The Primal-Dual Active Set (PDAS) Method for Dynamic Variational Inequalities Arising from the Fractured Bone Neoplasm Models

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Abstract:

The paper deals with efficient algorithms for dynamic variational inequalities arising from fractured neoplasm (benign and malignant tumors and cysts) growth models. Since the geometry of bones with neoplasms changes in time, therefore, mathematical models of tumor and cyst evolutions are shortly presented. Owing to a loading the bones with neoplasms are fractured. The models of fractured bones with neoplasms are based on the theory of dynamic contact problems without or with Coulomb or Tresca frictions. The numerical solutions of these part of problems are based on mortar methods for nonconforming meshes with dual Lagrange multipliers and the primal-dual active set algorithms for problems without and with friction are derived. It is shown that the propagation of the crack can be calculated with both remeshing and nodal relaxation; some crack growth criteria are also mentioned. Moreover, it is shown that generalized crack models lead to solve problems with nonpenetration conditions and the primal-dual active set method.

1 Introduction

In biology and medical sciences mathematical models play an important role. The role of mathematical models are then to explain a set of biomedical experiments and analyses, and to make certain predictions which will then be tested by further biomedical, biological or numerical experiments as well as further analyses of obtained data. During the last four decades, various neoplasms (cysts, benign and malign tumors) models have been developed, analyzed and discussed. They also need to take into considerations the facts that the tumour regions are changing in time and that their boundaries are unknown in advance, and they are denoted as free boundary problems and in the case of fractured bones it leads to solve problems based on variational inequalities.

By **neoplasm**, or **tumor**, is meant a mass of tissue that forms when cells divide uncontrollably, that is, by an overproduction of cells. Neoplasms are benign tumors, malignant tumors or cancers and cysts. Cancers are of several types due to their origin, that is, due to the tissue from which they arise and the type of cells involved. A cancer of white blood cells is called leukemia, cancers arising in muscles and connective tissue are called sarcoma, and a cancer originated from epithelial cells is called carcinoma. A bone tumors are represented by abnormal growth of cells within the bone that are of (i) noncancerous types, and we speak about **benign bone tumors**, or (ii) cancerous types, and we speak about **malignant bone tumors**. Bone tumors are of primary types, originating within the bone tissues, or of secondary types, which result from the spread cancer cells from the primary tumors located in other tissues in the human body and we speak about metastasis. Another type of neoplasms are **cysts**, expect that they are filled by fluid and that are formed either in bones or in soft tissues, respectively. Growing tumors replace healthy tissue with abnormal benign or malignant tissues. Benign tumors are not life-threatening, expecting such benign tumors that are changed into malignant tumors. Benign bone tumors as well as cysts do not metastasize, that is, they do not spread to other tissues but remain situated in the bone or in the other tissue.

Since bones are composed of hard mineralized tissues, they are more resistant to destruction than other soft tissues, but in some cases the loaded long bones, vertebra or jaw-bones with tumors and cysts can fracture. The classifications of neoplasms are published by the World Health Organization – WHO.

Cancers arise from one single tumor cell. The transformation from the normal cells into tumor cells are multistage processes, where the evolution of cells are regulated and controlled by genes constrained in their nucleus (Weinberg [22]). A special feature in tumor growth is proliferation. Proliferating cells are causes of the tumor volume which varying in time. A tumor contains different populations of cells, such as (i) proliferating cells, i.e., cells that undergo abnormally fast mitosis; (ii) necrotic cells, i.e., cells that died due to a luck of nutrion; (iii) quiescent cells, i.e., cells that are alived but their rate of mitosis is balanced by the rate of natural death.

In growing masses of abnormal cells remain clustered together and confined to the cavity we then speak about **benign tumors**. These types of neoplasms rise relatively slowly, approximately several millimeters per year. In the case that the neoplasms (tumors) have emerged of the cavity, by braking out through the basal membrane and then proliferating into the extracellular matrix, or stroma, then the tumors have been malignant, and we then speak about **malign tumors** or **cancers.** In some cases the cancer cells invade into the blood or the lymphatic vessels and then transported into another locations, where they create secondary tumors. About this process we speak about **metastasis process**. Malign tumors rise relatively very quickly approximately 1mm/day. A primary tumors are traced to mutated cells, from which during short time colonies of cells are formed. In all types of neoplasms a solid tumors can be detected when it reaches a size of several millimeters.

Cysts are pathological cavity lined by the own epithelium and in the cyst lumen filled by fluid or semi-fluid contents which are not created by the accumulation of pus materials and generally are formed by a connective tissue walls. In this study we will limit ourselves to the odontogenic cysts only. **Odontogenic cysts** are cysts of the jaw which are lined by an odontogenic epithelium (that is, avascular epithelial tissues). Odontogenic cysts are in general slow growing and represent in early states of evolution no great problem and treat to human life. When there are occurred in the bones, they are called central cysts, and when they are occurred in soft tissues they are called peripheral cysts.

2 Mathematical models of tumor and cystic growths

2.1 Mathematical models of tumor growths

In our study a continuum model will be used, and moreover, we limit ourselves to avascular and vascular models only. We will formulate our models in terms of cell densities, denoted by $u_p(\mathbf{x}, t)$, $u_q(\mathbf{x}, t)$ and $u_D(\mathbf{x}, t)$ for proliferating, quiescent and dead cells, respectively, where $\mathbf{x}$ denotes a spatial coordinate and t time, $t \in I$, $\overline{I} \in [t_0, t_p]$, $t_0 \geq 0$, $t_p > 0$ (see Cui and Friedman [4, 5], Friedman [7]).

We assume that proliferating cells divide as a rate, that is, they are limited by crowding effect of the total cell population, and therefore, that proliferating cells become quiescent at a rate $K_Q(u_c)$ that depends on the concentration $u_c(\mathbf{x}, t)$ of a generic nourishment having an influence on a tumor growth and that their death rate is $K_A(u_c)$, that also depends on $u_c(\mathbf{x}, t)$. On the other hand, the quiescent cells become necrotic at a rate $K_D(u_c)$ that depends also on the concentration $u_c(\mathbf{x}, t)$. The quiescent cells become proliferating at a rate $K_P(u_c)$ which also depends on the concentration of nutrient $u_c(\mathbf{x}, t)$. The density of proliferating cells is increasing due to proliferation at a rate $K_B(u_c)$ also depending on $u_c(\mathbf{x}, t)$. Finally, the dead cells are removed from the tumor, as they decompose, at a constant rate K_R. Since cells proliferate and dead cells are removed from the tumor, there exists a continuous motion of cells within the tumor, which is represented by a velocity $\mathbf{v}_T$. Denoting by $\Omega(t)$ a region occupied by a tumor at time t and $\partial\Omega(t)$ its boundary, then the conservation of mass laws for the densities of the proliferating cells $u_p(\mathbf{x}, t)$, the quiescent cells $u_q(\mathbf{x}, t)$ and the dead cells $u_D(\mathbf{x}, t)$ are as follows:

$$\frac{\partial u_p}{\partial t} + \mathrm{div}(u_p \mathbf{v}) = [K_B(u_c) - K_Q(u_c) - K_A(u_c)] \, u_p + K_P(u_c) u_q \,, \tag{2.1}$$

$$\frac{\partial u_q}{\partial t} + \mathrm{div}(u_q \mathbf{v}) = K_Q(u_c) u_p - [K_P(u_c) + K_D(u_c)] \, u_q \,, \tag{2.2}$$

$$\frac{\partial u_D}{\partial t} + \mathrm{div}(u_D \mathbf{v}) = K_A(u_c) u_p + K_D(u_c) u_q - K_R u_D \,. \tag{2.3}$$

Assuming that the tumor tissue is modelled by a porous medium and the moving cells as fluid flow, then the velocity $\mathbf{v}_T$ of fluid flow is related to the fluid pressure σ by the Darcy law, thus

$$\mathbf{v}_T = -\beta \nabla \sigma, \quad \text{where} \quad \beta > 0 \,. \tag{2.4}$$

Moreover, assuming that all cells are physically identical in volume and mass, therefore, their density is constant inside the tumor, that is,

$$u_p + u_q + u_D = N = \text{const.}$$

For simplicity, we can put $\beta = 1$ and $N = 1$.

To determine the appropriate equation for the concentration $u_c(\mathbf{x}, t)$, we must consider the context in which the tumor is growing, that is, in its avascular stage or in the process of angiogenesis or in its vascular stage. Next, due to our investigation of fractured long bone and/or of jaw-bone with tumor(s), it is possible to limit ourselves to avascular and vascular stages of tumor evolution only. Then, for an avascular evolution of tumors we find

$$\varepsilon_0 \frac{\partial u_c}{\partial t} = D_c \nabla^2 u_c - \lambda u_c, \quad \varepsilon_0 = \frac{T_{\text{diffusion}}}{T_{\text{growth}}} \,, \tag{2.5}$$

where D_c is a diffusion coefficient, about which is assumed to be constant, λ is the nutrient consumption rate, ε_0 is the ratio of the nutrient diffusion time scale to the tumor growth time scale, $T_{\text{diffusion}} \sim 1$ minute, while $T_{\text{growth}} \sim 1$ day, so that ε_0 is small. For a vascular evolution of tumors the Eq. (2.5) must be replaced by

$$\varepsilon_0 \frac{\partial u_c}{\partial t} = D_c \nabla^2 u_c + \Gamma(u_{cB} - u_c) - \lambda u_c \,, \tag{2.6}$$

where u_{cB} is the nutrient concentration in the vasculature, Γ is the rate of the blood-tissue transfer, so that $\Gamma(u_{cB} - u_c)$ represents the nutrient concentration after the process of angiogenesis.

In the case of vascularized tumors if we use the change of variables, that is, if we put

$$u_c - \frac{\Gamma u_{cB}}{\Gamma + \lambda} \to u_c, \quad \Gamma + \lambda \to \lambda, \tag{2.7}$$

then Eq. (2.6) is transformed to Eq. (2.5), that is, u_c in the avascular and vascular tumors are described by the same equation (2.5). Adding Eqs (2.1), (2.5) with (2.7), we find

$$\text{div } \mathbf{v} = K_B(u_c)u_p - K_R u_D\,,$$

and substituting $u_D = 1 - u_p - u_q$, then we obtain the following problem:

Problem ($\mathcal{P}_T$): Find u_c, u_p, u_q, σ satisfying the following system of equations

$$\varepsilon_0 \frac{\partial u_c}{\partial t} = D_c \nabla^2 u_c - \lambda u_c \quad \text{in} \quad \Omega(t),\ t > 0\,, \tag{2.8}$$

$$\frac{\partial u_p}{\partial t} - \nabla \sigma \cdot \nabla u_p = f(u_c, u_p, u_q) \quad \text{in} \quad \Omega(t),\ t > 0\,, \tag{2.9}$$

$$\frac{\partial u_q}{\partial t} - \nabla \sigma \cdot \nabla u_q = g(u_c, u_p, u_q) \quad \text{in} \quad \Omega(t),\ t > 0, \tag{2.10}$$

$$\Delta \sigma = -h(u_c, u_p, u_q) \quad \text{in} \quad \Omega(t),\ t > 0\,, \tag{2.11}$$

where

$$f(u_c, u_p, u_q) = [K_B(u_c) - K_Q(u_c) - K_A(u_c)]\, u_p + K_P(u_c)u_q - h(u_c, u_p, u_q)u_p,$$
$$g(u_c, u_p, u_q) = K_Q(u_c)u_p - [K_p(u_c) + K_D(u_c)]\, u_q - h(u_c, u_p, u_q)u_q\,,$$
$$h(u_c, u_p, u_q) = [K_B(u_c) + K_R]\, u_p + K_R u_q - K_R\,,$$

with the boundary conditions on $\partial\Omega(t)$

$$u_c = u_{c1} \quad \text{on} \quad \partial\Omega(t),\ t > 0, \tag{2.12}$$

$$\sigma = \gamma\kappa,\ \frac{\partial \sigma}{\partial n} = -v_n \quad \text{on} \quad \partial\Omega(t),\ t > 0, \tag{2.13}$$

and with the initial conditions

$$u_c(\mathbf{x}, t_0) = u_{c0}(\mathbf{x}) \quad \text{in} \quad \Omega(t_0),\ u_{c0}(\mathbf{x}) \geq 0, \tag{2.14}$$
$$u_p(\mathbf{x}, t_0) = u_{p0}(\mathbf{x}) \quad \text{in} \quad \Omega(t_0),\ u_{p0}(\mathbf{x}) \geq 0, \tag{2.15}$$
$$u_q(\mathbf{x}, t_0) = u_{q0}(\mathbf{x}) \quad \text{in} \quad \Omega(t_0),\ u_{q0}(\mathbf{x}) \geq 0, \tag{2.16}$$

where $u_{p0}(\mathbf{x}) + u_{q0}(\mathbf{x}) \leq 1$, and where u_{c1} is a constant concentration of nutrients, v_n is the velocity of the free boundary, κ is the mean curvature, γ is the surface tension coefficient and u_{c0}, u_{p0}, u_{q0} are given functions.

Under the assumption that the initial data are smooth and the initial and boundary data are consistent with the Eq. (2.8) at $\partial\Omega(t_0)$, we have the following result:

Theorem 1 *Let the initial data be sufficiently smooth, the physical data be constant and the consistency conditions be satisfied, then there exists a unique smooth solution to Problem ($\mathcal{P}_T$) for $t \in \overline{I} = [0, t_p]$.*

For the proof see Cui and Friedman [5].

2.2 Mathematical model of cystic growths

Our mathematical model of cystic growth is based on the important diffusive mechanisms, cell birth and death, the idea of osmosis, the balance between osmotic and hydrostatic pressure forces within

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the cyst structure and its neighboring tissue. By the **osmosis** we understand the diffusive process of permeability between two different liquids which are mutually separated by a porous membrane.

Let us assume that the cyst occupies the region, we denote it by Ω_c (e.g. it can be a sphere of radius R or of an arbitrary shape) with a thin epithelial rim of cells covering its surface. The lumen of the cyst is assumed to be filled by dead cellular material, consisting partly of osmotic material concentration C^+, with total mass S, generating an osmotic pressure P_0^+. Inside the cyst is observed the hydrostatic pressure, we denote it as P_h^+. The neighborhood of the cyst is created by a material, consisting of a fixed osmotic material of concentration C^-, generating an osmotic pressure P_0^-. The hydrostatic pressure here is P_h^-. According to the size of the cavity the thickness of the capsule and the epithelial layer can be neglected. The growth of radicular cysts is of about a few millimeters per year, while in the keratocyst's case their growths are several times higher. The osmotic pressure difference $\Delta P_0 = P_0^+ - P_0^-$ relates to the difference in osmolality Δm, that is,

$$\Delta P_0 = \Delta m R_g T \,, \tag{2.17}$$

where Δm is the molar concentration of "osmotic active" molecular per litre (~ 0.011 Osml $\equiv$ 0.011 mol), $R_g = 8.31$ J/mol.K is the ideal gas constant, T is the absolute temperature. We see that the osmotic pressure will be dependent on the deformation of the jaw. The osmotic pressure ΔP_0 is ~ 28.3 Nm^{-2}. Therefore, the osmotic process is also slow or relatively quick, but the passage of fluid (fluid passage) through the epithelial membrane in response to the differences between pressures inside the cyst and in its neighborhood is instantaneous. Hence, the hydrostatic pressure difference between the interior of the cyst and the neighborhood balances the osmotic pressure difference between the cyst interior and its neighborhood at the cyst rim, i.e.,

$$P_h^+ - P_h^- = P_0^+ - P_0^- \,, \tag{2.18}$$

where P_h^+, P_0^+ are the hydrostatic and osmotic pressures, respectively, inside the cyst and P_h^-, P_0^- are the hydrostatic and osmotic pressures, respectively, in its neighborhood.

