements (Sec. 3.1). Sections 3.2 and 3.3 then present monotone multigrid methods and show what modifications are necessary in order to use them as the inner QP solver in the trust-region algorithm. We close by giving numerical results showing the applicability of our solver.

2 Two-Body Contact in Finite Deformation Elasticity

This paper deals with contact problems between two elastic bodies undergoing large deformations. A prototype setting is depicted in Fig. 1. We identify the two bodies in their reference configurations with two compact sets $\Omega^{(1)}, \Omega^{(2)} \subset \mathbb{R}^d$, $d \in \{2, 3\}$. In the presence of body forces f and boundary forces h , as well as displacement boundary conditions, the bodies deform into new configurations. This deformation is denoted by functions $\varphi^{(i)} : \Omega^{(i)} \rightarrow \mathbb{R}^d$. We set $\Omega = \Omega^{(1)} \cup \Omega^{(2)}$ and $\varphi : \Omega \rightarrow \mathbb{R}^d$ such that $\varphi|_{\Omega^{(i)}} = \varphi^{(i)}$.

The displacements φ shall be taken from the space $\mathbf{H}^1(\Omega) = (H^1(\Omega))^d$ of d -valued, first-order Sobolev functions on Ω . We will sometimes use $\mathbf{H}_D^1(\Omega)$ to denote the affine subspace of $\mathbf{H}^1(\Omega)$ respecting the Dirichlet conditions.

In nonlinear mechanics it is important to bear in mind the distinction between material coordinates, defined on the reference configuration, and spatial

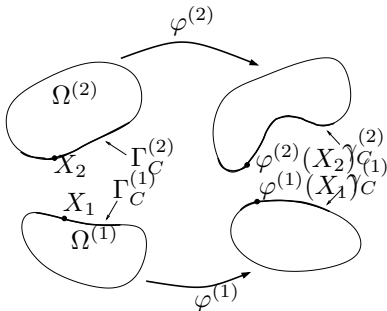


Figure 1: Geometry of the finite deformation two-body contact problem

coordinates on the deformed configuration. We will use upper case latin letters X, Y, \dots for material coordinates and lower case ones x, y, \dots for spatial ones.

The boundary of body $\Omega^{(i)}$ is denoted by $\Gamma^{(i)}$. It is composed of three disjoint parts $\Gamma_D^{(i)}, \Gamma_N^{(i)}, \Gamma_C^{(i)}$, such that $\Gamma_D^{(i)} \cup \Gamma_N^{(i)} \cup \Gamma_C^{(i)} = \Gamma^{(i)}$. We will apply Dirichlet and Neumann boundary conditions on $\Gamma_D^{(i)}$ and $\Gamma_N^{(i)}$, respectively. On $\Gamma_C^{(i)}$, we expect contact to occur. We set $\gamma^{(i)} = \varphi^{(i)}(\Gamma^{(i)})$ and $\gamma_C^{(i)} = \varphi^{(i)}(\Gamma_C^{(i)})$ for the deformed boundaries.

2.1 Nonlinear Elasticity

The material models considered in this article are fully nonlinear elastic ones. This means that the strain E is a quadratic function

$$E = \frac{1}{2}(\nabla u + \nabla u^T + \nabla u^T \nabla u)$$

of the displacements $u : \Omega \rightarrow \mathbb{R}^d$ defined by $u(X) = \varphi(X) - X$. Also the relationship between the strains E and the stresses σ will be a nonlinear one. In particular, we will look at general hyperelastic materials. There, the stress $\sigma : \Omega \rightarrow \mathbb{S}^d$, with \mathbb{S}^d the space of second-order symmetric d -dimensional tensors, can be expressed as the derivative of a stored energy function $J : \mathbf{H}_D^1(\Omega) \rightarrow \mathbb{R}$

$$\sigma = \frac{\partial J}{\partial E}.$$

Finding a solution of the continuity equation

$$-\operatorname{div} \sigma = f \tag{1}$$

is then equivalent to finding stationary points of the functional J [2]. Thus, nonlinear elasticity problems can be written as optimization problems. In what follows, there will be no further restrictions on J other than that it be twice differentiable.

