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DYNAMIC CONTACT PROBLEMS IN BONE NEOPLASM ANALYSES AND THE PRIMAL-DUAL ACTIVE SET (PDAS) METHOD

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Dedicated to Prof. Ivo Babuška, Dr. Milan Práger and Dr. Emil Vitásek on the occasion of their life jubilees.

Abstract: In the contribution growths of the neoplasms (benign and malignant tumors and cysts), located in a system of loaded bones, will be simulated. The main goal of the contribution is to present the useful methods and efficient algorithms for their solutions. Because the geometry of the system of loaded and possible fractured bones with enlarged neoplasms changes in time, the corresponding mathematical models of tumor's and cyst's evolutions lead to the coupled free boundary problems and the dynamic contact problems with or without friction. The discussed parts of these models will be based on the theory of dynamic contact problems without or with Tresca or Coulomb frictions in the visco-elastic rheology. The numerical solution of the problem with Coulomb friction is based on the semi-implicit scheme in time and the finite element method in space, where the Coulomb law of friction at every time level will be approximated by its value from the previous time level. The algorithm for the corresponding model of friction will be based on the discrete mortar formulation of the saddle point problem and the primal-dual active set algorithm. The algorithm for the Coulomb friction model will be based on the fixpoint algorithm, that will be an extension of the PDAS algorithm for the Tresca friction. In this algorithm the friction bound is iteratively modified using the normal component of the Lagrange multiplier. Thus the friction bound and the active and inactive sets are updated in every step of the iterative algorithm and at every time step corresponding to the semi-implicit scheme.

Keywords: dynamic contact problems, mathematical models of neoplasms - tumors and cysts, Coulomb and Tresca frictions, variational formulation, semi-implicit scheme, FEM, mortar aproximation, PDAS algorithm.

MSC: 65K10, 65C20, 65N15, 65N30, 74M15

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. During the last four decades, various neoplasms (cysts, benign and malign tumors) models have been developed, analyzed and discussed.

By **neoplasm** 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**. In some cases the cancer cells invade into the blood or the lymphatic vessels and then are transported into another locations, where they create secondary tumors. This process is known as the **metastasis process**. Malign tumors rise relatively very quickly approximately 1mm/day. In all types of neoplasms a solid tumors can be detected when it reaches a size of several millimeters. Bone tumors are of primary types, originating within the bone tissues, or of secondary types, that result from the spread cancer cells from the primary tumors located in other tissues in the human body and we speak about **metastasis**. 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. 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. By mitosis it is meant the process of cell division which results in the production of two daughter cells from an initial parent cell and that are identical with the parent cell.

Another type of neoplasms are **cysts** that are filled by fluid and that are formed either in bones or in soft tissues, respectively. **Cysts** are pathological cavity lined by the own epithelium and in the cyst lumen filled by fluid or semi-fluid contents, that 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-bone that are lined by an odontogenic epithelium (that is, avascular epithelial tissues). Odontogenic cysts are relatively slow growing and represent in early states of evolution no great problem and treat to human life. The main types are the radicular cysts, that grow relatively slowly and the keratocysts, that grow more rapidly.

2. Formulation of the problem

2.1. Formulation of the contact problem

Let the system of bones with neoplasms occupy a region $\Omega \in \mathbb{R}^N$, $N = 2, 3$, (Fig.1a,b,c), the geometry of which can be determined from the CT or MRI scans, respectively, and approximated by the visco-elasticity with short memory (Kelvin-Voigt type rheology).

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 (bones) 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 $\Gamma_c = \cup_{s,m}\Gamma_c^{sm}$, $\Gamma_c^{sm} = \partial\Omega^s \cap \partial\Omega^m$, $s \neq m$, $s, m \in \{1, \ldots, r\}$, 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 $\Omega(t) = \Omega \times I$ 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, spine, temporomandibular joints, etc.) as well as contact boundaries between the opposite boundaries in the fractures of bones and/or of vertebra. In the case of e.g. vertebra fracture, the domain denoted as Ω^s will be divided into two parts denoted by Ω_1^s and Ω_2^s (see Figs 1a-c).

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 $\mathbf{u} = (u_i)$, $\boldsymbol{\tau} = (\tau_i)$, $\tau_i = \tau_{ij} n_j$, $i, j = 1, \ldots, N$. 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 assume that the mapping $\mathcal{R}$ is

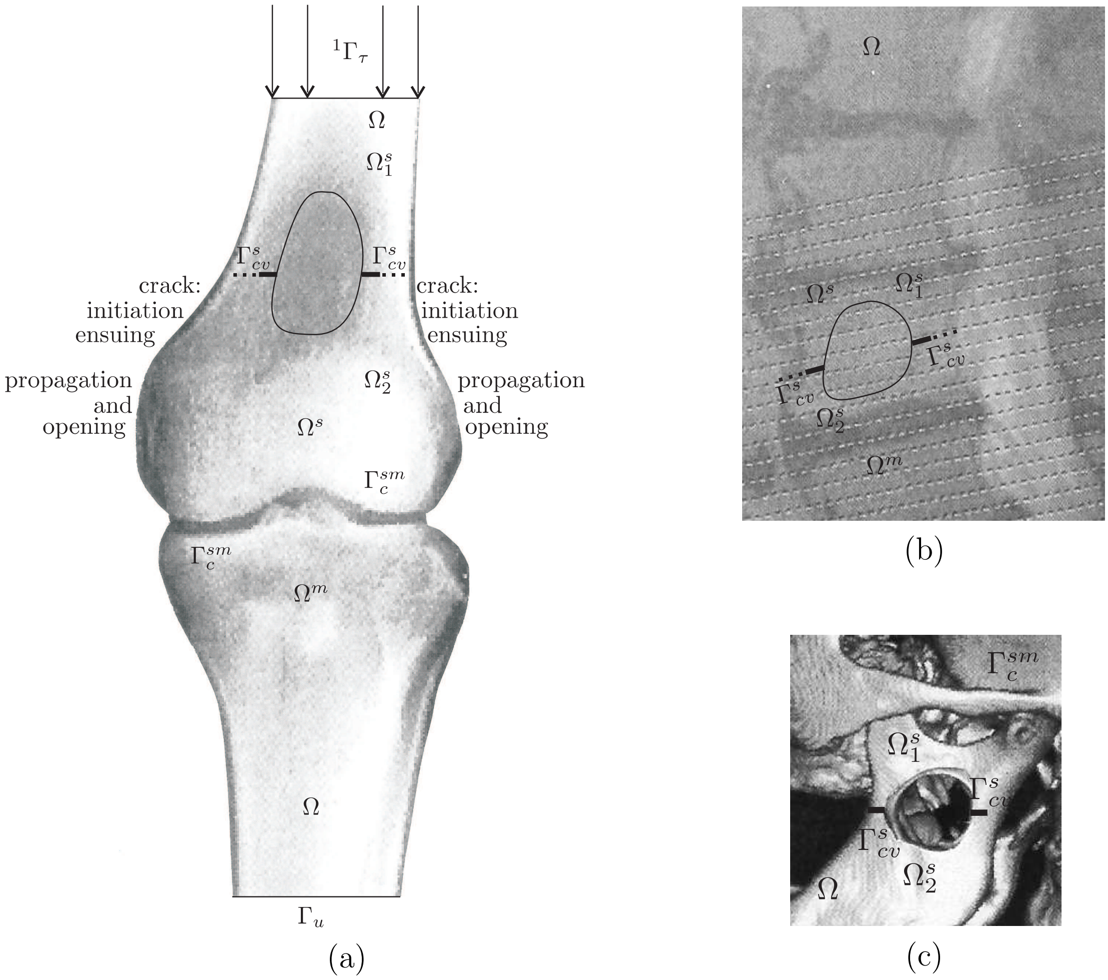

Figure 1: Mathematical models of the long bone and spine with tumors and the jaw-bone with cyst: crack initiation and ensuing crack propagation and crack opening are modelled on the basis of dynamic PDAS method for a crack problem with non-penetration: (a) the detail of knee joint with the tumor; (b) the detail of spine with the tumor; (c) the detail of jaw-bone with the cyst.

