On the calculation of crack paths in 3-dimensional anisotropic solids

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ABSTRACT. *One of the main interests of fracture mechanics is the prediction of crack propagation. While problems for plane scenarios are widely discussed in the literature, for real-world applications more interesting but still a hard problem is the fully three-dimensional case. Mathematical models for crack prediction are based on the asymptotic behavior of the displacements at the crack front, which is of well-known square-root type also in three dimensions. In this contribution we present the asymptotic decomposition of the displacements near an arbitrary curved crack front. By exploiting the structure of this expansion a representation of the change of potential energy caused by a small elongation of the crack surface is derived using methods of asymptotic analysis.*

INTRODUCTION

In this contribution we present ideas how fatigue crack growth in 3-dimensional anisotropic structures can be predicted using the GRIFFITH' energy principle: *A crack only starts to propagate if energy can be released.* The total energy is composed from the surface energy and the potential energy $\mathbf{U}$, the latter is the difference of the elastic energy and the work performed by external forces. Since the work of IRWIN the change of potential energy caused by a straight elongation of a crack in an isotropic two-dimensional homogeneous structure can be expressed in quadratic terms of the stress intensities at the crack tip. This result was generalized in the last decades to anisotropic and also inhomogeneous materials using methods of asymptotic analysis by many other authors [1, 2]. With the energy release rate at hand, quasi-static crack propagation can be calculated in linear elastic materials. Here, we generalize the ideas from [3] for a plane crack to a nearly arbitrary smooth crack geometry. For this, we introduce local coordinates at the crack front and give the asymptotic behavior of the displacement field. In local coordinates, we expand the results from [1] for two-dimensional problems and derive an asymptotic representation of the change of potential energy caused by a small elongation of the crack.

FORMULATION OF THE PROBLEM

Let $G \subset \mathbb{R}^3$ be a solid with polygonal boundary. We consider the problem of three-dimensional linear elasticity theory in the domain $\Omega := G \setminus \overline{\Xi}$, where Ξ (the crack) is a smooth two-dimensional sub-manifold of $\mathbb{R}^3$ with smooth boundary $\Gamma := \partial\Xi$ (the crack front) placed completely inside of G. We assume, that Ξ is simply connected and that the crack front Γ is a smooth curve. For a given self-balanced external loading $p = (p_1, p_2, p_3)^\top$ the displacement field $u = (u_1, u_2, u_3)^\top$ fulfills the equilibrium equations

$$\begin{aligned} -\nabla \cdot \sigma(u;x) &= 0, & x &\in \Omega, \\ \sigma(u;x) \cdot n(x) &= 0, & x &\in \Xi^+ \cup \Xi^-, \\ \sigma(u;x) \cdot n(x) &= p(x), & x &\in \partial\Omega \setminus \Xi^\pm, \end{aligned} \tag{1}$$

where $n = (n_1, n_2, n_3)^\top$ is the outward normal vector ($\top$ means transposition). With Ξ^+ and Ξ^- we denote the upper and lower surfaces of the crack, considered to be traction-free. The term $u \cdot n = u_i n_i$ denotes the inner product in the Euclidean space (with sum convention). The strain tensor with the Cartesian components evaluated for the displacement field at point x, $\varepsilon_{kl}(u;x) = \frac{1}{2}\big(\partial_{x_l} u_k(x) + \partial_{x_k} u_l(x)\big)$, $k, l = 1, 2, 3$, is related to the stress tensor by Hooke's law:

$$\sigma_{ij}(u;x) = \sum_{k,l=1}^{3} a_{ij}^{kl} \varepsilon_{kl}(u;x), \qquad i, j = 1, 2, 3.$$

The tensor $a = \left(a_{ij}^{kl}\right)$ contains the elastic moduli and is symmetric and positive.

