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Quadratic Programming Algorithm for Dual Solution of Mortar-based Contact Problems in Linear Elasticity

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Abstract

This paper presents an investigation into the numerical solution of linear elasticity contact problems utilizing the Finite Element Method for discretization, the Mortar method for handling non-penetration conditions, dual formulation for problem reduction, and optimal Quadratic Programming algorithms for scalable solution of dual problem. The study outlines the implementation of a computational pipeline for solving such problems and evaluates its performance on selected benchmark. The paper serves as an overview of the technique and can be regarded as a foundation for future enhancements or modifications to individual steps.

Keywords: finite elements, dual formulation, quadratic programming, Matlab, scalable algorithm, numerical solution

1 Introduction

Linear elasticity contact problems represent a significant area of study in computational mechanics, particularly in understanding the behavior of structures subject to contact forces. These problems arise in various engineering applications, ranging from automotive and aerospace industries to biomechanics and civil engineering. Understanding the interaction between solid bodies in contact is essential for designing reliable and efficient structures.

In linear elasticity contact problems, the objective is to analyze the deformation and stress distribution in solid bodies under external loads and constraints, while accounting for contact interactions between them. These interactions can give rise to complex phenomena such as friction, adhesion, and deformation discontinuities at the contact interfaces. However, the numerical solution of linear elasticity contact problems poses significant challenges due to the nonlinear nature of contact conditions, geometric complexities, and computational costs associated with large-scale simulations.

In this paper, we focus on the numerical solution of 2D linear elasticity contact problems using the Finite Element Method (FEM, [1]), Mortar method for contact detection [2], and optimal Quadratic Programming (QP) algorithms [3] for solving the dual formulation of the problem. We present a comprehensive review of the solution pipeline, covering the formulation of the problem, discretization techniques, handling of contact conditions, and solution algorithms. We are mainly interested in the scalability properties of presented numerical methods. To address this goal, we implemented the methodology in Matlab [4] and we demonstrate the scaling properties of individual ingredients on a selected benchmark.

Throughout the paper, we address the problem presented in Section 2 by introducing the geometry, material properties of the considered bodies, and present the discretized formulation of the problem in the form of constrained optimization problem. We specifically select a problem that can be easily meshed with any level of roughness, allowing us to study and present the scalability of the implementation based on the discretization parameter of the mesh. This section also briefly shows how Mortar method is utilized to deal with the definition of the non-penetration condition through linear inequality constraints. This step is crucial for handling non-conforming meshes, which is exactly our case. Section 3 introduces the dual problem, where the unknowns are Lagrange multipliers corresponding to the defined equality and inequality constraints. Here, the crucial step involves computing the pseudoinverse of the stiffness matrix, which can be avoided using smart factorization. Additionally, we include the scalability results of the used approach. Section 4 outlines the QP algorithm for solving the dual problem. We adopt the Semimonotonic Augmented Lagrangian Method (SMALBE) to enforce the equality conditions using penalization, while the inner problem with pure inequalities is addressed by the Modified Proportioning with Reduced Gradient Projection (MPRGP). This method is an active set method, where the problem on the free set is solved by Conjugate Gradient steps, and the solution process on the whole set is finally resolved by projection steps with a guaranteed decrease of the objective function. Finally, Section 5 presents the obtained numerical solution of the proposed problem and Section 6 concludes the paper.

2 The problem

The geometry of our benchmark is presented in Figure 1. We consider a rectangular beam A with a length of $l = 2\mathrm{m}$ and a height of $h = 0.25\mathrm{m}$, where the bottom left corner of the rectangle is at a height of $a = 0.5\mathrm{m}$. The rectangle is fixed on the left side using a Dirichlet boundary condition, and a force $F = 0.1\mathrm{GN}$ is applied downward at the upper right corner. The free deflection of the beam is restrained by a half of the ring B defined with center $S = [1\mathrm{m}, 0\mathrm{m}]$, inner radius $r_1 = 0.3\mathrm{m}$, and outer radius $r_2 = 0.49\mathrm{m}$. This body is fixed with a Dirichlet boundary condition on the bottom sides. The material of body A is defined by the Young's modulus of elasticity $E = 200\mathrm{GPa}$ and Poisson's ratio $\nu = 0.3$, while the material of body B has characteristics $E = 20\mathrm{GPa}$ and $\nu = 0.3$.