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, $[\mathbf{u}_t]^{sm} = (\mathbf{u}^s(\mathbf{x},t) - \mathbf{u}^m(\mathcal{R}(\mathbf{x},t))) - [\mathbf{u}]^{sm} \cdot \mathbf{n}^s$ is the jump in the tangential direction 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, $(\mathbf{t}_i^s)^T \boldsymbol{\tau}^s(\mathbf{x},t)\mathbf{t}_i^s = (\mathbf{t}_i^s)^T \boldsymbol{\tau}^m(\mathcal{R}(\mathbf{x},t))\mathbf{t}_i^s$, $i = N-1$, is satisfied.

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

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

where

$$\begin{aligned}\tau_{ij}^{\iota} =& \tau_{ij}^{\iota}(\mathbf{u}^{\iota}, \mathbf{u}'^{\iota}) = c_{ijkl}^{(0)\iota}(\mathbf{x}) e_{kl}(\mathbf{u}^{\iota}) + c_{ijkl}^{(1)\iota}(\mathbf{x}) e_{kl}(\mathbf{u}'^{\iota}) = \\ =& {}^{e}\tau_{ij}^{\iota}(\mathbf{u}^{\iota}) + {}^{\nu}\tau_{ij}^{\iota}(\mathbf{u}'^{\iota}), \quad i,j,k,l = 1,\ldots,N\,,\ \iota = 1,\ldots,r,\end{aligned} \tag{2}$$

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,

$$\begin{aligned}& c_{ijkl}^{(n)\iota} \in L^{\infty}(\Omega^{\iota}), \quad n = 0,1,\ \iota = 1,\ldots,r, \quad c_{ijkl}^{(n)\iota} = c_{jikl}^{(n)\iota} = c_{klij}^{(n)\iota} = c_{ijlk}^{(n)\iota}\,, \\ & c_{ijkl}^{(n)\iota} e_{ij} e_{kl} \geq c_{0}^{(n)\iota} e_{ij} e_{ij} \quad \forall e_{ij}, \quad e_{ij} = e_{ji} \quad \text{and a.e.} \quad \mathbf{x} \in \Omega^{\iota},\ c_0^{(n)\iota} > 0,\ \iota = 1,\ldots,r, \\ & c_{ijkl}^{(n)\iota} = \lambda^{(n)\iota}\delta_{ij}\delta_{ij} + \mu^{(n)\iota}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right), n = 0,1, \text{for the isotropic bone materials,}\end{aligned} \tag{3}$$

where a repeated index implies summation from 1 to N.

On the contact boundaries between neighbouring bones and the neighbouring faces in the case of bone fractures the following non-penetration conditions and the Coulomb friction conditions

$$\left.\begin{aligned}& [u_n]^{sm} \leq d^{sm},\ \tau_n^s = \tau_n^m \equiv \tau_n^{sm} \leq 0, \\ & \left([u_n]^{sm} - d^{sm}\right)\tau_n^{sm} = 0, \\ & [\mathbf{u}_t']^{sm} = \mathbf{0} \ \Rightarrow\ |\boldsymbol{\tau}_t^{sm}| \leq \mathcal{F}_c^{sm}\,|\tau_n^{sm}(\mathbf{u})|\,, \\ & [\mathbf{u}_t']^{sm} \neq \mathbf{0} \ \Rightarrow\ \boldsymbol{\tau}_t^{sm} = -\mathcal{F}_c^{sm}\,|\tau_n^{sm}(\mathbf{u})|\,\tfrac{[\mathbf{u}_t']^{sm}}{|[\mathbf{u}_t']^{sm}|},\end{aligned}\right\} (\mathbf{x},t) \in \cup_{e,m}\Gamma_c^{sm} \times I, \tag{4}$$

are given and on the boundary $\partial\Omega(t)$ the following conditions

$$\tau_{ij}n_j = P_i, \quad i,j = 1,\ldots,N, \quad (\mathbf{x},t) \in \Gamma_\tau(t) = \cup_{\iota=1}^{r}(\Gamma_\tau \cap \partial\Omega^{\iota}) \times I\,, \tag{5}$$

$$u_i = u_{2i}, \quad i = 1,\ldots,N, \quad (\mathbf{x},t) \in \Gamma_u(t) = \cup_{\iota=1}^{r}(\Gamma_u \cap \partial\Omega^{\iota}) \times I\,, \tag{6}$$

are prescribed and the initial conditions

$$\mathbf{u}^{\iota}(\mathbf{x},0) = \mathbf{u}_0^{\iota}(\mathbf{x}), \quad \mathbf{u}'^{\iota}(\mathbf{x},0) = \mathbf{u}_1^{\iota}(\mathbf{x}), \quad \mathbf{x} \in \Omega^{\iota}\,, \tag{7}$$

are given, 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 [4, 18, 20] and $\mathbf{u}_0$, $\mathbf{u}_1$ are the given functions, $\mathbf{u}_2 \neq 0$ 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 $d^{sm} \geq 0$ are the normalized gaps between the contact boundaries of Ω^s and Ω^m (e.g. of the joints or faces in the case of fractures) and between the two faces of the crack (i.e., Γ_c^s and Γ_c^m).

2.2. Formulation of coupled free boundary problems

Furthermore, we need to determine the evolution of neoplasms (tumors and cysts) in time, and then to determine the areas that are occupied by these tumors and cysts inside the system of bones, that create the investigated part of the human skeleton, and moreover, to determine their material compositions, all during the studied time period.

(A) The tumor growth case

The tumor's study and their growths are studied e.g. in [2, 3, 5] and in many others. Such models consist of a system of coupled partial differential equations and a mass conservation law. The problems then lead to solve the free boundary problems.

In the case of the tumor growth, we limit ourselves to avascular and vascular cases only. Let $u_c(\mathbf{x}, t)$ denote the concentration of cells, and let $u_p(\mathbf{x}, t)$, $u_q(\mathbf{x}, t)$ and $u_D(\mathbf{x}, t)$ denote the cell densities 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 [2, 3, 5]).

To determine the equation for the concentration $u_c(\mathbf{x}, t)$, we must consider two cases — the avascular stage and the vascular stage. Then, for an avascular evolution of tumors we find

$$\varepsilon_0 \frac{\partial u_c}{\partial t} = D_c \nabla^2 u_c - \lambda u_c, \quad \varepsilon_0 = \frac{T_{\text{diffusion}}}{T_{\text{growth}}}\,, \tag{8}$$

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. (8) must be replaced by

$$\varepsilon_0 \frac{\partial u_c}{\partial t} = D_c \nabla^2 u_c + \Gamma(u_{cB} - u_c) - \lambda u_c\,, \tag{9}$$

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. Tumor angiogenesis refers to the ability of a tumor to stimulate new blood vessel formation.

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

$$u_c - \frac{\Gamma u_{cB}}{\Gamma + \lambda} \to u_c, \quad \Gamma + \lambda \to \lambda\,, \tag{10}$$

then Eq. (9) is transformed to Eq. (8), that is, u_c in the avascular and vascular tumors are described by the same equation (8).