For the purpose of finite element computations we consider the two bodies $\Omega^{(1)}$ and $\Omega^{(2)}$ approximated by two conforming grids \mathcal{T}^1 and \mathcal{T}^2 . The sets of

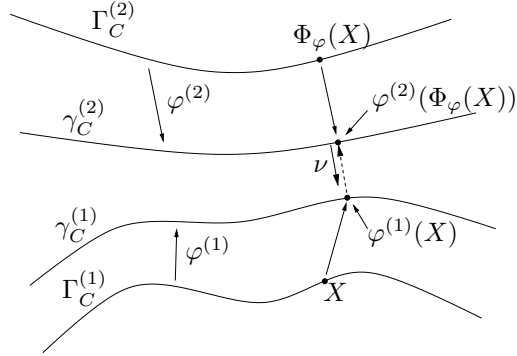


Figure 2: The nonlinear contact condition

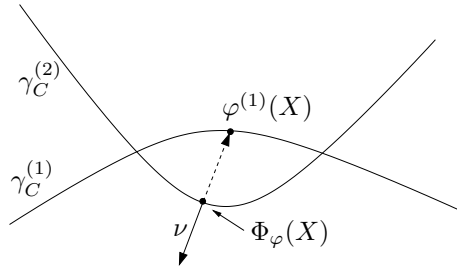


Figure 3: g is negative if the two bodies overlap

grid nodes are denoted by \mathcal{N}^1 and \mathcal{N}^2 , respectively. We will use standard first order Lagrangian finite element functions to discretize Problem (1). The space of all those functions on grid $\mathcal{T}^{(i)}$ will be called $S_h^{(i)}$.

2.2 Contact Conditions

If frictionless contact is to be modelled, the appropriate nonpenetration condition is simply that φ be injective on the interior of Ω . Even though mathematically elegant, this formulation is not very handable in an optimization context, where constraints on the solution are usually written in terms of equalities and inequalities. We therefore write the nonpenetration condition in a different way, taken from Laursen [10].

The first step is the parametrization of contact surface $\Gamma_C^{(2)}$ over contact surface $\Gamma_C^{(1)}$. For each point X on $\Gamma_C^{(1)}$ define $\Phi_\varphi(X) \in \Gamma_C^{(2)}$ by the closest-point projection in the deformed configuration

$$\Phi_\varphi(X) = \arg \min_{Y \in \Gamma_C^{(2)}} \|\varphi^{(1)}(X) - \varphi^{(2)}(Y)\|.$$

Remark 2.1 *There are situations where a point $x \in \gamma_C^{(1)}$ has more than one closest neighbor on $\gamma_C^{(2)}$. In that case it is sufficient to pick an arbitrary one of those for the definition of Φ_φ .*

Using the contact parametrization Φ_φ , we can define the gap function $g : \Gamma_C^{(1)} \rightarrow \mathbb{R}$ as

$$g(X) = \langle \nu_\varphi(X), [\varphi^{(1)}(X) - \varphi^{(2)}(\Phi_\varphi(X))] \rangle, \quad (2)$$

where we have used $\nu_\varphi = \nu \circ \varphi^{(2)} \circ \Phi_\varphi$ to denote the outward unit normals to γ_C^2 as a function on $\Gamma_C^{(1)}$. The condition of nonpenetration can now be stated as

$$0 \leq g(X) \quad \forall X \in \Gamma_C^{(1)}. \quad (3)$$

Keep in mind that g implicitly depends on the current deformation φ . Condition (3) is equivalent to injectivity of φ on $\mathring{\Omega}$, if both $\varphi^{(i)}$ are injective on the interiors of their respective domains. Evidently, $g(X)$ is nonnegative if $\varphi^{(1)}(X) \notin \mathring{\Omega}^{(2)}$ (Fig. 2). If, on the other hand, $\varphi^{(1)}(X) \in \mathring{\Omega}^{(2)}$, then from the definition of Φ_φ it follows that the vector from $\varphi^{(2)}(\Phi_\varphi(X))$ to $\varphi^{(1)}(X)$ appearing in (2) is a positive multiple of the *inside* surface normal of γ_C^2 at $\varphi^{(2)}(\Phi_\varphi(X))$. Thus, its scalar product with ν yields a negative value (Fig. 3).