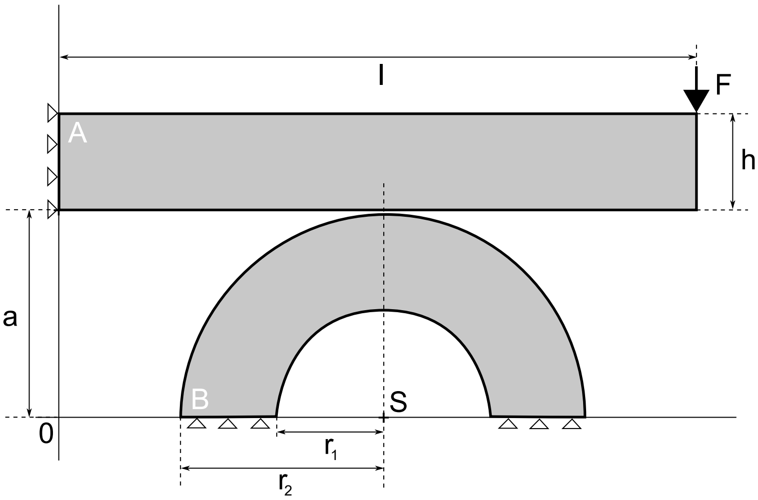

Figure 1: The geometry of contact problem.

We employ quadrilateral finite elements to discretize the problem. In constructing the mesh, we divide the rectangle into $8N_r$ squares along the x-axis and N_r squares along the y-axis. Similarly, for the ring, we partition the angle into equidistant $12N_h$ smaller angles and the radius into $2N_h$ equidistant intervals. By utilizing the discretization parameters $N_r, N_h \in \mathbb{N}$, we can adjust the number of nodes and corresponding finite elements accordingly. For the mesh example with $N_r = 4$ and $N_h = 3$, please refer to Figure 2. Here, we present also the solution deformations of the problem. This combination of parameters leads to the mesh with 313 nodes and the corresponding number of degrees of freedom (dof) $n = 626$.

The discretized problem is given by

$$u^* = \arg\min_{u \in \Omega} \frac{1}{2} u^T K u - f^T u, \tag{1}$$

where unknown $u \in \mathbb{R}^n$ denotes the discretized displacement of nodes, $K \in \mathbb{R}^{n,n}$ is given symmetric positive semidefinite stiffness matrix, $f \in \mathbb{R}^n$ is given vector of

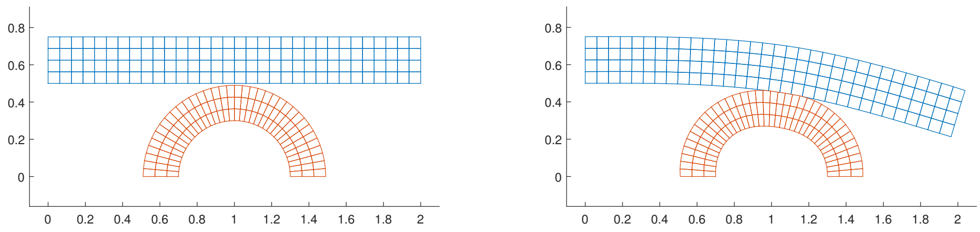

Figure 2: The mesh used for the discretization (left) and the solution of the problem (right).

discretized forces and feasible set $\Omega \subset \mathbb{R}^n$ constraints the solution to be feasible, i.e., the we are searching for the displacement which satisfies Dirichlet boundary condition and the non-penetration inequality condition. The Dirichlet boundary condition can be straightforwardly implemented as linear equality constraint $B_D u = 0$, where matrix $B_D \in \mathbb{R}^{m_E,n}$ includes 1 in each row for corresponding node with the defined boundary condition. Number $m_E \in \mathbb{N}$ is a number of nodes with prescribed non-zero displacement. See [5] for details. For the construction of the objects in equation (1), which represent the primal formulation, we utilize the Matlab library [6]. This library provides highly vectorized code, enabling efficient assembly of the sparse matrix K in linear time. The computational time for this step is depicted in Figure 3, where we present the performance for computing FEM objects for the rectangular body."