The cyst's epithelial layer keeps a constant mitotic rate. The rates of epithelial birth and death of the cell are balanced approximately to maintain a fixed rim thickness. Since the cyst grows, cells migrate towards the interior of cavity, where they die and since the degraded material driving the osmosis does not penetrate the epithelial layer (i.e. membrane) it then start to be a part of osmotic material. The osmotic material is trapped in the cavity of the cyst and only fluid can pass the semipermeable epithelial membrane. Let "s" be the total amount of degraded material inside the cyst. Then the rate of change of mass of osmotic material in the core in time, i.e. of "$\dot{s} = \frac{ds}{dt}$", is proportional to the surface area of the covering epithelium, we denote it as S_c, then we have

$$\frac{ds}{dt} = \beta S_c \,, \tag{2.19}$$

where β is a supply rate of the osmotic material, i.e., of degraded material into the cavity, and it can change according to the type of cyst. If β increases, the pathological change in the epithelium will increase the amount of osmotically material in the lumen of the cyst.

The jump in osmotic pressures across the epithelial lining is proportional to the concentration difference of osmotic material (degraded cells), i.e., it satisfies the so-called van Hoff equation

$$P_0^+ - P_0^- = \alpha(C^+ - C^-) \,, \tag{2.20}$$

where C^+ is the concentration of material inside the cyst, C^- is the concentration of material outside the cyst, $\alpha = R_g T$ is the proportional coefficient, where R_g is the ideal gas constant, T is the temperature (Tombs, Peacocke [20]).

The concentration of material inside the cyst, given as its total mass "s" divided by the cavity volume V_c, is

$$C^+ = \frac{s}{V_c} = \frac{s}{|\Omega_c|} \,, \tag{2.21}$$

where Ω_c represents the region occupied by the cyst, i.e., $V_c = |\Omega_c|$. When the cyst grows into a bony tissue, the bone is resorbed and the cyst grows as there it was no obstacle stopping it from expanding.

The hydrostatic pressure jump across the epithelial membrane balances the stresses in the semi-permeable membrane and the stresses on the cyst (cyst surface) from the neighboring bone tissue (which can be also a soft tissue). Thus

$$P_h^+ - P_h^- = f(\mathbf{r}, \dot{\mathbf{r}}) + f_b(\mathbf{r}, \dot{\mathbf{r}}), \qquad (2.22)$$

where f is the **physical stresses**, depending on the material properties of the cyst and the neighboring bone tissue, which in general is a function of a position vector $\mathbf{r}$ of the surface point, and $\dot{\mathbf{r}} = \frac{d\mathbf{r}}{dt}$ is the time derivative of $\mathbf{r}$, and f_b corresponds to the **biological stresses**, i.e., stresses due to biological processes, such as tension shifts in the epithelial lining due to the cell proliferation. These biological stresses may probably play an substantial role in keratocysts. The natures of these stresses in situ are not known currently, therefore, the term $f_b(\mathbf{r}, \dot{\mathbf{r}})$ can be omitted, i.e., $f_b(\mathbf{r}, \dot{\mathbf{r}}) = 0$.

Magar et al. [13] expect that the material of surrounding tissue is mixture of elastic and non-elastic (viscous) materials and that it can be modelled by a linear viscoelastic fluid of Maxwell type with a stiffness E and a viscosity ν. The total strain is the sum of the elastic and viscous strains and the total strain rate is the sum of its elastic and viscous strain rate

$$\varepsilon = \varepsilon^e + \varepsilon^\nu, \quad \dot{\varepsilon} = \dot{\varepsilon}^e + \dot{\varepsilon}^\nu,$$

where $\dot{\varepsilon} = \frac{d\varepsilon}{dt}$. Since $\dot{\varepsilon}^e = \frac{\dot{f}}{E}$, and $\dot{\varepsilon}^\nu = \frac{f}{\nu}$, we obtain

$$\dot{f} + \tau^{-1} f = E\dot{\varepsilon}, \qquad (2.23)$$

where $\tau = \frac{\nu}{E}$ is the so-called **relaxation time**.

From (2.20) we find $C^+ - C^- = \frac{1}{\alpha}(P_0^+ - P_0^-)$, i.e., the concentration difference $C^+ - C^-$ is the osmotic pressure difference divided by α. From (2.18) the osmotic pressure difference is equal to the hydrostatic pressure difference, i.e. $\frac{1}{\alpha}(P_0^+ - P_0^-) = \frac{1}{\alpha}(P_h^+ - P_h^-) = \frac{1}{\alpha} f(\mathbf{r}, \dot{\mathbf{r}})$, and therefore, the physical stresses $\frac{1}{\alpha} f(\mathbf{r}, \dot{\mathbf{r}}) = C^+ - C^-$. Hence, the concentration of degraded material

$$C^+ = C^- + \frac{1}{\alpha} f(\mathbf{r}, \dot{\mathbf{r}}), \qquad (2.24)$$

that is, it is a linear function of the stresses, since C^- and α are assumed to be constant.

Since $C^+ = \frac{s}{V_c(\mathbf{r})}$, then substituting $s = C^+ V_c(\mathbf{r})$ into (2.19), i.e., $\frac{ds}{dt} = \beta S_c$, and using (2.24), then after some modification, we obtain

$$\frac{\dot{V}_c}{\alpha} f(\mathbf{r}, \dot{\mathbf{r}}) \dot{\mathbf{r}} + \dot{V}_c C^- \dot{\mathbf{r}} + \frac{V_c}{\alpha} \dot{f}(\mathbf{r}, \dot{\mathbf{r}}) = \beta S_c, \qquad (2.25)$$

representing expression relating the cyst size, its shape and the physical stresses exerted by the stroma, where β is the core supply rate of osmotic material ($[\mathrm{mol/m^2.s}]$) and is different for radicular cysts and keratocysts for which is several times higher than for radicular cysts.

Since we model the material which is a mixture of fluid, collagenous capsule, and crystalline structures, than it can be described as Maxwell's fluid. Due to (2.23) the stresses satisfy

$$\tau \dot{f}(\mathbf{r}, \dot{\mathbf{r}}) + f(\mathbf{r}, \dot{\mathbf{r}}) = \nu \dot{\varepsilon}, \qquad (2.26)$$

as $\tau = \frac{\nu}{E}$. The problem will be complete, if the initial condition on $\mathbf{r}$ and f will be given. Thus, for $t = 0$

$$\mathbf{r}(0) = \mathbf{r}_0, \quad f(0) = f_0, \qquad (2.27)$$

where $\mathbf{r}_0$ and f_0 are given.

Assuming that the cyst is of a spherical shape, then $V_c = \frac{4}{3}\pi R^3$ and $S_c = 4\pi R^2$, where R is a radius of the cyst. For more details see Magar et al. [13], Ward et al. [21], Nedoma [18]. The problem can be solved by numerical methods for ODEs.

3 Stress-strain analysis of the fractured bone with neoplasms

3.1 Mathematical model

Let the bones with neoplasms be approximated by elastic or visco-elastic rheologies, respectively, and let occupy a region $\Omega \in \mathbb{R}^N$, $N = 2, 3$. (Fig.1a,b,c), the geometry of which was determined on the obtained results from the previous section. Further, we will limit ourselves to the linear elasticity and the visco-elasticity with short memory (Kelvin-Voigt type).

Let $I = (0, t_p)$, $t_p > 0$, be a time interval. Let $\Omega \subset \mathbb{R}^N$, $N = 2, 3$, be a region occupied by a system of bodies of arbitrary shapes Ω^ι such that $\Omega = \cup_{\iota=1}^r (\Omega^\iota \cup \Gamma_{cv}^\iota)$. Let Ω^ι have Lipschitz boundaries $\partial \Omega^\iota$ and let us assume that $\partial \Omega = \Gamma_\tau \cup \Gamma_u \cup \Gamma_c$, where the disjoint parts Γ_τ, Γ_u, Γ_c are open subsets. Moreover, let $\Gamma_\tau = {}^1\Gamma_\tau \cup {}^2\Gamma_\tau$, $\Gamma_u = {}^1\Gamma_u \cup {}^2\Gamma_u$ and $\Gamma_c = \cup_{s,m}\Gamma_c^{sm}$, $\Gamma_c^{sm} = \partial \Omega^s \cap \partial \Omega^m$, $s \neq m$, $s, m \in \{1, \dots, r\}$, Γ_c^{sm} represent the contact boundaries between the components of joints as well as between two opposite faces of cracks, $\Gamma_{cv} = \cup_s \Gamma_{cv}^s$, $\Gamma_{cv}^s \subset \partial \Omega_1^s \cap \partial \Omega_2^s$, represent virtual interfaces between regions Ω_1^s and Ω_2^s. It is evident that these boundaries are determined as results of the used neoplasm's growth models. Let $\Omega(t) = I \times \Omega$ denote the time-space domain and let $\Gamma_\tau(t) = \Gamma_\tau \times I$, $\Gamma_u(t) = \Gamma_u \times I$, $\Gamma_c(t) = \Gamma_c \times I$ denote the parts of its boundary $\partial \Omega(t) = \partial \Omega \times I$. In the study we will assume that the contact boundaries Γ_c^{sm} are between contact boundaries of joints (i.e., hip joints, knee joints, temporomandibular joints, etc.) as well as contact boundaries between the opposite boundaries in the fractures of bones and/or of vertebra.

Furthermore, let $\mathbf{n}$ denote the outer normal vector of the boundary, $u_n = u_i n_i$, $\mathbf{u}_t = \mathbf{u} - u_n \mathbf{n}$, $\tau_n = \tau_{ij} n_j n_i$, $\boldsymbol{\tau}_t = \boldsymbol{\tau} - \tau_n \mathbf{n}$ be normal and tangential components of displacement and stress vectors $\mathbf{u} = (u_i)$, $\boldsymbol{\tau} = (\tau_i)$, $\tau_i = \tau_{ij} n_j$, $i, j = 1, \dots, N$. Let $\mathbf{F}$, $\mathbf{P}$ be the body and surface forces, ρ the density. The respective time derivatives are denoted by "'". Let us denote by $\mathbf{u}' = (u_k')$ the velocity vector. To formulate the contact and friction conditions, let us introduce at each point of Γ_c^s the vectors $\mathbf{t}_i^s$, $i = N - 1$, spanning in the corresponding tangential plane. Let $\{\mathbf{n}^s, \mathbf{t}_i^s\}$, $i = 1, 2$, be an orthogonal basis in $\mathbb{R}^N$ for each point of Γ_c^s. To formulate the non-penetration condition we use a predefined relation between the points of the possible contact zones Γ_c. Therefore, we introduce a smooth mapping $\mathcal{R} : \Gamma_c^s \to \Gamma_c^m$ such that $\mathcal{R}(\Gamma_c^s) \subset \Gamma_c^m$, and we will assume that the mapping $\mathcal{R}$ is well defined and maps any $\mathbf{x} \in \Gamma_c^s$ to the intersection of the normal on Γ_c^s at $\mathbf{x}$ with Γ_c^m. Then $[\mathbf{u}]^{sm} := \mathbf{u}^s(\mathbf{x}, t) - \mathbf{u}^m(\mathcal{R}(\mathbf{x}, t))$, $[u_n]^{sm} := [\mathbf{u}]^{sm} \cdot \mathbf{n}^s$ is the jump in normal direction, $[\mathbf{u}_t]^{sm} = (\mathbf{u}^s(\mathbf{x}, t) - \mathbf{u}^m(\mathcal{R}(\mathbf{x}, t))) - [\mathbf{u}]^{sm} \cdot \mathbf{n}^s$ and $\tau_n^s = (\mathbf{n}^s)^T \boldsymbol{\tau}^s(\mathbf{x}, t)\mathbf{n}^s = (\mathbf{n}^s)^T \boldsymbol{\tau}^m(\mathcal{R}(\mathbf{x}, t))\mathbf{n}^s$ is the boundary stress in normal direction on the possible contact part, and moreover, $(\mathbf{t}_i^s)^T \boldsymbol{\tau}^s(\mathbf{x}, t)\mathbf{t}_i^s = (\mathbf{t}_i^s)^T \boldsymbol{\tau}^m(\mathcal{R}(\mathbf{x}, t))\mathbf{t}_i^s$, $i = N - 1$, must be ensured.

From the momentum conservation law the equation of motion is of the form

$$\rho \frac{\partial^2 u_i^\iota}{\partial t^2} = \frac{\partial \tau_{ij}^\iota}{\partial x_j} + F_i^\iota, \quad i, j = 1, \dots, N, \quad \iota = 1, \dots, r, \quad (\mathbf{x}, t) \in \Omega^\iota(t) = \Omega^\iota \times I, \qquad (3.1)$$

where for the linear elastic rheology

$$\tau_{ij}^\iota = \tau_{ij}^\iota(\mathbf{u}) = c_{ijkl}^{(0)\iota}(\mathbf{x})e_{kl}(\mathbf{u}^\iota), \quad e_{ij}(\mathbf{u}) = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right),$$

$$i, j, k, l = 1, \dots, N, \ \iota = 1, \dots, r, \qquad (3.2)$$

and for the linear visco-elastic rheology

$$\tau_{ij}^\iota = \tau_{ij}^\iota(\mathbf{u}^\iota, \mathbf{u}'^\iota) = c_{ijkl}^{(0)\iota}(\mathbf{x})e_{kl}(\mathbf{u}^\iota) + c_{ijkl}^{(1)\iota}(\mathbf{x})e_{kl}(\mathbf{u}'^\iota) =$$

$$= {}^e\tau_{ij}^\iota(\mathbf{u}^\iota) + {}^\nu\tau_{ij}^\iota(\mathbf{u}'^\iota), \quad i, j, k, l = 1, \dots, N, \ \iota = 1, \dots, r, \qquad (3.3)$$

where $c_{ijkl}^{(n)\iota}(\mathbf{x})$, $n = 0, 1$, are anisotropic elastic and viscous coefficients and $e_{ij}(\mathbf{u})$ are components of the small strain tensor, N is the space dimension. For the tensors $c_{ijkl}^{(n)\iota}(\mathbf{x})$, $n = 0, 1$, we assume that they satisfy the symmetric and Lipschitz conditions, that is,

$$c_{ijkl}^{(n)\iota} \in L^\infty(\Omega^\iota), \quad n = 0, 1, \ \iota = 1, \dots, r, \quad c_{ijkl}^{(n)\iota} = c_{jikl}^{(n)\iota} = c_{klij}^{(n)\iota} = c_{ijlk}^{(n)\iota},$$

$$c_{ijkl}^{(n)\iota}e_{ij}e_{kl} \geq c_0^{(n)\iota}e_{ij}e_{ij} \quad \forall e_{ij}, \quad e_{ij} = e_{ji} \quad \text{and a.e.} \quad \mathbf{x} \in \Omega^\iota, \quad c_0^{(n)\iota} > 0,$$

