Solution of contact problems between rough body surfaces with non matching meshes using a parallel mortar method

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November 8, 2018

Abstract

The mechanical behavior of fractures in solids, such as rocks, has strong implications for reservoir engineering applications. Deformations, and the corresponding change in solid contact area and aperture field, impact rock fracture stiffness and permeability thus altering the reservoir properties significantly. Simulating contact between fractures is numerically difficult as the non-penetration constraints lead to a nonlinear problem and the surface meshes of the solid bodies on the opposing fracture sides may be non-matching. Here we use a parallel mortar method to resolve the contact conditions between the non-matching surfaces, a three dimensional finite element formulation of linear elasticity and linearized contact conditions. The contact method is numerically stable and neither the solution nor the convergence depend on a penalty parameter. We present contact stresses, interior stresses and normal closure behavior for contact simulations of rough fractures, with geometries created from fractured granite specimens from the Grimsel test site in Switzerland. Our implementation uses open source software components which are designed for parallel computing in HPC environments.

Keywords: contact mechanics, geomechanics, fracture, contact, mortar

1 Introduction

Mechanical contact of rough surfaces of fractures or faults along discontinuities in the rock mass is of significant importance in reservoir engineering applications, such as enhanced geothermal systems (EGS) or CO\textsubscript{2} sequestration \cite{1, 34}. The mechanical contact determines normal and shear compliance of rock fractures, which govern the geomechanical reservoir behavior and thereby influence economical efficiency and risk (e.g., induced seismic hazards or CO\textsubscript{2} leakage) of the reservoir application in question \cite{26}. The mechanical behavior of rock fractures has therefore been studied extensively, with many studies focusing on surface topography \cite{4, 43, 40} and the influence of surface topography on the mechanical behavior of the fracture \cite{11, 30, 16, 29, 33, 38}.

Specifically, the surface topography determines the contact area distribution in the fracture for given loading conditions, and is thereby crucial when investigating fracture strength (fracture compliance in normal or shear direction). As a fracture is exposed to mechanical loading normal to the fracture, or loading is increased, fracture closure and load exhibit a nonlinear
relationship, with fracture closure increments becoming smaller with increasing load increments and displaying convergent behavior [4, 25, 13, 36, 38, 19]. This nonlinear closure behavior of fractures can be attributed to the increase in contact area with fracture closure, which increases the fracture stiffness.

The described rock fracture surface topographies are complex, with characteristic features on the sub-millimeter scale [40]. Therefore, computing the contact and deformation of two such fracture surfaces constitute a two- or multi-body contact problem, a problem class that even in standard finite element (FEM) setting with linearized contact, still poses a significant computational challenge to this day. This is for two reasons: First, the formulation of the non-penetration condition itself is nontrivial as the bodies in consideration normally have non-matching triangulations at the contact boundary. Secondly, the non-penetration condition at the a priori unknown contact zone between the bodies constrains the solution space of possible displacements, thereby introducing a nonlinearity. Simulation tools that resolve small-scale roughnesses, while allowing computation of contact stresses and stress variations in the rock mass, are rare. Most analytical or numerical studies at the laboratory or reservoir scale rely on simplifying assumptions and regularizations, such as averaging asperity scale processes with an empirical relationship, reduction to two dimensions, using variants of boundary element methods, not modeling explicitly the mechanical contact between two surfaces, treating the surfaces as two parallel plates, using penalty methods or only matching triangulations at the surface [4, 28, 7, 27, 9, 12, 32, 31, 24, 8].

In this work, we present a new parallel implementation of an approach that does not require any of the previously mentioned assumptions. The approach is conventional in as much as we employ linear elasticity and linearized contact conditions in the strong formulation [17]. However, when discretizing with finite elements, we use non-uniform meshes with non-matching surface meshes at the contact boundary and then employ a mortar projection to resolve the contact conditions across the non-matching contact surfaces. We follow [42] in that we use a mortar projection with dual Lagrange multipliers and apply a change of basis transform to the system, to effectively transform the two-body problem into a one-body problem. The formulation and discretization rest on a solid theoretical basis with proven numerical stability (see [5, 41, 42] and references cited therein) and can be extended to also include friction [21] and multigrid acceleration for the solution of the constrained system [42, 10, 21]. For rough rock surfaces, our mortar technique is particularly useful, since we have complex, non-matching triangulations at the contact boundary (see Figure 1) and an unknown contact zone. Still, we want to obtain accurate three-dimensional representations of a fracture with contact areas to model fluid flow in fractures. For this, penalty-based approaches are at a disadvantage, as the solution can be distorted by over-closure or additional convergence problems result from large penalty parameters. In the mortar case, the non-penetration condition is enforced locally in a weak sense. Thus, while locally some interpenetration is possible, the discretization error depends on the local mesh size and can, if needed, be reduced at will through local refinement.