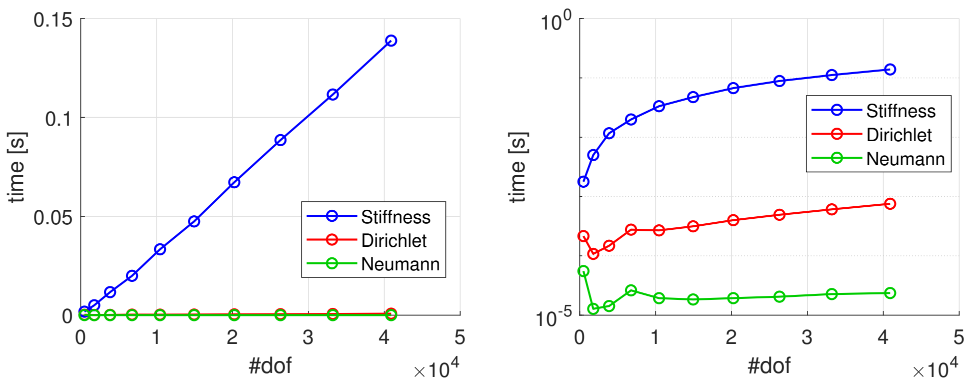

Figure 3: The computational time for assembling FEM objects of rectangle body in linear scale (left) and logarithmic scale (right). The results are the average of 100 runs.

The non-penetration condition is implemented using Mortar method [2]. In this case, we utilize our previous experiences and code [7]. To be more specific, we use the node-to-segment approach, where we use line segments of FEM discetization of the bottom side of rectangle and the top side of ring. Each node on one side of the contact interface is associated with one or more segments on the opposing side. The algorithm assembles non-penetration condition in form of linear inequalities $B_M u \leq c_M$, where $B_M \in \mathbb{R}^{m_I,n}$, $c_M \in \mathbb{R}^{m_I}$ and number $m_I \in \mathbb{N}$ is a number of identified linear inequalities. However, the precision of this linear approximation of non-penetration condition is constructed from the actual position of nodes, therefore to obtain better results, we implement pseudo-spatial approach, where we are slowly increasing the applied force and update the solution based on the corresponding response of displacement. After each time-step, we recompute the Mortar linearization. In our case, we use 10 steps. The scalability results of our implementation are presented in Figure 4. In this case, the master body (rectangle) provides the segments to which are nodes from the slave body (ring) projected. We obtained different number of contact segments using various values of discretization parameters N_r, N_h.

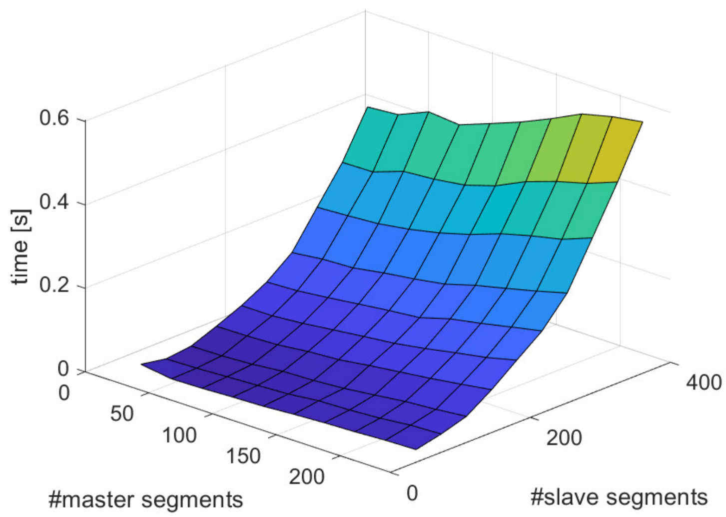

Figure 4: The computational time for assembling linear inequalities using Mortar method for different number of segments of master body (rectangle - bottom side) and slave body (ring - top side). The results are the average of 10 runs.