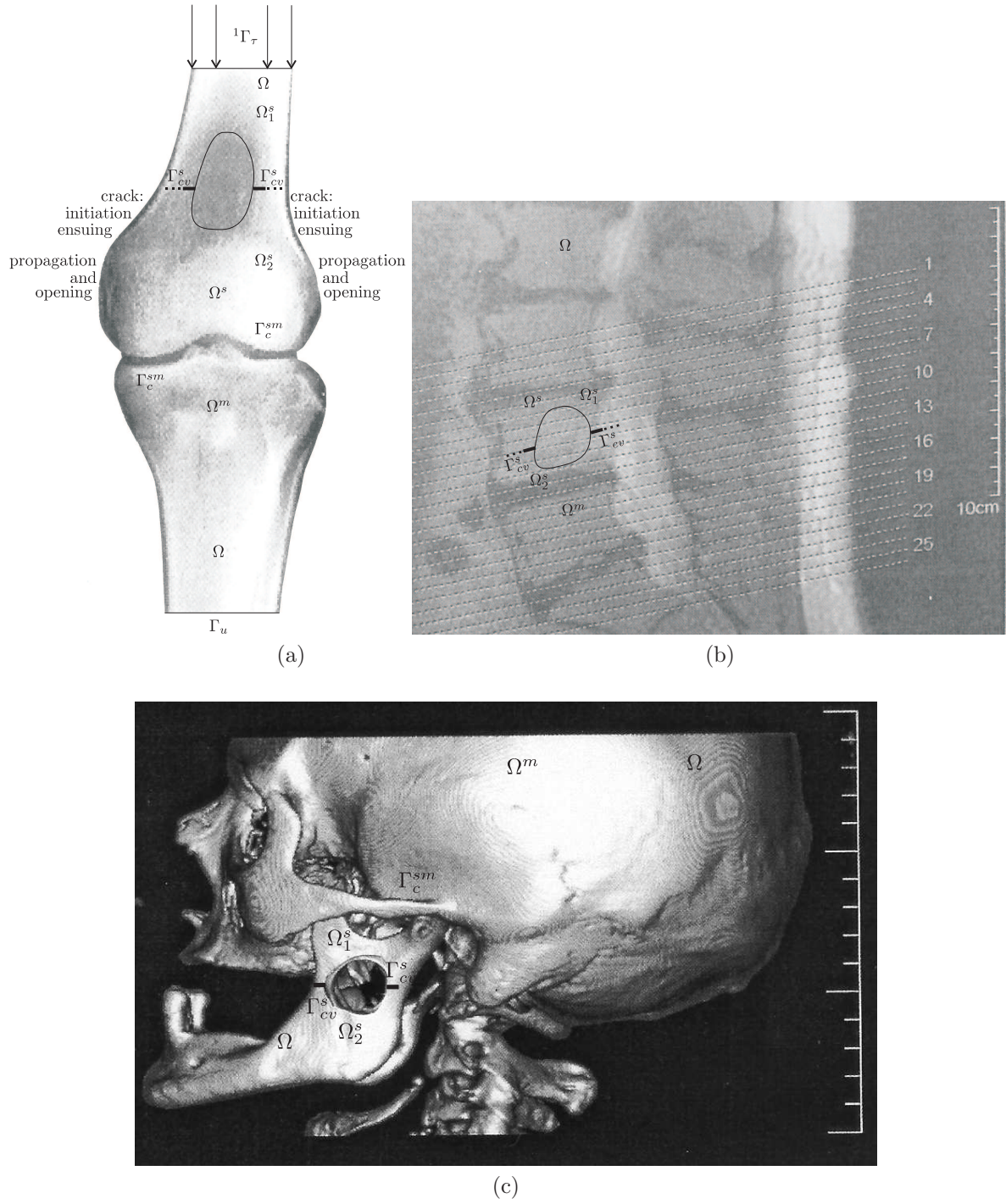$$\iota = 1, \dots, r, \qquad (3.4)$$

Figure 3.1: a, b,c Mathematical models of the long bone and spine with tumors and the jaw-bone with cyst: crack initiation and ensuing crack propagation and crack opening.

where a repeated index implies summation from 1 to N.

The problem to be solved has the following classical formulation:

Problem ($\mathcal{P}$): Let $N = 2, 3$, $r \geq 2$. Find a displacement vector $\mathbf{u}^\iota : \overline{\Omega}^\iota \times I \to \mathbb{R}^N$ satisfying Eqs (3.1) with Eq. (3.2) or (3.3) and the boundary and initial conditions

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$$\tau_{ij}n_j = P_i, \quad i,j = 1,\ldots,N, \quad (\mathbf{x},t) \in \Gamma_\tau(t) = \cup_{\iota=1}^r (\Gamma_\tau \cap \partial\Omega^\iota) \times I \,, \tag{3.5}$$

$$u_i = u_{2i}, \quad i = 1,\ldots,N, \quad (\mathbf{x},t) \in \Gamma_u(t) = \cup_{\iota=1}^r (\Gamma_u \cap \partial\Omega^\iota) \times I \,, \tag{3.6}$$

$$\left.\begin{array}{l} [u_n]^{sm} \le d^{sm}, \ \tau_n^s = \tau_n^m \equiv \tau_n^{sm} \le 0, \\ ([u_n]^{sm} - d^{sm})\,\tau_n^{sm} = 0, \boldsymbol{\tau}_t^{sm} = \mathbf{0}, \end{array}\right\} (\mathbf{x},t) \in \cup_{s,m}\Gamma_c^{sm} \times I, \tag{3.7}$$

in the case without friction and in the case with Coulombian friction

$$\left.\begin{array}{l} [u_n]^{sm} \le d^{sm}, \ \tau_n^s = \tau_n^m \equiv \tau_n^{sm} \le 0, \\ ([u_n]^{sm} - d^{sm})\,\tau_n^{sm} = 0, \\ [\mathbf{u}_t']^{sm} = \mathbf{0} \Rightarrow |\boldsymbol{\tau}_t^{sm}| \le \mathcal{F}_c^{sm}\,|\tau_n^{sm}(\mathbf{u})|, \\ [\mathbf{u}_t']^{sm} \ne \mathbf{0} \Rightarrow \boldsymbol{\tau}_t^{sm} = -\mathcal{F}_c^{sm}\,|\tau_n^{sm}(\mathbf{u})|\,\frac{[\mathbf{u}_t']^{sm}}{|[\mathbf{u}_t']^{sm}|}, \end{array}\right\} (\mathbf{x},t) \in \cup_{e,m}\Gamma_c^{sm} \times I, \tag{3.8}$$

$$\mathbf{u}^\iota(\mathbf{x},0) = \mathbf{u}_0^\iota(\mathbf{x}), \quad \mathbf{u}'^\iota(\mathbf{x},0) = \mathbf{u}_1^\iota(\mathbf{x}), \quad \mathbf{x} \in \Omega^\iota \,, \tag{3.9}$$

where $\boldsymbol{\tau}_t^{sm} \equiv \boldsymbol{\tau}_t^s = -\boldsymbol{\tau}_t^m$, $\mathcal{F}_c^{sm} = \mathcal{F}_c^{sm}(\mathbf{x},\mathbf{u}_t')$ is globally bounded, nonnegative, and satisfies the Carathéodory conditions (Eck et al. [6], Nedoma [17], Nedoma et al. [19]) and $\mathbf{u}_0$, $\mathbf{u}_1$ are the given functions, $\mathbf{u}_2(\ne 0$ on $^1\Gamma_u$ or $= 0$ on $^2\Gamma_u)$ has a time derivative $\mathbf{u}_2'$, and on $\cup\Gamma_c^{sm}$ due to the equilibrium of forces $\tau_{ij}(\mathbf{u}^s)n_j^s = -\tau_{ij}(\mathbf{u}^m)n_j^m$ and where $[\mathbf{v}]^{sm} = \mathbf{v}^s - \mathbf{v}^n$ is a jump (difference) of quantities $\mathbf{v}^s$ and $\mathbf{v}^m$ and d^{sm} is a gap, where

$$d^{sm}(\mathbf{x}) = \frac{\varphi^s(\mathbf{x}) - \varphi^m(\mathbf{x})}{\sqrt{1 + |\nabla\varphi^s(\mathbf{x})|^2}} \,,$$

where $\varphi^s, \varphi^m \in C^1$ are functions defined on an open subset Γ_c^{sm} of $\mathbb{R}^{N-1}$ parametrized the two contact boundaries, e.g. of joints in the first case, and the two opposite faces of the cracks in the second case. Thus the terms $d^{sm} \ge 0$ are the normalized gaps between the contact boundaries of Ω^s and Ω^m (e.g. of joints) and between the two faces of the crack (i.e., Γ_c^s and Γ_c^m).

Since the problem with Coulombian friction formulated in displacements is up-to-date an open problem, therefore, for the existence analysis the contact conditions of nonpenetration (Signorini conditions) will be formulated in velocities, that is,

$$[u_n']^{sm} \le 0, \quad \tau_n^s = \tau_n^m \equiv \tau_n^{sm} \le 0, \quad [u_n']^{sm}\tau_n^{sm} = 0 \,. \tag{3.10}$$

Let us introduce the spaces $L^{p,N}(\Omega)$, $p \in [1,+\infty)$, $L^\infty(\Omega)$, the Sobolev spaces $H^{1,N}(\Omega)$, $H_0^{1,N}(\Omega)$, $H^{\frac{1}{2},N}(\Gamma_c)$, $H_{00}^{\frac{1}{2},N}(\Gamma_c)$ by the usual way, and let $B(M)$ be the space of bounded functions endowed with the sup norm, and moreover, the spaces and sets

$$V_0 = \left\{ \mathbf{v}|\mathbf{v} \in \sqcap_{\iota=1}^r H^{1,N}(\Omega^\iota), \mathbf{v} = 0 \text{ a.e. on } \Gamma_u \right\},$$

$$V = \mathbf{u}_2 + V_0, \ \mathcal{V} = \mathbf{u}_2' + \mathcal{V}_0 = L^2(I;V), \quad K = \left\{ \mathbf{v} \in V|[v_n]^{sm} \le d^{sm} \text{ a.e. on } \Gamma_c^{sm} \right\},$$

$$\mathcal{K} = \left\{ \mathbf{v}|\mathbf{v} \in L^2(I;\sqcap_{\iota=1}^s H^{1,N}(\Omega^\iota)), \mathbf{v} = \mathbf{u}_2' \text{ on } \Gamma_u(t), [v_n]^{sm} \le 0 \text{ a.e. on } \Gamma_c^{sm}(t) \right\} \,.$$

Let $\rho^\iota \in C(\overline{\Omega}^\iota)$, $\rho^\iota \ge \rho_0^\iota > 0$, $c_{ijkl}^\iota \in L^\infty(\Omega^\iota)$, $\mathbf{F}^\iota, \mathbf{F}'^\iota \in L^2(I;L^{2,N}(\Omega^\iota))$, $\mathbf{P}, \mathbf{P}' \in L^2(I;L^{2,N}(\Gamma_\tau))$, $\mathbf{u}_0 \in K$, $\mathbf{u}_1 \in V$, $\mathbf{u}_2' \in L^2\left(I;\sqcap_{\iota=1}^r H^{1,N}(\Omega^\iota)\right)$, $d^{sm} \in H^{\frac{1}{2},N}(\Gamma_c^{sm})$, $d^{sm} \ge 0$ a.e. on Γ_c^{sm}, $\mathcal{F}_c^{sm} \in L^\infty(\Gamma_c^{sm})$, $\mathcal{F}_c^{sm} \ge 0$ a.e. on Γ_c^{sm}. In a special case if $\overline{\Gamma}_c^s = \partial\Omega^\iota \setminus \Gamma_u^s$ then instead of the space $H^{\frac{1}{2},N}(\Gamma_c^{sm})$ we will use the space $H_{00}^{\frac{1}{2},N}(\Gamma_c^{sm})$.

Then multiplying (3.1) by $\mathbf{v} - \mathbf{u}'$, where $\mathbf{v}$ are suitable test functions, integrating over $\Omega^\iota \times I$ for all ι, using the Green's theorems and boundary and contact conditions, then we obtain the following variational problem:

Problem $(\mathcal{P})_v$: Find a vector function $\mathbf{u} \in \mathcal{K}$ with $\mathbf{u}' \in \mathcal{K} \cap B(I;L^{2,N}(\Omega))$ and $\mathbf{u}(\cdot,0) = \mathbf{u}_0$, $\mathbf{u}'(\cdot,0) = \mathbf{u}_1$, such that for all $t \in I$

$$\int_I \Big\{ (\mathbf{u}''(t),\mathbf{v} - \mathbf{u}'(t)) + a^{(0)}(\mathbf{u}(t),\mathbf{v} - \mathbf{u}'(t)) + a^{(1)}(\mathbf{u}'(t),\mathbf{v} - \mathbf{u}'(t)) +$$

$$+ j(\mathbf{v}) - j(\mathbf{u}'(t)) \Big\} dt \ge \int_I (\mathbf{f}(t),\mathbf{v} - \mathbf{u}'(t))dt \quad \forall\mathbf{v} \in \mathcal{K}, \tag{3.11}$$

holds, where

$$(\mathbf{u}'', \mathbf{v}) = \sum_{\iota=1}^{r} (\mathbf{u}''^{\iota}, \mathbf{v}^{\iota}) = \int_{\Omega} \rho u_i'' v_i d\mathbf{x},$$

$$a^{(n)\iota}(\mathbf{u}^{\iota}, \mathbf{v}^{\iota}) = \sum_{\iota=1}^{r} a^{\iota}(\mathbf{u}^{\iota}, \mathbf{v}^{\iota}) = \int_{\Omega} c_{ijkl}^{(n)} e_{kl}(\mathbf{u}^{\iota}) e_{ij}(\mathbf{v}^{\iota}) d\mathbf{x}, \quad n = 0, 1,$$

$$(\mathbf{f}, \mathbf{v}) = \sum_{\iota=1}^{r} (\mathbf{f}^{\iota}, \mathbf{v}^{\iota}) = \int_{\Omega} \mathbf{F} \cdot \mathbf{v} d\mathbf{x} + \int_{\Gamma_{\tau}} \mathbf{P} \cdot \mathbf{v} ds,$$

$$j(\mathbf{v}) = \int_{\cup_{s,m} \Gamma_c^{sm}} \mathcal{F}_c^{sm} |\tau_n^{sm}(\mathbf{u}, \mathbf{u}')| \left([\mathbf{v}_t]^{sm}\right) ds,$$

and where the bilinear forms $a^{(n)}(\mathbf{u}, \mathbf{v})$, $n = 0, 1$, are symmetric in $\mathbf{u}$, $\mathbf{v}$ and satisfy $a^{(n)}(\mathbf{u}, \mathbf{u}) \geq c_0^{(n)} \|\mathbf{u}\|_{1,N}^2$, $c_0^{(n)} = \text{const} > 0$, $a^{(n)}(\mathbf{u}, \mathbf{v}) \leq c_1^{(n)} \|\mathbf{u}\|_{1,N} \|\mathbf{v}\|_{1,N}$, $c_1^{(n)} = \text{const} > 0$, $\mathbf{u}, \mathbf{v} \in V_0$, and moreover, where we assume that the initial data $\mathbf{u}_0$, $\mathbf{u}_1$ satisfy, e.g., the static contact multibody linear elastic problem (Nedoma [14]). The elastic problem is a special case of the above problem (for details see Eck et al. [6]) and will be discussed in more details in the subsection concerning the algorithms.

The proof of the existence of the solution is based on the penalization and regularization techniques and is modification of that of Eck et al. [6], Nedoma [16], and see also Cocou and Scarella [3].

3.2 Approximation of the problem by the Tresca model of friction

Let us assume that the Coulombian law of friction in every time level is approximated by its value g_c^{sm} from the previous time level, i.e., $g_c^{sm} \equiv \mathcal{F}_c^{sm} |\tau_n^{sm}(\mathbf{u}, \mathbf{u}')|) (t - \Delta t)$. Thus g_c^{sm} is a non-negative function and has a meaning of a given friction limit (or a given friction bound, representing the magnitude of the limiting friction traction at which slip originates), and where $-g_c^{sm}$ has a meaning of a given frictional force, and Δt is a time element. Thus this problem is approximated by another problem in which in every time level we will solve the dynamic contact problem with the given friction, called the Tresca model of friction.