ASYMPTOTIC DECOMPOSITION AT THE CRACK FRONT

Local curvilinear coordinates.
In order to derive the asymptotic decomposition of the displacement field near the crack front, we introduce local coordinates. In a (small) neighborhood T around the crack front Γ local curvilinear coordinates $y = (y_1, s, y_2)^\top$ of a point $P \in T$ are defined by the transformation

$$P = \Theta(y) = x(s) + y_1 n(s) - y_2 b(s)\,, \tag{2}$$

where t, n and $b = t \times n$ are the tangent, (outer) normal and binormal unit vectors on Ξ at point $x(s)$ with arc length s on the crack front, see figure 1.
Choosing a local positive coordinate system,

$$e_1(s) = t(s), \qquad e_2(s) = -n(s), \qquad e_3(s) = -b(s),$$

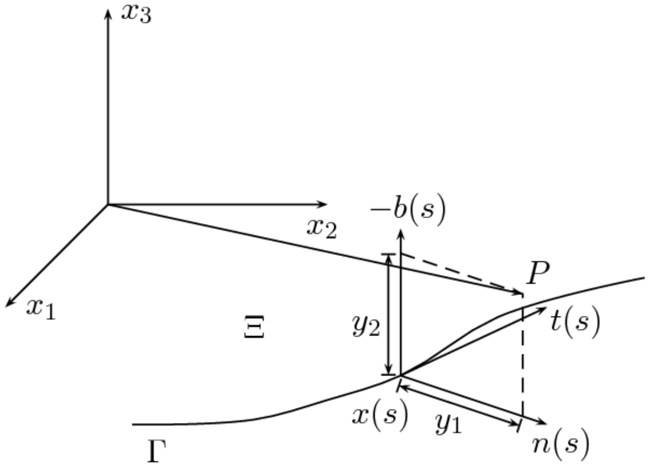

Figure 1: Point P in local coordinates near the crack front Γ.

the FRENET-SERRET formulas from differential geometry [4] lead to

$$\frac{\mathrm{d}t}{\mathrm{d}s}(s) = -\kappa(s)n(s), \qquad \frac{\mathrm{d}n}{\mathrm{d}s}(s) = \kappa(s)t(s) + \tau(s)b(s), \qquad \frac{\mathrm{d}b}{\mathrm{d}s}(s) = -\tau(s)n(s),$$

where $\kappa(s)$ is the curvature and $\tau(s)$ is the torsion of the curve Γ (the crack front) at arc length s. A covariant basis $\{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3\}$ of (positive orientated) curvilinear coordinates at a point $\Theta(y) = x \in T$ is given by $\mathbf{g}_j(y) = \partial_{y_j}\Theta(y)$, here

$$\mathbf{g}_1(y) = n(s), \quad \mathbf{g}_2(y) = \big(1 + y_1\kappa(s)\big)t(s) + \tau(s)\big(y_1 b(s) + y_2 n(s)\big), \quad \mathbf{g}_3(y) = -b(s).$$

The components $g_{ij}(y) := \mathbf{g}_i(y) \cdot \mathbf{g}_j(y)$ of the RIEMANNIAN metric tensor are

$$\big(g_{ij}(y)\big) = \begin{pmatrix} 1 & y_2\tau(s) & 0 \\ y_2\tau(s) & \Big(\big(1 + y_1\kappa(s)\big)^2 + \big(y_1^2 + y_2^2\big)\tau(s)^2\Big) & -y_1\tau(s) \\ 0 & -y_1\tau(s) & 1 \end{pmatrix}.$$

The contravariant basis, defined by the relation $\mathbf{g}^i \cdot \mathbf{g}_j = \delta_{ij}$ with the KRONECKER symbol δ_{ij}, can also be explicitly calculated:

$$\mathbf{g}^1(y) = n(s) - \frac{y_2\tau(s)}{\sqrt{g(y)}}t(s), \quad \mathbf{g}^2(y) = \frac{1}{\sqrt{g(y)}}t(s), \quad \mathbf{g}^3(y) = -b(s) + \frac{y_1\tau(s)}{\sqrt{g(y)})}t(s)$$

where $\sqrt{g(y)} = \big(1 + y_1\kappa(s)\big)$ is the JACOBIAN, see e.g. [5]. Because Ξ is considered to be smooth, local coordinates are uniquely defined at any arc length s. Nevertheless, the determinant $\sqrt{g(y)}$ of the JACOBIAN matrix vanishes at $y_1 = -\frac{1}{\kappa(s)}$ and the transformation (2) is valid only in a possibly small vicinity around the crack front.