3 Dual problem

Instead of solving the optimization problem (1), we solve the corresponding dual problem

$$\lambda^* = \arg \min_{\lambda \in \Omega_{\text{dual}}} \frac{1}{2} \lambda^T F \lambda - \lambda^T d, \tag{2}$$

with symmetric positive semidefinite Hessian matrix $F \in \mathbb{R}^{m,m}$ and new linear term $d \in \mathbb{R}^m$ given by

$$F = BK^+B^T, \;\; d = BK^+f - c, \tag{3}$$

and feasible set composed from lower bounds and linear equality constraints

$$\Omega_{\text{dual}} = \{\lambda \in \mathbb{R}^m : \ \lambda_I \geq 0 \ \text{ and } \ R^T B^T \lambda = R^T b\}. \tag{4}$$

The size of the dual is the number of constraints of primal problem, i.e., $m = m_E + m_I$ and B, c, λ are composed from equality and inequality constraints

$$B = \begin{bmatrix} B_D \\ B_M \end{bmatrix} \in \mathbb{R}^{m,n}, \quad c = \begin{bmatrix} 0 \\ c_M \end{bmatrix} \in \mathbb{R}^m, \quad \lambda = \begin{bmatrix} \lambda_E \\ \lambda_I \end{bmatrix} \in \mathbb{R}^m. \tag{5}$$

Matrix $R \in \mathbb{R}^{r,n}$ is a matrix of basis vectors of $\ker K$. In the case of linear elasticity, this object can be constructed using analytic formula.

The dual problem (2) is equivalent to the original (primal) problem (1), see [3]. After solving dual problem (2), one can reconstruct the solution of primal problem (1) using

$$x^* = K^+(f - B^T \lambda^*) - R\alpha^*, \tag{6}$$

where $\alpha^* \in \mathbb{R}^r$ are Lagrange multipliers of dual problem corresponding to equality constraints. The numerical algorithm, which we are using, is returning this vector.

From the computational point of view, the dual problem is much more smaller than the primal problem (i.e., number of degrees of freedom n is lower than the number of constraints m), therefore the solution of this problem should be cheaper. With respect to "no free lunch" theorem, the price which has to be paid is hidden in the computation of (3), i.e., the computation of pseudoinverse of stiffness matrix. The straightforward implementation in Matlab involves using the command "pinv", which computes and assembles the pseudoinverse. However, despite the original stiffness matrix being sparse and the number of non-zero elements depending linearly on the number of nodes, the assembled pseudoinverse turns out to be dense. Furthermore, the assembly process is computationally expensive. In fact, for sufficiently large problems, this computation dominates the solution process.

To avoid this difficulty, we adopt idea from [8], where authors do not assemble the preudoinverse, but "only" computed the Cholesky decomposition modified by the usage of so-called fixing node. In our implementation, we choose the fixing nodes based on the spectral decomposition of the graph of given mesh. With the decomposition of K, the application of matrix multiplication K^+v can be implemented as a solution of the system of linear equations. In the case of Cholesky decomposition, we perform the linearly scaling reduction of variables twice. Following this trick, the assembly of objects in (3) and (6) consist of solution of linear systems with multiple right hand-side vectors.

To demonstrate the efficiency of proposed method, please, see Figure **??**, where we compare the computation with pseudoinverse computed by Matlab command "pinv" and our implementation of Cholesky decomposition with fixing nodes. For demonstration purpose, we are working only with the stiffness matrix corresponding to the rectangle varying N_r.

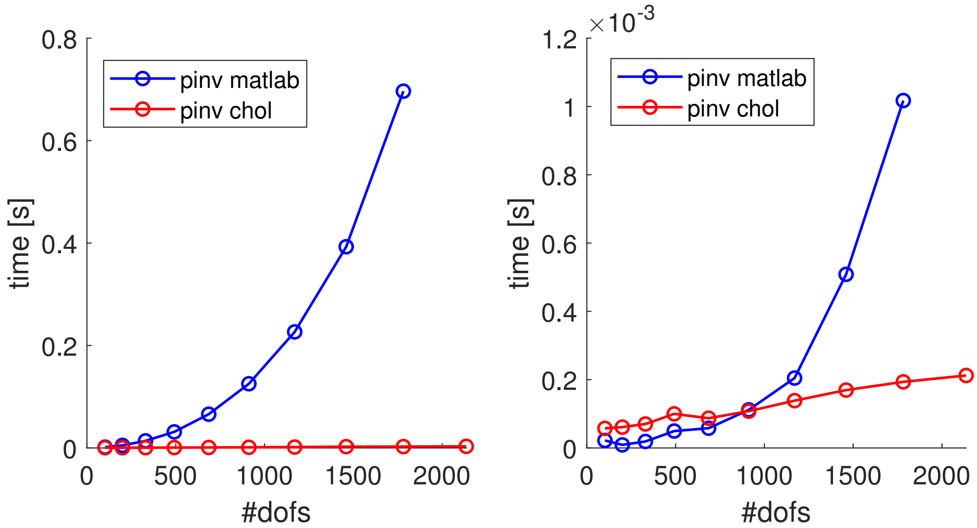

Figure 5: The computational time for assembling the pseudoinverse by Matlab command "pinv" compared to the computation of Cholesky decomposition (left) and the multiplication of the pseudoinverse with a random vector (right). The results are the average of 10 runs.