Multiplying (3.1) by $\mathbf{v} - \mathbf{u}$, integrating over $\Omega = \cup_{\iota=1}^{r} (\Omega^{\iota} \cup \Gamma_{cv}^{\iota})$, using the Green theorem, the boundary conditions and contact conditions in displacements, then we have

Problem $(\mathcal{P}_0)_v$**:** Find a displacement field $\mathbf{u} : \overline{I} \to V$ such that $\mathbf{u}(t) \in K$ for a.e. $t \in I$, and

$$(\mathbf{u}''(t), \mathbf{v} - \mathbf{u}(t)) + a^{(0)}(\mathbf{u}(t), \mathbf{v} - \mathbf{u}(t)) + a^{(1)}(\mathbf{u}'(t), \mathbf{v} - \mathbf{u}(t)) +$$
$$+ j(\mathbf{v}) - j(\mathbf{u}(t)) \geq (\mathbf{f}(t), \mathbf{v} - \mathbf{u}(t)) \quad \forall \mathbf{v} \in K, \, t \in I, \tag{3.12}$$

$$\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), \mathbf{u}'(\mathbf{x}, 0) = \mathbf{u}_1(\mathbf{x}), \tag{3.13}$$

where we assume that the initial data $\mathbf{u}_0$, $\mathbf{u}_1$ are given functions as above, and where

$$(\mathbf{u}'', \mathbf{v}) = \sum_{\iota=1}^{r} (\mathbf{u}''^{\iota}, \mathbf{v}^{\iota}) = \int_{\Omega} \rho u_i'' v_i d\mathbf{x},$$

$$a^{(n)}(\mathbf{u}, \mathbf{v}) = \sum_{\iota=1}^{r} a^{(n)\iota}(\mathbf{u}^{\iota}, \mathbf{v}^{\iota}) = \int_{\Omega} c_{ijkl}^{(n)} e_{kl}(\mathbf{u}) e_{ij}(\mathbf{v}) d\mathbf{x}, \, n = 0, 1,$$

$$(\mathbf{f}, \mathbf{v}) = \sum_{\iota=1}^{r} (\mathbf{f}^{\iota}, \mathbf{v}^{\iota}) = \int_{\Omega} F_i v_i d\mathbf{x} + \int_{\Gamma_{\tau}} P_i v_i ds,$$

$$j(\mathbf{v}) = \int_{\cup_{s,m} \Gamma_c^{sm}} g_c^{sm} [\mathbf{v}_t]^{sm} ds,$$

where the bilinear forms $a^{(n)}(\mathbf{u}, \mathbf{v})$, $n = 0, 1$, are symmetric in $\mathbf{u}$, $\mathbf{v}$ and satisfy $a^{(n)}(\mathbf{u}, \mathbf{u}) \geq c_0^{(n)} \|\mathbf{u}\|_{1,N}^2$, $c_0^{(n)} = \text{const} > 0$, $a^{(n)}(\mathbf{u}, \mathbf{v}) \leq c_1^{(n)} \|\mathbf{u}\|_{1,N} \|\mathbf{v}\|_{1,N}$, $c_1^{(n)} = \text{const} > 0$, $\mathbf{u}, \mathbf{v} \in V_0$.

Problem $(\mathcal{P}_0)_v$ is equivalent with the following problem:

Problem $(\mathcal{P})_v$: Find a vector function $\mathbf{u} \in B(I; \sqcap_{\iota=1}^r H^{1,N}(\Omega^\iota))$ with $\mathbf{u}(\cdot, t) \in \mathcal{K}$, for a.e. $t \in I$, $\mathbf{u}' \in L^2(I; \sqcap_{\iota=1}^r H^{1,N}(\Omega^\iota)) \cap L^\infty(I; \sqcap_{\iota=1}^r L^{2,N}(\Omega^\iota))$, $\mathbf{u}'(\cdot, t_p) \in L^{2,N}(\Omega)$, such that for all $\mathbf{v} \in \sqcap_{\iota=1}^r H^{1,N}(\Omega^\iota(t))$ with $\mathbf{v}(\cdot, t) \in \mathcal{K}$ a.e. in I the following inequality

$$\int_I \left\{ (\mathbf{u}''(t), \mathbf{v} - \mathbf{u}'(t)) + a^{(0)}(\mathbf{u}(t), \mathbf{v} - \mathbf{u}'(t)) + a^{(1)}(\mathbf{u}'(t), \mathbf{v} - \mathbf{u}'(t)) + \right.$$
$$\left. + j(\mathbf{v}) - j(\mathbf{u}'(t)) \right\} dt \geq \int_I (\mathbf{f}(t), \mathbf{v} - \mathbf{u}'(t)) dt \,, \tag{3.14}$$

with $\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x})$, $\mathbf{u}'(\mathbf{x}, 0) = \mathbf{u}_1(\mathbf{x})$, holds.

To prove the existence of the solution of Problem $(\mathcal{P})_v$ the decomposition $\mathbf{v} - \mathbf{u} = \mathbf{v} - \mathbf{u} + \mathbf{u}' - \mathbf{u}' = \mathbf{w} - \mathbf{u}'$ will be also used. Next, the test function $\mathbf{v}$ will correspond with the test function $\mathbf{v} - \mathbf{u} + \mathbf{u}'$. The proof of the existence of the solution is based on the penalization and regularization techniques and is parallel to that of Eck et al. [6, Chapter 4].

3.3 Numerical solution and the algorithm

Let $\Omega = \cup_{\iota=1}^r (\Omega^\iota \cup \Gamma_{cv}^\iota)$ be approximated by $\Omega_h = \cup_{\iota=1}^r (\Omega_h^\iota \cup \Gamma_{cvh}^\iota)$ (a polygon in 2D and a polyhedron in 3D) with the boundary $\partial \Omega_h = \Gamma_{\tau h} \cup \Gamma_{uh} \cup \Gamma_{ch}$. Let $I = (0, t_p)$, $t_p > 0$, let $m > 0$ be an integer, then $\Delta t = t_p/m$, $t_i = i\Delta t$, $i = 0, \ldots, m$. Let $\{\mathcal{T}_{h, \Omega_h}\}$ be a regular family of finite element partitions $\mathcal{T}_h$ of $\overline{\Omega}_h$ compatible to the boundary subsets $\overline{\Gamma}_{\tau h}$, $\overline{\Gamma}_{uh}$ and $\overline{\Gamma}_{ch}$. Let $V_h \subset V$ be the finite element space of linear elements corresponding to the partition $\mathcal{T}_h$, $K_h = V_h \cap K$ the set of continuous piecewise linear functions that vanish at the nodes of $\overline{\Gamma}_{uh}$ and whose normal components are non-positive at the nodes on $\cup_{s,m} \Gamma_c^{sm}$; K_h is a nonempty, closed, convex subset of $V_h \subset V$. Let $\mathbf{u}_{0h} \in K_h$, $\mathbf{u}_{1h} \in V_h$ be an approximation of $\mathbf{u}_0$ or $\mathbf{u}_1$. Let the end points $\overline{\Gamma}_{\tau h} \cup \overline{\Gamma}_{uh}$, $\overline{\Gamma}_{uh} \cup \overline{\Gamma}_{ch}$, $\overline{\Gamma}_{\tau h} \cup \overline{\Gamma}_{ch}$, coincide with the vertices of T_{hi}. Since the frictional term is assumed to be approximated by its value in the previous time level, the frictional term is approximated by a given friction limit. Then in every time level we have the following discrete problem:

Problem $(\mathcal{P})_h$: Find a displacement field $\mathbf{u}_h : \overline{I} \to V_h$ with $\mathbf{u}_h(0) = \mathbf{u}_{0h}, \mathbf{u}_h'(0) = \mathbf{u}_{1h}$, such that for a.e. $t \in I$, $\mathbf{u}_h(t) \in K_h$

$$(\mathbf{u}_h''(t), \mathbf{v}_h - \mathbf{u}_h(t)) + a^{(0)}(\mathbf{u}_h(t), \mathbf{v}_h - \mathbf{u}_h(t)) + a^{(1)}(\mathbf{u}_h'(t), \mathbf{v}_h - \mathbf{u}_h(t)) +$$
$$+ j(\mathbf{v}_h) - j(\mathbf{u}_h(t)) \geq (\mathbf{f}_h(t), \mathbf{v}_h - \mathbf{u}_h(t)) \quad \forall \mathbf{v}_h \in K_h, \quad \text{a.e.} \, t \in I \,, \tag{3.15}$$

where

$$(\mathbf{u}_h'', \mathbf{v}_h) = \sum_{\iota=1}^r (\mathbf{u}_h''^\iota, \mathbf{v}_h^\iota) = \int_{\Omega_h} \rho u_{hi}'' v_{hi} d\mathbf{x} \,,$$

$$a^{(n)}(\mathbf{u}_h, \mathbf{v}_h) = \sum_{\iota=1}^r a^{(n)\iota}(\mathbf{u}_h^\iota, \mathbf{v}_h^\iota) = \int_{\Omega_h} c_{ijkl}^{(n)} e_{kl}(\mathbf{u}_h) e_{ij}(\mathbf{v}_h) d\mathbf{x}, \quad n = 0, 1,$$

$$(\mathbf{f}_h, \mathbf{v}_h) = \sum_{\iota=1}^r (\mathbf{f}_h^\iota, \mathbf{v}_h^\iota) = \int_{\Omega_h} F_i v_{hi} d\mathbf{x} + \int_{\Gamma_{\tau h}} P_i v_{hi} ds,$$

$$j(\mathbf{v}_h) = \sum_{\iota=1}^r j^\iota(\mathbf{v}_h^\iota) = \int_{\cup_{s,m} \Gamma_{ch}^{sm}} g_{ch}^{sm} |[\mathbf{v}_{ht}]^{sm}| ds \equiv \langle g_{ch}^{sm}, |[\mathbf{v}_{ht}]^{sm}| \rangle_{\Gamma_{ch}^{sm}} \,.$$

To prove the existence of discrete solution $\mathbf{u}_h$ the technique similar of that as in the continuous case, based on the decomposition $\mathbf{v}_h - \mathbf{u}_h = \mathbf{v}_h - \mathbf{u}_h + \mathbf{u}_h' - \mathbf{u}_h' = \mathbf{w}_h - \mathbf{u}_h'$, the penalty and regularization techniques are used. In the next the test function $\mathbf{v}$ will correspond with $\mathbf{v} + \mathbf{u}' - \mathbf{u}$ in (3.12) and $\mathbf{v}_h$ with $\mathbf{v}_h + \mathbf{u}_h' - \mathbf{u}_h$ in (3.15) after used decomposition.

Algorithm

The algorithm will be based on the semi-implicit scheme in time and the finite elements in space. Let $m > 0$ be an integer, then $\Delta t = t_p/m$, $t_i = i\Delta t$, $i = 0, 1, \ldots, m$. Approximating the derivatives by the differences, i.e., $\mathbf{u}_h'' = \frac{\mathbf{u}_h^{i+1} - 2\mathbf{u}_h^i + \mathbf{u}_h^{i-1}}{\Delta t^2}$, $\mathbf{u}_h' = \frac{\mathbf{u}_h^{i+1} - \mathbf{u}_h^i}{\Delta t}$, and setting $\mathbf{u}_h^i = \mathbf{u}_h(t_i)$, $\Delta \mathbf{u}_h^i = \mathbf{u}_h(t_i) - \mathbf{u}_h(t_{i-1})$, $\mathbf{u}_h^{i+1} \equiv \mathbf{u}_h$, $g_{ch}^{sm} = g_{ch}^{sm}(t_i) = \mathcal{F}_c^{sm}\left(\Delta t^{-1}[\Delta \mathbf{u}_{th}^i]^{sm}\right) \left|\tau_n^{sm}\left(\mathbf{u}_h^i, \frac{\Delta \mathbf{u}_h^i}{\Delta t}\right)\right|$, $(\mathbf{F}(t_{i+1}), \mathbf{v}_h) = \Delta t^2 (\mathbf{f}_h(t_{i+1}), \mathbf{v}_h) + (2\mathbf{u}_h^i - \mathbf{u}_h^{i-1}, \mathbf{v}_h) + \Delta t a_h^{(1)}(\mathbf{u}_h^i, \mathbf{v}_h)$, $\mathbf{F}(t_{i+1}) \equiv \mathbf{f}_h$, then after some algebra in every time level $t = t_{i+1}$ we have to solve the following problem:

Problem $(\mathcal{P}_A)_h$**:** Find $\mathbf{u}_h \in K_h$, a.e. $t = t_{i+1} \in I$, such that

$$A(\mathbf{u}_h, \mathbf{v}_h - \mathbf{u}_h) + j(\mathbf{v}_h) - j(\mathbf{u}_h) \geq (\mathbf{f}_h, \mathbf{v}_h - \mathbf{u}_h), \quad \forall \mathbf{v}_h \in K_h, \ t = t_{i+1} \in I, \tag{3.16}$$

where for the visco-elastic and elastic cases

$$A(\mathbf{u}_h, \mathbf{v}_h) = (\mathbf{u}_h, \mathbf{v}_h) + \Delta t^2 a^{(0)}(\mathbf{u}_h, \mathbf{v}_h) + \Delta t a^{(1)}(\mathbf{u}_h, \mathbf{v}_h) \text{ for the viscoelastic case,}$$

$$A(\mathbf{u}_h, \mathbf{v}_h) = (\mathbf{u}_h, \mathbf{v}_h) + \Delta t^2 a^{(0)}(\mathbf{u}_h, \mathbf{v}_h) \text{ for the elastic case,}$$

$$j(\mathbf{v}_h) = \Delta t^2 \int_{\cup_{s,m} \Gamma_c^{sm}} g_{ch}^{sm} |[\mathbf{v}_{ht}]^{sm}| \, ds,$$

where g_{ch}^{sm} is the approximate given frictional limit. According to the above assumptions about the bilinear forms $a_h^{(n)}(\cdot, \cdot)$, $n = 0, 1$, and since $\rho \geq \rho_0 > 0$, then the bilinear form $A(\mathbf{u}_h, \mathbf{v}_h)$ is also symmetric in $\mathbf{u}_h$ and $\mathbf{v}_h$ and

$$A(\mathbf{u}_h, \mathbf{u}_h) \geq a_0 \|\mathbf{u}_h\|_{1,2}^2, \quad a_0 = \text{const.} > 0,$$

$$|A(\mathbf{u}_h, \mathbf{v}_h)| \leq a_1 \|\mathbf{u}_h\|_{1,2} \|\mathbf{v}_h\|_{1,2}, \quad a_1 = \text{const.} > 0, \ \mathbf{u}_h, \mathbf{v}_h \in V_h,$$

hold.

The discretization error will be a function of the time step Δt and the mesh size h and thus the truncation error of the time and spatial discretization must tend to zero (Bathe [1], Belytschko et al. [2], Nedoma [17], Nedoma et al. [19]). From the stability analysis for the critical time step size we have

$$\Delta t \leq \Delta t_{\text{crit}} = \gamma \frac{h^{(n)}}{\pi} \left(\frac{\rho^{(n)}}{E^{(n)}}\right), \tag{3.17}$$

where $h^{(n)}$ is the diameter of the corresponding (n)-th element, $h^{(n)} = c^{(n)} T_n$, T_n is the smallest period of the finite discretization with n degrees of freedom, $c^{(n)}$ is a dilatational wave velocity in the (n)-th material element, $\rho^{(n)}$ and $E^{(n)}$ are (average) values of the density and the Young modulus on the (n)-th element and γ is a reduction factor determining from numerical experiments. Moreover, the algorithm is also consistent of order two, because the truncation error is of order Δt^2 in the displacements. Hence, the algorithm is convergent.

The mortar discretization

To give a saddle point formulation it is usually to introduce a Lagrange multiplier space $M = M_n \times M_t$, being the dual space of the trace space $W = \sqcap_s H^{\frac{1}{2},N}(\Gamma_c^s)$ (i.e., the trace space of V_0 restricted to $\cup_s \Gamma_c^s$) and its dual $W' = \sqcap_s H^{-\frac{1}{2},N}(\Gamma_c^s)$, assuming that Ω^ι, $\iota = 1, \ldots, r$, are domains with sufficiently smooth boundaries $\partial \Omega^\iota$, and the bilinear form $b(\cdot, \cdot)$ on the product space $V_0 \times M$. In the case if $\overline{\Gamma}_c^s = \partial \Omega^s \setminus \Gamma_u^s$ we must use $H_{00}^{\frac{1}{2},N}(\Gamma_c^s)$ instead of $H^{\frac{1}{2},N}(\Gamma_c^s)$.

