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Computational micromechanics model for the convection of a cracks population in a brittle material

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Abstract

We stated in Sánchez et al. (Proc. 15th IMACS World Congress, Vol. 5, 1997, p. 513), the objective rate law governing the general evolution, nucleation, growth and convection, of a diluted 3D population of arbitrarily oriented, penny-shaped, non-interacting stable microcracks that is dragged along the flow of a regular motion of a simple continuous body of brittle material.

This requires the prior analysis of the convection process in the hypothesis of ignoring crack nucleation. It follows that the evolution of the microcrack population is here due only to the rotation of the crack planes as a consequence of the deformation processes of the microcracked brittle solid.

The determinant role of this case in the general evolution problem, is also so in its numerical treatment.

In this paper, use is made of the Bubnov–Galerkin spectral method with respect to the angular variable defining the orientation of a crack to numerically solve the mathematical model of the pure convection of microcracks in the no-nucleation hypothesis.

The paper is completed with three applications. The corresponding microcracks evolutions have been graphically displayed showing a behaviour that agrees with the expected.

Indications about the computer codes implementing the numerical algorithm are included in an appendix.

Keywords: Microcrack evolution; Brittle material; Computational micromechanics model; Galerkin method (method of spherical harmonics); Pseudospectral method

1. Introduction

Our objective is the analysis concerning the convection process of non-interacting stable microcracks embedded in a matrix in the hypothesis of ignoring crack nucleation.

In a simple body B of brittle material a diluted 3D population of penny-shaped microcracks will be dragged along the flow of a regular motion $t \to \phi_t$. We assume implicitly that cracks move without getting out of their planes so that the orientation of an individual crack following the material movement is given

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by an inextensible vector, normal to its plane not necessarily a unit. The non-interacting microcracks approximation will be adopted.

We will also assume the no-nucleation no-growth hypothesis. In this hypothesis the radius of each penny-shaped microcrack remains constant along the motion.

We prove that the evolution of the microcrack population is here due to the rotation of the crack planes as a consequence of the deformation processes of the microcracked solid.

We consider the analysis of this case as an indispensable step towards more complex models.

Our point of view considers a microspace $\wp$ attached to each point of the brittle microcracked solid B. This microspace is in general, a Cartesian product of submanifolds of R^3 in which the internal parameters needed to describe the microcrack population evolution vary.

The evolution process is then described in terms of the new body $B \times \wp$. A motion of $B \times \wp$ is a curve $(t \to B_t \times \wp)$ defined by an evolution operator that extends the flow of our motion by joining as a second operator a smooth flow describing the evolution of the internal parameters. Therefore, the Lie differentiation would be available for these generalised flows on $B_t \times \wp$ with its objectivity properties including even the "diffeomorphism-like" spatial covariance objectivity (Simo, 1988).

In the general case, the extra microscopic variables needed to describe the microcrack pattern (Krajcinovic and Lemaitre, 1987) would be the radius, or the area, of the crack that defines the shape of each penny-shaped crack in the elastic matrix, the material coordinates of the crack center defining the position of each defect, and the normal to the crack plane defining its orientation. Our approach allows us to consider the evolution of the microspace as a "product" of evolution operators depending on the microcrack variables.

Once the general evolution laws are stated, and the mathematical model is correctly posed, a multidimensional pseudospectral numerical method blending different approximations in each of the submanifolds in the microspace (Canuto et al., 1988) can be used to approximately solve the problem respecting the conceived structure. The change of orientation of a crack is not influenced by the other microvariables consequently, its contribution to the general evolution of the microcrack population can be studied separately. The numerical implementation of this model, problem that we solve in this paper, will be essential in the numerical solution of the general model which will be a finite expansion in terms of the tensor product basis of the functional spaces involved in the pseudospectral method.

2. Microcrack population evolution law

2.1. General considerations and notation

We consider a regular motion $t \to \phi_t$ of a simple continuous body of brittle material B.

The collection of orientation preserving diffeomorphisms $\phi_{t,s} = \phi_t \circ \phi_s^{-1}$ mapping $\phi_s(B) = B_s$ onto $\phi_t(B) = B_t$, is the time-dependent flow, the evolution operator, of the spatial velocity vector field $\mathbf{v}$ of our motion.

Both the time-independent configuration of the body B and the present time configuration B_s, will be reference configurations.

"Determinism" is expressed by the Chapman–Kolmogorov law (Marsden and Hughes, 1983) $\phi_{\tau,t} \circ \phi_{t,s} = \phi_{\tau,s}$ and $\phi_{s,s} =$ identity for all τ, t, $s \in R$ for which the flow $\phi_{\tau,s}$ is defined.

We write $x = \phi_{t,s}(X, t)$, so that points in B_s, and also in B, will be denoted by capital letters. Coordinate systems on the ambient space R^3 are denoted by $\{x^i\}$ while those on B or B_s are denoted by $\{X^I\}$. The corresponding spatial and material local bases in the tangent and the cotangent spaces are denoted by $\{\mathbf{e}_i(x)\}$, $\{\mathrm{d}x^i\}$, $\{\mathbf{E}_i(X)\}$ and $\{\mathrm{d}X^I\}$ respectively. The usual inner product in R^3 will be denoted by $(\bullet|\bullet)$.

$\Phi_{t,s}$ represents the deformation gradient of the flow. For each $X \in B_s$, $\Phi_{t,s}(X)$ is the two-point tensor $T_X\phi_{t,s}$, the linear isomorphism from $T_X B_s$ to $T_x B_t$ tangent to the flow at X. Its matrix with respect to the local bases $\{\mathbf{E}_i(X)\}$ and $\{\mathbf{e}_i(x)\}$ is

$$(\Phi_{t,s})^i_K(X) = \frac{\partial \phi^i_{t,s}}{\partial X^K}(X)$$

A vector **a** engraved on the body at the point X in B_s, is transformed within the first order into the vector $\Phi_{t,s}(\mathbf{a})$ engraved on the body at the point $x = \phi_{t,s}(X)$ in B_t at time t. [1] Thusat the microcrack scale the general flow $\phi_{t,s}$ induces a convection whose evolution operator is $\Phi_{t,s}$. [2] Thislinear local flow generates other evolution linear local operators, $\Phi^{\mathrm{T}}_{t,s}$ the transposed of the deformation gradient and the so-called spatial deformation gradients, $\Phi^{-1}_{t,s} = \Phi_{s,t}$ and $\Phi^{-\mathrm{T}}_{t,s} = (\Phi^{-1}_{t,s})^{\mathrm{T}}$ that also satisfy the Chapman–Kolmogorov law.

In particular $\Phi^{-\mathrm{T}}_{t,s} = \left(T_x\phi^{-1}_{t,s}\right)^{\mathrm{T}} : T^*_X B_s \to T^*_x B_t$, with matrix

$$\left(\Phi^{-\mathrm{T}}_{t,s}(x)\right)^i_I = \frac{\partial\left(\phi^{-1}_{t,s}\right)^I}{\partial x^i}(x)$$

with respect to the dual local bases, $\{\mathrm{d}X^I\}$ and $\{\mathrm{d}x^i\}$ plays an important role in this paper.

2.2. Analysis of deformation

As was mentioned before, the orientation of an individual crack following the material movement is given by a vector **n**, normal to its plane not necessarily a unit. This vector is inextensible throughout the evolution process because the orientation of the microcrack does not depend on the length of **n**. Functions depending on the orientation must be zero degree homogeneous. Consequently they only need to be defined on S^2, the unit sphere of R^3, in which case they must have the same value for any unit vector and its opposite, vectors defining the same orientation. [3] To allow the extra microscopic degrees of freedom necessary to define the orientation of the crack we modify the containing space R^3 by "adding" the microspace S^2. The modified space is then $R^3 \times S^2$ and the corresponding new body $B \times S^2$.

[1] Indeed, the material vector $\mathbf{a} = XP \in T_X R^3$ is flow-dragged to $\phi_{t,s}(\mathbf{a}) = \phi_{t,s}(P) - \phi_{t,s}(X)$. The components of this convected vector can be described by a Taylor expansion

$$(\phi_{t,s}\mathbf{a}) = \phi_{t,s}(P) - \phi_{t,s}(X) = \sum_K (\Phi_{t,s})^i_K(X)\mathbf{a}^K + \cdots$$

[2] Using the chain rule in $\phi_{\tau,t} \circ \phi_{t,s} = \phi_{\tau,s}$ we have for all $X \in B_s$

$$T_{\phi_{t,s}(X)}\phi_{\tau,t} \circ T_X\phi_{t,s} = T_X\phi_{\tau,s}$$

that is

$$\Phi_{\tau,t}(\phi_{t,s}(X)) \circ \Phi_{t,s}(X) = \Phi_{\tau,s}(X)$$

so that $\Phi_{\tau,t} \circ \Phi_{t,s} = \Phi_{\tau,s}$ and $\Phi_{s,s} = \mathrm{i}d$ for all τ, t, $s \in R$ for which the flow $\Phi_{\tau,s}$ is defined.