The use of this mortar technique has previously been hindered by the absence of an efficient way to compute the projection operator. The assembly of the operator requires the detection of intersections between the non-matching surface meshes, which is a complex task in parallel, as the portions of the intersecting meshes might reside on different compute nodes. Only with the relatively recent introduction of the MOONolith library [22] has this task become feasible for parallel computing. Using MOONolith, the projection operator is assembled with libMesh [18] and custom components of the MOOSE framework [13].

This, and the reliance on a finite element formulation, makes it feasible to apply the method to a wide range of problems, since the method can be incorporated into the vast number of available finite element software packages. Here, we combine the projection operator with custom components from PETSc [2] and the MOOSE framework [13] to conduct our numerical experiments. However, and even though we use a new parallel implementation of a mortar-
based contact method, the focus of this article is not on software, but on establishing a new method and tool for studying contact in the geoscience community.

We thus put a strong focus on the formulation of the rock, or other solid, contact conditions, in particular the non-penetration condition in its strong, weak and discretized form (Equations 9, 16, 24). To our knowledge, this is the first application of a parallel two-body contact method that uses a mortar technique for non-matching rock surfaces in three dimensions.

This paper is organized as follows. In Section 2, we formulate the two-body contact problem. Then we introduce the mortar projection and its discrete assembly, followed by the change of basis transformations to solve the resulting system. In Section 3, we show the characteristic boundary stresses from Hertzian contact and simulations of rough fractures, subjected to increasing the normal load, which exhibit the characteristic nonlinear closing behavior of a fracture under increased normal stress.

2 Methods

In the following section we introduce the two-body contact problem, the mortar approach at the contact boundaries and the basis transformations needed to solve the two-body problem. An example for two-body contact on non matching grids is shown in Figure 1, where the mesh discretization on the fracture surface is shown for a cylindrical specimen with a fracture normal to the cylinder axis in the center.

Figure 1: Mesh used for the numerical simulations with: A) The two specimen halves which are separated by the fracture; B) The rough fracture surface of the lower specimen half. C) Normal view on the two non-matching meshes of the fracture surfaces.

2.1 Contact formulation

We give a brief introduction to the formulation of the contact problem and its finite element discretization. For the most part we follow the formulations in [42, 10] and we refer the reader to these articles and the references cited therein for a more in-depth introduction.

We consider a master body $\Omega^m \subset \mathbb{R}^3$ and a slave body $\Omega^s \subset \mathbb{R}^3$. The boundary $\Gamma^\alpha$, $\alpha \in \{m, s\}$ of each body consists of three non overlapping parts: of a Neumann boundary $\Gamma^N$, a Dirichlet boundary $\Gamma^D_\alpha$ and a boundary $\Gamma^C_\alpha$, where the possible contact occurs. The displacement field on the bodies $u := [u^m, u^s]$ is separated into displacements on the master and slave body, respectively. The material of $\Omega^\alpha$ is considered to be linear elastic. Hooke’s tensor $(E^{\alpha}_{ijml})$, $1 \leq i, j, l, m \leq 3$ is used to formulate the stresses $\sigma$ given by Hooke’s law, using the index $\cdot_j$ to abbreviate derivatives with respect to $x_j$:

$$\sigma_{ij}(u^\alpha) = E^{\alpha}_{ijml}u^\alpha_{l,m}. \quad (1)$$
We assume that a bijective mapping $\Phi : \Gamma^s_C \rightarrow \Gamma^m_C$ exists, which maps the points on the slave side of the boundary to the possible contact point on the master side. We then define the vector field of normal directions $n^\Phi$:

$$n^\Phi : \Gamma^s \rightarrow S^2, \quad n^\Phi(x) := \begin{cases} \Phi(x) - x & \text{if } \Phi(x) \neq x \text{ (no contact)} \\ n^s(x) & \text{otherwise} \end{cases}$$

The gap function $g : \mathbb{R}^3 \rightarrow \mathbb{R}, x \mapsto |\Phi(x) - x|$ then measures the width of the gap between the two bodies in the normal direction (i.e., aperture of the fracture in geophysics) and we also define the point-wise jump $[u] := (u^s - u^m \circ \Phi) \cdot n^\Phi$, which is to be smaller than the gap $g$: $[u] \leq g$. This condition is only meaningful in the linearized contact setting, where the bodies are close together and the outer normals $n^\alpha, \alpha \in \{m,s\}$ are parallel, i.e. we have $n^s := n^\Phi$ and $n^m := -n^s$.