We assume 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 $u_c(\mathbf{x},t)$. 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 $K_P(u_c)$ that 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 $K_B(u_c)$ that 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 $\mathbf{v}$. Denoting by $\omega_n(t)$ a region occupied by a tumor at time t and $\partial\omega_n(t)$ 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:

$$\frac{\partial u_p}{\partial t} + \operatorname{div}(u_p\mathbf{v}) = [K_B(u_c) - K_Q(u_c) - K_A(u_c)]\, u_p + K_P(u_c)u_q\,, \tag{11}$$

$$\frac{\partial u_q}{\partial t} + \operatorname{div}(u_q\mathbf{v}) = K_Q(u_c)u_p - [K_P(u_c) + K_D(u_c)]\, u_q\,, \tag{12}$$

$$\frac{\partial u_D}{\partial t} + \operatorname{div}(u_D\mathbf{v}) = K_A(u_c)u_p + K_D(u_c)u_q - K_R u_D\,. \tag{13}$$

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

$$\mathbf{v} = -\beta\nabla\sigma, \quad \text{where} \quad \beta > 0\,. \tag{14}$$

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 $N = 1$.

Adding Eqs (11), (8) with (10), we find

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

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

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

$$\varepsilon_0\frac{\partial u_c}{\partial t} = D_c\nabla^2 u_c - \lambda u_c \qquad \text{in} \quad \omega_n(t),\ t > 0\,, \tag{15}$$

$$\frac{\partial u_p}{\partial t} - \nabla\sigma\cdot\nabla u_p = f(u_c,u_p,u_q) \qquad \text{in} \quad \omega_n(t),\ t > 0\,, \tag{16}$$

$$\frac{\partial u_q}{\partial t} - \nabla\sigma\cdot\nabla u_q = g(u_c,u_p,u_q) \qquad \text{in} \quad \omega_n(t),\ t > 0, \tag{17}$$

$$\Delta\sigma = -h(u_c,u_p,u_q) \qquad \text{in} \quad \omega_n(t),\ t > 0\,, \tag{18}$$

where

$$
\begin{aligned}
f(u_c, u_p, u_q) &= [K_B(u_c) - K_Q(u_c) - K_A(u_c)]\, u_p + K_P(u_c)u_q - h(u_c, u_p, u_q)u_p, \\
g(u_c, u_p, u_q) &= K_Q(u_c)u_p - [K_p(u_c) + K_D(u_c)]\, u_q - h(u_c, u_p, u_q)u_q\,, \\
h(u_c, u_p, u_q) &= [K_B(u_c) + K_R]\, u_p + K_R u_q - K_R\,,
\end{aligned}
$$

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

$$
u_c = u_{c1} \qquad \text{on} \quad \partial\omega_n(t),\ t > 0, \tag{19}
$$

$$
\sigma = \gamma\kappa,\ \frac{\partial\sigma}{\partial n} = -v_n \qquad \text{on} \quad \partial\omega_n(t),\ t > 0, \tag{20}
$$

and with the initial conditions

$$
u_c(\mathbf{x}, t_0) = u_{c0}(\mathbf{x}) \qquad \text{in} \quad \omega_n(t_0),\ u_{c0}(\mathbf{x}) \geq 0, \tag{21}
$$

$$
u_p(\mathbf{x}, t_0) = u_{p0}(\mathbf{x}) \qquad \text{in} \quad \omega_n(t_0),\ u_{p0}(\mathbf{x}) \geq 0, \tag{22}
$$

$$
u_q(\mathbf{x}, t_0) = u_{q0}(\mathbf{x}) \qquad \text{in} \quad \omega_n(t_0),\ u_{q0}(\mathbf{x}) \geq 0, \tag{23}
$$

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. (15) at $\partial\omega_n(t_0)$, we have the following result [3]:

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 $t \in \overline{I} = [0, t_p]$.*

(B) The case of the cystic growths

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

$$\Delta P_0 = \Delta m R_g T \sim 28.3 \ Nm^{-2}\,, \tag{24}$$

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. For 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.,

$$P_h^+ - P_h^- = P_0^+ - P_0^- = \alpha(C^+ - C^-), \quad \alpha = R_g T\,, \tag{25}$$

where the van Hoff equation was used, where α is the proportional coefficient R_g is the ideal gas constant, T is the temperature [21].

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 cummulated in the cavity of the cyst and only fluid can pass the semi-permeable 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

$$\frac{ds}{dt} = \beta S_c\,, \tag{26}$$

where β is a supply rate of the osmotic material and it can change according to the type of cyst.

The hydrostatic pressure jump across the epithelial membrane balances the stresses in the semi-permeable membrane and the stresses on the cyst from the neighboring bone tissue. Thus

$$P_h^+ - P_h^- = f(\mathbf{r}, \dot{\mathbf{r}}) + f_b(\mathbf{r}, \dot{\mathbf{r}})\,, \tag{27}$$

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**. 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., $f_b(\mathbf{r}, \dot{\mathbf{r}}) = 0$.

Ward et al. [23] 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,i.e., $\varepsilon = \varepsilon^e + \varepsilon^\nu$, $\quad \dot{\varepsilon} = \dot{\varepsilon}^e + \dot{\varepsilon}^\nu$, where $\dot{\varepsilon} = \frac{d\varepsilon}{dt}$. Since $\dot{\varepsilon}^e = \frac{\dot{f}}{E}$, and $\dot{\varepsilon}^\nu = \frac{f}{\nu}$, then we obtain

$$\dot{f} + \tau^{-1} f = E\dot{\varepsilon}\,, \tag{28}$$

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

From (25) 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

$$C^+ = C^- + \frac{1}{\alpha} f(\mathbf{r}, \dot{\mathbf{r}})\,, \tag{29}$$

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

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

$$C^+ = \frac{s}{v_c} = \frac{s}{|\omega_c|}\,, \tag{30}$$

where ω_c represents the region occupied by the cyst, i.e., $v_c = |\omega_c|$. When the cyst grows in a bony tissue, the bone is resorbed and the cyst grows as there it was no obstacle stopping it from expanding. Because $C^+ = \frac{s}{v_c(\mathbf{r})}$, then substituting $s = C^+ v_c(\mathbf{r})$ into (26), i.e., $\frac{ds}{dt} = \beta S_c$, and using (29), then after some modification, we obtain

$$\frac{\dot{v}_c}{\alpha} f(\mathbf{r}, \dot{\mathbf{r}})\dot{\mathbf{r}} + \dot{v}_c C^- \dot{\mathbf{r}} + \frac{v_c}{\alpha} \dot{f}(\mathbf{r}, \dot{\mathbf{r}}) = \beta S_c\,, \tag{31}$$

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 ([mol/m^2.s]) and is different for the radicular cysts and the 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 (28) the stresses satisfy

$$\tau \dot{f}(\mathbf{r}, \dot{\mathbf{r}}) + f(\mathbf{r}, \dot{\mathbf{r}}) = \nu\dot{\varepsilon}\,, \tag{32}$$

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

$$\mathbf{r}(0) = \mathbf{r}_0, \quad f(0) = f_0\,, \tag{33}$$

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 [23, 21, 19]. The problem can be solved by numerical methods for ODEs.

The biological materials of both types of tumors and both types of cysts are assumed to be near a fluids for which $\mu^{(0)} = 0$. When at $t \in I$ the shape of the cyst is known, it is possible to estimate a probable evolution of the cyst, and moreover, to determine a probable time of a cyst origin, similarly as in the previous case.

3. Stress-strain analysis of the loaded bone system with neoplasms

3.1. Mathematical model and its solution

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 (1)–(3) and the contact conditions with the Coulomb friction (4), the boundary conditions (5)–(6) and initial conditions (7), where we assume that the geometry of ω_n and ω_c at $t = 0$ and the corresponding material coefficients were determined and that all anisotropic elastic and viscous coefficients satisfy the symmetric and Lipschitz conditions (3).