[3] Any continuous function f on S^2, has a continuous extension $\tilde{f}$ to $R^3 - 0 = R^3_*$ defined by $\tilde{f}(\mathbf{n}) = f(\mathbf{n}/\|\mathbf{n}\|)$ which is positively homogeneous of degree zero.

Conversely, any continuous function g on R^3_* positively homogeneous of degree zero is of the form $g = \tilde{f}$ where its generator f is the restriction $g|_{S^2}$ of g to the unit sphere S^2.

When g is zero degree homogeneous, its generator f must satisfy for every $\mathbf{n} \in S^2$, the property $f(\mathbf{n}) = f(-\mathbf{n})$, therefore in order to define g, it suffices to give the values $f(\mathbf{n})$ of its generator on the subset A of S^2 described in Cartesian coordinates by $A = (1,0,0) \cup D^1 \cap H^+_2 \cup S^2 \cap H^+_3$, where H^+_i represents the half space $x_i > 0$ $(i = 2,3)$, and D^1 is the unit disk in the plane $H_3 = 0$.

Thereafter, this function is extended to S^2 by writing $f(\mathbf{n}) = f(-\mathbf{n})$, for every **n** in S^2 that is not in A, and in a final step to R^3_* recalling that the values at **n** and $(\mathbf{n}/\|\mathbf{n}\|) \in S^2$ must be equal.

The functions depending on the orientation are zero degree homogeneous in R^3_* and assuming adequate properties of differentiability, they will satisfy the Eulers theorem that will still hold when their generators on S^2 are considered. This fact will be used in some of the coordinates computations later on. In general, we shall not distinguish between f and $\tilde{f}$.

A state of our physical system at time t is a couple $(x, \mathbf{n}_t) \in B_t \times S^2$, defined by the spatial point x and a normal unit vector $\mathbf{n}_t$ to the plane of the crack. Let $\varphi_{t,s}$ be the evolution operator $(X, \mathbf{n}_s) \rightarrow (x, \mathbf{n}_t)$ that maps a state at time s to what the state would be at time t after time $t-s$ has elapsed. $\varphi_{t,s} = (\phi_{t,s}, \psi_{t,s}) : B_s \times S^2 \rightarrow B_t \times S^2$ is made up with the flow $\phi_{t,s}$ of $\mathbf{v}$ and the flow $\psi_{t,s}$ of $\mathbf{w}$, the time-dependent vector field on S^2 defining the rate of change in orientations of the microcrack population convected by the flow. By studying the motion of an individual crack that follows the material movement, we define the evolution operator $\psi_{t,s}$ that relates, for a fixed particle $X \in B_s$ and any size of crack opening, the unit normal $\mathbf{n}_s$ to the plane Σ_s of a microcrack at time s, to $\mathbf{n}_t$ the unit normal, to the plane $\Sigma_t = \Phi_{t,s}(X) \cdot \Sigma_s$, that contains the microcrack at time t when is convected by the material from B_s to B_t without opening new surface area.

$\mathbf{n}_s$ can be described in terms of the one form α_s such that $\alpha_s \wedge \mu = \omega$, where ω and μ are the volume elements defining the canonical orientation in R^3 and S^2 respectively (see Chapter 2, Box 2.1 of Marsden and Hughes (1983)). We say that α_s is the unit normal to Σ_s. The same unit normal thought of as a vector $\mathbf{n}_s$, satisfies that μ is the interior product $\mu = \mathrm{i}_{\mathbf{n}_s}\omega$, of $\mathbf{n}_s$ and ω.

If $\mathbf{n}_s$ is described in terms of α_s, $\mathbf{n}_t$ will be described in terms of $\alpha_t = (\phi_{t,s})_* \alpha_s$, the push-forward of α_s.

By definition $\alpha_t = (\phi_{t,s}^{-1})^* \alpha_s$ so that

$$\alpha_t(x)(\mathbf{e}_a) = \alpha_s\left(\phi_{t,s}^{-1}(x)\right)\left(T_x\phi_{t,s}^{-1}\right)(\mathbf{e}_a) = \alpha_s\left(\phi_{t,s}^{-1}(x)\right)\left(\Phi_{t,s}^{-1}(x)\right)(\mathbf{e}_a)$$

with

$$\Phi_{t,s}^{-1}(x)(\mathbf{e}_a) = \frac{\partial \phi_{t,s}^{-1}}{\partial x^a}(x) = \sum_A \frac{\left(\partial \phi_{t,s}^{-1}\right)^A}{\partial x^a}\mathbf{E}_A$$

and

$$(\alpha_t)_a(x) = \sum_A (\alpha_s)_A\left(\phi_{t,s}^{-1}(x)\right)\frac{\left(\partial \phi_{t,s}^{-1}\right)^A}{\partial x^a}(x)$$

thus we have

$$\alpha_t(x) = \Phi_{t,s}^{-\mathrm{T}}(x)\left(\alpha_s \circ \phi_{t,s}^{-1}\right)(x)$$

Going back to $\mathbf{n}_s$ with the adequate isomorphisms, we see that $\Phi_{t,s}^{-\mathrm{T}} \cdot \mathbf{n}_s$ defines a normal vector to Σ_t not necessarily a unit.

Considering that $\mathbf{n}_t$ is a unit, we got

$$\mathbf{n}_t = \psi_{t,s}(\mathbf{n}_s) = \frac{\Phi_{t,s}^{-\mathrm{T}}(\mathbf{n}_s)}{\|\Phi_{t,s}^{-\mathrm{T}}(\mathbf{n}_s)\|} \tag{1}$$

Once the evolution operator $\psi_{t,s}$ is defined, we need to find the unique time-dependent field of contravariant vectors $\mathbf{w}$ over S^2, spatial velocity vector field of our motion. [4] $\mathbf{w}_t(\mathbf{n})$ is the tangent vector at $\psi_{s,s}(\mathbf{n}_s) = \mathbf{n}_s$ to the curve $(t \rightarrow \psi_{t,s}(\mathbf{n}_s))$, and is defined for all $\mathbf{n}$ in S^2 by

$$\mathbf{w}_t(\mathbf{n}) = \frac{\mathrm{d}}{\mathrm{d}t}\left[\psi_{t,s}(\mathbf{n}_s)\right]_{|_{t=s}} = \frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{\Phi_{t,s}^{-\mathrm{T}}\mathbf{n}_s}{\|\Phi_{t,s}^{-\mathrm{T}}\mathbf{n}_s\|}\right]_{|_{t=s}} \tag{2}$$

[4] Usually what is given is the time-varying vector field $\mathbf{w}_t$ defining the law of motion and the corresponding evolution operator $\psi_{t,s}$ is defined by

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}(\psi_{t,s}(\mathbf{n})) = \mathbf{w}_t(\psi_{t,s}(\mathbf{n})) \\ \psi_{s,s}(\mathbf{n}) = \mathbf{n} \end{cases}$$

Introducing the auxiliary functions $g : x \to \|x\|^{-1} = (x|x)^{-1/2}$, C^∞ for $x \neq 0$, and $f(t) = \Phi_{t,s}^{-\mathrm{T}}\mathbf{n}_s$ we can write

$$\frac{\Phi_{t,s}^{-\mathrm{T}}\mathbf{n}_s}{\|\Phi_{t,s}^{-\mathrm{T}}\mathbf{n}_s\|} = f(t)(g \circ f)(t)$$

Recalling that

$$g'(x)u = -\frac{1}{\|x\|^3}(x|u)$$

and

$$f'(t) = \frac{\mathrm{d}\Phi_{t,s}^{-\mathrm{T}}}{\mathrm{d}t}\mathbf{n}_s$$

we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{\Phi_{t,s}^{-\mathrm{T}}\mathbf{n}_s}{\|\Phi_{t,s}^{-\mathrm{T}}\mathbf{n}_s\|}\right] = f'(t)(g \circ f)(t) + f(t)(g \circ f)'(t) = f'(t)(g \circ f)(t) - \frac{1}{\|f'(t)\|^3}\left(f(t)|f'(t)\right)$$

so that

$$\frac{\mathrm{d}\mathbf{n}_t}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{\Phi_{t,s}^{-\mathrm{T}}\mathbf{n}_s}{\|\Phi_{t,s}^{-\mathrm{T}}\mathbf{n}_s\|}\right] = \frac{\frac{\mathrm{d}\Phi_{t,s}^{-\mathrm{T}}}{\mathrm{d}t}\mathbf{n}_s}{\|\Phi_{t,s}^{-\mathrm{T}}\mathbf{n}_s\|} - \frac{\left(\Phi_{t,s}^{-\mathrm{T}}\mathbf{n}_s | \frac{\mathrm{d}\Phi_{t,s}^{-\mathrm{T}}}{\mathrm{d}t}\mathbf{n}_s\right)}{\|\Phi_{t,s}^{-\mathrm{T}}\mathbf{n}_s\|^3}\Phi_{t,s}^{-\mathrm{T}}\mathbf{n}_s \tag{3}$$

The material derivative of $\Phi_{t,s}$ is (Malvern, 1969)

$$\frac{\mathrm{d}\Phi_{t,s}}{\mathrm{d}t} = \mathrm{grad}\,\mathbf{v} \cdot \Phi_{t,s}$$

where grad $\mathbf{v}$ represents the gradient in configuration B_t of the spatial velocity field.