The displacement field $u : \Omega \to \mathbb{R}^3$ with (smooth enough) components u_i can be transformed to curvilinear coordinates by the defining relation

$$u(x) = u_i(x)\mathbf{e}_i = \widehat{u}_i(y)\mathbf{g}^i(y) \quad \text{for all} \quad x = \Theta(y), \qquad \|y'\| \ll 1.$$

Vector fields in global CARTESIAN coordinates $x = (x_1, x_2, x_3)^\top$ are related to the standard unit basis of $\mathbb{R}^3$: $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$. While this basis is fixed in $\mathbb{R}^3$, the displacement field can be identified by the vector of its CARTESIAN components $u(x) = (u_1(x), u_2(x), u_3(x))^\top$ at any point $x \in \mathbb{R}^3$. This is no longer true in curvilinear coordinates, where the functions $\widehat{u}_i(y)$ represent the covariant components of the displacement vector over the contravariant basis $\{\mathbf{g}^1(y), \mathbf{g}^2(y), \mathbf{g}^3(y)\}$ which varies with $\Theta(y) = x \in T$. We identify the vector $\widehat{u} = (\widehat{u}_i)$ with the vector of its covariant components whereas $\widehat{\mathbf{u}} := \widehat{u}_i\mathbf{g}^i$ is the (physical) displacement vector, see e.g. [5] for more details.

We formulate the equilibrium equations (1) in curvilinear coordinates. The derivatives of a vector field in curvilinear coordinates are defined by the relations

$$\partial_j v_i(x) = \Big(\widehat{v}_{k\|l}[\mathbf{g}^k]_i[\mathbf{g}^l]_j\Big)(y), \qquad x = \Theta(y), \qquad [\mathbf{g}^k]_i := \mathbf{g}^k \cdot \mathbf{e}_i\,,$$

(always with sum convention), the covariant derivative is defined by

$$\widehat{v}_{i\|j} := \widehat{\partial}_j\widehat{v}_i - \Gamma^p_{ij}\widehat{v}_p \qquad \text{with the CHRISTOFFEL symbols} \qquad \Gamma^p_{ij} := \mathbf{g}^p \cdot \partial_i\mathbf{g}_j.$$

Remark, that the choice of the basis as shown in figure 1 specifies the enumeration of derivatives as follows:

$$\nabla_y\widehat{v} = \Big(\widehat{\partial}_1\widehat{v}, \widehat{\partial}_2\widehat{v}, \widehat{\partial}_3\widehat{v}\Big), \qquad \widehat{\partial}_1\widehat{v} = \frac{\partial\widehat{v}}{\partial y_1}, \qquad \widehat{\partial}_2\widehat{v} = \frac{\partial\widehat{v}}{\partial s}, \qquad \widehat{\partial}_3\widehat{v} = \frac{\partial\widehat{v}}{\partial y_2}.$$

The CHRISTOFFEL symbols Γ^p_{ij} of the second kind can be expressed in terms of the metric tensor by CHRISTOFFEL symbols of the first kind,

$$\Gamma_{ijq} := \frac{1}{2}\left(\partial_j g_{iq} + \partial_i g_{jq} - \partial_q g_{ij}\right),$$

by the relation $\Gamma^p_{ij} = g^{pq}\Gamma_{ijq}$ where $(g^{pq}) = (g_{ij})^{-1}$. The (covariant) components of the strain tensor in curvilinear coordinates are defined by the relation

$$\widehat{\varepsilon}_{ij}(\widehat{u}; y) := \varepsilon_{kl}(u; x)[\mathbf{g}_i(y)]_k[\mathbf{g}_j(y)]_l, \qquad \widehat{\varepsilon}_{ij}(\widehat{u}; y) = \frac{1}{2}\left(\widehat{u}_{i\|j} + \widehat{u}_{j\|i}\right), \qquad i, j = 1, 2, 3,$$

and similar the (contravariant) components of the stress tensor are

$$\widehat{\sigma}^{ij}(\widehat{u}; y) := \sigma_{kl}(u; x)[\mathbf{g}^i(y)]_k[\mathbf{g}^j(y)]_l\,, \qquad i, j = 1, 2, 3.$$

In curvilinear coordinates HOOKE's law reads:

$$\begin{aligned}\widehat{\sigma}^{ij}(\widehat{u};y) &= \sigma_{kl}(u;x)[\mathbf{g}^i(y)]_k[\mathbf{g}^j(y)]_l = a_{kl}^{pq}\varepsilon_{pq}(u;x)[\mathbf{g}^i(y)]_k[\mathbf{g}^j(y)]_l \\ &= a_{kl}^{pq}\widehat{\varepsilon}_{mn}(\widehat{u};y)[\mathbf{g}^m(y)]_p[\mathbf{g}^n(y)]_q[\mathbf{g}^i(y)]_k[\mathbf{g}^j(y)]_l =: \widehat{a}_{ij}^{mn}(y)\widehat{\varepsilon}_{mn}(\widehat{u};y)\end{aligned}$$