For the contact conditions we need stresses and displacements with respect to the outer normal direction and the tangential direction $t$:

$$\begin{align*}
\sigma^\alpha_n &= n^\alpha \cdot \sigma_{ij}(u^\alpha) \cdot n^\alpha_j, \\
\sigma^\alpha_t &= \sigma(u^\alpha) \cdot n^\alpha - \sigma_n \cdot n^\alpha, \\
\sigma_n &= \sigma_n \leq 0 \text{ on } \Gamma_C.
\end{align*}$$

With this we state the contact problem in its strong form: We assume that the body is in an equilibrium state (Eq. 4) with body forces $f$, Dirichlet boundary conditions (Eq. 5), Neumann boundary conditions with pressure $p_i$ (Eq. 6) and contact boundary conditions (Eq. 7). In the right column we have the contact conditions, where Equation 9 is the non-penetration condition, Equation 10 is the complementary condition and Equation 11 states that we have no stresses in tangential directions, i.e., we are considering frictionless contact.
\[
\sigma_n(u^m \circ \Phi) = \sigma_n(u^s) \quad \text{on } \Gamma_C \quad (8)
\]
\[
[u] \leq g \quad \text{on } \Gamma_C \quad (9)
\]
\[
([u] - g)\sigma_n(u^s) = 0 \quad \text{on } \Gamma_C \quad (10)
\]
\[
\sigma_T = 0 \quad \text{on } \Gamma_C. \quad (11)
\]

For the weak formulation we use the space \( \mathbf{X} := H^1_0(\Omega^m) \times H^1_0(\Omega^s) \), where \( H^1_0(\Omega_\alpha), \alpha \in \{m, s\} \) are the Sobolev spaces, satisfying the Dirichlet boundary conditions (Eq. 5) and we define the bilinear form \( a(u, v) \):

\[
a(u, v) := \sum_{\alpha \in \{m, s\}} \int_{\Omega^\alpha} E_{ijkl} u_{k,j} v_{l,m} \, dx \quad w, v \in \mathbf{X},
\]

and the linear form \( f(v) := (v, f)_{0,\Omega} + (v, p)_0,\Gamma_s \). Furthermore, we introduce the convex set of admissible displacements \( \mathcal{K} \subseteq \mathbf{X} \):

\[
\mathcal{K} := \{ u \in \mathbf{X} | [u] \leq g \}. \quad (13)
\]

Here the inequality needs to be interpreted pointwise. We can now state the contact problem in its weak form as the minimum of the energy functional \( J(u) := \frac{1}{2} a(u, u) - f(u) \): Find a \( u \in \mathcal{K} \) such that:

\[
J(u) \leq J(v), \quad \forall v \in \mathcal{K}. \quad (14)
\]

We end this subsection by introducing the finite element spaces \( \mathbf{X}_h := \mathbf{X}_h(\Omega^m) \times \mathbf{X}_h(\Omega^s) \) associated to \( \mathbf{X} \) and appropriate triangulations \( T_h^m \) and \( T_h^s \) of \( \Omega^m \) and \( \Omega^s \) with mesh width \( h \). Using the basis functions \( \phi_i \) of \( \mathbf{X}_h \) we define

\[
A := a(\phi_i e_k, \phi_j e_l) \quad \text{and} \quad f_h \quad \text{with} \quad (f_h)_{ji} := f(\phi_i e_k), \quad i, j = 1, \ldots, N; k, l = 1, \ldots, 3, \quad (15)
\]

where \( N \) is the number of nodes of the meshes \( T_h^\alpha, \alpha \in m, s \) and \( (e_i)_{i=1,2,3} \) are the standard basis vectors in \( \mathbb{R}^3 \). \( A \in \mathbb{R}^{3N \times 3N} \) is usually referred to as the stiffness matrix and \( f_h \in \mathbb{R}^{3N} \) as the right-hand side in the FEM context. The following subsections show, how the discretized system is solved by applying a change of basis on \( A \). A weak and discretized version \( g_h \) of \( g \) is obtained as a byproduct of the computation of the mortar projection routine.