Since the problem with Coulomb 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,

$$[u_n']^{sm} \leq d^{sm}, \quad \tau_n^s = \tau_n^m \equiv \tau_n^{sm} \leq 0, \quad ([u_n']^{sm} - d^{sm})\tau_n^{sm} = 0\,. \tag{34}$$

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

$$\begin{aligned}
&V_0 = \left\{\mathbf{v} | \mathbf{v} \in \sqcap_{\iota=1}^r H^{1,N}(\Omega^\iota), \mathbf{v} = 0 \text{ a.e. on } \Gamma_u\right\},\\
&V = \mathbf{u}_2 + V_0,\ \mathcal{V} = \mathbf{u}_2' + \mathcal{V}_0 = L^2(I; V),\quad K = \{\mathbf{v} \in V | [v_n]^{sm} \leq d^{sm} \text{ a.e. on } \Gamma_c^{sm}\},\\
&\mathcal{K} = \left\{\mathbf{v} | \mathbf{v} \in L^2(I; \sqcap_{\iota=1}^s H^{1,N}(\Omega^\iota)), \mathbf{v} = \mathbf{u}_2' \text{ on } \Gamma_u(t),\ [v_n]^{sm} \leq 0 \text{ a.e. on } \Gamma_c^{sm}(t)\right\}.
\end{aligned}$$

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

The variational formulation of Problem $(\mathcal{P})$ will be obtained by the usual way. Thus,

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

$$\begin{aligned}
&(\mathbf{u}''(t), \mathbf{v} - \mathbf{u}(t)) + a^{(0)}(\mathbf{u}(t), \mathbf{v} - \mathbf{u}(t)) + a^{(1)}(\mathbf{u}'(t), \mathbf{v} - \mathbf{u}(t)) + j(\mathbf{v}) - j(\mathbf{u}(t)) \geq\\
&\geq (\mathbf{f}(t), \mathbf{v} - \mathbf{u}(t)) \quad \forall \mathbf{v} \in K,\ t \in I\,,
\end{aligned} \tag{35}$$

$$\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), \mathbf{u}'(\mathbf{x}, 0) = \mathbf{u}_1(\mathbf{x})\,, \tag{36}$$

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

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

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

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

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

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 $\mathbf{u}_0$, $\mathbf{u}_1$ are given functions (e.g. they can be determined as solutions of static elastic contact problems).

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 used. The proof of the existence of the solution is based on the penalization and regularization techniques and is modification of that of [4].

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.

The corresponding variational problem is the following:

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

$$(\mathbf{u}''(t), \mathbf{v} - \mathbf{u}(t)) + a^{(0)}(\mathbf{u}(t), \mathbf{v} - \mathbf{u}(t)) + a^{(1)}(\mathbf{u}'(t), \mathbf{v} - \mathbf{u}(t)) + j(\mathbf{v}) - j(\mathbf{u}(t)) \geq$$
$$\geq (\mathbf{f}(t), \mathbf{v} - \mathbf{u}(t)) \quad \forall \mathbf{v} \in K,\ t \in I\,, \tag{37}$$
$$\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), \mathbf{u}'(\mathbf{x}, 0) = \mathbf{u}_1(\mathbf{x})\,, \tag{38}$$

where the initial data $\mathbf{u}_0$, $\mathbf{u}_1$ are given functions, and where $(\mathbf{u}'', \mathbf{v})$, $a^{(n)}(\mathbf{u}, \mathbf{v})$, $n = 0, 1$, $(\mathbf{f}, \mathbf{v})$ are defined above, and

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

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

The proof of the existence of the solution is based on the penalization and regularization techniques and is modification of that of [4], where the decomposition as above will be used.

3.3. Numerical solution

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 approximations 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. $t \in I$, $\mathbf{u}_h(t) \in K_h$

$$
\begin{aligned}
&(\mathbf{u}_h''(t), \mathbf{v}_h - \mathbf{u}_h(t)) + a^{(0)}(\mathbf{u}_h(t), \mathbf{v}_h - \mathbf{u}_h(t)) + a^{(1)}(\mathbf{u}_h'(t), \mathbf{v}_h - \mathbf{u}_h(t)) + \\
&+ j(\mathbf{v}_h) - j(\mathbf{u}_h(t)) \geq (\mathbf{f}_h(t), \mathbf{v}_h - \mathbf{u}_h(t)) \quad \forall \mathbf{v}_h \in K_h, \quad \text{a.e.}\, t \in I\,, \qquad (39)
\end{aligned}
$$

where

$$
\begin{aligned}
(\mathbf{u}_h'', \mathbf{v}_h) &= \sum_{\iota=1}^r (\mathbf{u}_h''^\iota, \mathbf{v}_h^\iota) = \int_{\Omega_h} \rho u_{hi}'' v_{hi} d\mathbf{x}\,, \\
a^{(n)}(\mathbf{u}_h, \mathbf{v}_h) &= \sum_{\iota=1}^r a^{(n)\iota}(\mathbf{u}_h^\iota, \mathbf{v}_h^\iota) = \int_{\Omega_h} c_{ijkl}^{(n)} e_{kl}(\mathbf{u}_h) e_{ij}(\mathbf{v}_h) d\mathbf{x}, \quad n=0,1, \\
(\mathbf{f}_h, \mathbf{v}_h) &= \sum_{\iota=1}^r (\mathbf{f}_h^\iota, \mathbf{v}_h^\iota) = \int_{\Omega_h} F_i v_{hi} d\mathbf{x} + \int_{\Gamma_{\tau_h}} P_i v_{hi} ds, \\
j(\mathbf{v}_h) &= \sum_{\iota=1}^r j^\iota(\mathbf{v}_h^\iota) = \int_{\cup_{s,m}\Gamma_{ch}^{sm}} g_{ch}^{sm} \left|[\mathbf{v}_{ht}]^{sm}\right| ds \equiv \langle g_{ch}^{sm}, |[\mathbf{v}_{ht}]^{sm}| \rangle_{\Gamma_{ch}^{sm}}\,.
\end{aligned}
$$

To prove the existence of discrete solution $\mathbf{u}_h$ the technique similar of that as in the continuous case, where the decomposition parallel as above, the penalty and regularization techniques are used.

3.4. 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 $\mathbf{u}_h^i = \mathbf{u}_h(t_i)$, $\Delta \mathbf{u}_h^i = \mathbf{u}_h(t_i) - \mathbf{u}_h(t_{i-1})$, $\mathbf{u}_h^{i+1} \equiv \mathbf{u}_h$, $g_{ch}^{sm} = g_{ch}^{sm}(t_i) = \mathcal{F}_c^{sm}(\Delta t^{-1}[\Delta \mathbf{u}_{th}^i]^{sm}) \left| \tau_n^{sm}\left(\mathbf{u}_h^i, \frac{\Delta \mathbf{u}_h^i}{\Delta t}\right)\right|$, $(\mathbf{F}(t_{i+1}), \mathbf{v}_h) = \Delta t^2 (\mathbf{f}_h(t_{i+1}), \mathbf{v}_h) + (2\mathbf{u}_h^i - \mathbf{u}_h^{i-1}, \mathbf{v}_h) + \Delta t a_h^{(1)}(\mathbf{u}_h^i, \mathbf{v}_h)$, $\mathbf{F}(t_{i+1}) \equiv \mathbf{f}_h$, 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

$$A(\mathbf{u}_h, \mathbf{v}_h - \mathbf{u}_h) + j(\mathbf{v}_h) - j(\mathbf{u}_h) \geq (\mathbf{f}_h, \mathbf{v}_h - \mathbf{u}_h), \quad \forall \mathbf{v}_h \in K_h,\ t = t_{i+1} \in I\,, \tag{40}$$

where

$$\begin{aligned} A(\mathbf{u}_h, \mathbf{v}_h) &= (\mathbf{u}_h, \mathbf{v}_h) + \Delta t^2 a^{(0)}(\mathbf{u}_h, \mathbf{v}_h) + \Delta t a^{(1)}(\mathbf{u}_h, \mathbf{v}_h)\,, \\ j(\mathbf{v}_h) &= \Delta t^2 \int_{\cup_{s,m}\Gamma_c^{sm}} g_{ch}^{sm}\, |[\mathbf{v}_{ht}]^{sm}|\, ds, \end{aligned}$$