Let every polygonal domain Ω_h^ι, $\iota = 1, \ldots, r$, be covered by a triangulation $\mathcal{T}_{h,\Omega^\iota}$ in such a way that on the contact boundaries Γ_{ch}^s the points of Γ_{ch}^s and Γ_{ch}^m are not identical, therefore, the mesh sizes $h_s \neq h_m$ and the global meshsize h is $h = \max\{h_s, h_m\}$.

Let us introduce the discrete approximation of the Lagrange multiplier space $M_{hH} = M_{hn} \times M_{Ht}$, where

Case I:

$$W_{hH}\left(\cup_s\Gamma^s_{ch}\right) =W_{hn}\left(\cup_s\Gamma^s_{ch}\right) \times W_{Ht}\left(\cup_s\Gamma^s_{ch}\right) =$$
$$=\left\{\mathbf{v}^s_h\cdot\mathbf{n}^s|_{\cup_s\Gamma^s_{ch}}, \mathbf{v}_h\in V_h\right\}\times\left\{\mathbf{v}^s_h\cdot\mathbf{t}^s|_{\cup_s\Gamma^s_{ch}}, \mathbf{v}_h\in V_h\right\},$$
$$M_{hn} =\Big\{\mu_{hn}\in W_{hn}\left(\cup_s\Gamma^s_{ch}\right), \int_{\Gamma^s_c}\mu_{hn}\psi_h ds\geq 0,$$
$$\forall\psi_h\in W_{hn},\ \psi_n\geq 0\ \text{a.e. on every}\ \Gamma^s_{ch}\Big\},$$

$$M_{Ht} =\Big\{\mu_{Ht}\in W_{Ht}\left(\cup_s\Gamma^s_{ch}\right), \int_{\Gamma^s_{ch}}\boldsymbol{\mu}_{Ht}\boldsymbol{\psi}_H ds -\int_{\Gamma^s_{ch}}g^{sm}_{ch}|\psi_H|ds\leq 0,$$
$$\forall\boldsymbol{\psi}_H\in W_{Ht}\left(\cup_s\Gamma^s_{ch}\right)\Big\},$$

Case II:

$$W_{hH}\left(\cup_s\Gamma^s_{ch}\right) =W_{hn}\left(\cup_s\Gamma^s_{ch}\right) \times W_{Ht}\left(\cup_s\Gamma^s_{ch}\right) =$$
$$=\left\{\boldsymbol{\mu}_{hH}|_{\Delta_r}\in\left[P_0(\Delta_r)\right]^{N-1},\ 0\leq r\leq n(h^s)\right\},$$
$$M_{hn} =\left\{\mu_{hn}\in W_{hn}\left(\cup_s\Gamma^s_{ch}\right), \mu_{hn}\geq 0\ \text{a.e. on every}\ \Gamma^s_{ch}\right\},$$
$$M_{Ht} =\Big\{\boldsymbol{\mu}_{Ht}\in W_{Ht}\left(\cup_s\Gamma^s_{ch}\right), \int_{\Gamma^s_{ch}}\boldsymbol{\mu}_{Ht}\boldsymbol{\psi}_H ds -\int_{\Gamma^s_{ch}}g^{sm}_{ch}|\psi_H|ds\leq 0,$$
$$\forall\boldsymbol{\psi}_H\in W_{Ht}\left(\cup_s\Gamma^s_{ch}\right)\Big\},$$

where $\Gamma^s_{ch}=\cup^{\overline{p}}_{p=1}\Gamma^{sp}_{ch}$, $\Gamma^{sp}_{ch}=\cup_r\Delta_r$, $\Delta_r=(q_r,q_r+h_p)$, $r=0,1,\ldots,m-1$, $m=m(h_p)$, where h_p is a step of mesh in the $p-th$ segment of Γ^s_{ch} for $N=2$; or Δ_r are the faces of polyhedron, $r=0,1,\ldots,m-1$, $m=m(h_p)$, for $N=3$. Let

$$b(\boldsymbol{\mu}_{hH},\mathbf{v}_h)=\langle\mu_{hn},[\mathbf{v}_h\cdot\mathbf{n}]^s-d^{sm}\rangle_{\cup\Gamma^s_{ch}}+\int_{\cup_s\Gamma^s_{ch}}g^{sm}_{ch}\boldsymbol{\mu}_{Ht}\cdot[\mathbf{v}_{ht}]^s ds,$$
$$\boldsymbol{\mu}_{hH}\in M_{hH},\ \mathbf{v}_h\in V_{0h},$$

where $[\mathbf{v}_h\cdot\mathbf{n}]^{sm}=v^s_{hn}(\mathbf{x},t)-v^m_{hn}(\mathcal{R}^{sm}(\mathbf{x},t))$, $[\mathbf{v}_{ht}]^{sm}=\mathbf{v}^s_{ht}(\mathbf{x},t)-\mathbf{v}^m_{ht}(\mathcal{R}^{sm}(\mathbf{x},t))$, where $\mathcal{R}^{sm}:$ $\Gamma^s_{ch}(t)\mapsto\Gamma^m_{ch}(t)$, at $t\in I$, is a bijective map satisfying $\Gamma^s_{ch}(t)\subset\mathcal{R}^{sm}(\Gamma^s_{ch}(t))$, $t\in I$, and where $\langle\cdot,\cdot\rangle_{\Gamma^s_{ch}}$ denotes the duality pairing between W_{hH} and M_{hH}.

Then we have the following problem:

Problem $(\mathcal{P})_h$: At every time level find $(\boldsymbol{\lambda}_{hH},\mathbf{u}_h)\in M_{hH}\times V_h$ satisfying

$$A(\mathbf{u}_h,\mathbf{v}_h)+b(\boldsymbol{\lambda}_{hH},\mathbf{v}_h)=(\mathbf{f}_h,\mathbf{v}_h)\quad\forall\mathbf{v}_h\in V_h=\sqcap^r_{\iota=1}V^\iota_h,\ t\in I,$$
$$b(\boldsymbol{\mu}_{hH}-\boldsymbol{\lambda}_{hH},\mathbf{v}_h)\leq\langle d^{sm},\mu_{hn}-\lambda_{hn}\rangle_{\cup\Gamma^s_{ch}}\quad\forall\boldsymbol{\mu}_{hH}\in M_{hH},\ t\in I. \tag{3.18}$$

For the existence and uniqueness it is necessary to ensure that $\{\boldsymbol{\mu}_{hH}\in M_{hH},b(\boldsymbol{\mu}_{hH},\mathbf{v}_h)=0,\forall\mathbf{v}_h\in V_h\}=\{\oslash\}$, which for the Case I is obvious and for the Case II the technique of Haslinger et al. [9], with using the discrete Babuška-Brezzi "inf-sup" condition, is used.

Proposition 1 *Let* $-\tau_n(\mathbf{u})\in M_{hn}$. *Then the problem (3.18) has a unique solution* $(\boldsymbol{\lambda}_{hH},\mathbf{u}_h)\in M_{hH}\times V_h$, *a.e.* $t\in I$. *Moreover, we have*

$$\lambda^s_{hn}=-\tau^s_n(\mathbf{u}_h)\quad and\quad g^s_c\boldsymbol{\lambda}^s_{Ht}=-\boldsymbol{\tau}^s_t(\mathbf{u}_h),$$

where $\mathbf{u}_h$ *is the solution of the discrete primal problem and* $g^s_c\equiv g^{sm}_{ch}$.

The primal-dual active set (PDAS) method. As usual in the mortar approach the interface Γ_{ch}^{sm} has two sides, the "slave" side from Ω_h^s and the "master" side from Ω_h^m. The interface Γ_{ch}^{sm} is assumed to be a union of edges in the 2D case and of faces in the 3D case.

Wohlmuth and Krause [24] introduced the modification of the space $V_h = V_h^s \times V_h^m \subset V$ by such a way that the nodal basis function on the mortar side will be biorthogonal with respect to the piecewise linear basis on the slave side. Thus the non-penetration condition $[\mathbf{u} \cdot \mathbf{n}]^s \leq d^{sm}$ will be replaced by its weak discrete form

$$\int_{\cup \Gamma_{ch}^s} [\mathbf{u}_h \cdot \mathbf{n}]^s \varphi_p ds \leq \int_{\cup \Gamma_{ch}^s} d_p^s \varphi_p ds, \quad p \in S, \tag{3.19}$$

giving a coupling between the vertices on the slave side and the master side, where S is the set of all vertices in the potential contact part on the slave side. We introduce a basis transformation of the basis of V_h in such a way that the weak non-penetration condition (3.19) in the new basis (the so-called dual basis) only deals with the vertices on the slave side.

In the mortar approach, the Lagrange multiplier space is approximated by its $(N-1)$-dimensional mesh resulting from the N-dimensional triangulation on the slave side. Here we will use discontinuous piecewise linear nodal basis functions for the dual Lagrange multiplier. The discrete Lagrange multiplier space M_{hH} can be spanned as $M_{hH}^s = \text{span}\{\psi_i \mathbf{e}_k, i = 1, \ldots, n_c, k = 1, \ldots, N\}$, $s \in \{1, \ldots, r\}$, where ψ_i is the i-th scalar dual basis function, $\mathbf{e}_k$ is the k-th unit vector, n_c is the number of nodes on the slave side of $\overline{\Gamma}_{ch}^s$, i.e., the number of freedom of the space M_{hH} in each component. Denoting $\{\varphi_j\}$, $j = 1, \ldots, m$, the standard piecewise linear basis on the slave side (i.e., the basis of a component $W_{hH}(\Gamma_c^{sm})$), we have

$$\int_{\Gamma_{ch}^s} \varphi_j \psi_i ds = \delta_{ij} \int_{\Gamma_{ch}^s} \varphi_j ds, \quad 1 \leq i, j \leq m, \tag{3.20}$$

where δ_{ij} is the Kronecker delta. Let W_{hH}^s be the vector valued trace space of V_{0h} restricted to $\cup_s \Gamma_{ch}^s$. Then for each $\mathbf{v}_h = \sum_i \gamma_i \varphi_i \in W_{hH}$ the discrete scalar product $\mathbf{v}_h \cdot \mathbf{n}_h = \sum_i (\gamma_i \cdot \mathbf{n}_i) \varphi_i$, where $\mathbf{n}_i$ denotes the outer normal of Ω^s at the node i. Similarly, for each $\boldsymbol{\mu}_h = \sum_i \boldsymbol{\alpha}_i \psi_i \in M_{hH}$ the discrete product $\boldsymbol{\mu}_h \cdot \mathbf{n}_h = \sum_i (\boldsymbol{\alpha}_i \cdot \mathbf{n}_i) \psi_i$. Let us define

$$M_{hH}^{s+} := \left\{ \boldsymbol{\mu}_{hH} \in M_{hH}^s | \langle \boldsymbol{\mu}_{hH}, \mathbf{v}_h \rangle \geq 0, \mathbf{v}_h \in W_h^{s+} := \{\mathbf{v}_h \in W_{hH}^s | \mathbf{v}_h \cdot \mathbf{n}_h \geq 0\} \right\}.$$

Hüeber and Wohlmuth [11] show that

$$M_{hH}^{s+} := \left\{ \boldsymbol{\mu}_{hH} = \sum_{i=1}^m \boldsymbol{\alpha}_i \psi_i | \boldsymbol{\alpha}_i \in \mathbb{R}^N, \boldsymbol{\alpha}_i = \alpha_i^n \mathbf{n}_i^s, \alpha_i^n \in \mathbb{R}, \alpha_i^n \geq 0, i \leq m \right\},$$

and that M_{hH}^{s+} is not a conforming approach for the Lagrange multiplier space.

Finally, we define

$$M_{hH}^+ = \sqcap_s M_{hH}^{s+},$$
$$b(\boldsymbol{\mu}_{hH}, \mathbf{v}_h) = \langle \boldsymbol{\mu}_{hH}, [\mathbf{v}_h]^s \rangle_{\cup \Gamma_{ch}^s}.$$

For completeness, the discrete convex subset $K_h \subset V_h$ will be then defined as

$$K_h := \left\{ \mathbf{v}_h \in V_h | b(\boldsymbol{\mu}_{hH}, \mathbf{v}_h) \leq \int_{\Gamma_{ch}^s} d_h^{sm} (\boldsymbol{\mu}_{hH} \cdot \mathbf{n}_h) ds, \boldsymbol{\mu}_{hH} \in M_{hH}^+ \right\},$$

where d_h^{sm} is a suitable approximation of d^{sm} on W_{hH}.

The discrete mortar formulation of the saddle point problem (3.18) for every time level is defined as follows:

Problem $(\mathcal{P}_{sp})_{dm}$**:** At every time level find $\mathbf{u}_h \in V_h$, $\boldsymbol{\lambda}_{hH} \in M_{hH}^+$, a.e. $t \in I$, $\boldsymbol{\lambda}_{hH} = (\lambda_{hn}, \boldsymbol{\lambda}_{Ht})$, satisfying

$$A(\mathbf{u}_h, \mathbf{v}_h) + b(\boldsymbol{\lambda}_{hH}, \mathbf{v}_h) = (\mathbf{f}_h, \mathbf{v}_h) \quad \forall \mathbf{v}_h \in V_h, \ t \in I,$$
$$b(\boldsymbol{\mu}_{hH} - \boldsymbol{\lambda}_{hH}, \mathbf{v}_h) \leq \langle d^{sm}, (\boldsymbol{\mu}_{hH} - \boldsymbol{\lambda}_{hH}) \cdot \mathbf{n}_h \rangle_{\cup \Gamma_{ch}^s} \quad \forall \boldsymbol{\mu}_{hH} \in M_{hH}^+, \ t \in I, \tag{3.21}$$

where

$$A(\mathbf{u}_h, \mathbf{v}_h) = (\mathbf{u}_h, \mathbf{v}_h) + \Delta t^2 a^{(0)}(\mathbf{u}_h, \mathbf{v}_h) + \Delta t a^{(1)}(\mathbf{u}_h, \mathbf{v}_h) \text{ for the viscoelastic case,}$$

$$A(\mathbf{u}_h, \mathbf{v}_h) = (\mathbf{u}_h, \mathbf{v}_h) + \Delta t^2 a^{(0)}(\mathbf{u}_h, \mathbf{v}_h) \text{ for the elastic case,}$$

$$b(\boldsymbol{\mu}_{hH}, \mathbf{v}_h) = \langle \boldsymbol{\mu}_{hH}, [\mathbf{v}_h]^s \rangle_{\cup \Gamma_{ch}^s} \quad \forall \mathbf{v}_h \in V_h, \ \boldsymbol{\mu}_{hH} \in M_{hH}.$$

In the frictionless case the tangential stress component on the contact boundary $\cup \Gamma_c^{sm}$ is zero, then $\boldsymbol{\lambda}_{Ht} = 0$, and therefore, $M_{hH} = M_{hn}$. The Lagrange multipliers λ_{hn} are the approximations of the contact forces $-\boldsymbol{\tau}(\mathbf{u}_h) \cdot \mathbf{n} = -(n_j n_k \tau_{jk}(\mathbf{u}_h))$ which are necessary to adjust the contact displacements on the contact boundary $\cup \Gamma_{ch}^{sm}$.

Let us denote the nodal parameters $\mathbf{u}_h$ by $\mathbf{U}$, of λ_{hn} by $\boldsymbol{\Lambda}_{hn}$, and since for the frictionless case the tangential stress component on the contact boundary $\cup \Gamma_{ch}^{sm}$ is zero, then $\boldsymbol{\lambda}_{Ht} = \mathbf{0}$, and thus $\boldsymbol{\Lambda}_{Ht} = \mathbf{0}$.