4 Algorithms

In our implementation, we use SMALBE (Semimonotonic Augmented Lagrangian method for constrained QP, [3]) to solve the problem (2). The SMALBE is a Uzawa-type algorithm which generates the approximations for the Lagrange multipliers corresponding to equality constraints of the dual problem in the outer loop and solves auxiliary problems with bounds constraints in the inner loop. Application of the specific update rule for the penalty parameter results in convergence of the feasibility error that is independent of the conditioning of the equality constraints. The basic scheme has been proposed in [9], where authors adapted the augmented Lagrangian method to the solution of problems with a general cost function subject to general equality constraints and simple bounds, however, using the properties of quadratic objective function, stronger convergence results can be achieved [10]. The optimality of the algorithm was shown in [3] and [11]. For the survey and possible extension to quadratic constraints, see [12].

The inner problem is solved by active-set algorithm proposed by [3]. The basic version was proposed independently by [13] and [14] and can be considered as a modification of the well-known Polyak algorithm. One of the key ingredient is the estimation of the decrease of objective function during the gradient projections [15]. Later in [16], authors combined the proportioning algorithm with the gradient projections [17], they use the constant $\Gamma > 0$, the test to decide about leaving the face, and three types of steps to generate convergent monotone algorithm. The algorithm is based on using the free, chopped, and projected gradients to minimize the cost function on the free set using Conjugate Gradient (CG) steps and afterwards on the active set using shortened CG step and projected gradient steps. The switching between these processes is realized by the proportioning condition.

We implemented algorithms in Matlab environment. For the demonstration, we fix the discretization of ring $N_h = 15$, which results in number of dofs corresponding to ring $n_r = 11222$ and number of contact segments of top side equal to 180. Figure 7 demonstrates the scalability of the approach and our implementation.

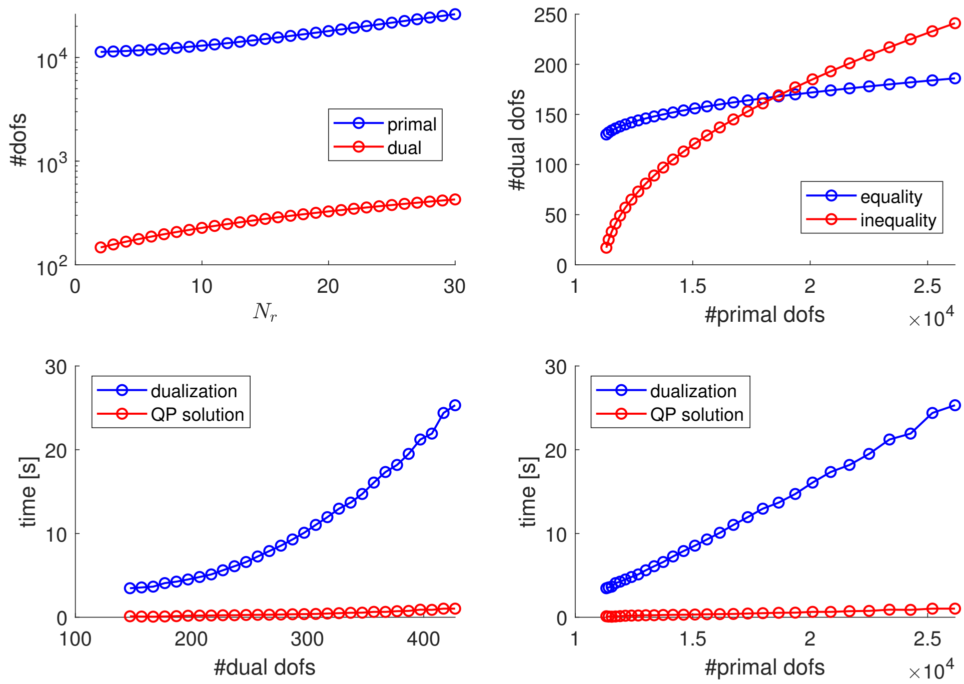

Figure 6: Scaling of the method and implementation with change of the discretization parameter of rectangle body N_r. The size of the dual problem is much more lower than the size of primal problem (top left, logarithmic scale), the number of Dirichlet equality constraints and Mortar inequality constraints (top right), the dependency of the dualization time and the solution time of optimization problem depending on the size of dual problem (bottom left), and the dependency between the size of primal problem and the computational time.