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

$$\begin{aligned} A(\mathbf{u}_h, \mathbf{u}_h) &\geq a_0 \|\mathbf{u}_h\|_{1,2}^2, && a_0 = \text{const.} > 0, \\ |A(\mathbf{u}_h, \mathbf{v}_h)| &\leq a_1 \|\mathbf{u}_h\|_{1,2} \|\mathbf{v}_h\|_{1,2}, && a_1 = \text{const.} > 0,\ \mathbf{u}_h, \mathbf{v}_h \in V_h, \end{aligned}$$

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 [1, 18, 20]. From the stability analysis for the critical time step size we have

$$\Delta t \leq \Delta t_{\text{crit}} = \gamma \frac{h^{(n)}}{\pi} \left(\frac{\rho^{(n)}}{E^{(n)}} \right)\,, \tag{41}$$

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 determined from the 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.

3.4.1. 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 $\overline{\Gamma}_c^s = \cup_{\iota=1}^r (\partial\Omega^\iota \cap \Gamma_c^s) \setminus \Gamma_u^s$ 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}^{sm} 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 $h = \max_{\Omega_h}\{h_s, h_m\}$.

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

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

$$\begin{aligned} M_{Ht} = & \Big\{\mu_{Ht} \in W_{Ht}(\cup_s\Gamma_{ch}^s), \int_{\Gamma_{ch}^s} \boldsymbol{\mu}_{Ht}\boldsymbol{\psi}_H ds - \int_{\Gamma_{ch}^s} g_{ch}^{sm}|\boldsymbol{\psi}_H| ds \leq 0, \\ & \forall \boldsymbol{\psi}_H \in W_{Ht}(\cup_s\Gamma_{ch}^s)\Big\}, \end{aligned}$$

Let

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

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

Then we have the following problem:

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

$$\begin{aligned} & A(\mathbf{u}_h, \mathbf{v}_h) + b(\boldsymbol{\lambda}_{hH}, \mathbf{v}_h) = (\mathbf{f}_h, \mathbf{v}_h) && \forall \mathbf{v}_h \in V_h = \sqcap_{\iota=1}^r V_h^\iota,\ t \in I, \\ & b(\boldsymbol{\mu}_{hH} - \boldsymbol{\lambda}_{hH}, \mathbf{v}_h) \leq \langle d^{sm}, \mu_{hn} - \lambda_{hn}\rangle_{\cup\Gamma_{ch}^s} && \forall \boldsymbol{\mu}_{hH} \in M_{hH},\ t \in I. \end{aligned} \tag{42}$$

For the existence and uniqueness it is necessary to ensure that $\{\boldsymbol{\mu}_{hH} \in M_{hH}, b(\boldsymbol{\mu}_{hH}, \mathbf{v}_h) = 0, \forall \mathbf{v}_h \in V_h\} = \{\emptyset\}$.

Proposition 1 *Let* $-\tau_n(\mathbf{u}) \in M_{hn}$. *Then the problem (42) has a unique solution* $(\boldsymbol{\lambda}_{hH}, \mathbf{u}_h) \in M_{hH} \times V_h$, *a.e.* $t \in I$. *Moreover, we have*

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

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

3.4.2. Matrix formulation and the PDAS method

As usual in the mortar approach the contact boundary Γ^{sm}_{ch} has two sides, the "slave" side from the Ω^s_h and the "master" side from the Ω^m_h. The contact boundaries Γ^{sm}_{ch} are assumed to be a union of faces in the 3D case.

Let us assume that the space V is approximated by the discrete finite element space V_h of linear elements corresponding to the partition $\mathcal{T}_h$ and let $V_h = V^s_h \times V^m_h \subset V$ be introduced by such a way that the nodal basis functions on the mortar side will be biorthogonal with respect to the piecewise linear basis on the slave side.[1]

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. In this case the discontinuous piecewise linear nodal basis functions for the dual Lagrange multiplier will be used. The discrete Lagrange multiplier space M_{hH} can be spanned as $M^s_{hH} = \text{span}\{\psi_i \mathbf{e}_k,\ i = 1, \ldots, n_c,\ k = 1, \ldots, N\}$, $s \in \{1, \ldots, r\}$, where ψ_i is the i-th scalar dual basis function, $\mathbf{e}_k$ is the k-th unit vector, i.e., components of the unit Cartesian basis, n_c is the number of nodes on the slave side of $\overline{\Gamma}^s_{ch}$, i.e., the number of freedom of the space M_{hH} in each component.

Let W^s_{hH} be the vector valued trace space of V_{0h} restricted to $\cup_s \Gamma^s_{ch}$. Then for each $\mathbf{v}_h = \sum_i \gamma_i \varphi_i \in W_{hH}$ the discrete scalar product $\mathbf{v}_h \cdot \mathbf{n}^s_h = \sum_i (\gamma_i \cdot \mathbf{n}^s_i)\varphi_i$, where $\mathbf{n}^s_i$ 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 $\boldsymbol{\mu}_h \cdot \mathbf{n}^s_h = \sum_i (\boldsymbol{\alpha}_i \cdot \mathbf{n}^s_i)\psi_i$. Let us define

$$M^{s+}_{hH} := \left\{ \boldsymbol{\mu}_{hH} \in M^s_{hH} | \, \langle \boldsymbol{\mu}_{hH}, \mathbf{v}_h \rangle \geq 0, \mathbf{v}_h \in W^{s+}_h \right\}\,,$$

where

$$W^{s+}_h := \{\mathbf{v}_h \in W_{hH}(\cup \Gamma^s_{ch}) | \mathbf{v}_h \cdot \mathbf{n}^s_h \geq 0\}$$

and

$$W_{hH} = W_{hH}(\cup_s \Gamma^s_{ch}) = W_{hn}(\cup_s \Gamma^s_{ch}) \times W_{Ht}(\cup_s \Gamma^s_{ch}) =$$

$$= \{\mathbf{v}_h \cdot \mathbf{n}^s|_{\cup \Gamma^s_{ch}}, \mathbf{v}_h \in V_h\} \times \{\mathbf{v}_h \cdot \mathbf{t}^s|_{\cup \Gamma^s_{ch}}, \mathbf{v}_h \in V_h\}$$

[1] Let $\{\psi_i\}^m_{i=1}$ be a suitable dual basis and $\{\varphi_j\}^m_{j=1}$ be the standard piecewise linear basis on the slave side, i.e., the basis of $W_{hH}(\Gamma^{sm}_{sh})$. We say that ψ_i and φ_j are biorthogonal if $\int_{\Gamma^{sm}_{ch}} \varphi_j \psi_i \, ds = \delta_{ij} \int_{\Gamma^{sm}_{ch}} \varphi_j \, ds,\ \ 1 \leq i, j \leq m,\ \ \delta_{ij}$ is the Kronecker delta.