### 2.2 Mortar-Approach

We begin this section by introducing the trace spaces \( \mathbf{X}_h(\Gamma_C^m) \) of \( \mathbf{X}_h(\Omega^m) \) and \( \mathbf{X}_h(\Gamma_C^s) \) of \( \mathbf{X}_h(\Omega^s) \) on the contact boundaries of the master and slave bodies. The aim of our mortar approach is to replace the strong non-penetration condition in Equation 9 in such a way, that we only allow for penetration in the normal direction in a weak sense:

\[
\int_{\Gamma_C} ([u] - g) \lambda_h^F d\gamma \leq 0 \quad \forall \lambda_h^F \in L_h,
\]

where \( L_h \) is a dual space of \( M_h := \mathbf{X}_h(\Gamma_C^s) \), defined as:

\[
L_h := \{ \lambda_h = \lambda_h^M \cdot n^\Phi | \lambda_h^M \in M_h, \int_{\Gamma_C} \lambda_h^M \lambda^s d\gamma \geq 0, \forall \lambda^s \in \mathbf{X}_h(\Gamma_C^s), \lambda^s \geq 0 \}. \quad (17)
\]

The intent of this definition is that the positivity of the \( \lambda \)'s ensures that the weak non-penetration condition is equivalent to the strong one asymptotically. However, in practice the weak non-penetration condition is difficult to enforce: First, in the discrete setting the elements \( u^m_h \in \mathbf{X}_h(\Gamma_C^m) \) and \( u^s_h \in \mathbf{X}_h(\Gamma_C^s) \) that would have to form the jump \([u]\), are apart and second, even if they were in contact, i.e. \( g = 0 \), they would have non-matching nodes. Hence,
an additional operator is needed to relate the nodes of the master side to the slave side of the contact boundary - our mortar projection $\Psi$. The construction of $\Psi$ is deduced in "reverse" by assuming the previously introduced mapping $\Phi$, which is part of the solution, already exists. We demand that for the mapping $\Psi : \Gamma_0^s \rightarrow \Gamma_S^s$ and the test space $M_h := X_h(\Gamma_C^s)$, the following $L^2$-orthogonality holds for all elements $u_h^m \circ \Phi \in X_h(\Gamma_C^s)$:

$$\int_{\Gamma_C^s} (\Psi(u_h^m \circ \Phi) - u_h^m \circ \Phi) m_h \, d\gamma = 0, \ \forall m_h \in M_h.$$  \hfill (18)

As we need a discrete representation $T$ of $\Psi$, we reformulate the weak equality (Eq. 18) using the $L^2$-scalar product $(\cdot, \cdot)_{L^2(\Gamma_C^s)}$ to:

$$\langle \Psi(u_h^m \circ \Phi), m_h \rangle_{L^2(\Gamma_C^s)} = \langle u_h^m \circ \Phi, m_h \rangle_{L^2(\Gamma_C^s)}, \ \forall m_h \in M_h,$$  \hfill (19)

and introduce the bases $(\lambda_i^m)_{i=1,...,N_m}$, $(\lambda_i^s)_{i=1,...,N_s}$, $(\lambda_i^{M_h})_{i=1,...,N^{M_h}}$, of $X_h(\Gamma_0^m)$, $X_h(\Gamma_0^s)$ and $M_h$, with $N_m, N_s = N^{M_h}$ being the dimension of each space. Then we write the elements $u_h^m \circ \Phi$, $\Psi(u_h^m \circ \Phi)$ and $m_h$ in the basis representations $u_h^m \circ \Phi = \sum_{i=1,...,N_m} v_i(\lambda_i^m \circ \Phi)$, $\Psi(u_h^m \circ \Phi) = \sum_{j=1,...,N_s} w_j(\lambda_j^s \circ \Phi)$, $m_h = \sum_{k=1,...,N_s} l_k(\lambda_k^{M_h})$, and reformulate Equation 19 to:

$$\left( \sum_{j=1,...,N_m} v_j(\lambda_j^m \circ \Phi), \lambda_k^{M_h} \right)_{L^2(\Gamma_C^s)} = \left( \sum_{i=1,...,N_s} w_i(\lambda_i^s \circ \Phi), \lambda_k^{M_h} \right)_{L^2(\Gamma_C^s)}, \ \forall k = 1,...,N^s.$$  \hfill (20)

We now define $D := (d_{ki})_{k,i=1,...,N^s}$ and $B := (b_{kj})_{k=1,...,N^m,j=1,...,N^s}$ through:

$$d_{ki} := (\lambda_i^s, \lambda_k^{M_h})_{L^2(\Gamma_C^s)} \, Id = \int_{\Gamma_C^s} \lambda_i^s \lambda_k^{M_h} \, d\gamma \, Id \ \text{ and}$$  \hfill (21)

$$b_{kj} := (\lambda_k^{M_h} \circ \Phi, \lambda_j^s)_{L^2(\Gamma_C^s)} \, Id = \int_{\Gamma_C^s} (\lambda_k^{M_h} \circ \Phi) \lambda_j^s \, d\gamma \, Id,$$  \hfill (22)