The Eq. (3.21a) for every $t \in I$ in the matrix form is of the form

$$\mathbb{A}_h \mathbf{U} + \mathbb{B}_h \boldsymbol{\Lambda}_{hH} = \mathbb{F}_h. \tag{3.22}$$

To determine the structure of $\mathbb{B}_h$, we decompose the set of all vertices in every time level into three disjoint parts $\mathcal{N}$, $\mathcal{M}$ and $\mathcal{S}$, where $\mathcal{S}(\dim n_V)$ denotes all vertices on the possible contact part on the slave side, $\mathcal{M}(\dim n_{cn})$ all vertices of the possible contact part of the master side, and $\mathcal{N}$ all the other one. The strong formulation of the non-penetration condition will be replaced by its weak discrete form

$$\int_{\cup \Gamma_{ch}^{sm}} [\mathbf{u}_h \cdot \mathbf{n}]^s \psi_p ds \le \int_{\cup \Gamma_{ch}^{sm}} d_h^s \psi_p ds, \quad p \in \mathcal{S}. \tag{3.23}$$

This condition connects points of sets $\mathcal{S}$ and $\mathcal{M}$. We introduce a basis in a new transformation of the basis of the space V_h in such a way that the weak non-penetration condition (3.23) in the new basis only deals with the vertices on the slave side (see Hüeber, Wohlmuth [11], Wohlmuth and Krause [24], Nedoma [16, 17], Nedoma et al. [19]).

Introducing the transformation $\varphi = (\varphi_{\mathcal{N}}, \varphi_{\mathcal{M}}, \varphi_{\mathcal{S}})^T$, then the matrices and vectors in (3.22) will be decomposed in the sense of the used decomposition as follows

$$\begin{bmatrix} \mathbb{A}_{\mathcal{N}\mathcal{N}} & \mathbb{A}_{\mathcal{N}\mathcal{M}} & \mathbb{A}_{\mathcal{N}\mathcal{S}} & \mathbb{O} \\ \mathbb{A}_{\mathcal{M}\mathcal{N}} & \mathbb{A}_{\mathcal{M}\mathcal{M}} & \mathbb{A}_{\mathcal{M}\mathcal{S}} & -\mathbb{M}^T \\ \mathbb{A}_{\mathcal{S}\mathcal{N}} & \mathbb{A}_{\mathcal{S}\mathcal{M}} & \mathbb{A}_{\mathcal{S}\mathcal{S}} & \mathbb{D} \end{bmatrix} \begin{bmatrix} \mathbb{U}_{\mathcal{N}} \\ \mathbb{U}_{\mathcal{M}} \\ \mathbb{U}_{\mathcal{S}} \\ \boldsymbol{\Lambda}_{\mathcal{S}} \end{bmatrix} = \begin{bmatrix} \mathbb{F}_{\mathcal{N}} \\ \mathbb{F}_{\mathcal{M}} \\ \mathbb{F}_{\mathcal{S}} \end{bmatrix}, \tag{3.24}$$

where elements of $\mathbb{B}_h$ are defined by $\mathbb{B}_h[p, q] = \int_{\cup \Gamma_{ch}^s} \varphi_p \psi_q ds \mathbb{I}_N = \delta_{pq} \int_{\cup \Gamma_{ch}^s} \varphi_p ds$, $p = 1, \ldots, n_V$, $q = 1, \ldots, n_{cn}$, and where $\mathbb{I}_N$ denotes the identity matrix in $\mathbb{R}^{N \times N}$. The basis functions satisfy the condition of biorthogonality (3.20). The matrix $\mathbb{M}$ represents coupling between the traces of the finite element shape functions on the master side "m" and the shape functions for the Lagrange multiplier on the slave side "s, that is,

$$\mathbb{M}[p, q] = \langle \varphi_p, \psi_q \rangle \mathbb{I}_N, \quad p \in \mathcal{S}, \ q \in \mathcal{M}, \tag{3.25}$$

where $\mathbb{I}_N$ is the identity matrix in $\mathbb{R}^{N \times N}$. The matrix $\mathbb{M}$ is the block matrix and $\mathbb{D}$, due to the biorthogonality, is the block diagonal matrix with

$$\mathbb{D}[p, q] = \langle \varphi_p, \psi_q \rangle \mathbb{I}_N, \quad p = q \in \mathcal{S}. \tag{3.26}$$

The matrix $\mathbb{B}_h$ in every time level is of the form $\mathbb{B}_h = (\mathbb{O}, -\mathbb{M}^T, \mathbb{D})^T$. By $\mathbb{A}_{k,l}$, $k, l \in \{\mathcal{N}, \mathcal{M}, \mathcal{S}\}$ we denote the block matrices associated with the basis functions of the free structure nodes (i.e., $\mathcal{N}$), the potential contact nodes of the master side (i.e., $\mathcal{M}$) and the potential contact nodes on the slide side (i.e., $\mathcal{S}$). The entries of vectors $\mathbb{U}$ and $\mathbb{F}$ for $k \in \{\mathcal{N}, \mathcal{M}, \mathcal{S}\}$ are denoted by $\mathbb{U}_k$ and $\mathbb{F}_k$, respectively.

Introducing $\hat{\mathbb{M}} = \mathbb{D}^{-1} \mathbb{M}$ and a new modified basis $\Phi = (\Phi_{\mathcal{N}}, \Phi_{\mathcal{M}}, \Phi_{\mathcal{S}})^T$ instead of the basis $\varphi = (\varphi_{\mathcal{N}}, \varphi_{\mathcal{M}}, \varphi_{\mathcal{S}})^T$, that is,

$$\Phi = (\Phi_{\mathcal{N}}, \Phi_{\mathcal{M}}, \Phi_{\mathcal{S}})^T = \begin{bmatrix} \mathbb{I}_N & \mathbb{O} & \mathbb{O} \\ \mathbb{O} & \mathbb{I}_N & \hat{\mathbb{M}}^T \\ \mathbb{O} & \mathbb{O} & \mathbb{I}_N \end{bmatrix} \begin{bmatrix} \varphi_{\mathcal{N}} \\ \varphi_{\mathcal{M}} \\ \varphi_{\mathcal{S}} \end{bmatrix} = Q\varphi, \tag{3.27}$$

then
$$\mathbb{U} = Q^T \hat{\mathbb{U}},$$

where $\hat{\mathbb{U}}$ is the vector of coefficients with respect to the transformed basis Φ.

Then the modified stiffness matrix $\hat{\mathbb{A}}_h$ associated with the transformed basis Φ is of the form

$$\hat{\mathbb{A}}_h = Q\mathbb{A}_h Q^T =$$
$$= \begin{bmatrix} \mathbb{A}_{\mathcal{NN}} & \mathbb{A}_{\mathcal{NM}} + \mathbb{A}_{\mathcal{NS}}\hat{\mathbb{M}} & \mathbb{A}_{\mathcal{NS}} \\ \mathbb{A}_{\mathcal{MN}} + \hat{\mathbb{M}}^T\mathbb{A}_{\mathcal{SN}} & \mathbb{A}_{\mathcal{MM}} + \mathbb{A}_{\mathcal{MS}}\hat{\mathbb{M}} + \hat{\mathbb{M}}^T\mathbb{A}_{\mathcal{SM}} + \hat{\mathbb{M}}^T\mathbb{A}_{\mathcal{SS}}\hat{\mathbb{M}} & \mathbb{A}_{\mathcal{MS}} + \hat{\mathbb{M}}^T\mathbb{A}_{\mathcal{SS}} \\ \mathbb{A}_{\mathcal{SN}} & \mathbb{A}_{\mathcal{SM}} + \mathbb{A}_{\mathcal{SS}}\hat{\mathbb{M}} & \mathbb{A}_{\mathcal{SS}} \end{bmatrix}$$

and the vector $\hat{\mathbb{F}}_h$ is of the form

$$\hat{\mathbb{F}}_h = Q\mathbb{F}_h = (\mathbb{F}_\mathcal{N}, \ \mathbb{F}_\mathcal{M} + \hat{\mathbb{M}}^T\mathbb{F}_\mathcal{S}, \ \mathbb{F}_\mathcal{S})^T.$$

The weak non-penetration condition associated with the transformed basis Φ is of the form (Nedoma [16, 17], Nedoma et al. [19])

$$\hat{\mathbb{U}}_{n,p} \equiv (\mathbf{n}_p^s)^T \mathbb{D}[p,p]\hat{\mathbb{U}}_p \leq d_p^{sm} \quad \forall p \in \mathcal{S}, \tag{3.28}$$

where $d_p^{sm} = \int_{\cup_s \Gamma_c^s} d_h^{sm}\psi_p ds$, $p \in \mathcal{S}$, as the coefficients at $\hat{\mathbb{U}}_q$, $q \in \mathcal{M}$, are nullified. The matrix $\hat{\mathbb{B}}_h$, associated with the transformed basis Φ, is then of the form $\hat{\mathbb{B}}_h = Q\mathbb{B}_h = (\mathbb{O}, \mathbb{O}, \mathbb{D})^T$.

Thus, in every time level, we will solve the following problem

$$\hat{\mathbb{A}}_h\hat{\mathbb{U}} + \hat{\mathbb{B}}_h\mathbf{\Lambda}_{hH} = \hat{\mathbb{F}}_h,$$
$$\hat{\mathbb{U}}_{n,p} \leq d_p^{sm}, \mathbf{\Lambda}_{hn,p} \geq 0, (\hat{\mathbb{U}}_{n,p} - d_p^{sm})\mathbf{\Lambda}_{hn,p} = 0, \quad \forall p \in \mathcal{S}, \ t \in I,$$
$$\mathbf{\Lambda}_{Ht,p} = \mathbf{0}, \quad \forall p \in \mathcal{S}, \ t \in I, \tag{3.29}$$

where (3.29b–d) is the Karush-Kuhn-Tucker conditions of a constrained optimization problem for inequality constraints,

$$\mathbf{\Lambda}_{hn,p} = \mathbf{n}_p^{sT}\hat{\mathbb{D}}[p,p]\mathbf{\Lambda}_{hH}(p), \quad \mathbf{\Lambda}_{hH}(p) \in \mathbb{R}^N,$$
$$\mathbf{\Lambda}_{Ht,p} = \mathbf{\Lambda}_{hH}(p) - (\mathbf{\Lambda}_{hH}(p) \cdot \mathbf{n}_p^s)\mathbf{n}_p^s = (\mathbf{\Lambda}_{hH}(p) \cdot \mathbf{t}_p^s)\mathbf{t}_p^s.$$

A primal-dual active set (PDAS) algorithm - the frictionless case

Hintermüller et al. [10] present a method how to find the correct "active" subset $\mathcal{A}$ of vertices from $\mathcal{S}$, and Nedoma [16, 17], Nedoma et al. [19] applied the method for dynamic contact problems, where is assumed that the bodies Ω^s, Ω^m are in mutual contact.

Let us decompose the set $\mathcal{S}$ as $\mathcal{S} = \mathcal{A} \cup \mathcal{I}$, where $\mathcal{A}$ is the active set and $\mathcal{I}$ is the inactive set. Let us put

$$C_n(\hat{\mathbb{U}}_{n,p}, \mathbf{\Lambda}_{hn,p}) = \mathbf{\Lambda}_{hn,p} - \max\left\{0, \mathbf{\Lambda}_{hn,p} + c_1(\hat{\mathbb{U}}_{n,p} - d_p^{sm})\right\}, \quad c_1 = \text{const.} > 0,$$

then (3.29b–d) can be expressed as

$$C_n(\hat{\mathbb{U}}_{n,p}, \mathbf{\Lambda}_{hn,p}) = 0, \quad p \in \mathcal{S}.$$

Thus, at every time $t \in I$ Eq. (3.29) can be rewritten as

$$\hat{\mathbb{A}}_h\hat{\mathbb{U}} + \hat{\mathbb{B}}_h\mathbf{\Lambda}_{hH} = \hat{\mathbb{F}}_h,$$
$$C_n(\hat{\mathbb{U}}_{n,p}, \mathbf{\Lambda}_{hn,p}) = 0,$$
$$\mathbf{\Lambda}_{Ht,p} = \mathbf{0} \tag{3.30}$$

for all vertices $p \in \mathcal{S}$ and $t \in I$.

Decomposing the set $\mathcal{S}$ as $\mathcal{S} = \mathcal{A} \cup \mathcal{I}$, where $\mathcal{A}$ is the active set and $\mathcal{I}$ is the inactive set, then the algorithm of our problem in every level leads to **the primal-dual active set (PDAS) algorithm** of the form (Nedoma [16, 17], Nedoma et al. [19]):

Algorithm ($\mathcal{FL}$):

STEP 1. Initiate the active set $\mathcal{A}_1$ and the inactive set $\mathcal{I}_1$, such that $\mathcal{S} = \mathcal{A}_1 \cup \mathcal{I}_1$, $\mathcal{A}_1 \cap \mathcal{I}_1 = \emptyset$, put the initial value $(\hat{\mathbb{U}}^0, \mathbf{\Lambda}_{hH}^0)$, $c_1 \in (10^3, 10^4)$ and set $k = 1$.

STEP 2. If $(\hat{\mathbb{U}}^{k-1}, \mathbf{\Lambda}_{hH}^{k-1})$ and $\mathcal{A}_k$, $\mathcal{I}_k$ are known, then find the primal-dual pair $(\hat{\mathbb{U}}^k, \mathbf{\Lambda}_{hH}^k)$ such that

$$
\begin{aligned}
&\hat{\mathbb{A}}_h \hat{\mathbb{U}}^k + \hat{\mathbb{B}}_h \mathbf{\Lambda}_{hH}^k = \hat{\mathbb{F}}_h \,, \\
&\hat{\mathbb{U}}_{n,p}^k = d_p^{sm} \quad \text{for all } p \in \mathcal{A}_k \,, \\
&\mathbf{\Lambda}_{hn,p}^k = \mathbf{0} \quad \text{for all } p \in \mathcal{I}_k \,, \\
&\mathbf{\Lambda}_{Ht,p}^k = \mathbf{0} \quad \text{for all } p \in \mathcal{S} .
\end{aligned}
\tag{3.31}
$$

STEP 3. Set $\mathcal{A}_{k+1}$ and $\mathcal{I}_{k+1}$ by

$$
\begin{aligned}
\mathcal{A}_{k+1} &= \left\{ p \in \mathcal{S} : \mathbf{\Lambda}_{hn,p}^k + c_1(\hat{\mathbb{U}}_{n,p}^k - d_p^{sm}) > 0 \right\} \,, \\
\mathcal{I}_{k+1} &:= \left\{ p \in \mathcal{S} : \mathbf{\Lambda}_{hn,p}^k + c_1(\hat{\mathbb{U}}_{n,p}^k - d_p^{sm}) \le 0 \right\} .
\end{aligned}
$$

STEP 4. **If** $\mathcal{A}_{k+1} = \mathcal{A}_k$ **then** STOP **else** $k = k + 1$; **goto** STEP 2;
where the active $\mathcal{A}_k$ and inactive $\mathcal{I}_k$ sets are associated with the transformed basis Φ.

The system (3.31) can be simplified by using the decomposition of the set of vertices $\mathcal{S}$ on the slave side in each step k of the PDAS algorithm into the disjoint active and inactive sets as $\mathcal{S} = \mathcal{A}_k \cup \mathcal{I}_k$. Since $\hat{\mathbb{B}}_h = (\mathbb{O}, \mathbb{O}, \mathbb{D})^T$, we decompose the diagonal matrix $\mathbb{D}$ into

$$
\mathbb{D} = \begin{bmatrix} \mathbb{D}_{\mathcal{I}_k} & \mathbb{O} \\ \mathbb{O} & \mathbb{D}_{\mathcal{A}_k} \end{bmatrix}, \quad \text{since } \mathcal{S} = \mathcal{A}_k \cup \mathcal{I}_k .
$$

According to the definition of $\hat{\mathbb{U}}_{n,p}$, we introduce the matrix $\mathbb{N}_{\mathcal{A}_k} \in \mathbb{R}^{|\mathcal{A}_k| \times N|\mathcal{A}_k|}$, where $|\mathcal{A}_k|$ denotes the number of vertices in $\mathcal{A}_k$, by

$$
\mathbb{N}_{\mathcal{A}_k} = \begin{bmatrix} \ddots & & \mathbb{O} & \\ & w_{pp}\mathbf{n}_{p,1}^s & \cdots & w_{pp}\mathbf{n}_{p,N}^s \\ & \mathbb{O} & & \ddots \end{bmatrix}, \quad p \in \mathcal{A}_k \,,
$$

where w_{pp} denotes an abbreviation for $\mathbb{D}[p,p]_{1,1} = \cdots = \mathbb{D}[p,p]_{N,N} = \int_{\Gamma_{ch}^s} \varphi_p ds$, having the meaning of a weighting factor.