We also have

$$\frac{\mathrm{d}\Phi_{t,s}^{\mathrm{T}}}{\mathrm{d}t} = \Phi_{t,s}^{\mathrm{T}} \cdot (\mathrm{grad}\,\mathbf{v})^{\mathrm{T}} \tag{4}$$

and [5]

$$\frac{\mathrm{d}\Phi_{t,s}^{-\mathrm{T}}}{\mathrm{d}t} = -(\mathrm{grad}\,\mathbf{v})^{\mathrm{T}} \cdot \Phi_{t,s}^{-\mathrm{T}}$$

[5] From the evident identity

$$\Phi_{t,s}^{\mathrm{T}}(X) \circ \Phi_{t,s}^{-\mathrm{T}}(x) = \mathrm{i}d_{T_X^* B_s}$$

we get

$$0 = \Phi_{t,s}^{\mathrm{T}}(X) \circ \frac{\mathrm{d}\Phi_{t,s}^{-\mathrm{T}}}{\mathrm{d}t}(x) + \frac{\mathrm{d}\Phi_{t,s}^{\mathrm{T}}}{\mathrm{d}t}(X) \circ \Phi_{t,s}^{-\mathrm{T}}(x)$$

where 0 denotes the zero operator.

Suppressing the arguments and solving for $\mathrm{d}\Phi_{t,s}^{\mathrm{T}}/\mathrm{d}t$

$$\frac{\mathrm{d}\Phi_{t,s}^{\mathrm{T}}}{\mathrm{d}t} = -\Phi_{t,s}^{\mathrm{T}} \circ \frac{\mathrm{d}\Phi_{t,s}^{-\mathrm{T}}}{\mathrm{d}t} \circ \Phi_{t,s}^{\mathrm{T}}$$

and plugging it in the LHS of Eq. (4), we get

$$\frac{\mathrm{d}\Phi_{t,s}^{-\mathrm{T}}}{\mathrm{d}t} = -(\mathrm{grad}\,\mathbf{v})^{\mathrm{T}} \cdot \Phi_{t,s}^{-\mathrm{T}}$$

so that

$$\frac{d\mathbf{n}_t}{dt} = -\frac{(\operatorname{grad}\mathbf{v})^{\mathrm{T}} \cdot \Phi_{t,s}^{-\mathrm{T}}}{\|\Phi_{t,s}^{-\mathrm{T}}\mathbf{n}_s\|}\mathbf{n}_s + \frac{\left(\left((\operatorname{grad}\mathbf{v})^{\mathrm{T}} \cdot \Phi_{t,s}^{-\mathrm{T}}\right)\mathbf{n}_s | \Phi_{t,s}^{-\mathrm{T}}\mathbf{n}_s\right)}{\|\Phi_{t,s}^{-\mathrm{T}}\mathbf{n}_s\|^3}\Phi_{t,s}^{-\mathrm{T}}\mathbf{n}_s$$

Putting $t = s$ and remembering that $\Phi_{s,s} = \mathrm{id}_{T_x^* B_s}$ and $\mathbf{n}_s = \mathbf{n}_t$, we get finally the expression defining the spatial velocity vector field of our motion on S^2.

$$\mathbf{w}(\mathbf{n}) = \left((\operatorname{grad}\mathbf{v})^{\mathrm{T}} \cdot \mathbf{n}|\mathbf{n}\right)\mathbf{n} - (\operatorname{grad}\mathbf{v})^{\mathrm{T}} \cdot \mathbf{n} \tag{5}$$

Also on R^3_* when the normal vector $\mathbf{n}$ is not a unit, but it is inextensible we get.

$$\mathbf{w}(\mathbf{n}) = \frac{\left((\operatorname{grad}\mathbf{v})^{\mathrm{T}} \cdot \mathbf{n}|\mathbf{n}\right)}{\|\mathbf{n}\|^2}\mathbf{n} - (\operatorname{grad}\mathbf{v})^{\mathrm{T}} \cdot \mathbf{n} \tag{6}$$

that we can write

$$\mathbf{w}(\mathbf{n}) = A\mathbf{n} - (\operatorname{grad}\mathbf{v})^{\mathrm{T}} \cdot \mathbf{n} \tag{7}$$

with

$$A = \frac{\left((\operatorname{grad}\mathbf{v})^{\mathrm{T}} \cdot \mathbf{n}|\mathbf{n}\right)}{\|\mathbf{n}\|^2}$$

A is a real zero degree homogeneous function of $\mathbf{n}$ so that $(\mathbf{n}|\operatorname{grad}_{\mathbf{n}} A) = 0$ (Euler's theorem).

In both cases, $(\mathbf{w}(\mathbf{n})|\mathbf{n}) = 0$, expressing that $\mathbf{n}$ being inextensible, remains orthogonal to its velocity, relation that will hold as long as $\|\mathbf{n}\|$ is constant along the motion.

Once the vector field $(\mathbf{v}, \mathbf{w}) : B_t \times S^2 \to T_{(x,\mathbf{n})}(R^3 \times S^2) = (R^3)_x \times T_{\mathbf{n}}S^2$ tangent at time t to the flow $\varphi_{t,s}$ is defined, the push-forward and pull-back operators induced by $\varphi_{t,s}$, or any of its components $\phi_{t,s}$ and $\psi_{t,s}$, can be defined in the usual way; and as a consequence, we can find Lie derivatives of smooth time changing tensor fields along these flows.

2.3. Mathematical description of the microcrack population

We postulate the existence of a time-dependent real function $N(x, t, \mathbf{n})$, defined at time t on $B_t \times S^2$, representing for any size of microcracks, the time evolution of the density of the distribution of the normal vectors to the microcracks per unit volume, per unit of solid angle of S^2. Physically, $N(x, t, \mathbf{n})$ is interpreted as the density (number) of microcracks per unit volume at x, per unit solid angle at $\mathbf{n}$ at time t.

For a fixed spatial point x, $N(x, t, \mathbf{n})$ is a comodular scalar, the unique component of a time-dependent two-exterior differential form β_t on S^2 and must satisfy

$$N(x, t, \mathbf{n}) = N(x, t, -\mathbf{n}) \tag{8}$$

As we have mentioned before, N can be extended to R^3_* maintaining the zero degree homogeneity property by writing for $\mathbf{n} \neq \mathbf{0}$

$$N(x, t, \mathbf{n}) = N\left(x, t, \frac{\mathbf{n}}{\|\mathbf{n}\|}\right)$$

therefore, assuming that N is C^1 in R^3_*, the Euler's theorem holds. [6]

$$(\mathbf{n}|\text{grad}_{\mathbf{n}} N) = 0 \tag{9}$$

Equality that is also true when $\mathbf{n}$ is a unit vector.

In the sequel, $\mathbf{n}$ will denote either a unit vector, or an inextensible vector, not necessarily a unit. [7]

2.4. Objective convected rate of the density of normals distribution

To estimate the change in $N(x,t,\mathbf{n})$ when we convect $\mathbf{n}$, according to the flow $\psi_{t,s}$, we state in the no-nucleation hypothesis the conservation law

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\psi_{t,s}(P)} \beta_t = 0 \tag{10}$$

where P is any nice open set of S^2 (see e.g. Marsden and Hughes (1983) and Abraham et al. (1988))

Using the generalised transport theorem

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\psi_{t,s}(P)} \beta_t = \int_{\psi_{t,s}(P)} \mathscr{L}_{\mathbf{w}_t}\beta_t \tag{11}$$

we have,

$$\int_{\psi_{t,s}(P)} \mathscr{L}_{\mathbf{w}_t}\beta_t = 0 \tag{12}$$

for any P, condition that we will express in local differential form as

$$\mathscr{L}_{\mathbf{w}_t}\beta_t = 0 \tag{13}$$

after this localisation process we get (Sánchez et al., 1997) [8]

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[6] Considerations of N being a distribution not necessarily differentiable in the usual way do not affect the problem.
We can use the following characterisation of a homogeneous distribution. $N \in D'(R^n)$ is homogeneous of degree $p \in R$, iff

$$\sum_{i=1}^{n} x_i \frac{\partial N(x,t,\mathbf{n})}{\partial x_i} = pN(x,t,\mathbf{n})$$

N being a zero degree homogeneous distribution should satisfy Eq. (9) in the distributional sense.