where $Id \in \mathbb{R}^{3\times 3}$ is the identity operator. We then reformulate Equation 20 as

$$Bv = Dw,$$  \hfill (23)

and with $T := D^{-1}B$ we get the discrete representation of the mortar transfer operator. Its purpose is to represent elements of $X_h(\Gamma_C^s)$ in $X_h(\Gamma_C^s)$ in a meaningful way using $\Phi$ and the $L^2$-orthogonality in Equation 18. Using $T$, it is now possible to formulate the non-penetration condition (compare Eq. 9) in its discrete form at the nodes $p$ on the slave side $\Gamma_C^s$:

$$\{(u_h^m)^p - (Tu_h^m)^p \cdot n_p^s - (g_h)^p \leq 0, \ \ p = 1,...,N^s.$$  \hfill (24)

Here, $(u_h^m)^p$ and $(u_h^m)^p \in \mathbb{R}^3$ denote local nodal vectors, whereas $g_h = (g_p)_{p=1,...,N^s}$ is the weighted gap vector defined as:

$$g_p := (D^{-1}g')^p, \quad (g')^p := \left( \int_{\Gamma_C^s} \lambda_p^{M_h} g \, d\gamma \right) n_p^s, \ \ p = 1,...,N^s.$$  \hfill (25)

Note that computing the entries $d_{ki}$ and $b_{kj}$, which are surface integrals on a trace space, is nontrivial: Apart from computing an approximation to $\Phi$, one needs to find suitable quadrature points on $\text{supp}(\lambda_i^s) \cap \text{supp}(\lambda_i^m \circ \Phi)$, which is especially tedious in cluster computing when the meshes $T_h^s$ and $T_h^m$ are distributed across several compute nodes. We use the library MOONoLith to obtain the quadrature points, as well as $\Phi$, $n^s$ and $g_h$, and we refer to [22] for an in-depth description of the required procedures, i.e. detection of intersections between the non matching meshes, load distribution and parallel communication.
(Remark 1). By defining the bilinear form \( b : H^{-\frac{1}{2}}(\Gamma_C^s) \times H^\frac{1}{2}(\Gamma_C^s) \to \mathbb{R} \), where \( \langle \cdot , \cdot \rangle \) denotes the dual pairing, the contact problem can be formulated as a saddle point problem. Find \((\lambda_h^L, u_h) \in H^{-\frac{1}{2}}(\Gamma_C^s) \times H^\frac{1}{2}(\Gamma_C^s)\) such that:

\[
\begin{align*}
    a(u_h, v_h) + b(\lambda_h^L, v_h) &= f(v_h), \quad \forall v_h \in X_h, \quad (26) \\
    b(\lambda_h^L, u_h) &\leq \langle \lambda_h^L, g \rangle, \quad \forall \lambda_h^L \in L_h. \quad (27)
\end{align*}
\]

One can show that a uniform inf-sup condition holds and under additional mild assumptions the following a-priori error estimate between the discrete solution \((\lambda_h^L, u_h)\) and the real solution \((\lambda, u)\) can be proven:

\[
||u - u_h|| + ||\lambda - \lambda_h^L||_{H^{-1/2}(\Gamma_C^s)} \leq C h^\frac{3}{2} + \alpha \sum_{k \in \mathbb{N}_m} |u^k|_{H^\frac{3}{2} + \alpha(\Omega^k)}, \forall \alpha \in (0, 1/2), \quad (28)
\]

with \(u^k \in H^{\frac{3}{2} + \alpha}(\Omega^k)\). See also [10] and the references cited therein.

(Remark 2). If \(M_h = X_h(\Gamma_C^s)\) holds, the assembly of the Operator \(T\) requires the inversion of \(D\). To avoid this computation, we choose a subspace \(M^b \not\subset X_h(\Gamma_C^s)\), which is spanned by biorthogonal basis functions \(\lambda_j^s\) that fulfill the biorthogonality relation:

\[
(\lambda^s_i, \lambda^b_j)_{L^2(\Gamma_C^s)} = \int_{\Gamma_C^s} \lambda^s_i \lambda^b_j d\gamma = \delta_{ij} \int_{\Gamma_C^s} \lambda^s_i d\gamma, \quad (29)
\]

where \(\delta_{ij}\) is the Kronecker delta. This way, the inverse of \(D\) is simply an inverted diagonal matrix (see also [41][42][21]).

(Remark 3). Our approach (Eq. [16]) differs from the classic Mortar approach [6], where the non-penetration condition is formulated as

\[
\int_{\Gamma_C^s} ((|u| - g)\lambda_h^M d\gamma \leq 0 \quad \forall \lambda \in M_h. \quad (30)
\]

That is, the test space \(M_h\) is a subspace of, or the same space as the trace space \(X_h(\Gamma_C^s)\).