The associated tangential vectors are then given by $\mathbf{t}_p^\xi \perp \mathbf{n}_p^s$ and $\mathbf{t}_p^\eta = \mathbf{t}_p^\xi \times \mathbf{n}_p^s$ with $\|\mathbf{n}_p^s\| = \|\mathbf{t}_p^\xi\| = \|\mathbf{t}_p^\eta\| = 1$. We define the matrix $\mathbb{T}_{\mathcal{A}_k} \in \mathbb{R}^{|\mathcal{A}_k| \times N|\mathcal{A}_k|}$, by

$$
\mathbb{T}_{\mathcal{A}_k} = \begin{bmatrix} \ddots & & \mathbb{O} & \\ & t_{p,1}^{(m)} & t_{p,2}^{(m)} & t_{p,3}^{(m)} \\ & \mathbb{O} & & \ddots \end{bmatrix} \in \mathbb{R}^{|\mathcal{A}_k| \times 3|\mathcal{A}_k|}, \quad m = \xi, \eta, \ p \in \mathcal{A}_k
$$

for $N = 3$ and by

$$
\mathbb{T}_{\mathcal{A}_k} = \begin{bmatrix} \ddots & & \mathbb{O} & \\ & -n_{p,2}^s & & n_{p,1}^s \\ & \mathbb{O} & & \ddots \end{bmatrix} \in \mathbb{R}^{|\mathcal{A}_k| \times 2|\mathcal{A}_k|}, \quad p \in \mathcal{A}_k
$$

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for $N = 2$ as $\mathbf{t}_p^s \perp \mathbf{n}_p^s$.

The algebraic representation of (3.31) after some modification leads to

$$
\begin{bmatrix}
\hat{\mathbb{A}}_{\mathcal{N}\mathcal{N}} & \hat{\mathbb{A}}_{\mathcal{N}\mathcal{M}} & \hat{\mathbb{A}}_{\mathcal{N}\mathcal{I}_k} & \hat{\mathbb{A}}_{\mathcal{N}\mathcal{A}_k} \\
\hat{\mathbb{A}}_{\mathcal{M}\mathcal{N}} & \hat{\mathbb{A}}_{\mathcal{M}\mathcal{M}} & \hat{\mathbb{A}}_{\mathcal{M}\mathcal{I}_k} & \hat{\mathbb{A}}_{\mathcal{M}\mathcal{A}_k} \\
\hat{\mathbb{A}}_{\mathcal{I}_k\mathcal{N}} & \hat{\mathbb{A}}_{\mathcal{I}_k\mathcal{M}} & \hat{\mathbb{A}}_{\mathcal{I}_k\mathcal{I}_k} & \hat{\mathbb{A}}_{\mathcal{I}_k\mathcal{A}_k} \\
0 & 0 & 0 & \mathbb{N}_{\mathcal{A}_k} \\
\mathbb{T}_{\mathcal{A}_k}\hat{\mathbb{A}}_{\mathcal{A}_k\mathcal{N}} & \mathbb{T}_{\mathcal{A}_k}\hat{\mathbb{A}}_{\mathcal{A}_k\mathcal{M}} & \mathbb{T}_{\mathcal{A}_k}\hat{\mathbb{A}}_{\mathcal{A}_k\mathcal{I}_k} & \mathbb{T}_{\mathcal{A}_k}\hat{\mathbb{A}}_{\mathcal{A}_k\mathcal{A}_k}
\end{bmatrix}
\cdot
\begin{bmatrix}
\hat{\mathbb{U}}_{\mathcal{N}}^k \\
\hat{\mathbb{U}}_{\mathcal{M}}^k \\
\hat{\mathbb{U}}_{\mathcal{I}_k}^k \\
\hat{\mathbb{U}}_{\mathcal{A}_k}^k
\end{bmatrix}
=
\begin{bmatrix}
\hat{\mathbb{F}}_{\mathcal{N}} \\
\hat{\mathbb{F}}_{\mathcal{M}} \\
\hat{\mathbb{F}}_{\mathcal{I}_k} \\
d_{\mathcal{A}_k}^{sm} \\
\mathbb{T}_{\mathcal{A}_k}\hat{\mathbb{F}}_{\mathcal{A}_k}
\end{bmatrix}, \qquad (3.32)
$$

with $\mathbb{T}_{\mathcal{A}_k} = (\mathbb{T}_{\mathcal{A}_k}^{\xi}, \mathbb{T}_{\mathcal{A}_k}^{\eta})^T$ for $N = 3$, where k denotes the index of the active set step, $d_{\mathcal{A}_k}^{sm}$ denotes the vector containing the entries d_p^{sm} associated with the active vertex $p \in \mathcal{A}_k$, $\mathbf{\Lambda}_{hH}$ can be locally eliminated. Since $\hat{\mathbb{B}}_h = (0, 0, \mathbb{D})^T$, then $\hat{\mathbb{B}}_h^k \mathbf{\Lambda}_{hH}^k = (0, 0, \mathbb{D}\mathbf{\Lambda}_{hHS}^k)^T$, where

$$
\mathbf{\Lambda}_{hHS}^k = \mathbb{D}^{-1}\left[\hat{\mathbb{F}}_{\mathcal{S}} - \hat{\mathbb{A}}_{\mathcal{S}\mathcal{N}}\hat{\mathbb{U}}_{\mathcal{N}}^k - \hat{\mathbb{A}}_{\mathcal{S}\mathcal{S}}\hat{\mathbb{U}}_{\mathcal{S}}^k - \left(\hat{\mathbb{A}}_{\mathcal{S}\mathcal{M}} + \hat{\mathbb{A}}_{\mathcal{S}\mathcal{S}}\hat{\mathbb{M}}\right)\hat{\mathbb{U}}_{\mathcal{M}}^k\right]. \qquad (3.33)
$$

Moreover, since $\mathbf{\Lambda}_{\mathcal{I}_k}^k = \mathbf{0}$, and since $\mathbb{T}_{\mathcal{A}_k}\mathbb{D}_{\mathcal{A}_k}\mathbf{\Lambda}_{\mathcal{A}_k} = 0$, where $\mathbb{D}_{\mathcal{A}_k}$ is a diagonal matrix for all $p \in \mathcal{A}_k$, therefore, $\mathbf{\Lambda}_{\mathcal{A}_k} = \mathbf{0}$. Thus, we determine $\left(\hat{\mathbb{U}}_{\mathcal{N}}^k, \hat{\mathbb{U}}_{\mathcal{M}}^k, \hat{\mathbb{U}}_{\mathcal{I}_k}^k, \hat{\mathbb{U}}_{\mathcal{A}_k}^k\right)^T$ from (3.32) and $\mathbf{\Lambda}_{hHS}^k$ from (3.33).

A primal-dual active set (PDAS) algorithm – the 3D case with friction of Tresca type

In the 3D model with the Tresca friction if the displacements $\mathbf{u}_h$ are known, the Lagrange multiplier $\mathbf{\Lambda}_{hH} = (\Lambda_{hn}, \mathbf{\Lambda}_{Ht})$ can be computed directly from (3.22), that is,

$$
\mathbf{\Lambda}_{hH} = \mathbb{D}^{-1}(\mathbb{F}_h - \mathbb{A}_h\mathbf{U})_S, \qquad (3.34)
$$

where the subscript S denotes that we use only the entries of the vector corresponding to the nodes $p \in S$. For the normal and tangential components of the multiplier $\mathbf{\Lambda}_{hH}$ and of the relative decomposition $\mathbf{u}_h$ for a node point $p \in S$, we have

$$
u_{hn,p} = \mathbf{u}_p^T\mathbf{n}_p \in \mathbb{R}, \quad \mathbf{u}_{Ht,p} = (\mathbf{u}_p^T\mathbf{t}_{1p}, \quad \mathbf{u}_p^T\mathbf{t}_{2p})^T \in \mathbb{R}^2,
$$
$$
\mathbf{\Lambda}_{hn,p}^s = (\mathbf{n}_p^s)^T\mathbb{D}[p,p]\mathbf{\Lambda}_{hH}(p) \in \mathbb{R}, \quad \mathbf{\Lambda}_{hH}(p) \in \mathbb{R}^3,
$$
$$
\mathbf{\Lambda}_{Ht,p}^s = \mathbf{\Lambda}_{hH}(p) - (\mathbf{\Lambda}_{hH}(p) \cdot \mathbf{n}_p^s)\mathbf{n}_p^s = \left(\mathbf{\Lambda}_{hH}(p) \cdot \mathbf{t}_p^s\right)\mathbf{t}_p^s =
$$
$$
= \left(\mathbf{\Lambda}_{hH}^T(p)\mathbb{D}[p,p]\mathbf{t}_{1,p}^s, \quad \mathbf{\Lambda}_{hH}^T(p)\mathbb{D}[p,p]\mathbf{t}_{2,p}^s\right)^T \in \mathbb{R}^2.
$$

Then the discrete conditions for normal contact are given by (3.29b,c,d) and the discrete Coulomb friction conditions are given by

$$
\begin{aligned}
\left|\mathbf{\Lambda}_{Ht,p}^s(p)\right| &\leq \mathcal{F}_c^{sm}\left|\mathbf{\Lambda}_{hn,p}^s\right| \\
\left|\mathbf{\Lambda}_{Ht,p}^s(p)\right| &< \mathcal{F}_c^{sm}\left|\mathbf{\Lambda}_{hn,p}^s\right| \Rightarrow \mathbf{u}_{ht,p} = \mathbf{0} \\
\left|\mathbf{\Lambda}_{Ht,p}^s(p)\right| &= \mathcal{F}_c^{sm}\left|\mathbf{\Lambda}_{hn,p}^s\right| \Rightarrow \exists\vartheta \geq 0 \quad \text{such that } \mathbf{\Lambda}_{Ht,p}^s = -\vartheta\mathbf{u}_{ht,p}
\end{aligned} \qquad \text{for all } p \in S, \qquad (3.35)
$$

where for the Tresca friction model $\mathcal{F}_c^{sm}|\mathbf{\Lambda}_{hn,p}^s| \equiv g_{ch,p}^s \in H^{-\frac{1}{2}}(\Gamma_c^s)$, $g_{ch,p}^s \geq 0$, $g_{ch,p}^s = \int_{\Gamma_{ch}^s} g_{ch}^s\varphi_p ds$. For $g_{ch,p}^s = 0$ the condition (3.35) leads to homogeneous Neumann boundary conditions in tangential direction. Let $g_{ch,p}^s > 0$, then the condition (3.35) is equivalent to $C_t\left(\hat{\mathbb{U}}_{t,p}, \mathbf{\Lambda}_{Ht,p}^s\right) = 0$ for all $p \in S$, where

$$
\begin{aligned}
C_t\left(\hat{\mathbb{U}}_{t,p}, \mathbf{\Lambda}_{Ht,p}^s\right) &= \\
&= \max\left(g_{ch,p}^s, |\mathbf{\Lambda}_{Ht,p}^s + c_2\hat{\mathbb{U}}_{t,p}|\right)\mathbf{\Lambda}_{Ht,p}^s - g_{ch,p}^s\left(\mathbf{\Lambda}_{Ht,p}^s + c_2\hat{\mathbb{U}}_{t,p}\right), \quad c_2 > 0, \qquad (3.36)
\end{aligned}
$$

which will be starting point of the algorithm, that will be based on a Newton-type algorithm for the solution $C_t(\hat{\mathbb{U}}_{t,p}, \mathbf{\Lambda}_{Ht,p}^s) = 0$. As it was shown in Hintermüller et al. [10] the max-function and the Euclidean norm are semi-smooth, and therefore, a semi-smooth Newton method can be used. If the

Euclidean norm $\left|\mathbf{\Lambda}_{Ht,p}^s + c_2 \hat{\mathbb{U}}_{t,p}\right| = 0$, then $\max\left(g_{ch,p}^s, |\mathbf{\Lambda}_{Ht,p}^s + c_2 \hat{\mathbb{U}}_{t,p}|\right) = g_{ch,p}^s$ and the Euclidean norm vanishes. Hence, the derivative of the Euclidean norm only occurs for points that are differentiable in the classical sense. The analysis of the generalized derivative of $C_t(\hat{\mathbb{U}}_{t,p}, \mathbf{\Lambda}_{Ht,p}^s)$ (see Hüeber et al. [12]) shows that the nodes of $\mathcal{S}$ are separated into the active set $\mathcal{A}_{Ht,k}$ and the inactive set $\mathcal{I}_{Ht,k}$, where

$$\mathcal{A}_{Ht,k} := \left\{p \in S; |\mathbf{\Lambda}_{Ht,p}^{s,k-1} + c_2 \hat{\mathbb{U}}_{t,p}^{k-1}| - g_{ch,p}^s > 0\right\}, \tag{3.37}$$

$$\mathcal{I}_{Ht,k} := \left\{p \in S; |\mathbf{\Lambda}_{Ht,p}^{s,k-1} + c_2 \hat{\mathbb{U}}_{t,p}^{k-1}| - g_{ch,p}^s \leq 0\right\}. \tag{3.38}$$

This separation of nodes of S into the active $\mathcal{A}_{Ht,k}$ and inactive $\mathcal{I}_{Ht,k}$ sets is provided by the characteristic function in the generalized derivative of $C_t(\cdot, \cdot)$. The case if $g_{ch,p} = 0$ is in details analyzed in Hüeber et al. [12].

Summing all results for the frictionless contact problem and for the Tresca friction case, then Problem $(\mathcal{P})$ can be rewritten as

$$\hat{\mathbb{A}}_h \hat{\mathbb{U}} + \hat{\mathbb{B}}_h \mathbf{\Lambda}_{hH} = \hat{\mathbb{F}}_h,$$

$$C_n\left(\hat{\mathbb{U}}_{n,p}, \mathbf{\Lambda}_{hn,p}\right) = 0,$$

$$C_t(\hat{\mathbb{U}}_{t,p} \mathbf{\Lambda}_{Ht,p}) = 0 \tag{3.39}$$

for all vertices $p \in \mathcal{S}$ and $t \in I$.