	N	$\#nodes$	$\#elements$	$\#dofs$	$\#segments$
rectangle	30	7471	7200	14942	240
ring	15	5611	5400	11222	180
total		13082	12600	26164	

Table 1: Parameters of the largest problem.

5 Final results

In this final section, we present the solution for the largest problem considered in this paper. We solved the problem with the parameters presented in Table 1. The assembly of the FEM objects took 0.087 seconds, the computation of the Cholesky decomposition of the stiffness matrix took 0.078 seconds, the sum of the Mortar computations in all steps amounted to 2.064 seconds, the dualization in all steps took 26.6858 seconds, and all dual QP problems were solved in 1.0739 seconds.

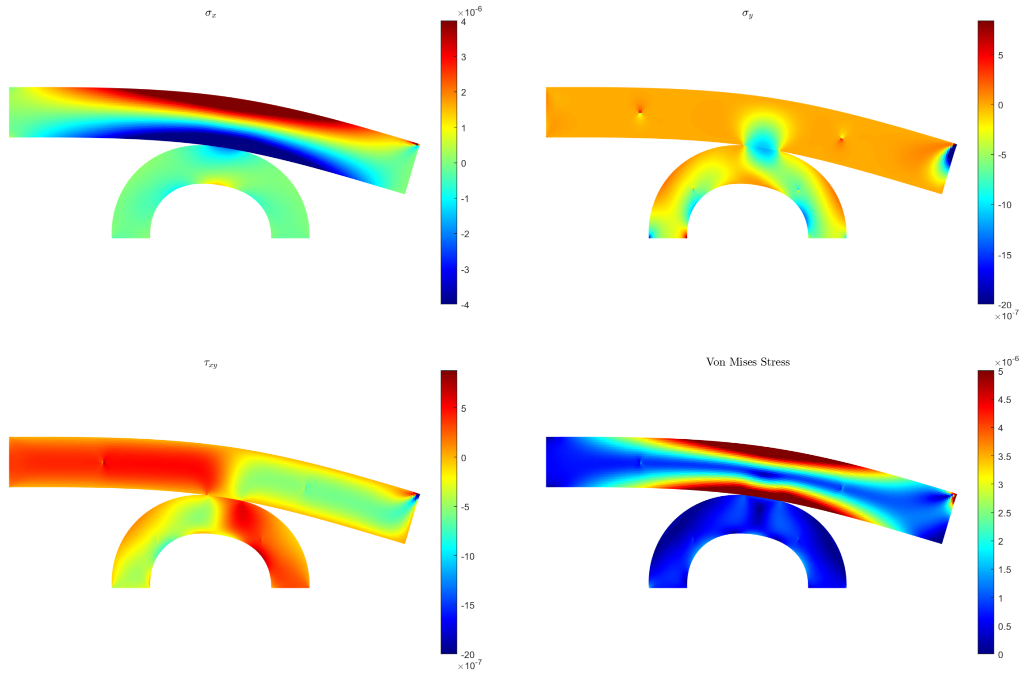

Figure 7: Normal stress, Shear stress, and Von Mises stress for the selected benchmark with parameters in Table 1.

All results presented in this paper have been computed in Matlab R2020a on personal computer with processor *AMD Ryzen 5 3600 6-Core* and *32 GB DDR4* RAM.

6 Conclusion

In this paper, we have briefly shared our experiences with implementing a pipeline for solving linear elasticity contact problems using the Mortar method, dual formulation, and optimal QP algorithms. While the results appear promising, the true potential of dualization becomes evident when applied in parallel computation and combined with the Finite Element Tearing and Interconnecting Method (FETI, [18]). This approach distributes the computation of the pseudoinverse to computational nodes, significantly improving the efficiency of the method. Our aim is to achieve results similar to those in previous works [19], [20], but this time incorporating friction and non-linear elasticity.

Acknowledgements

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