Rewriting the divergence of the stress tensor in curvilinear coordinates, the equilibrium equations (1) near the crack front read

$$-\widehat{\sigma}^{ij}(\widehat{u};y)\|_j = 0, \quad x=\Theta(y)\in T, \qquad \widehat{\sigma}^{ij}(\widehat{u};y)\widehat{n}_j = 0, \quad x=\Theta(y)\in\Xi^{\pm}, \tag{3}$$

with the components $\widehat{\sigma}^{ij}\|_j := \widehat{\partial}_j\widehat{\sigma}^{ij} + \Gamma_{pj}^i\widehat{\sigma}^{pj} + \Gamma_{jq}^j\widehat{\sigma}^{iq}$ for $i=1,2,3$, see [5] for more details on curvilinear coordinates.

Asymptotic expansion at the crack front.

From nowadays classical results it is known, that also in three dimensions the displacement field has an asymptotic expansion of square-root type at the crack front: $\widehat{u} \sim r^{1/2}\Phi(\varphi;s)$, where $\big(r\cos(\varphi), r\sin(\varphi)\big)^\top = y'$ are polar coordinates in the y'-plane at arc length s (see e.g. [4, 6, 7] and the literature cited there). If we rewrite the elasticity equations (3) in operator notation,

$$\mathscr{L}(y,\nabla_y)\widehat{u}(y) = 0, \quad x=\Theta(y)\in T, \quad \mathscr{N}(y,\nabla_y)\widehat{u}(y)=0, \quad x=\Theta(y)\in\Xi^{\pm}, \tag{4}$$

we can expand the elasticity operator into a series:

$$\big\{\mathscr{L}(y,\nabla_y),\mathscr{N}(y,\nabla_y)\big\} = \sum_{k=0}^{\infty}\Big\{r^{k-2}\mathcal{L}^k(\varphi,\partial_\varphi,r\partial_r,s,\partial_s), r^{k-1}\mathcal{N}^k(\varphi,\partial_\varphi,r\partial_r,s,\partial_s)\Big\}.$$

The first operator $\mathcal{L}^0(\varphi,\partial_\varphi,r\partial_r,s,\partial_s) = \mathcal{L}^0(\varphi,\partial_\varphi,r\partial_r,s) = \mathscr{L}^0(\nabla_{y'},s)$ does not involve derivatives of the arc length and is a homogeneous second-order operator with constant coefficients, namely the elastic moduli transformed to curvilinear coordinates at arc length s at the crack front. Exploiting (4), longer calculations show, that the asymptotic decomposition of the displacement field reads

$$\begin{aligned}\widehat{u}(y) = r^{1/2}\sum_{j=1}^{3}K_{j,1}(s)\Phi_{j,1}^0(\varphi) + r^{3/2}\sum_{j=1}^{3}\bigg(&K_{j,1}(s)\Phi_{j,1}^1\big(\ln(r),\varphi\big) \\ &+ \partial_s K_{j,1}(s)\Phi_{j,1}^2\big(\ln(r),\varphi\big) + K_{j,3}(s)\Phi_{j,3}^0(\varphi)\bigg) + \mathcal{O}\left(r^2\right),\end{aligned}$$

where $K_{j,1}(s)$ are the classical stress intensity factors (SIFs) and $K_{j,3}(s)$ higher-order coefficients. The functions $r^{1/2}\Phi_{j,1}^0$ are solutions of the pure two-dimensional homogeneous problem

$$\mathcal{L}^0(\varphi,\partial_\varphi,r\partial_r,s)r^{\Lambda}\Phi(\varphi) = r^{\Lambda}\mathcal{L}^0(\varphi,\partial_\varphi,\Lambda,s)\Phi(\varphi) = 0, \qquad \varphi\in(-\pi,\pi), \tag{5}$$

$$\mathcal{N}^0(\pm\pi, \partial_\varphi, r\partial_r, s) r^\Lambda \Phi(\pm\pi) = r^\Lambda \mathcal{N}^0(\pm\pi, \partial_\varphi, \Lambda, s)\Phi(\pm\pi) = 0. \tag{6}$$