[7]

$$\mathscr{L}_{\mathbf{w}_t}\beta_t = \frac{\partial \beta_t}{\partial t} + (L_{\mathbf{w}_t}\beta_t)$$

where L is the autonomous Lie derivative (Marsden and Hughes, 1983).

[8] Recalling the definition of divergence of a vector field $\mathbf{V}$ on an orientable manifold $\mathbf{X}$ with volume form μ, as the comodular scalar such that $L_{\mathbf{V}}(\mu) = (\text{div}_\mu \mathbf{V})\mu$ and the equality

$$\mathrm{v}(\alpha \wedge \beta) = L_{\mathbf{V}}(\alpha) \wedge \beta + \alpha \wedge L_{\mathbf{V}}(\beta)$$

we have

$$L_{\mathbf{w}_t}\beta_t = L_{\mathbf{w}_t}(N\mu) = (L_{\mathbf{w}_t}N)\mu + NL_{\mathbf{w}_t}\mu = \left(L_{\mathbf{w}_t}N\mu + N\text{div}_\mu \mathbf{w}_t\right)\mu = \left((\text{grad}_\mu N|\mathbf{w}_t) + N\text{div}_\mu \mathbf{w}_t\right)\mu$$

Using the Hodge star operator we get

$$(L_{\mathbf{w}_t}\beta_t)^* = \text{grad}_\mu N|\mathbf{w}_t + N\text{div}_\mu \mathbf{w}_t$$

In our case (non-autonomous Lie derivative)

$$(\mathscr{L}_{\mathbf{w}_t}\beta_t)^* = \frac{\partial N}{\partial t} + (L_{\mathbf{w}_t}\beta_t)^* = \frac{\partial N}{\partial t} + \left(\text{grad}_\mu N|\mathbf{w}_t\right) + N\text{div}_\mu \mathbf{w}_t$$

$$(\mathscr{L}_{\mathbf{w}_t}\beta_t)^* = \frac{\partial N}{\partial t} + (\mathbf{w}_t|\mathrm{grad}_{\mathbf{n}} N) + N\mathrm{div}_{\mathbf{n}}\,\mathbf{w}_t = 0 \tag{14}$$

Going back to the expression (7) where we had defined $\mathbf{w}_t(\mathbf{n})$, we see that

$$\mathrm{div}_{\mathbf{n}}\,\mathbf{w}_t = \mathrm{div}_{\mathbf{n}}\,(A\mathbf{n}) - \mathrm{div}_{\mathbf{n}}\left[(\mathrm{grad}_x\,\mathbf{v})^{\mathrm{T}} \cdot \mathbf{n}\right]$$

and [9]

$$\mathrm{div}_{\mathbf{n}}\,(A\mathbf{n}) = A\mathrm{div}_{\mathbf{n}}\,\mathbf{n} + (\mathbf{n}|\mathrm{grad}_{\mathbf{n}} A) = A\mathrm{div}_{\mathbf{n}}\,\mathbf{n} = 3A\mathrm{div}_{\mathbf{n}}\left[(\mathrm{grad}_x\,\mathbf{v})^{\mathrm{T}} \cdot \mathbf{n}\right] = (\mathrm{div}_x\,\mathbf{v})$$

thus we have

$$\mathrm{div}_{\mathbf{n}}\,\mathbf{w}_t = 3A - (\mathrm{div}_x\,\mathbf{v}) \tag{15}$$

We also have

$$(\mathbf{w}_t|\mathrm{grad}_{\mathbf{n}} N) = (A\mathbf{n}|\mathrm{grad}_{\mathbf{n}} N) - ((\mathrm{grad}_x\,\mathbf{v})^{\mathrm{T}}\mathbf{n}|\mathrm{grad}_{\mathbf{n}} N) = -((\mathrm{grad}_x\,\mathbf{v})^{\mathrm{T}}\mathbf{n}|\mathrm{grad}_{\mathbf{n}} N) \tag{16}$$

plugging the LHS of Eqs. (15) and (16) into Eq. (14) gives us the equation.

$$(\mathscr{L}_{\mathbf{w}_t}\beta_t)^* = \frac{\partial N}{\partial t} - ((\mathrm{grad}_x\,\mathbf{v})^{\mathrm{T}}\mathbf{n}|\mathrm{grad}_{\mathbf{n}} N) + \frac{3N}{\|\mathbf{n}\|^2}(\mathbf{n}|(\mathrm{grad}_x\,\mathbf{v})^{\mathrm{T}}\mathbf{n}) - N\mathrm{div}_x\,\mathbf{v} = 0 \tag{17}$$

3. Formulation of the model

We assume that for each (x,t), $N : \mathbf{n} \to N(t,x,\mathbf{n})$ with $\mathbf{n} \in S^2$, is an element of the Hilbert space $L^2(S^2)$, with the usual inner product $(\bullet,\bullet)$ and associated norm $\|\bullet\|_2$.

N is the trace over S^2 of an element also denoted N, that belongs to $H^1(R^3_*)$. More precisely, the generator of N, varies in the subspace V of $L^2(S^2)$ consisting of all functions satisfying the homogeneity condition $N(t,x,\mathbf{n}) = N(t,x,-\mathbf{n})$.

The convected time rate equation (14), defines a homogeneous linear convection PDE (E) with convection velocity $\mathbf{w}(x,t,\mathbf{n})$, $x \in B_t$, $t \geqslant 0$ and $\mathbf{n} \in S^2$, that with the zero degree homogeneity condition, and the corresponding initial condition, defines the evolution problem (18)

$$\begin{cases} \frac{\partial N}{\partial t} + (\mathbf{w}_t|\mathrm{grad}_{\mathbf{n}} N) + N\mathrm{div}_{\mathbf{n}}\,\mathbf{w}_t = 0 \quad (\mathrm{E}) \\ N(t,x,\mathbf{n}) = N(t,x,-\mathbf{n}) \quad (\text{zero degree condition}) \\ N_0(x,r,\mathbf{n}) \quad \text{is known} \end{cases} \tag{18}$$

Introducing the linear (spatial) differential operator

$$L(x,t,\mathbf{n}) = \left((\mathrm{grad}_x\mathbf{v})^{\mathrm{T}}\mathbf{n}|\mathrm{grad}_{\mathbf{n}}\right) - \left[\frac{3}{\|\mathbf{n}\|^2}\left(\mathbf{n}|(\mathrm{grad}_x\mathbf{v})^{\mathrm{T}}\mathbf{n}\right) - \mathrm{div}_x\,\mathbf{v}\right]Id_{|V} \tag{19}$$

[9] Recalling that A is a real zero degree homogeneous function of $\mathbf{n}$ so that $(\mathbf{n}|\mathrm{grad}_{\mathbf{n}} A) = 0$.
Also from

$$(\mathrm{grad}_x\,\mathbf{v})^{\mathrm{T}} \cdot \mathbf{n} = \sum_{m,a} \frac{\partial \mathbf{v}_m}{\partial x^a}\mathbf{n}^m \mathbf{e}_a$$

we have

$$\mathrm{div}_{\mathbf{n}}\left[(\mathrm{grad}_x\,\mathbf{v})^{\mathrm{T}} \cdot \mathbf{n}\right] = \sum_{m,a} \frac{\partial\left(\frac{\partial \mathbf{v}_m}{\partial x^a}\mathbf{n}^m\right)}{\partial \mathbf{n}_a} = \sum_{m,a} \frac{\partial \mathbf{v}_m}{\partial x^a}\frac{\partial \mathbf{n}^m}{\partial \mathbf{n}_a} = \sum_{m,a} \frac{\partial \mathbf{v}_m}{\partial x^a}\delta_{m,a} = \sum_m \frac{\partial \mathbf{v}_m}{\partial x^m}$$

where $Id_{|V}$ is the identity operator of $L^2(S^2)$ restricted to V, Eq. (17) can be written as

$$\frac{\partial N}{\partial t}(t,x,\mathbf{n}) = L(x,t,\mathbf{n})N(t,x,\mathbf{n}) \tag{20}$$

Clearly $D(L)$ the domain of L, is contained in $L^2(S^2)$.