Remark 2.2 *Note that in general the set*

$$\mathcal{K} = \{\varphi \in \mathbf{H}_D^1(\Omega) \mid 0 \leq g(X) \text{ for all } X \in \Gamma_C^{(1)}\}$$

of admissible displacements is not convex!

3 An SQP-Trust-Region Algorithm

SQP and trust-region algorithms are well-known in optimization theory [7]. They are designed to solve problems of the type

$$\text{minimize } J(x) \text{ subject to } c_i(x) \leq 0, \quad (4)$$

where the c_i are a set of smooth scalar constraint functions. Most literature presents SQP and trust-region methods in a finite-dimensional context. Since our problem will eventually be posed in a finite-element space, we will do the same. In this section, x will designate a vector in the finite-dimensional space \mathbb{R}^n .

Common to both SQP and trust-region methods is the use of model functions J_k to mimic the local behaviour of the functional J around iterates x_k . The model functions are usually quadratic,

$$J_k(x) = x^T H_k x + b_k x. \quad (5)$$

A new iterate x_{k+1} is then produced by minimizing the quadratic functional (5). The most straightforward variant, which is the one we will use, takes the Hessian

and the gradient of J at x_k for H_k and b_k , respectively. In the absence of constraints this yields the standard Newton method.

Consider now the case where J is to be minimized on a set K bounded by nonlinear equations

$$K = \{x \in \mathbb{R}^n \mid c_i(x) \leq 0, \quad 0 \leq i < m\}, \quad (6)$$

the $c_i : \mathbb{R}^n \rightarrow \mathbb{R}$ being a set of m smooth constraint functions. The SQP approach is to linearize the inequality constraints at each iteration step. Therefore, at the current iteration x_k , K is replaced by

$$K_k = \{x \in \mathbb{R}^n \mid (x - x_k) \cdot \nabla c_i(x_k) \leq -c_i(x_k), \quad 0 \leq i < m\}.$$

This new set K_k is bounded by hyperplanes. In particular, this means that K_k is convex. Minimizing a functional on K_k is thus considerably easier than minimizing over K . Nevertheless, under suitable assumptions, we can expect x_k to approach a solution of (4) as $k \rightarrow \infty$ [3].

The quadratic model functions J_k defined by (5) cannot generally be assumed to be convex. This means that the quadratic problem

$$\text{minimize } J_k \text{ on } K_k$$

may not have a solution, if K_k is not bounded. Trust-region methods therefore constrain the problem further by additionally imposing

$$x_{k+1} \in K_k^{\text{tr}} = \{x \mid \|x - x_k\| \leq \rho\}$$

for a suitable radius $\rho > 0$. The set K_k^{tr} is called the trust-region. The norm used for its definition is arbitrary. In view of the use of a monotone multigrid method we will use the infinity-norm. Various heuristics are available for controlling the trust-region radius ρ .

A considerable amount of convergence theory has been published for SQP and trust-region methods [3, 7]. Under quite general conditions it can be shown that the algorithms converge globally to first-order critical points of J on K . In fact, due to the close relationship with Newton methods, under suitable assumptions the convergence speed is even locally quadratic.

In FE problems, the assembly of the Hessians H_k and gradients b_k can be done efficiently, and the algorithm will spend most of its time solving the quadratic programs. For large scale applications it is therefore of great importance to have a fast QP solver. In the following we will show how a special basis of S_h can be chosen in which the K_k take the form of hypercubes. This will allow the use of a monotone multigrid method, which, under certain conditions, can solve the QPs with multigrid complexity.

3.1 Linearized Contact Conditions

In this section we describe an approximate linearization of the contact condition (3) which is required at each SQP step. We then show how to discretize

this linear condition using mortar elements. We denote the configuration at the k -th SQP step as φ_k , and the contact parameterization Φ_φ with respect to φ_k as Φ_{φ_k} .