Similar (non-homogeneous) equations can be found for the higher-order terms [6]. Besides energy solutions, there exist singular solutions $r^{-1/2}\Psi$ of problem (5) - (6). In order to formulate a fracture criterion the first pairs of this power-law solutions,

$$U^0_{j,1}(y') := r^{1/2}\Phi^0_{j,1}(\varphi), \qquad V^0_{j,1}(y') := r^{-1/2}\Psi^0_{j,1}(\varphi), \qquad j = 1, 2, 3$$

have to be normalized in a mechanical reliable sense. Due to [8], the *energy* solutions can be chosen to

$$\frac{1}{2}\Big[U^0_{1,1}\Big](-y_1) = Cr^{1/2}\mathbf{e}_3, \quad \frac{1}{2}\Big[U^0_{2,1}\Big](-y_1) = Cr^{1/2}\mathbf{e}_1, \quad \frac{1}{2}\Big[U^0_{3,1}\Big](-y_1) = Cr^{1/2}\mathbf{e}_2$$

where $[u](y_1) := u(y_1, +0) - u(y_1, -0)$ is the jump over the crack and C a material constant. Using this so-called *strain basis* of power-law solutions, the first SIF is related directly to opening of the crack, the second to sliding of the crack surfaces in the y'-plane and the third to out-of-plane sliding of the crack surfaces. The singular solutions can be chosen in such a way, that

$$\int_{-\pi}^{\pi} \mathcal{N}^0(1/2)\Phi^0_{j,1}(\varphi)\cdot\Psi^0_{i,1}(\varphi) - \Phi^0_{j,1}(\varphi)\cdot\mathcal{N}^0(-1/2)\Psi^0_{i,1}(\varphi)\,d\varphi = \delta_{ij}, \qquad i, j = 1, 2, 3.$$

where $\mathcal{N}^0(\Lambda) := \mathcal{N}^0(\varphi, \partial_\varphi, \Lambda, s)$ [6]. Also in three dimensions SIFs can be calculated using singular weight functions. There exist solutions ζ^j of the homogeneous equations (1) with singular asymptotic behavior at the crack front:

$$\widehat{\zeta}^j(H; y) = H(s)V^0_{j,1}(y') + \ldots = H(s)r^{-1/2}\Psi^0_{j,1}(\varphi) + \ldots, \qquad \|y'\| \to 0,$$

and for smooth functions $H(s)$ the following integral representation holds [3, 6]:

$$\int_{\partial\Omega\setminus\Xi^\pm} p(x)\cdot\zeta^j(H; x)\,dS = \int_\Gamma H(s)K_{j,1}(s)\,ds\,, \qquad j = 1, 2, 3. \tag{7}$$

Griffith' ENERGY CRITERION

As previously discussed, crack propagation can be predicted using the energy criterion [9, 10]. For this it is necessary to calculate the change of potential energy $\Delta\mathbf{U}$ for small crack elongations. Let $\Xi(t)$ be the elongated crack with new crack front

$$\Gamma(t) := \Big\{x(s) + t\Big(h(s)\cos\big(\vartheta(s)\big)n(s) - h(s)\sin\big(\vartheta(s)\big)b(s)\Big) : x(s) \in \Gamma\Big\}$$

Here, $t \geq 0$ is a time-like parameter and $0 \leq th(s) \ll 1$ is the length of the crack shoot in the y'-plane to direction $\vartheta(s)$. We assume, that h and ϑ are smooth functions of the arc length s. To calculate the change of potential energy for small $th(s) \ll 1$, we use the method of matched asymptotic expansions [10]. The principle idea is the following. For a small elongation $th(s)$, the displacement field u^t at time t will not differ too much from the displacement field $u = u^0$ at time $t = 0$ in some distance to the crack front $\Gamma(t)$, hence we approximate u^t by an *outer expansion*

$$u^t(x) \sim u^0(x) + \zeta^1(a^1; x) + \zeta^2(a^2; x) + \zeta^3(a^3; x) + \dots$$

where the functions $a^j = a^j(t, s)$ have to be determined. Near the crack front, the influence of the propagated crack on the solution u^t will be more significant and to detect this at arc length s, we change local coordinates to $\xi = t^{-1}y'$. Sending $t \to 0$ the outer boundary moves to infinity and very close to the crack front we approximate the displacement field by an *inner expansion*