Thus problem (18) is equivalent to the Cauchy problem

$$\begin{cases} \frac{\partial N}{\partial t} = L(N) & \text{with} \quad N \in V \\ N_0 & \text{is known} \end{cases} \tag{21}$$

where $N_0 : \mathbf{n} \to N_0(\mathbf{n})$ is in V and $\mathbf{n}$ varies in S^2.

4. Numerical implementation of the model

4.1. Method of spherical harmonics

We will use the Bubnov–Galerkin weighted residual method to solve approximately problem (21) by reducing it to a Cauchy problem for a system of ordinary differential equations.

The geometry of the problem suggest to choose the spherical harmonic functions

$$(\{q_{m,k}\};\ m = 0,1,2,\ldots;\ k = 0,\pm 1,\pm 2,\ldots,\pm m)$$

an orthonormal complete system on the unit sphere S^2 equipped with the usual inner product and norm (Neri, 1971), as possible basis functions.

After taking the classical spherical coordinates chart in S^2, only the angular coordinates $\sigma = (\varphi, \psi) \in \Sigma = [0, 2\pi] \times [0, \pi]$ intervene in the transformed equation. [10] The approximation $F_M(t,\sigma)$ with $M \in N$ to the solution $N(t,\sigma)$ is sought in Q_M the linear subspace of $L^2(\Sigma)$ spanned by the spherical harmonics of degree up to M.

$$F_M(t,\sigma) = \sum_{m=0}^{M} \sum_{k=-m}^{+m} c_{m,k}(t) q_{m,k}(\sigma) \tag{22}$$

The basis functions are selected so that the trial functions, satisfy the homogeneity condition that is expressed in spherical coordinates by

$$F_M(t,\pi+\varphi,\pi-\psi) = F_M(t,\varphi,\psi)$$

turning into

$$F_M(t,\pi+\varphi,\pi-\psi) = (-1)^M F_M(t,\varphi,\psi)$$

when plugged in Eq. (22).

This condition is fulfilled by the family $(\{q_{2m,k}\};\ m = 0,1,2,\ldots;\ k = 0,\pm 1,\ldots,\pm 2m)$ of the even degree spherical harmonic functions. This family is an orthonormal complete system on V, consequently our approximating space will be Q'_M the subspace of Q_{2M} spanned by the family of the even degree spherical harmonic functions up to the truncation level $2M$, and the trial functions will be defined by the truncated series

[10] The system $\{q_{m,k}\}$ $m = 0,1,2,\ldots$; $k = 0,\pm 1,\pm 2,\ldots,\pm m$ is an orthonormal complete set on $L^2(\Sigma)$, so that

$$(q_{m,k}(\sigma), q_{r,s}(\sigma)) = \int_{\sigma\in\Sigma} q_{m,k}(\sigma) q_{r,s}(\sigma)\,\mathrm{d}\sigma = \delta_{m,r}\delta_{k,s}$$

where $\mathrm{d}\sigma = \sin\psi\,\mathrm{d}\psi\,\mathrm{d}\varphi$ is the unit sphere measure in spherical coordinates.

$$F_{2M}(t,\sigma) = \sum_{m=0}^{M} \sum_{k=-2m}^{+2m} c_{2m,k}(t) q_{2m,k}(\sigma) \tag{23}$$

4.2. The approximating system of ODE

The $(2M+1)(M+1)$ expansion coefficients $c_{2m,k}$ are determined from the condition expressing in $L^2(\Sigma)$ the orthogonality of the residual

$$R_E(F_M(t,\sigma)) = \frac{\partial F_M(t,\sigma)}{\partial t} - L(t,\sigma) \tag{24}$$

and each of the $(2M+1)(M+1)$ basis functions $q_{2n,l}$ with $n = 0, 1, 2, \ldots$; and $l = 0, \pm 1, \ldots, \pm 2n$

$$(R_E(F_M(t,\sigma)), q_{2m,k}(\sigma)) = \int_{\sigma\in\Sigma} \left(\frac{\partial F_M(t,\sigma)}{\partial t} - L(t,\sigma) \right) q_{2m,k}(\sigma)\,\mathrm{d}\sigma = 0 \tag{25}$$

Taking into consideration the orthonormal properties of the spherical harmonics functions and the expression in Cartesian coordinates of the operator L, we get the set of ordinary differential equations

$$\left\{ \begin{array}{l} n = 0, 1, \ldots, M;\ l = 0, \pm 1, \ldots, \pm 2n \\ \dot{c}_{2n,l}(t) = \left(\sum_{i=1}^{3} \frac{\partial \mathbf{v}_i}{\partial x_i} \right) c_{2n,l}(t) + \sum_{i,j=1}^{3} \frac{\partial \mathbf{v}_j}{\partial x_i} \sum_{m=0}^{M} \left(\sum_{k=-2m}^{k=2m} c_{2m,k}(t) \int_\Sigma \mathbf{n}_j \frac{\partial q_{2m,k}(\sigma)}{\partial \mathbf{n}_i} q_{2n,l}(\sigma)\,\mathrm{d}\sigma \right) \\ \qquad -3 \sum_{i,j=1}^{3} \frac{\partial \mathbf{v}_j}{\partial x_i} \sum_{m=0}^{M} \left(\sum_{k=-2m}^{k=2m} c_{2m,k}(t) \int_\Sigma \frac{\mathbf{n}_i \mathbf{n}_j}{\|\mathbf{n}\|^2} q_{2m,k}(\sigma) q_{2r,s}(\sigma)\,\mathrm{d}\sigma \right) \end{array} \right. \tag{26}$$

Denoting

$$D_{i,j,m,k,r,s} = \int_\Sigma \mathbf{n}_j \frac{\partial q_{2m,k}(\sigma)}{\partial \mathbf{n}_i} q_{2r,s}(\sigma)\,\mathrm{d}\sigma \tag{27}$$

$$B_{i,j,m,k,r,s} = \int_\Sigma \frac{\mathbf{n}_i \mathbf{n}_j}{\|\mathbf{n}\|^2} q_{2m,k}(\sigma) q_{2r,s}(\sigma)\,\mathrm{d}\sigma \tag{28}$$

and

$$A_{i,j,m,k,r,s} = D_{i,j,m,k,r,s} - 3B_{i,j,m,k,r,s}$$

the system of ODE defining the expansion coefficients can be written in the more compact way,

$$\left\{ \begin{array}{l} n = 0, 1, \ldots, M;\ l = 0, \pm 1, \ldots, \pm 2n \\ \dot{c}_{2n,l}(t) = \left(\sum_{i=1}^{3} \frac{\partial \mathbf{v}_i}{\partial x_i} \right) c_{2n,l}(t) + \sum_{i,j=1}^{3} \frac{\partial \mathbf{v}_j}{\partial x_i} \sum_{m=0}^{M} \sum_{k=-2m}^{k=2m} c_{2m,k}(t) A_{i,j,m,k,n,l} \end{array} \right. \tag{29}$$

4.3. The coefficients $A_{i,j,m,k,r,s}$

The integral expression

$$A_{i,j,m,k,r,s} = \int_\Sigma \left(\mathbf{n}_j \frac{\partial q_{2m,k}(\sigma)}{\partial \mathbf{n}_i} - 3 \frac{\mathbf{n}_i \mathbf{n}_j}{\|\mathbf{n}\|^2} q_{2m,k}(\sigma) \right) q_{2r,s}(\sigma)\,\mathrm{d}\sigma \tag{30}$$

defining the coefficients $A_{i,j,m,k,r,s}$ depends only upon the basis functions and is not time-dependent.

In order to evaluate these coefficients, we begin writing

$$\frac{\partial q_{2m,k}(\sigma)}{\partial \mathbf{n}_i} = \frac{\partial q_{2m,k}(\sigma)}{\partial \varphi}\frac{\partial \varphi}{\partial \mathbf{n}_i} + \frac{\partial q_{2m,k}(\sigma)}{\partial \psi}\frac{\partial \psi}{\partial \mathbf{n}_i} \tag{31}$$

then we split $D_{i,j,m,k,r,s}$ as the sum of the two integrals

$$D1_{i,j,m,k,r,s} = \int_\Sigma \mathbf{n}_j q_{2r,s}(\sigma)\frac{\partial q_{2m,k}(\sigma)}{\partial \varphi}\frac{\partial \varphi}{\partial \mathbf{n}_i}\,\mathrm{d}\sigma$$

$$D2_{i,j,m,k,r,s} = \int_\Sigma \mathbf{n}_j q_{2r,s}(\sigma)\frac{\partial q_{2m,k}(\sigma)}{\partial \psi}\frac{\partial \psi}{\partial \mathbf{n}_i}\,\mathrm{d}\sigma$$

Using closed forms of the spherical harmonics $q_{2m,k}$ in terms of φ and ψ (Korn and Korn, 1961) and the following expressions of the components of $\mathbf{n}$ in spherical coordinates

$$\mathbf{n}_i = \|\mathbf{n}\|(\delta_{i,1}\cos\varphi + \delta_{i,2}\sin\varphi + \delta_{i,3})((\delta_{i,1}+\delta_{i,2})\sin\psi + \delta_{i,3}\cos\psi)$$

$(i = 1, 2, 3)$, we find expressions of each one of the four partial derivatives in the RHS of Eq. (31) as a product of two factors depending each one of them only on one of the variables φ and ψ.