It can be shown ([20]) that M_{hH}^{s+} can be written as

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

Finally,

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

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

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

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

Then the discrete mortar formulation of the saddle point problem for every time level is defined as follows:

Problem $(\mathcal{P}_{sp})_{dm}$**:** In 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

$$\begin{aligned} A(\mathbf{u}_h, \mathbf{v}_h) + b(\boldsymbol{\lambda}_{hH}, \mathbf{v}_h) &= (\mathbf{f}_h, \mathbf{v}_h) \quad \forall \mathbf{v}_h \in V_h,\ t \in I , \\ b(\boldsymbol{\mu}_{hH} - \boldsymbol{\lambda}_{hH}, \mathbf{v}_h) &\leq \langle d^{sm}, (\boldsymbol{\mu}_{hH} - \boldsymbol{\lambda}_{hH}) \cdot \mathbf{n}_h \rangle_{\cup \Gamma_{ch}^s} \quad \forall \boldsymbol{\mu}_{hH} \in M_{hH}^{+},\ t \in I, \end{aligned} \tag{43}$$

where

$$\begin{aligned} A(\mathbf{u}_h, \mathbf{v}_h) =& (\mathbf{u}_h, \mathbf{v}_h) + \Delta t^2 a^{(0)}(\mathbf{u}_h, \mathbf{v}_h) + \Delta t a^{(1)}(\mathbf{u}_h, \mathbf{v}_h) , \\ b(\boldsymbol{\mu}_{hH}, \mathbf{v}_h) =& \langle \boldsymbol{\mu}_{hH}, [\mathbf{v}_h]^s \rangle_{\cup \Gamma_{ch}^s} \quad \forall \mathbf{v}_h \in V_h,\ \boldsymbol{\mu}_{hH} \in M_{hH} . \end{aligned}$$

Let us decompose the set of all vertices of triangulation $\mathcal{T}_h = \cup_{i=1}^r \mathcal{T}_h^i$ into three disjoint parts $\mathcal{N}, \mathcal{M}, \mathcal{S}$, where $\mathcal{S}$ is a set of vertices on all $\mathcal{T}_h^s \cap \Gamma_{ch}^{sm}$, and $\mathcal{M}$ is a set of vertices on all $\mathcal{T}_h^m \cap \Gamma_{ch}^{sm}$, and $\mathcal{N}$ is a set of all the other one. The strong formulation of the non-penetration condition will be replaced by its weak discrete form

$$\int_{\cup \Gamma_{ch}^{sm}} [\mathbf{u}_h \cdot \mathbf{n}]^s \psi_p ds \leq \int_{\cup \Gamma_{ch}^{sm}} d_h^s \psi_p ds, \quad p \in \mathcal{S} , \tag{44}$$

that coupled the vertices on the slave side and the master side. Using a transformation of the basis of the space V_h in such a way that the weak non-penetration condition (44) in the new basis only deals with the vertices on the slave side. Moreover, the elimination of the Lagrange multiplicators $\boldsymbol{\Lambda}_{hH}$ can be easy made (see [11, 18, 20]). In this new basis the first equation of Problem $(\mathcal{P}_{sp})_{dm}$ for every $t \in I$ will be expressed in the matrix form, that with respect to the sets $\mathcal{N}, \mathcal{M}, \mathcal{S}$, after using the modified basis bellow defined, after some modification ([18, 20]), we obtain the modified system

$$\hat{\mathbb{A}}_h \hat{\mathbf{U}}_h + \hat{\mathbb{B}}_h \hat{\mathbf{\Lambda}}_{hH} = \hat{\mathbb{F}}_h \,, \tag{45}$$

where $\hat{\mathbf{U}}_h$ is the displacement vector of nodal parameter with respect to the modified basis Φ, and where the modified stiffness matrix is of the form

$$\hat{\mathbb{A}}_h = Q\mathbb{A}_h Q^T = \begin{bmatrix} \mathbb{A}_{\mathcal{N}\mathcal{N}} & \mathbb{A}_{\mathcal{N}\mathcal{M}} + \mathbb{A}_{\mathcal{N}\mathcal{S}}\hat{\mathbb{M}} & \mathbb{A}_{\mathcal{N}\mathcal{S}} \\ \mathbb{A}_{\mathcal{M}\mathcal{N}} + \hat{\mathbb{M}}^T\mathbb{A}_{\mathcal{S}\mathcal{N}} & \begin{matrix}\mathbb{A}_{\mathcal{M}\mathcal{M}} + \mathbb{A}_{\mathcal{M}\mathcal{S}}\hat{\mathbb{M}} + \\ +\hat{\mathbb{M}}^T\mathbb{A}_{\mathcal{S}\mathcal{M}} + \hat{\mathbb{M}}^T\mathbb{A}_{\mathcal{S}\mathcal{S}}\hat{\mathbb{M}}\end{matrix} & \mathbb{A}_{\mathcal{M}\mathcal{S}} + \hat{\mathbb{M}}^T\mathbb{A}_{\mathcal{S}\mathcal{S}} \\ \mathbb{A}_{\mathcal{S}\mathcal{N}} & \mathbb{A}_{\mathcal{S}\mathcal{M}} + \mathbb{A}_{\mathcal{S}\mathcal{S}}\hat{\mathbb{M}} & \mathbb{A}_{\mathcal{S}\mathcal{S}} \end{bmatrix}$$

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

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

$\hat{\mathbb{B}}_h = Q.(\mathbf{0}, -\mathbb{M}^T, \mathbf{0})^T = (\mathbb{O}, \mathbb{O}, \mathbb{D})^T$, and $\hat{\mathbb{M}}^T = \mathbb{D}^{-1}\mathbb{M}$, $\mathbb{M} = (\mathbb{M}[p,q])$, where $\mathbb{M}[p,q] = \int_{\cup\Gamma_{ch}^{sm}} \varphi_p\psi_q ds\, \mathbb{I}_3$, $p, \in \mathcal{S}, q \in \mathcal{M}$, and $\mathbb{D} = (\mathbb{D}[p,q])$, $\mathbb{D}[p,q] = \delta_{pq}\mathbb{I}_3 \cdot \int_{\cap\Gamma_{ch}^{sm}} \varphi_p\psi_q\, ds$, $p = q \in \mathcal{S}$, and where the used modified basis is of the form

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

If the displacement $\hat{\mathbb{U}}_h$ is known, then the Lagrange multiplier can be computed directly from (45) and then

$$\hat{\mathbf{\Lambda}}_{hH} = \mathbb{D}^{-1}(\hat{\mathbb{F}}_h - \hat{\mathbb{A}}_h\hat{\mathbb{U}}_h)_S. \tag{46}$$

The algebraic representation of the weak nonpenetration condition is associated with the transformed basis Φ is of the form ([10],[12])

$$\hat{\mathbb{U}}_{hn,p} \equiv (\mathbf{n}_p^s)^T\mathbb{D}[p,p]\hat{\mathbb{U}}_{hp} \le d_p^{sm} \quad \forall p \in \mathcal{S}\,, \tag{47}$$

where $d_p^{sm} = \int_{\cup_s\Gamma_c^s} d_h^{sm}\psi_p ds$, $p \in \mathcal{S}$, and the coefficients at $\hat{\mathbb{U}}_{hq}$, $q \in \mathcal{M}$, are nullified.