(Remark 4). As long as \(M_h = X_h(\Gamma_C^s)\) holds, \(\Psi\) is the \(L^2\)-projection of the elements \(u^k \circ \Phi\) onto \(X_h(\Gamma_C^s)\). If we choose \(M^b\) from above as multiplier space, we also speak of pseudo-\(L^2\)-projections [11].

### 2.3 Change of basis

We apply an orthogonal transformation \(O\) and a mortar transformation \(Z\) on the assembled discrete finite element system. The purpose of \(O\) is to rotate the local coordinate systems at the nodes of the slave boundary \(\Gamma_C^s\), in the direction of the local normals, whereas the purpose of \(Z\) is to algebraically transform the two-body problem into a one-body problem, thereby decoupling the non-penetration constraints \(|u| \leq g\) (Eq. [9]). The solution can then be obtained from a quadratic optimization problem with \(A := (OZ) A (OZ)^T\) and \(f := (OZ) f_h\): Find a \(\hat{u}\) such that

\[
\frac{1}{2} \hat{u}' A \hat{u} - \hat{f}' \hat{u} \quad \text{is minimal}, \quad (31)
\]

with: \(\hat{u} \leq g_h. \quad (32)
\]

To construct \(O\) and \(Z\), we label the nodes of the discretized finite element system with three index sets \(\mathcal{M}, \mathcal{S}\) and \(\mathcal{I}\). The indices of the nodes on the boundary \(\Gamma_C^m\) on the master side are in \(\mathcal{M}\), those at the slave side in \(\mathcal{S}\) and the indices of the remaining nodes in the interior are in \(\mathcal{I}\). For the orthogonal transformation \(O\), we then use outer normals \(n^i_s, i \in \mathcal{S}\) at nodes of the slave
side of the contact boundary to compute local householder transformations. These transform
the local coordinate systems on the slave side of the contact boundary in such a way, that the
first coordinate of each nodal vector points in the direction of the local normals:

\[ \mathbb{R}^{3N \times 3N} \ni O := a_{ij} = \begin{cases} id_{3 \times 3} - \frac{2}{(n_i \cdot n_j)n_i^t(n_j)^t}, & i = j \text{ and } i \in S \\ id_{3 \times 3}, & i = j \text{ and } i \in I \cup M \\ 0, & \text{else.} \end{cases} \] (33)

This has the effect that the constraints, introduced by the gap function \( g \), only need to be
considered on the first coordinate in each local coordinate system (see also [23, 20, 42]).

The second transformation \( Z \) uses the mortar operator \( T \) from the previous section and is
formed in the following way:

\[ Z := \begin{bmatrix} Id_I & 0 & 0 \\ 0 & Id_M & T^t \\ 0 & 0 & Id_S \end{bmatrix} \in \mathbb{R}^{3N \times 3N}. \] (34)

The multiplication with \( Z \) transfers the displacements of the master nodes to the slave nodes
and transforms the two-body problem into a one-body problem. To illustrate this, we apply the
operator \( Z^{-t} \) to the solution \( \hat{u} \):

\[ \begin{bmatrix} Id_I & 0 & 0 \\ 0 & Id_M & 0 \\ 0 & -T & Id_S \end{bmatrix} u = \begin{bmatrix} u_I \\ u_M \\ -Tu_M + u_S \end{bmatrix} = \begin{bmatrix} \hat{u}_I \\ \hat{u}_M \\ \hat{u}_S \end{bmatrix} =: \hat{u} \in \mathbb{R}^{3N}. \] (35)

The constraints of the transformed system are now only on the third component \( \hat{u}_S \) of the
transformed solution vector \( \hat{u} \) (compare also with Eq. (24)). We solve the system with solvers of
the semismooth Newton class [15]. Another particular appeal of this transformation is, that it
is also suitable to employ monotone multigrid methods of optimal complexity [23, 21, 11] for
the solution of the system.

2.4 Implementation

We implement the discrete mortar projection \( T \), the gap function \( g_h \) and the orthogonal trans-
f ormation \( O \) as userobjects in the MOOSE framework [13], employing MOoNoLith [22] and
libMesh [18]. We have augmented the MOOSE framework with the semismooth Newton solver
from the PETSc SNES framework [3] to solve the transformed system. All components are
open source and designed for parallel computing.

3 Numerical experiments

3.1 Hertzian contact

Contact methods are commonly validated with variants of the Hertzian contact problem, a term
which stems from a study by Heinrich Hertz in which he derived analytical solutions from two
bodies in contact which have elliptic contact interfaces [14]. Here we set up a two-body problem
in which a half sphere is in contact with a cube. Valid contact methods need to replicate the
characteristic parabolic shape of the boundary stresses, as can be observed for the approach
presented in Figure 3.