This factorisation is particularly adequate for the evaluation process.

In particular we get

$$\frac{\partial \varphi}{\partial \mathbf{n}_i} = -\frac{1}{\|\mathbf{n}\|\sin\psi}[-\delta_{i,1}\sin\varphi + \delta_{i,2}\cos\varphi]$$

and

$$\frac{\partial \psi}{\partial \mathbf{n}_i} = -\frac{1}{\|\mathbf{n}\|}(\delta_{i,1}\cos\varphi + \delta_{i,2}\sin\varphi + \delta_{i,3})((\delta_{i,1}+\delta_{i,2})\cos\psi - \delta_{i,3}\sin\psi)$$

With all this, we obtain expressions of $D1_{i,j,m,k,r,s}$, $D2_{i,j,m,k,r,s}$ and $B_{i,j,m,k,r,s}$ as products of integrals depending only on one of the variables φ and ψ.

Plugging these products in $A_{i,j,m,k,r,s} = D1_{i,j,m,k,r,s} + D2_{i,j,m,k,r,s} - 3B_{i,j,m,k,r,s}$, we write an integral expression of the elements $A_{i,j,m,k,r,s}$ as sum of products of integrals that can be all of them evaluated using a regular Gauss integration technique.

4.4. The initial conditions

We have assumed that the density function $N_0 : \mathbf{n} \to N_0(\mathbf{n})$ representing the initial distribution of the normal vectors to the microcracks per unit volume, per unit of solid angle in the reference configuration is an element of $V \subseteq L^2(S^2)$. Let $S_{M,K}$ be the following symmetric linear combination of even degree spherical harmonic functions, degree $2M$ and order K,

$$\begin{cases} M = 0, 1, \ldots, K;\ l = 0, 1, \ldots, 2M \\ S_{M,K}(\sigma) = \sum_{m=0}^{M-1}\sum_{k=-2m}^{+2m} a_{2m,k}\,q_{2m,k}(\sigma) + \sum_{k=-K}^{+K} a_{2M,k}\,q_{2M,k}(\sigma) \end{cases} \tag{32}$$

The objective is to determine the expansion coefficients in the finite series (32) that best approximate $N_0(\sigma)$.

When

$$a_{2m,k} = \int_\Sigma N_0(\sigma)q_{2m,k}(\sigma)\,\mathrm{d}\sigma \tag{33}$$

Eq. (32) is the partial sums sequence of

$$\begin{cases} m = 0, 1, \ldots, ;\ k = 0, \pm 1, \ldots, \pm 2m \\ N_0(\sigma) = \sum_{m=0}^{\infty} \sum_{k=-2m}^{+2m} a_{2m,k}\, q_{2m,k}(\sigma) \end{cases} \tag{34}$$

the unique Fourier series of $N_0(\sigma)$ with respect to the system $(\{\sigma \to q_{2m,k}(\sigma)\};\ m = 0, 1, 2, \ldots;\ k = 0, \pm 1, \ldots, \pm 2m)$.

The truncated Fourier series, is among the linear combinations (32), the one that best approximates $N_0(\sigma)$ in the norm $\| \bullet \|_2$, and in that case, the partial sums sequence converges to $N_0(\sigma)$ in $L^2(\Sigma)$.

The initial conditions $c_{2m.k}(0)$ for Eq. (29) are the coefficients $a_{2m,k}$ defined in Eq. (33), that we will find approximately.

We have also considered the possibility of using the Fejèr sums of the partial sums sequence $S_{M,K}$ of the Fourier series.

$$\begin{cases} M = 0, 1, \ldots, K;\ l = 0, 1, \ldots, 2M \\ S_{M,K}(\sigma) = \sum_{m=0}^{M-1} \sum_{k=-2m}^{+2m} c_{2m,k}(0) q_{2m,k}(\sigma) + \sum_{k=-K}^{+K} c_{2M,k}(0) q_{2M,k}(\sigma) \end{cases} \tag{35}$$

This Fejèr sums sequence, is the arithmetic means of $\{S_{M,K}\}$

$$\begin{cases} M = 0, 1, \ldots, K;\ l = 0, 1, \ldots, 2M \\ \tilde{F}_{M,K}(\sigma) = \frac{1}{M^2+K+1} \sum_{m=0}^{M} \sum_{k=0}^{K} S_{m,k}(\sigma) \end{cases} \tag{36}$$

and also converges to $N_0(\sigma)$. We can also represent this sequence, as a linear combination of the type (32) with coefficients

$$a_{2m,k} = \left(1 - \frac{m^2 - |k|}{M^2 + K + 1}\right) c_{2m,k}(0) \tag{37}$$

These sums are a classical way of smoothing the higher orders Fourier coefficients.

4.5. The approximating Cauchy problem

The system of ordinary differential equations (29)

$$\begin{cases} n = 0, 1, \ldots, M;\ l = 0, \pm 1, \ldots, \pm 2n \\ \dot{c}_{2n,l}(t) = \left(\sum_{i=1}^{3} \frac{\partial \mathbf{v}_i}{\partial x_i}\right) c_{2n,l}(t) + \sum_{i,j=1}^{3} \frac{\partial \mathbf{v}_j}{\partial x_i} \sum_{m=0}^{M} \sum_{k=-2m}^{k=2m} c_{2m,k}(t) A_{i,j,m,k,n,l} \end{cases}$$

together with the values $c_{2n,l}(0)$ of the expansion coefficients of the Fourier series of $N_0(\sigma)$ in Q'_M

$$c_{2n,l}(0) = \int_{\Sigma} N_0(\sigma) q_{2n,l}(\sigma)\, d\sigma$$

define in Cartesian coordinates, the Cauchy problem determining the evolution of the time-dependent expansion coefficients $c_{2n,l}(t)$ of the trial function $F_{2M}(t, \sigma)$, approximating the solution $N(t, \sigma)$ to problem (21).

5. Examples of application and analysis of results

Assuming an initial microcrack population N_0, the code has been tested with three classical examples, simple traction in the direction of one coordinate axis, the simple shear problem, and a rigid motion, so verifying the material frame indifference behaviour of our approach.

In these experiments the spatial velocity vector field **v** has been imposed, supplying the different codes with the corresponding motions, the initial distribution, and whatever they may require.

In the future, when all these routines act combined in the cracking package of routines, the program will provide these data.

5.1. Simple traction

Let B be an elementary prismatic block of brittle material (Fig. 1) with edges parallel to the axes of the Cartesian coordinate system $[X^i]$ on B. We will denote by $[x^i]$, the coordinate system on the ambient space R^3. If we apply a constant surface traction q along the X^1-axis, the spatial velocity vector field **v** of the corresponding motion is represented by,

$$\mathbf{v} = \begin{pmatrix} \alpha x^1 \\ -v\alpha x^2 \\ -v\alpha x^3 \end{pmatrix}$$

where $\alpha = q/E$ is a constant and E and v are the Young modulus and the Poisson ratio respectively.

The gradient and the divergence of the spatial velocity are,

$$\operatorname{grad}\mathbf{v} = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & -v\alpha & 0 \\ 0 & 0 & -v\alpha \end{pmatrix}; \qquad \operatorname{div}_X \mathbf{v} = \alpha(1-2v)$$

Assuming an initial microcrack population with a uniform distribution of normals of constant density $N_0(\mathbf{n}) = 2.24$ per unit volume, per unit of solid angle of S^2, the evolution of the density distribution of normals of the population due to the deformation of B under this motion, is depicted in Fig. 2a–f.

$N(\mathbf{n})$, the number of microcracks per unit volume, per unit of solid angle of S^2 with normal vector $\mathbf{n} = (\varphi, \psi) \in [0, 2\pi] \times [0, \pi/2]$ is represented in the vertical axis. The total number of cracks will remain constant throughout the evolution in the no-nucleation hypothesis.