Taylor expansion of the gap function g around φ_k gives

$$g_k(\varphi) = g(\varphi_k) + ((Dg)(\varphi_k))(\varphi - \varphi_k). \quad (7)$$

In general Dg can be obtained as the Gâteaux derivative

$$\begin{aligned} (Dg)(\varphi_k)(v) &= \lim_{t \rightarrow 0} \frac{g(\varphi_k + tv) - g(\varphi_k)}{t} \\ &= \lim_{t \rightarrow 0} \frac{1}{t} \left[\left\langle \nu_{\varphi_k + tv}, (\varphi_k^{(1)} + tv^{(1)}) - (\varphi_k^{(2)} + tv^{(2)}) \circ \Phi_{\varphi_k + tv} \right\rangle \right. \\ &\quad \left. - \left\langle \nu_{\varphi_k}, \varphi_k^{(1)} - \varphi_k^{(2)} \circ \Phi_{\varphi_k} \right\rangle \right]. \quad (8) \end{aligned}$$

Remember that in general Φ_φ as a function of φ is neither continuous nor single-valued. We thus make the simplifying assumption that $\Phi_{\varphi_k + tv}$ can be approximated by Φ_{φ_k} and further that $\nu_{\varphi_k + tv}$ can be approximated by ν_{φ_k} . This allows us to cancel several terms in (8) and we are left with

$$(Dg)(\varphi_k)(v) = \langle \nu_{\varphi_k}, v^{(1)} - v^{(2)} \circ \Phi_{\varphi_k} \rangle.$$

Plugging this expression into (7), our pseudo-linearized contact condition reads

$$0 \leq g(\varphi_k) + \langle \nu_{\varphi_k}, (\varphi^{(1)} - \varphi_k^{(1)}) - (\varphi^{(2)} - \varphi_k^{(2)}) \circ \Phi_{\varphi_k} \rangle.$$

Written in terms of corrections $d_k = \varphi - \varphi_k$, this last inequality becomes

$$\langle -\nu_{\varphi_k}, d^{(1)} - d^{(2)} \circ \Phi_{\varphi_k} \rangle \leq g(\varphi_k),$$

and is well-known from two-body contact problems in *linear* elastomechanics. It is therefore appropriate to use a discretization from this field. Wohlmuth and Krause [14] used a special mortar formulation which we will adopt here. It guarantees optimal *a priori* error estimates. Let $d_{h,k}$ be a function from the space of first-order Lagrangian finite elements S_h . We call d_h a *weakly linearly admissible* correction with respect to φ_k if

$$\int_{\gamma_k^{(1)}} \langle -\nu_{\varphi_k}, d^{(1)} - d^{(2)} \circ \Phi_{\varphi_k} \rangle \psi \, ds \leq \int_{\gamma_k^{(1)}} g(\varphi_k) \psi \, ds$$

for all test functions ψ from a suitable space M defined on $\gamma_k^{(1)}$. M is called a mortar space. In [14] it is shown that a stable discretization for M is the space M_h of *dual basis mortar functions*. They enjoy the property that there is a basis Ψ such that for any $\psi_p \in \Psi$ and any nodal basis function θ_q of $S_h|_{\gamma_k^{(1)}}$

$$\int_{\gamma_k^{(1)}} \psi_p \theta_q \, ds = \delta_{pq} \int_{\gamma_k^{(1)}} \theta_q \, ds \quad (9)$$

holds. Let $u^{(1)}$ and $u^{(2)}$ be the vectors of normal displacement on $\gamma_k^{(1)}$ and $\gamma_k^{(2)}$, respectively, and set $\mathbf{g} = (g_p)$, with $g_p = \int_{\gamma_k^{(1)}} g(\varphi_k) \psi_p ds$ for all $p \in \mathcal{N} \cap \gamma_k^{(1)}$. The discrete version of the set K_k can then be written algebraically as

$$K_{h,k} = \{u \in \mathbb{R}^n \mid \mathbf{M}u^{(2)} - \mathbf{D}u^{(1)} \leq \mathbf{D}\mathbf{g}\} \quad (10)$$

with

$$\mathbf{M} = (m_{pq}) = \int_{\gamma_k^{(1)}} (\theta_p^{(2)} \circ \Phi_{\varphi_k}) \psi_q ds$$

and

$$\mathbf{D} = (d_{pq}) = \int_{\gamma_k^{(1)}} \theta_p^{(1)} \psi_q ds,$$

where $\theta_i^{(1)}$ and $\theta_i^{(2)}$ denote the restrictions of the nodal basis functions of the transformed FE space $S_h(\varphi_k(\Omega))$ on $\gamma_k^{(1)}$ and $\gamma_k^{(2)}$, respectively. Note that due to the orthogonality property (9), \mathbf{D} is a diagonal matrix, whereas \mathbf{M} is not.