3.2 Contact between two rough rock surfaces

The capability of the presented methodology to solve contact problems between highly complex
surface topographies is demonstrated in a numerical experiment with a rock specimen taken
Figure 3: Hertzian contact problem: A) Setup of the Hertzian contact problem, showing a half-sphere which is pressed into a flat surface; and B) Resulting contact stress distribution on the flat surface.

from the Grimsel Test Site in Switzerland. The fracture geometries are adapted from previous studies [37, 35, 38] and are embedded in a cylindrical rock specimen consisting of granodiorite rock (Fig. 1). Here, an increasing compressive load is applied to the specimen cylinder top in the axial direction (z-direction), while displacement in the z-direction is fixed to zero with a Dirichlet boundary condition on the cylinder bottom. The diameter of the cylinder is 122mm and the material is defined to be linear elastic with Youngs Modulus \( E = 10 \text{MPa} \) and Poisson ratio \( \nu = 0.33 \). Fracture surfaces were digitized with photogrammetric techniques [40, 39, 38], which produce a mesh of triangular elements at the body surface. From the surface mesh, a volumetric mesh of tetrahedral elements can be generated for the solid bodies with the software TRELIS. The upper body contains 101'637 nodes, the lower body 98'866 nodes, which results in 601'509 degrees of freedom for the simulation. The upper contact boundary consists of 8793 nodes, the lower one has 7898 nodes. Since the meshes are non-uniform, these numbers are difficult to relate to a resolution, which is by definition a measure that only applies to uniform meshes. We would argue however, that non-uniformness gives us at least the same, or even higher, "effective" resolution as a uniform mesh, since the nodes are distributed more effectively according to the complexity of the rock surface (see Figure 1). The simulations themselves ran on 4 nodes (2 x Intel Xeon E5-2650 v3 @ 2.30GHz) with 10 CPU’s each, on the cluster of the Institute of Computational Science in Lugano, Switzerland.

In this section aperture is defined as the values of the gap function \( g \), which reside on the nodes of the slave side. In its implementation \( g \) differs from theory, as on a finite element mesh, normals are defined on the surfaces of the element sides and not at the nodes. The direction of \( g \) is therefore computed as the average of the normals of all sides of the mesh surrounding each node of the contact side. Still, we believe this to be a more accurate description of the distance between the fracture surfaces than a simple projection in the normal \((0, 0, -1)^t\)-direction and we thus use the value of \( g \) as aperture. For the assembly of the mortar operator, only intersections up to a reasonable distance of 0.21mm are detected and the maximum value of the aperture is fixed at 0.21mm. This does not impact the accuracy of the contact method, as the displacements of the rock are smaller than this maximum value (compare also with Figure 9).

Figure 5 shows the closure of the fracture aperture field under increasing normal loads from 0.25 to 20 MPa. The aperture field is highly heterogeneous across the interface with isolated regions of small apertures, for example, right of the center of the surface. Increasing the confining stress transforms the field significantly: At 0.25 MPa, only few parts of the surface are in contact and the apertures across large parts of the surface are at the maximum value of 0.21mm. The aperture field then decreases significantly for a confining stress of 2 MPa and even more so at 10 MPa. There are regions however, which do not close, so that apertures of
Figure 4: Histograms of the aperture distribution at increasing confining stresses of 0.25, 2, 10 and 20 MPa. As the confining stress increases, areas with high aperture become less frequent, while frequency of low aperture regions increases.

at least 0.21mm remain, even when the confining stress is further increased to 20 MPa. The closing of the fracture is again illustrated in Figure 6 where we show a cross section of the fracture during closure with the open part of the fracture depicted in yellow. At 0.25 MPa, there are only few contact areas and a large part of the fracture is still open. One can observe how the fracture closes more and more with increasing normal stress until, at 20 MPa, the only open areas are essentially those, where the fracture geometry indicates cavities. In Figure 4, we illustrate the overall behavior of the aperture field during closure. As the confining stress increases, the histogram is shifted to the left and the aperture field is distributed around a lower mean.

Hence, our method replicates the closure of the fracture in contact, free of over-closure. Studying the aperture field, the cross-section and the aperture histogram (Figure 5, 6, 4), we

Figure 5: View of the different aperture fields under increasing confining stresses of 0.25, 2, 10 and 20 MPa.
Figure 6: Left: 3D representation of the approximately horizontal fracture. Right: 2D view of the fracture shown on the left. Open regions of the fracture are shown in yellow.