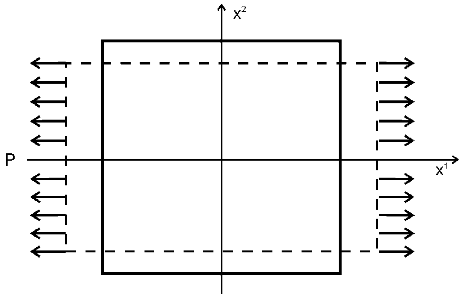

Fig. 1. Simple traction along the X^1-axis.

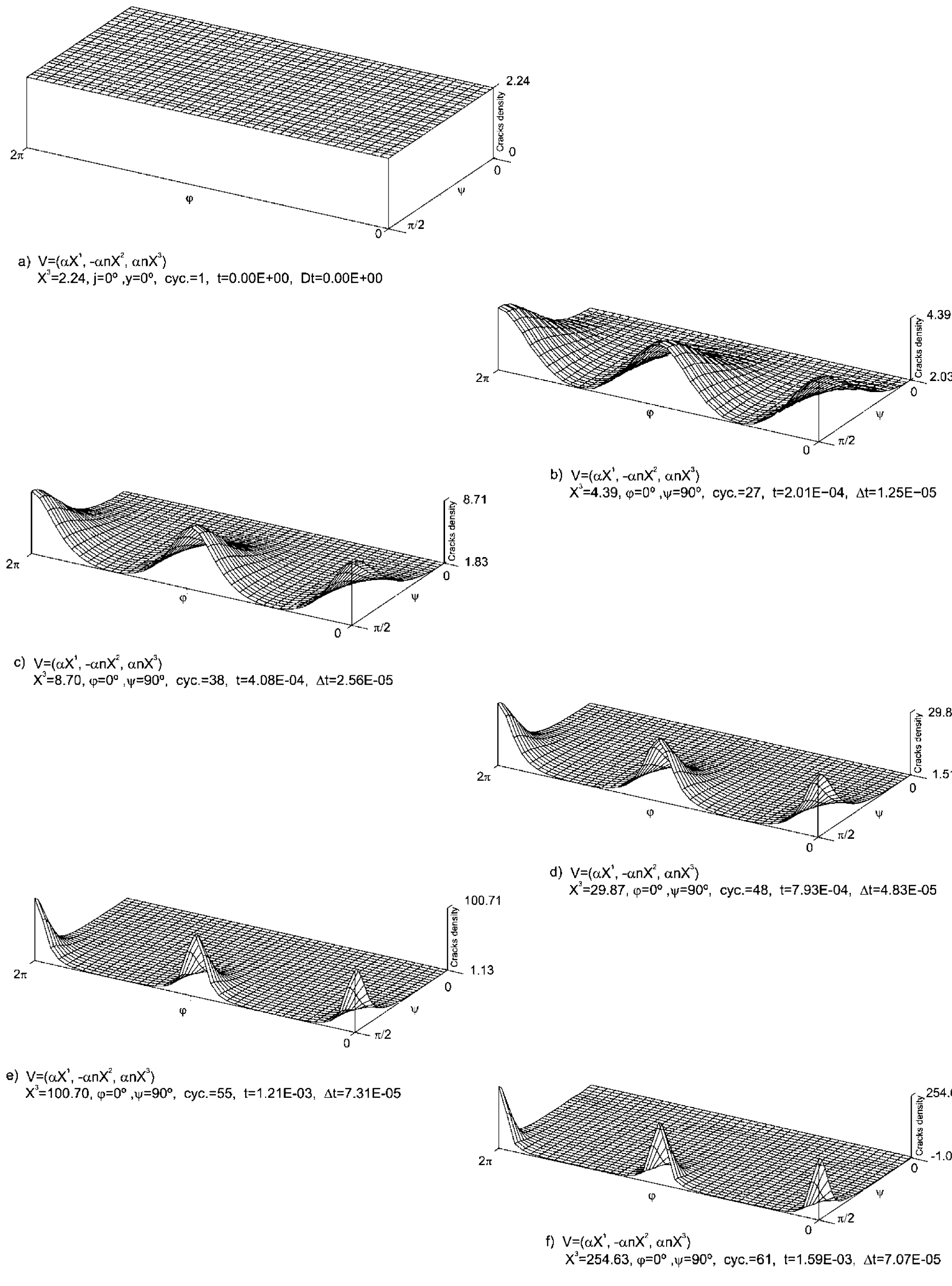

Fig. 2. Evolution of a microcracks population under simple traction along X^1.

The initial distribution is represented in Fig. 2(a). Each figure represents a picture of the evolution corresponding to a progressively increasing tensile or conventional strain. We start imposing a tensile strain

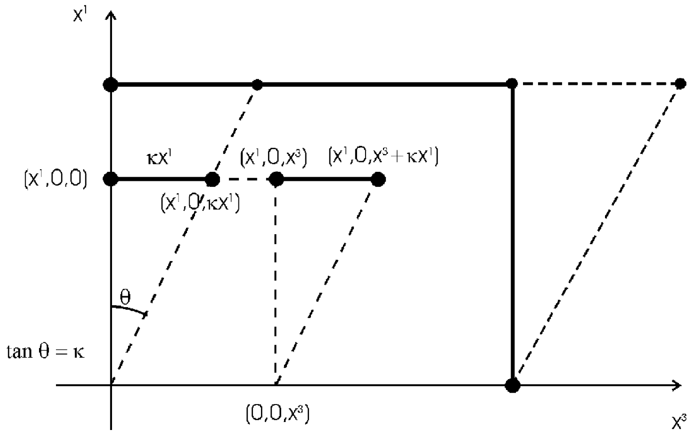

Fig. 3. Deformation under simple shear in the plane X^1X^3 along X^3.

of a 20% [11] Fig. 2b, that is gradually raised up to 40% (Fig. 2c), 80% (Fig. 2d), 120% (Fig. 2e) and 160% (Fig. 2f). [12]

The corresponding uniaxial tension $T = q\mathbf{e}_1$ along the X^1-axis with unit vector $\mathbf{e}_1 = (1,0,0)$; $((\varphi,\psi) = \{(0,\pi/2),(\pi,\pi/2)\})$, causes an increment in the number of microcracks with orientation parallel to $(0,\pi/2)$ or $(\pi,\pi/2)$, directions of maximum tensile stress.

The closer to this orientation the greater the density, and this number increases keeping the same shape as the deformation increases (Fig. 2b–f).

5.2. Simple shear problem

Simple shear in the plane X^1X^3 along X^3. The stress tensor of simple shear with slip plane perpendicular to the X^2-axis and slip direction parallel to the X^3-axis with shearing strain κ is

$$\Sigma = \begin{pmatrix} 0 & 0 & \mu\kappa \\ 0 & 0 & 0 \\ \mu\kappa & 0 & 0 \end{pmatrix}$$

where $\mu = E/2(1+v)$ is the Lame's coefficient.

The deformation $x = \phi(X,t)$ is (Fig. 3).

$$(x^1,x^2,x^3) = (X^1,X^2,X^3 + \kappa X^1)$$

The corresponding displacement vector field

$$\mathbf{v} = \begin{pmatrix} 0 \\ 0 \\ \kappa x^1 \end{pmatrix}$$

Assuming that κ is a linear function of t ($\kappa = \alpha t$, where α is a constant), we get the motion and the spatial velocity

[11] Total elongation of the specimen $0.2L$.

[12] The deformations imposed to the specimen are obviously ideal, a 2% tensile strain of a steel bar would be considered already very high, these non-realistic deformations far beyond any real behaviour, only intend to test the model and the algorithm.

$$(x^1, x^2, x^3) = (X^1, X^2, X^3 + \alpha t X^1)$$

$$\mathbf{v}(x, t) = (0, 0, \alpha x^1)$$

The corresponding gradient and divergence are,

$$\text{grad}\,\mathbf{v} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \alpha & 0 & 0 \end{pmatrix}; \ \text{div}_X\,\mathbf{v} = 0$$

With an initial microcrack population of constant density of normals $N_0(\mathbf{n}) = 22.45$ per unit volume, per unit of solid angle of S^2, the evolution of the population undergoing this motion, is represented in the following Fig. 4a–f.

Assuming that $\alpha > 0$, the major principal stress direction is $(1, 0, 1)$; $((\varphi, \psi) = \{(0, \pi/4), (2\pi, \pi/4)\})$, corresponding to the major principal stress $\mu\alpha$, and consequently there is an increase in the number of microcracks with orientation parallel to the maximum tensile stress. The direction $(0, 1, 0)$; $((\varphi, \psi) = \{(\pi/2, \pi/2), (3\pi/2, \pi/2)\})$, corresponds to the intermediate principal stress 0 and $(1, 0, -1)$; $((\varphi, \psi) = (\pi, \pi/4))$, the minor principal stress direction corresponding to the compression $-\mu\alpha$.