$$u^t\big(t^{-1}y', s\big) = u^t(\xi, s) \sim t^{1/2} w^1(\xi, s) + \dots .$$

For any arc length s the functions $w^1(\cdot, s)$ are solutions of the homogeneous elasticity problem in the plane with a semi-infinite kinked crack (compare to (4)):

$$\mathscr{L}^0(\nabla_\xi, s) w^1(\xi, s) = 0, \quad \xi \in \Omega^h_\infty, \qquad \mathscr{N}^0(\nabla_\xi, s) w^1(\xi, s) = 0, \quad \xi \in \partial\Omega^h_\infty,$$

where $\Omega^h_\infty := \mathbb{R}^2 \setminus \big(\Xi_\infty \cup \Upsilon_h\big(\vartheta(s)\big)\big)$ is an unbounded domain with a semi-infinite crack $\Xi_\infty := \{\xi : \xi_1 \le 0, \xi_2 = 0\}$ and crack shoot $\Upsilon_h\big(\vartheta(s)\big) := \big\{\xi : 0 < \xi_1 \le h(s)\cos\big(\vartheta(s)\big), \xi_2 = \xi_1 \tan\big(\vartheta(s)\big)\big\}$. This is a pure two-dimensional problem depending on s. Scaling $\boldsymbol{\xi} := h^{-1}\xi$, we arrive at a problem in a domain with a kink of fixed length one. Here, we can use the results in [1, 2]: There exist solutions with singular asymptotic decomposition at infinity:

$$\eta^j(\boldsymbol{\xi}) = U^0_{j,1}(\boldsymbol{\xi}) + \sum_{i=1}^{3} M_{i,j}\big(\vartheta(s); h\big) V^0_{i,1}(\boldsymbol{\xi}) + \dots, \qquad |\boldsymbol{\xi}| \to +\infty. \tag{8}$$

and shown in [2, 10] there holds

$$M_{i,j}(\vartheta; h) = -h^{1/2} \sum_{\pm} \left(\int_{\Upsilon^\pm(\vartheta)} \eta^i(\boldsymbol{\xi}) \cdot \mathscr{N}^0(\nabla_{\boldsymbol{\xi}}) U^0_{j,1}(\boldsymbol{\xi})\, d\mathbf{S} \right) =: h^{1/2} M_{i,j}(\vartheta).$$

Inner and outer expansion approximate the same solution u^t only in different regions and must coincide for small $|y'|$ and large $|\xi|$. Both approximations have asymptotic decompositions for $r \to 0$ and $|\xi| \to +\infty$, respectively, in terms of power-law solutions. Rewriting the decomposition (8) in local coordinates, we find

$$t^{1/2} w^1(\xi; s) = \sum_{j=1}^{3} K_{j,1}(s) U^0_{j,1}(y') + t \left(h(s) \sum_{i,j=1}^{3} K_{j,1}(s) M_{i,j}\big(\vartheta(s)\big) V^0_{i,1}(y') \right) + \dots .$$

Matching the decompositions of the *inner* and *outer* expansions, both coincide if

$$a^j(s) := h(s)\sum_{i=1}^{3} K_{i,1}(s) M_{i,j}\big(\vartheta(s)\big).$$

With CLAPEYRON's theorem and inserting the *outer* expansion, the change of potential energy can be calculated to

$$\begin{aligned}\Delta\mathbf{U} = \mathbf{U}(\Xi(t)) - \mathbf{U}(\Xi(0)) &= -\frac{1}{2}\int_{\partial\Omega} p(x)\cdot\big(u^t(x) - u^0(x)\big)\,ds \\ &= -\frac{1}{2}t\left(\sum_{j=1}^{3}\int_{\partial\Omega_0} p(x)\cdot V^{j,1}\big(a^{j,1};x\big)\,ds\right) + \dots \\ &= -\frac{1}{2}t\left(\int_{\Gamma} h(s)\left(\sum_{i,j=1}^{3} K_{i,1}(s) M_{i,j}\big(\vartheta(s)\big) K_{j,1}(s)\right)\,ds\right) + \dots .\end{aligned}$$

This is a generalization of the results in [1, 2, 3] to the fully three-dimensional case with nearly arbitrary crack geometries.

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