3.2 Monotone Multigrid Methods

Monotone multigrid methods were presented by Kornhuber [8]. They solve convex minimization problems without the need for any regularization, and converge globally and with asymptotic multigrid convergence rates. Kornhuber and Krause [9] applied them to single-body contact problems.

It is customary to introduce monotone multigrid methods as a subspace correction technique. Given the problem

$$\text{minimize } J \text{ on } K \quad (11)$$

with

$$K = \{v \in S_h \mid v(p) \in [a_p, b_p] \quad \forall p \in \mathcal{N}\}, \quad (12)$$

where $-\infty \leq a_p \leq b_p \leq \infty$, the idea is to span S_h by a set of search directions from the set $\Lambda = \Lambda_0 \cup \Lambda_c$. The Λ_0 are the standard nodal basis functions, sufficient by themselves to span S_h , whereas the coarse grid corrections from the set Λ_c are used to accelerate convergence. Then loop over all directions λ_i in Λ and solve the problem

$$\text{minimize } J(s) = J(w_{i-1} + s\lambda_i) \text{ on } K$$

where the $w_i = \sum_{k < i} s_k \lambda_k$ are the previous iterates.

If J is a quadratic functional, the algorithm can be interpreted in terms of linear multigrid theory. The loop over Λ_0 is equivalent to a projected Gauß-Seidel iteration. This kind of iterative method is only convergent if the set K has tensor-product structure [5], and the same requirement carries over to monotone multigrid methods. The coarse grid corrections Λ_c can be chosen to be the standard coarse grid nodal basis functions. To minimize in their directions then means a coarse grid Gauß-Seidel iteration which projects onto a

suitable coarsification of K . Details on how to construct the coarse sets K_j can be found in [8].

If Problem (11) is convex, it was shown in [8] that the monotone multigrid algorithm converges globally to the unique minimizer. In other cases, however, it is easy to see that the algorithm may get stuck at first-order critical points of J . Numerical evidence suggests that this does not impair the overall convergence of the SQP-trust-region algorithm with a monotone multigrid method used to solve the QPs. Also, modifications of the standard SQP idea exist which are proven to be globally convergent even if the inner QP is only solved up to a first-order critical point [11].

3.3 Transforming the Ansatz Space

Monotone multigrid methods only work if the admissible set K_k is bounded by box constraints. In our case K_k is the intersection between the trust-region K_k^{tr} and the set of linearly admissible deformations $K_{h,k}$ (10). Since we defined the trust-region using the ∞ -norm, it is bounded by box constraints. However, it is easy to see that $K_{h,k}$ is not. Indeed, taking into account Def. (10), since the matrix M is not diagonal it couples the obstacles for several variables.

Wohlmuth and Krause [14] used the following trick to overcome this problem. Let Θ be the standard nodal basis of $S_h(\varphi(\Omega))$, split up as

$$\Theta = \{\theta^{(1)}, \theta_C^{(1)}, \theta^{(2)}, \theta_C^{(2)}\}^T,$$

where $\theta_C^{(1)}, \theta_C^{(2)}$ are the hat functions of grid nodes on the contact boundaries $\gamma_k^{(1)}$ and $\gamma_k^{(2)}$, and $\theta^{(1)}, \theta^{(2)}$ are the hat functions in the interiors of $\Omega^{(1)}$ and $\Omega^{(2)}$, respectively. Now introduce the transformed basis

$$\hat{\Theta} = \begin{pmatrix} I & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & (D^{-1}M)^T & 0 & I \end{pmatrix} \begin{pmatrix} \theta^{(1)} \\ \theta_C^{(1)} \\ \theta^{(2)} \\ \theta_C^{(2)} \end{pmatrix}.$$

Set $u_p \in \mathbb{R}^d$ the displacement at a vertex $p \in \mathcal{N}$. In the basis $\hat{\Theta}$, the set $K_{h,k}$ of admissible displacements reads

$$\hat{K}_{h,k} = \{u = (u_p)_{p \in \mathcal{N}} \mid \langle \nu, u_p \rangle \leq g_p \quad \forall p \in \gamma_k^{(1)}\},$$

and the obstacles decouple into small d -dimensional problems.