The PDAS algorithm for the contact problem with friction in the Tresca sense is as follows:

Algorithm $(\mathcal{T})$:
STEP 1: Initiate the active sets $\mathcal{A}_{hn,1}$, $\mathcal{A}_{Ht,1}$ and the inactive sets $\mathcal{I}_{hn,1}$, $\mathcal{I}_{Ht,1}$ such that $\mathcal{S}_n = \mathcal{A}_{hn1} \cup \mathcal{I}_{hn1}$, $\mathcal{S}_t = \mathcal{A}_{Ht1} \cup \mathcal{I}_{Ht1}$, $\mathcal{A}_{hn1} \cap \mathcal{I}_{hn1} = \emptyset$, $\mathcal{A}_{Ht1} \cap \mathcal{I}_{Ht1} = \emptyset$ and put the initial value $(\hat{\mathbb{U}}^0, \mathbf{\Lambda}_{hH}^0)$, $c_1, c_2 \in (10^3, 10^4)$ and set $k = 1$, $c_1 > 0$, $c_2 > 0$, $m \in \mathbb{N}$.
STEP 2: Define the active and inactive sets

$$\mathcal{A}_{hn,k} := \left\{p \in S; \mathbf{\Lambda}_{hn,p}^{s,k-1} + c_1\left(\hat{\mathbb{U}}_{n,p}^{k-1,m} - d_p^{sm}\right) > 0\right\},$$

$$\mathcal{I}_{hn,k} := \left\{p \in S; \mathbf{\Lambda}_{hn,p}^{s,k-1} + c_1\left(\hat{\mathbb{U}}_{n,p}^{k-1,m} - d_p^{sm}\right) \leq 0\right\},$$

$$\mathcal{A}_{Ht,k} := \left\{p \in S; \left|\mathbf{\Lambda}_{Ht,p}^{s,k-1} + c_2 \hat{\mathbb{U}}_{t,p}^{k-1,m}\right| - g_{ch,p}^s > 0\right\},$$

$$\mathcal{I}_{Ht,k} := \left\{p \in S; \left|\mathbf{\Lambda}_{Ht,p}^{s,k-1} + c_2 \hat{\mathbb{U}}_{t,p}^{k-1,m}\right| - g_{ch,p}^s \geq 0\right\},$$

STEP 3: For $i = 1, \ldots, m$, compute the generalized derivative in the sense of a semi-smooth Newton method, i.e.,

$$\hat{\mathbb{U}}_{hH}^{k,i} = G\left(\hat{\mathbb{U}}_{hH}^{k,i-1}, \mathcal{A}_{hn,k}, \mathcal{I}_{hn,k}, \mathcal{A}_{Ht,k}, \mathcal{I}_{Ht,k}, \hat{\mathbb{U}}_{hH}^{k-1,m}, \mathbf{\Lambda}_{hH}^{k-1}\right),$$

where by the symbol G we denote the generalized derivative in the sense of a semi-smooth Newton method.
STEP 4: If $\left|\hat{\mathbb{U}}_{hH}^{k,m} - \hat{\mathbb{U}}_{hH}^{k,0}\right| / \left|\hat{\mathbb{U}}_{hH}^{k,m}\right| < \varepsilon$ **then** STOP.
STEP 5: Compute the Lagrange multiplier due to (3.34), that is,

$$\mathbf{\Lambda}_{hH,k} = \hat{\mathbb{D}}^{-1}\left(\hat{\mathbb{F}}_{hS} - \hat{\mathbb{A}}_{hS} \hat{\mathbb{U}}_{hH}^{k,m}\right).$$

STEP 6: Set $\hat{\mathbb{U}}_{hH}^{k+1,0} = \hat{\mathbb{U}}_{hH}^{k,m}$, $k = k + 1$ and **goto STEP 2.**

Similarly as in the frictionless case the system (3.39) can be rewritten, if we decompose the set of vertices S on the slave side in each step k of the PDAS algorithm into the disjoint active and inactive sets (for more details see Hüeber et al. [12]). Since due to the dual Lagrange multiplier space, $\mathbf{\Lambda}_{hH}$ can be eliminated locally.

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A primal-dual active set (PDAS) algorithm – the 3D case with Coulomb friction

The algorithms can be based on the fixpoint algorithm or on the full Newton method (Hüeber et al. [12]).

The Fixpoint Algorithm ($\mathcal{FP}$) is the extension of the above PDAS algorithm for Tresca friction, in which the friction bound $g_{ch,p}^s = \mathcal{F}_c^{sm}|\mathbf{\Lambda}_{n,p}^s|$ is iteratively modified using the normal component of the Lagrange multiplier. Thus, we have the following algorithm, that the friction bound and the active and inactive sets are updated in every step.

Algorithm ($\mathcal{FP}$):

STEP 1: Initiate the initial value $\left(\hat{\mathbb{U}}^{0,0}, \mathbf{\Lambda}_{hH}^0\right)$, $c_1, c_2 \in (10^3, 10^4)$ and set $k = 1, m \in \mathbb{N}$.

STEP 2: Set $k_c = k - 1$ and update the friction bound by $g_{ch,p}^{s,k_c} = \mathcal{F}_c^{sm} \max\{0, \mathbf{\Lambda}_{n,p}^{s,k_c}\}, p \in S$.

STEP 3: Define the active sets $\mathcal{A}_{hn,k}$, $\mathcal{A}_{Ht,k}$ and the inactive sets $\mathcal{I}_{hn,k}$, $\mathcal{I}_{Ht,k}$ by

$$\mathcal{A}_{hn,k} := \left\{ p \in S; \mathbf{\Lambda}_{hn,p}^{s,k-1} + c_1\left(\hat{\mathbb{U}}_{n,p}^{k-1,m} - d_p^{sm}\right) > 0 \right\},$$

$$\mathcal{I}_{hn,k} := \left\{ p \in S; \mathbf{\Lambda}_{hn,p}^{s,k-1} + c_1\left(\hat{\mathbb{U}}_{n,p}^{k-1,m} - d_p^{sm}\right) \leq 0 \right\},$$

$$\mathcal{A}_{Ht,k} := \left\{ p \in S; \left|\mathbf{\Lambda}_{Ht,p}^{s,k-1} + c_2\hat{\mathbb{U}}_{t,p}^{k-1,m}\right| - g_{ch,p}^{s,k_c} > 0 \right\},$$

$$\mathcal{I}_{Ht,k} := \left\{ p \in S; \left|\mathbf{\Lambda}_{Ht,p}^{s,k-1} + c_2\hat{\mathbb{U}}_{t,p}^{k-1,m}\right| - g_{ch,p}^{s,k_c} \leq 0 \right\}.$$

STEP 4: For $i = 1, \ldots, m$, compute the generalized derivative in the sense of a semi-smooth Newton method

$$\hat{\mathbb{U}}_{hH}^{k,i} = G\left(\hat{\mathbb{U}}_{hH}^{k,i-1}, \mathcal{A}_{hn,k}, \mathcal{I}_{hn,k}, \mathcal{A}_{Ht,k}, \mathcal{I}_{Ht,k}, \hat{\mathbb{U}}_{hH}^{k-1,m}, \mathbf{\Lambda}_{hH}^{k-1}\right),$$

where the symbol G has the same meaning as above.

STEP 5: Compute the Lagrange multiplier due to (3.34) as

$$\mathbf{\Lambda}_{hH}^k = \hat{\mathbb{D}}^{-1}\left(\hat{\mathbf{F}}_{hS} - \hat{\mathbb{A}}_{hS}\hat{\mathbb{U}}_{hH}^{k,m}\right).$$

STEP 6: If $\left\|\hat{\mathbb{U}}_{hH}^{k,m} - \hat{\mathbb{U}}_{hH}^{k_c,m}\right\| / \left\|\hat{\mathbb{U}}_{hH}^{k,m}\right\| < \varepsilon$ **then** STOP.

STEP 7: Set $\hat{\mathbb{U}}_{hH}^{k+1,0} = \hat{\mathbb{U}}_{hH}^{k,m}$ and $k = k + 1$ and **goto** STEP 2.

If $m = \infty$, we obtain the exact version of the algorithm, in the previous case we speak about inexact algorithm. The algorithm is convergent for small coefficient of friction (see Eck et al. [6]).

The Full Newton method is very advantageous method due to its fast convergence, the derivation of which see, e.g., in Hüeber et al. [12]. This fast convergence is due to the fact that the friction bound is updated in the Newton iteration.

4 Numerical algorithm for opening the crack as the first stage of bone fractures

With a persistent growth of the neoplasms, the possibility of fracture rises can be expected. Firstly, in locations with highest stresses the crack initiations can be occurred (Fig. 1a,b,c), and with continuous loading the cracks start to opening and propagate, up-to the moment when the bone fractures.

In the real situations it is very difficult to determine the location of a crack, its initiation, its further opening and propagation, and in which direction. In the literature many crack initiation, crack propagation and kinking criteria were introduced. These criteria depend on the material properties and also depend on the length of possible fractures. Some of them are based on critical values of stress and strain or on the use of a damage law and a critical damage parameter to determine the location of the crack initiation. Since in our case the length of cracks are relatively short, the crack initiation criterion can be based on a critical stress-value for a given material.
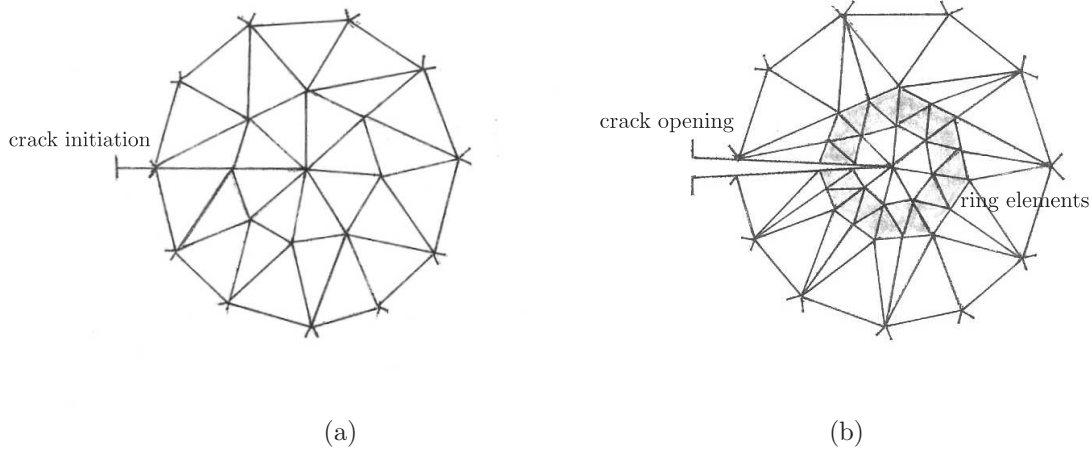
Figure 4.1: Location of the crack and the mesh around the crack tip: a) crack initiation; b) crack opening.

To determine the areas of possible fracture zones, we firstly determine the areas with maximal principle stresses, and therefore, the places where cracks are initiated. Thus we need to check, at each time step, when the crack is start to propagate and in which direction. In the first case the crack propagation criteria will be used, while in the second one the crack kinking criteria will be used. When a crack propagate through a mesh, the accuracy at the crack tip will be of great importance for determination of a possible fracture. Many numerical tools were developed to improve the accuracy at the crack tip. Since the stress field is singular in the vicinity of the crack tip, a concentric mesh around the crack tip can be coupled with singular elements, which can be used to model the stress field singularity (Whiteman and Akin [23], Nedoma [15, 18]). An other approach is based on the strain energy release rate, where a construction of ring elements in the neighborhood of the crack tip (Fig. 2b), is also used. Finally mesh refinement around the crack tip is necessary to keep a better precision in the vicinity of the crack. Since the crack propagates, the crack tip moves along and the areas in the vicinity of crack are changed; thus, a new mesh is created and refined only in areas at the front of the propagated crack. For more details see Whiteman and Akin [23], Gdontos [8], Nedoma [18].

A location of a crack and its initiation and further opening are given in Fig. 2a,b. Many numerical algorithms have been applied to improve the accuracy at the crack tip and to determine a crack propagation direction. With a great advantage the automatic remeshing procedure at the crack tip, with a thickening of the mesh at the crack tip and using singular elements to model the singular stress-strain fields, can be used (Figs 3a,b,c). To determine a crack propagation direction we compute eigenvalues and eigenvectors of the stress tensor in all determined mesh points nearest to the crack tip, i.e., we determine the principal stresses and their directions. The final direction of the crack propagation will be obtained as a weighted average of each direction with respect to the distance between the mesh point and the crack tip. Moreover, stress intensity factors, that is, strength singularity at the crack tip, can be used for determination of a crack propagation. E.g., for Mode I loading, these stress intensity factors are compared with a critical value K_{Ic} of the bone material.

From the fracture mechanics it is known that high values of strain energy W_e and high values of stresses indicate the places of possible initiation of fractures. Therefore, they can be used to prevent crack growth, and that the crack grows and propagates in the direction that minimizes the strain energy W_e. Let us introduce the strain energy density $w_e = \frac{dW_e}{dV}$, where dV is an element of volume. Since the strain energy W_e is proportional to the square of stress, and since the stress at the crack tip has singularity $\frac{1}{\sqrt{r}}$, then the strain energy density has also singularity $\sim \frac{1}{\sqrt{r}}$, where r is the distance of mesh points to the crack tip. Then at each time step in every mesh point we compute W_e and thus,
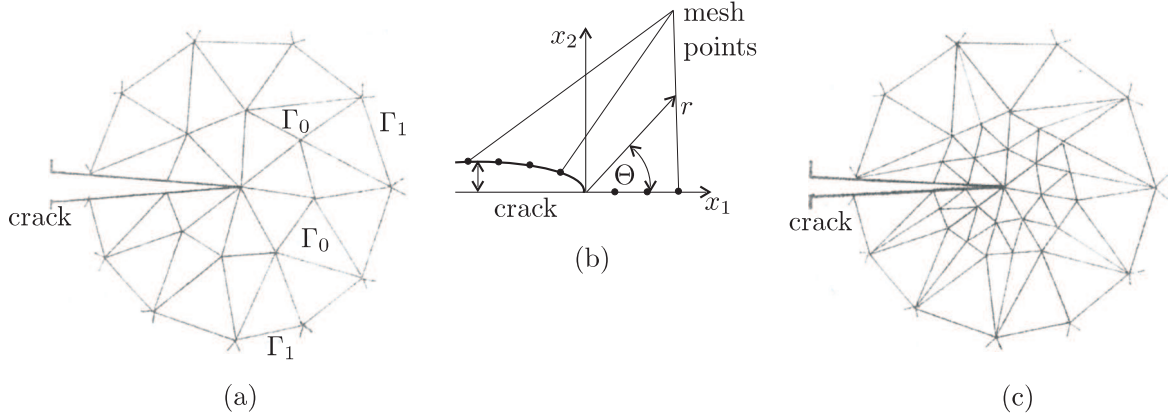
Figure 4.2: Construction of the mesh at the crack tip: (a) the mesh near the crack tip; (b) the mesh in the local coordinate system at the crack tip; (c) the design of the mesh for the h- and h-p-versions of the finite element method.

using the strain energy density w_e, the strain energy density factor $S = rw_e$, where r is the distance of the mesh point and the crack tip. The parameter S will be computing by using rings of elements around the crack tip (Fig. 2b). The kinking angle ϑ_0 can be found as the local minimum of $S(\vartheta)$, that is,

$$\left(\frac{\partial S}{\partial \vartheta}\right)_{\vartheta=\vartheta_0} = 0; \quad \left(\frac{\partial^2 S}{\partial \vartheta^2}\right)_{\vartheta=\vartheta_0} \geq 0 \,.$$

The parameter S, e.g. in isotropic bone materials, can be found analytically as follows:

$$S = rw_e = r\left(\frac{1+\nu}{2E}\right)\left[\tau_{11}^2 + \tau_{22}^2 + \tau_{33}^2 - \frac{\nu}{1+\nu}(\tau_{11} + \tau_{22} + \tau_{33})^2 + 2\tau_{12}^2\right] \,,$$

where E is the Young modulus and ν is the Poisson's ratio.

Another crack growth criteria are (i) the so-called real crack extension and the virtual crack extension criteria, which are based on the definition of the strain energy release rate G, $G = -\frac{\partial \Pi}{\partial A}$, where Π is the total potential energy and A represents the crack area, and/or (ii) the path independent J integral method (Gdoutos [8], Nedoma [18]).

With opening the crack, at the crack faces, we denote them by ${}^i\Gamma_c^s$, $i = 1, 2$, the contact conditions of Signorini type with or without Coulombian friction will be prescribed. The numerical realization of such problem corresponds to formulation of a generalized crack problem, formulated by using the nonpenetration (Signorini type) conditions. Such problem leads to solve the contact problems and the PDAS method both discussed in the previous section. In general the dynamic contact problems lead to solve hyperbolic variational inequalities by finite element methods and the PDAS algorithms, discussed in the previous section. It is evident that the evolutionary mesh will be created and refined only at the tip of the cracks and in the areas where it is needed in order to optimise calculations of the mesh and it is unrefined in the rest of the initial mesh.

Acknowledgements

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