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

$$\begin{aligned} &\hat{\mathbb{A}}_h\hat{\mathbb{U}}_h + \hat{\mathbb{B}}_h\mathbf{\Lambda}_{hH} = \hat{\mathbb{F}}_h, \\ &\hat{\mathbb{U}}_{hn,p} \le d_p^{sm}, \mathbf{\Lambda}_{hn,p} \ge 0, (\hat{\mathbb{U}}_{hn,p} - d_p^{sm})\mathbf{\Lambda}_{hn,p} = 0, \quad \forall p \in \mathcal{S},\ t \in I, \end{aligned} \tag{48}$$

where the second line represents the Karush-Kuhn-Tucker conditions of a constrained optimization problem for inequality constraints, with the discrete Tresca friction conditions and with the discrete friction conditions

$$\begin{aligned} \left|\mathbf{\Lambda}_{Ht,p}^s(p)\right| &\le g_p^s \ (= \mathcal{F}_c^{sm}\left|\mathbf{\Lambda}_{hn,p}^s\right|), \\ \left|\mathbf{\Lambda}_{Ht,p}^s(p)\right| &< g_p^s \ (= \mathcal{F}_c^{sm}\left|\mathbf{\Lambda}_{hn,p}^s\right|) \Rightarrow \mathbf{u}_{ht,p} = \mathbf{0}, \end{aligned}$$

$$
\begin{aligned}
\left|\mathbf{\Lambda}^s_{Ht,p}(p)\right| = & g^s_p \; (= \mathcal{F}^{sm}_c \left|\mathbf{\Lambda}^s_{hn,p}\right|) \Rightarrow \exists \vartheta \geq 0 \\
& \text{such that } \; \mathbf{\Lambda}^s_{Ht,p} = -\vartheta \mathbf{u}_{ht,p}, \quad \text{for all } p \in S,
\end{aligned} \tag{49}
$$

where for the Tresca friction model $\mathcal{F}^{sm}_c|\mathbf{\Lambda}^s_{hn,p}| \equiv g^s_p \in H^{-\frac{1}{2}}(\Gamma^s_c)$, $g^s_p \geq 0$, $g^s_p = \int_{\Gamma^s_{ch}} g^s_{ch}\varphi_p ds$, and where

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

For $g^s_p = 0$ the condition (49) leads to homogeneous Neumann boundary conditions in tangential direction.

PDAS algorithm for 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 (49a), that is,

$$
\mathbf{\Lambda}_{hH} = \mathbb{D}^{-1}(\hat{\mathbb{F}}_h - \hat{\mathbb{A}}_h \hat{\mathbb{U}})_S \,, \tag{50}
$$

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

$$
\begin{aligned}
\hat{\mathbb{U}}_{hn,p} &= \hat{\mathbb{U}}^T_p \mathbf{n}_p \in \mathbb{R}, \quad \hat{\mathbb{U}}_{Ht,p} = (\hat{\mathbb{U}}^T_p \mathbf{t}_{1p}, \quad \hat{\mathbb{U}}^T_p \mathbf{t}_{2p})^T \in \mathbb{R}^2, \\
\mathbf{\Lambda}^s_{hn,p} &= (\mathbf{n}^s_p)^T \mathbb{D}[p,p]\mathbf{\Lambda}_{hH}(p) \in \mathbb{R}, \quad \mathbf{\Lambda}_{hH}(p) \in \mathbb{R}^3, \\
\mathbf{\Lambda}^s_{Ht,p} &= \mathbf{\Lambda}_{hH}(p) - (\mathbf{\Lambda}_{hH}(p) \cdot \mathbf{n}^s_p)\mathbf{n}^s_p = \left(\mathbf{\Lambda}_{hH}(p) \cdot \mathbf{t}^s_p\right) \mathbf{t}^s_p = \\
&= \left(\mathbf{\Lambda}^T_{hH}(p)\mathbb{D}[p,p]\mathbf{t}^s_{1,p}, \; \mathbf{\Lambda}^T_{hH}(p)\mathbb{D}[p,p]\mathbf{t}^s_{2,p}\right)^T \in \mathbb{R}^2 \,.
\end{aligned}
$$

Let $g^s_p > 0$, then the condition (49) is equivalent to $C_t\left(\hat{\mathbb{U}}_{t,p}, \mathbf{\Lambda}^s_{Ht,p}\right) = 0$ for all $p \in S$, where

$$
C_t\left(\hat{\mathbb{U}}_{ht,p}, \mathbf{\Lambda}^s_{Ht,p}\right) = \max\left(g^s_{ch,p}, |\mathbf{\Lambda}^s_{Ht,p} + c_2\hat{\mathbb{U}}_{ht,p}|\right)\mathbf{\Lambda}^s_{Ht,p} - g^s_p\left(\mathbf{\Lambda}^s_{Ht,p} + c_2\hat{\mathbb{U}}_{ht,p}\right), \; c_2 > 0 \,, \tag{51}
$$

which will be a starting point of the algorithm, that will be based on a Newton-type algorithm for the solution of $C_t(\hat{\mathbb{U}}_{ht,p}, \mathbf{\Lambda}^s_{Ht,p}) = 0$. As it was shown in [7] the max-function and the Euclidean norm are semi-smooth, and therefore, a semi-smooth Newton method can be used. If the Euclidean norm $\left|\mathbf{\Lambda}^s_{Ht,p} + c_2\hat{\mathbb{U}}_{ht,p}\right| = 0$, then $\max\left(g^s_{ch,p}, |\mathbf{\Lambda}^s_{Ht,p} + c_2\hat{\mathbb{U}}_{ht,p}|\right) = g^s_{ch,p}$ 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 $C_t(\hat{\mathbb{U}}_{ht,p}, \mathbf{\Lambda}^s_{Ht,p})$ (see [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

$$\mathcal{A}_{Ht,k} := \left\{ p \in S; |\mathbf{\Lambda}^{s,k-1}_{Ht,p} + c_2 \hat{\mathbb{U}}^{k-1}_{ht,p}| - g^s_{ch,p} > 0 \right\} , \tag{52}$$

$$\mathcal{I}_{Ht,k} := \left\{ p \in S; |\mathbf{\Lambda}^{s,k-1}_{Ht,p} + c_2 \hat{\mathbb{U}}^{k-1}_{ht,p}| - g^s_{ch,p} \leq 0 \right\} . \tag{53}$$

Since $\hat{\mathbb{B}}_h = (\mathbb{O}, \mathbb{O}, \mathbb{D})^T$, we decompose the matrix $\mathbb{D}$ into

$$\mathbb{D} = \left[\begin{array}{cc} \mathbb{D}_{\mathcal{I}_k} & \mathbb{O} \\ \mathbb{O} & \mathbb{D}_{\mathcal{A}_k} \end{array} \right] , \text{ since } \ \mathcal{S} = \mathcal{A}_k \cup \mathcal{I}_k .$$

This decomposition 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 [12].

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

$$\begin{aligned} \hat{\mathbb{A}}_h \hat{\mathbb{U}}_h + \hat{\mathbb{B}}_h \mathbf{\Lambda}_{hH} &= \hat{\mathbb{F}}_h , \\ C_n \left(\hat{\mathbb{U}}_{hn,p}, \mathbf{\Lambda}_{hn,p} \right) &= 0 , \\ C_t (\hat{\mathbb{U}}_{ht,p} \mathbf{\Lambda}_{Ht,p}) &= 0 \end{aligned} \tag{54}$$

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

STEP 2: Define the active and inactive sets

$$\begin{aligned} \mathcal{A}_{hn,k} &:= \left\{ p \in S; \mathbf{\Lambda}^{s,k-1}_{hn,p} + c_1 \left(\hat{\mathbb{U}}^{k-1,m}_{n,p} - d^{sm}_p \right) > 0 \right\} , \\ \mathcal{I}_{hn,k} &:= \left\{ p \in S; \mathbf{\Lambda}^{s,k-1}_{hn,p} + c_1 \left(\hat{\mathbb{U}}^{k-1,m}_{n,p} - d^{sm}_p \right) \leq 0 \right\} , \\ \mathcal{A}_{Ht,k} &:= \left\{ p \in S; \left| \mathbf{\Lambda}^{s,k-1}_{Ht,p} + c_2 \hat{\mathbb{U}}^{k-1,m}_{t,p} \right| - g^s_{ch,p} > 0 \right\} , \\ \mathcal{I}_{Ht,k} &:= \left\{ p \in S; \left| \mathbf{\Lambda}^{s,k-1}_{Ht,p} + c_2 \hat{\mathbb{U}}^{k-1,m}_{t,p} \right| - g^s_{ch,p} \geq 0 \right\} , \end{aligned}$$

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

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

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 (51), that is,

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

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

PDAS algorithm for the 3D case with Coulomb friction. The algorithms can be based on the fixpoint algorithm or on the full Newton method ([12]). We limit ourselves to the fixpoint algorithm only.