Figure 7: Top view of the lower fracture surface for confining stresses of 2, 10 and 20 MPa. Color indicates the vertical stresses $\sigma_{zz}$.

Figure 8: Color indicates von Mises stresses around contact points during closure of the fracture at confining stresses of 0.25, 1 and 2 MPa.

see that even at confining stresses of 10 and 20 MPa, the fracture is far from closed. Small cavities and channels still exist and the deformed fracture geometries can be used for simulating fluid flow under increasing confining stresses. The development of the vertical stresses is shown in Figure 7. The vertical stresses develop around the few contact points for an axial load of 0.25 MPa and spread over the contact surface when loads of more than 10 MPa are applied. Comparing Figures 5 and 7, we can observe, that the first vertical stresses form around regions with small apertures (dark parts), which become more pronounced when the confining stresses are increased. In Figure 8, we show a cross section of the fracture with the von Mises stresses developing at the contact nodes under increasing loads. In contrast to simpler contact models, we are able to observe, that the stresses develop from the contact surface in non-orthogonal
directions in the interior of the body. This enables the observation of stress concentrations and stress shadows around contact regions.

While this study focuses primarily on contact detection, normal stresses, aperture field development and fracture closure, intricate knowledge of stress field variation around the contact zone is of imminent importance. This is the case, as localized stress variations around zones of contact can lead to plastic deformation and failure, which permanently alter the mechanical and hydraulic behavior of the fracture [36]. The extent of stress concentrations around contact zones depends on both external load as well as on fracture surface topographies. The presented approach therefore enables an estimation of stress extrema for fracture topographies commonly encountered in specific rock types.

Rock fractures subjected to normal loading show a characteristic nonlinear fracture closure curve, where fracture closure becomes increasingly smaller for the same load increment, until it approaches the behavior of elastic deformation in a solid body [4, 25, 43, 36, 38, 19]. The fracture closure curve obtained from our numerical experiment is shown in Figure 9 for increasing axial loads from 0.25 to 20 MPa. Here, we increased the axial load incrementally in steps of 0.25 MPa from 0 to 2 MPa and then in steps of 1 MPa from 2 to 20 MPa. The fracture closure (displacement) is measured as the average displacement of nodes in zones of about 1 mm thickness, approximately 2.5 cm above and 2.5 cm below the fracture. Displacement is measured at such a small distance from the fracture to avoid large heterogeneities in displacement due to the heterogeneous distribution of surface height and contact over the fracture surface. To exclude elastic displacement due to the axial load on the lower specimen half, the average displacements of the zone in the lower specimen half are subtracted from the upper zone (see also [38]). The curve in Figure 9 shows, that the displacements become smaller when the confining stresses become larger, eventually leading to a linear relationship between axial load and displacement. The shape of the curve can be explained by noting that an increase in loading results in more areas of the fracture being in contact, increasing the overall resistance to the confining stress until a quasi-linear elastic response is reached. This is a well known characteristic of loading curves and, together with the obtained boundary stresses for the Hertzian contact, underlines the soundness of our approach.

![Figure 9: Simulated loading curve, showing displacement (i.e., fracture closure) versus axial load.](image)
4 Conclusions

We presented a parallel mortar approach to compute contact between two rough fracture surfaces with non-matching meshes, employing linear elasticity and linearized contact conditions. Unlike penalty methods, neither solution nor convergence depend on an external parameter and over-closure of the fracture is not a concern. To test our approach, we used complex fracture geometries, obtained from a real granite rock. The high-resolution 3D fracture geometries were resolved from a rock specimen that had undergone laboratory experiments. We have demonstrated the validity of our method by reproducing the boundary stresses for Hertzian contact and the characteristic nonlinear closing behavior of a fracture under increasing normal loads. The presented methodology enables investigation of the stress field development and its variations in the solid bodies, fracture aperture field, contact area and other behavior for arbitrary complex surface geometries.

Our implementation uses open source software components that are designed for parallel computing. In particular, we used MOOSE for the finite element assembly and MOONolith for the computation of the mortar transfer operator. Together with our contact formulation, we can extend our method in three directions: First, extend our formulation of frictionless contact to include friction as in [21, 10]. Second, use our formulation as a stepping stone for a wide class of more efficient multigrid obstacle solvers [21, 10]. And third, leveraging our implementation in MOOSE, to simulate fluid flow with the deformed fracture in a fluid structure interaction approach, which we have outlined in [29].

Acknowledgements

We gratefully acknowledge funding by the Swiss Competence Center for Energy Research - Supply of Electricity (SCCER-SoE) and by the Werner Siemens Foundation.

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