When implementing a multigrid method in this basis, the coarse grid correction spaces and the corresponding coarse admissible sets have to be transformed as well. Details can be found in [14] and [12].

4 Numerical Results

In this last section we show numerical results obtained with our new algorithm. In order to demonstrate its advantages, we will use a standard benchmark prob-

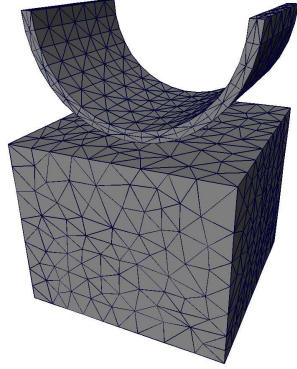


Figure 4: Coarse grid for the 3d example

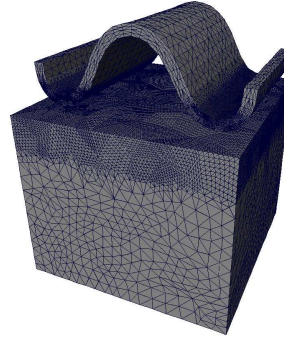


Figure 5: Solution after three refinement steps

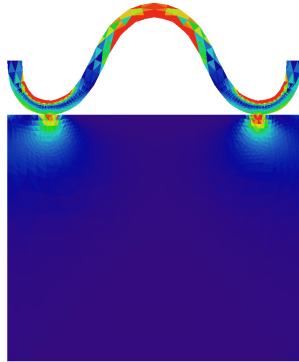


Figure 6: Cut through the von-Mises stress field

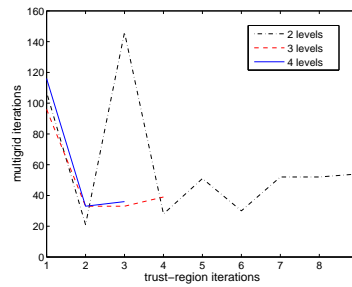


Figure 7: Multigrid iterations per trust-region step on each level. See text for an explanation of the peak in the curve for level 2.

lem, which has been used by other groups in the past (see e.g. [4] for a 2d variant). The example consists of an elastic ring being pressed onto an equally elastic foundation (Fig. 4). The material is Neo-Hookean with material parameters $E = 10^3, \nu = 0.3$ for the ring and $E = 10^8, \nu = 0.3$ for the block. The latter is clamped on its vertical sides, and a downward displacement is applied to the top ends of the ring. In order to show that the solver works on arbitrary grids, we have chosen an unstructured tetrahedral grid, containing 1409 vertices.

The Neo-Hookean energy functional is not defined for deformations that induce inverted elements. Therefore, when large displacement boundary conditions are prescribed, it is sometimes necessary to apply them in several loading steps. Generally, the number of steps needed depends on the size of the elements and on the convergence properties of the solver. Since our solver is globally convergent (cf. Sec. 3), we can choose the load increments arbitrarily large, as long as no element gets inverted. Loading was performed in eight steps for the example in Fig. 4. Since the coarse grid by itself is already quite large, we use the inner-point solver IPOpt [?] to solve the coarse grid problems. Inner-point methods are fast on problems of the size of the coarse grid, but scale badly for larger problems.

After having applied the full displacement, we refine and iterate on each level. We measure multigrid convergence in the energy norm of the associated linear elasticity problem, and trust-region convergence in the infinity-norm. Fig. 5 shows the solution on a grid that has been refined once uniformly and then another two times locally around the areas of actual contact. Fig. 6 shows a cut through the von-Mises stress field of the same solution. The final solution, containing 400578 degrees of freedom was obtained after about three and a half hours on a 1.7Ghz single-processor machine.

Fig. 7 shows the number of multigrid steps necessary for each trust-region iteration. Several things can be inferred from this chart. First of all, the trust-region solver converges quickly. After nine steps necessary to solve the problem on the second grid level, it only needs four resp. three on the subsequent levels. Secondly, the multigrid convergence rates are grid level independent. This was to be expected from multigrid methods, and shows the usefulness of the algorithm for large-scale problems. The peak in the second-level curve is due to the fact that the corresponding trust-region iteration had to be redone twice until a suitable trust-region radius ρ was found.

All results in this chapter have been obtained using the DUNE [1] numerics system.

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