The Fixpoint Algorithm ($\mathcal{FP}$) is the extension of the above PDAS algorithm for the 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 $k = 1$, $k_0 \in \mathbb{N}$, $m \in \mathbb{N}$.

STEP 2: If $mod_{k_0}(k-1) = 0$, 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

$$\begin{aligned}
\mathcal{A}_{hn,k} &:= \left\{p \in S; \mathbf{\Lambda}_{hn,p}^{s,k-1} + c_1\left(\hat{\mathbb{U}}_{n,p}^{k-1,m} - d_{p}^{sm}\right) > 0\right\} ,\\
\mathcal{I}_{hn,k} &:= \left\{p \in S; \mathbf{\Lambda}_{hn,p}^{s,k-1} + c_1\left(\hat{\mathbb{U}}_{n,p}^{k-1,m} - d_{p}^{sm}\right) \leq 0\right\} ,\\
\mathcal{A}_{Ht,k} &:= \left\{p \in S; \left|\mathbf{\Lambda}_{Ht,p}^{s,k-1} + c_2\hat{\mathbb{U}}_{t,p}^{k-1,m}\right| - g_{ch,p}^{s,k_c} > 0\right\} ,\\
\mathcal{I}_{Ht,k} &:= \left\{p \in S; \left|\mathbf{\Lambda}_{Ht,p}^{s,k-1} + c_2\hat{\mathbb{U}}_{t,p}^{k-1,m}\right| - g_{ch,p}^{s,k_c} \leq 0\right\} .
\end{aligned}$$

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 (51) as

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

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 [6]).

3.5. Fracture of bones with neoplasms

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 is fractured. In the real situations it is very difficult to determine the location of a crack, its initiation, its further opening and propagation and to determine the direction of its future propagation.

The geometry of the investigated system of bones with neoplasms is determined from the CT or MRI scan data. The locations of the acting contraction forces and their directions will be determined from the anatomy knowledges and their magnitudes (in N) will be determined from the cross-sectional area of the muscles (in mm^2), the averaged activation ratio, and a certain constant (in N/mm^2). On the bases of these CT or MRI data the finite element mesh will be generated. The contact boundaries will be approximated by such a way that the contact boundary is discretized from the both sides corresponding to the neighboring subdomains Ω^s and Ω^m, from the slave side and the master side, and then the unilateral contact conditions will be satisfied in all vertices of $\mathcal{T}_h^s \cap \Gamma_{ch}^{sm}$ from the slave side and in all vertices of $\mathcal{T}_h^m \cap \Gamma_{ch}^{sm}$ from the master side.

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 started 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 further propagate, 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. 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. 2a,b), 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

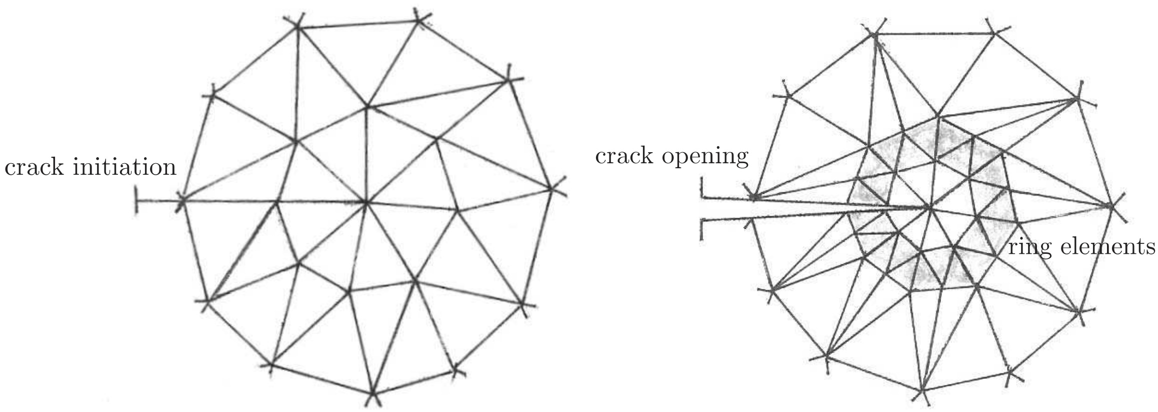

Figure 2: Location of the crack and the mesh around the crack tip: a) crack initiation; b) crack opening.

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.

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. 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. Very useful algorithms are based on the dynamic contact problems with friction. Therefore, the PDAS algorithms discussed above can also be used for numerical studies of opening of cracks and fractures in loaded bones with neoplasms. Numerically, simpler versions of the free boundary problems can be firstly studied for the symmetric neoplasms.

4. Conclusion

At present about tumor's studies exist more than two millions research papers, predominantly of the oncological studies from the medical point of views, and only relatively small part of these papers are devoted to mathematical problems of oncology. Majority of these mathematical papers are devoted to studies on the response of a vascular tumor to chemotherapeudic treetments and effects of drug resistance, to studies on a tumor-induced angiogenesis, on a tumor-immune system dynamics and minority of these papers are devoted to mathematical modelling of tumor's growth. These research works are connected with Profs A. Friedman, S. Cui, H. Byrne, L. Preziosi, M. A. Chaplain, S. J. Chapman, T. Roose, A. R. A. Andersson and many others. They analyzed the problems mathematically and under some assumptions on the physical parameters of the models, they prove the existence and the uniqueness of the solution of some free boundary problems. The studied models are predominantly assumed to be spherically symmetric.

The author, together with his co-workers, studied the problems concerning with the biomechanical problems of artificial replacements of human's joints, and moreover, e.g. a fractured lumbar spine, where the fracture passes practically horizontally through the vertebra, where the internal stabilized device was applied. Such a fracture is observed between the vertebra $Th12$ and $L3$, and is known as the Chance's fracture. The aim of this study was to obtain some knowledge about the situation and the behavior of fractured parts of the vertebra on their common contact boundary (because minor movements stimulate healing of the fracture), where the mathematical model was based on the contact problem in non-linear elasticity, where the non-linear elastic coefficients are strain dependent (see e.g. Nedoma et al. (2011) and the author's references presented here).

The PDAS method was firstly presented in the papers of Hintermüller et al. (2002), (2004), (2005) and in Wohlmuth and Krause (2003), Hüeber and Wohlmuth (2005), Hlaváček (2006) and many others, where the static contact problems with or without given friction were studied. Later Hüeber et al. (2008) applied the PDAS algorithm for $3D$ static contact problems with Coulomb friction, where they present two algorithms based on the fixpoint algorithm and on the full Newton method. Hüeber et al. (2005) studied the dynamic contact problem, where the Newmark algorithm with the PDAS algorithm was used. The author studied the quasi-static and dynamic problems with or without friction close of the nineties in connection with geodynamic problems, based on linear or non-linear elastic, thermo-(visco-)elastic and thermo-visco-plastic Bingham rheologies (Nedoma (1998a), (2005), (2006), (2010), (2012) and later in biomechanics (Nedoma (1998b), (2004), (2006), (2012) and Nedoma et al. (2011) and the author's references presented here. The PDAS algorithm presented in the paper is a continuations of results obtained in previous author's papers connected with the quasi-static and dynamic contact problems with or without friction in thermo-(visco-)elasticity. The presented PDAS algorithm as well as the PDAS algorithms of the previous mentioned papers are based on the author's idea and represent the own author's results. The novelty of these algorithms is that they practically pursue the techniques of proofs of dynamic problem with or without Coulomb (or Tresca) friction. From the medical point of view the aim of this paper is to give an optimal algorithm for application in connection with further oncological studies and in application concerned with a computer-aided orthopedic surgery. The presented method can be used also in geodynamic problems as well as in problems of technology.

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