The changes of the number of cracks for these three orientations are a consequence of the hypothesis of the conservation law (10)—no-nucleation—stable cracks.

5.3. Rigid motion

In order to test the material frame indifference behaviour of our model, we have applied the code to a rigid deformation, given by the transformation $\xi(x) = Qx + \mathbf{c}$, where Q is a proper orthogonal matrix and $\mathbf{c}$ is a constant vector.

We have considered a rotation about the X^1-axis with constant angular velocity ω.

$\mathbf{c} = \mathbf{0}$ and matrix Q is then

$$Q = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\omega t & -\sin\omega t \\ 0 & \sin\omega t & \cos\omega t \end{pmatrix}$$

The spatial velocity vector field $\mathbf{v}$ will be given by

$$\mathbf{v} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\omega \\ 0 & \omega & 0 \end{pmatrix} \begin{pmatrix} X^1 \\ X^2 \\ X^3 \end{pmatrix} = \begin{pmatrix} 0 \\ -\omega X^3 \\ \omega X^2 \end{pmatrix}$$

The gradient and the divergence of $\mathbf{v}$ are,

$$\text{grad}\,\mathbf{v} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\omega \\ 0 & \omega & 0 \end{pmatrix}; \ \text{div}_X\,\mathbf{v} = 0$$

Assuming an initial microcrack population that follows a binormal distribution with mean vector $(\pi, \pi/4)$ and standard deviation $(\pi/18, \pi/6)$ (Fig. 5), the convection of the population for a complete rotation about the X^1-axis has been studied.

The different results appear in Fig. 6a–f where the evolution of the population for the intermediate angles $\pi/3$, $2\pi/3$, π, $4\pi/3$, $5\pi/3$, and 2π has been represented, showing clearly that the microcrack population, has not been affected by the motion.

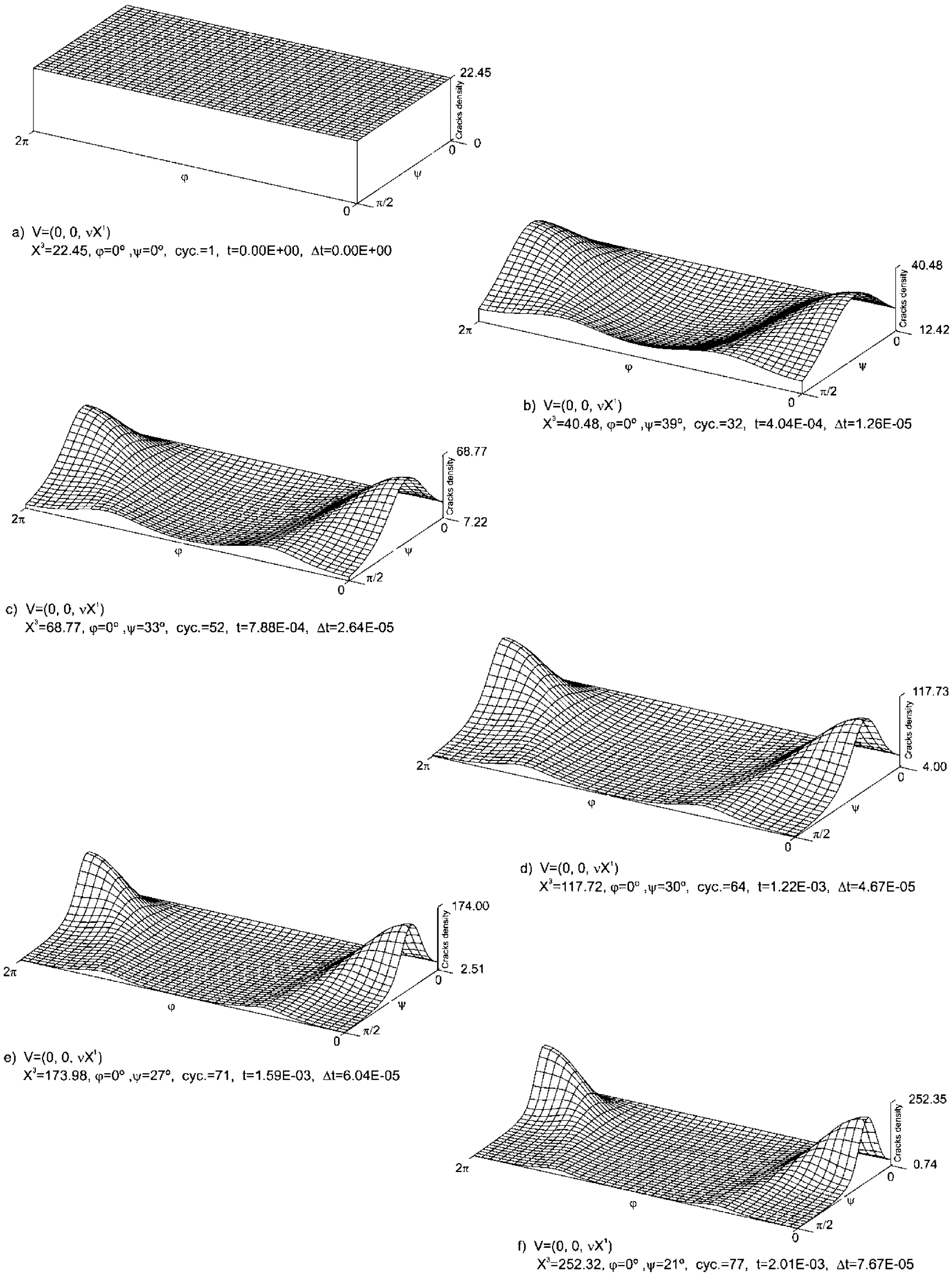

Fig. 4. Microcracks distributions for simple shear in the plane X^1X^3 along X^3.

6. Conclusions

This paper deals with the analysis of the convection process of non-interacting stable microcracks embedded in a matrix in the hypothesis of ignoring crack nucleation.

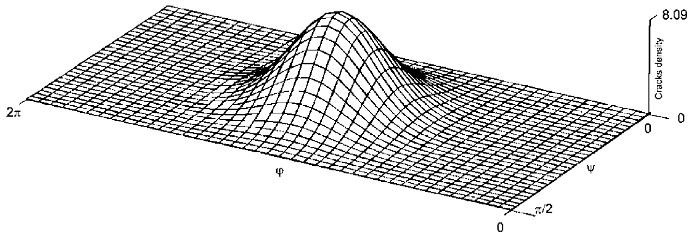

Fig. 5. Initial distribution for the case "rotation about the X^1-axis".

One first conclusion of the analysis of the Lie derivative convected rate of the density of orientations of cracks function, is that the evolution of the microcrack population is here due only to the rotation of the crack planes as a consequence of the deformation processes of the microcracked solid.

The idea underlying this analysis is that micromechanical study of damage and of continuum mechanics as a whole can be approached in a computational fashion. In this sense, this paper is considered an important contribution to a general formulation of a microfracture model for brittle cracking.

Our mathematical approach of the general problem combined with the use of pseudospectral methods to numerically solve the problem, suggest that the numerical implementation of the model discussed in this paper, will be essential in the numerical approach of the general model through the tensor product basis of the Cartesian product of the functional spaces in the microvariables involved in the description of the microcrack pattern.

The corresponding algorithm will be a set of routines simulating the microcracks behaviour within a high rate simulation computer program of brittle cracking.

Appendix A. Some computational details

A.1. The general flow of computations

In this section, we outline the role that should play the evolution of the microcracks population, in a structural dynamics stress analysis code.

The time dependence on the evolution of the crack population equation (E) comes through the stresses in the present model and so, it is coupled to the stress vs. strain relationship and through it, also to the conservation laws.

However, many computer codes would treat (E) as uncoupled at each step to the conservation laws (Zukas, 1992) with the usual technique of changing its coefficients in due manner at the next time step.

A typical high rate simulation code will advance time steps by switching back and forth from a conservation laws program (CLP) to subroutines simulating the material behaviour (MBR).

By and large, the CLP obtains from the MBR a discrete version of the stress field σ_n at a certain time t_n and computes among several quantities an update ϵ_{n+1} of the strain that together with some history variables stored, constitute the main input of the MBR.

These behaviour routines, work in a kind of implicit overall scheme. They need to start up a convenient guessed update of the chosen field, which is compared at some point with a computed update of that field. Should both fields agree the update process as a whole is declared finished and, as a result a special update σ_{n+1} of the stress field is determined, among other updates, and put into the CLP.

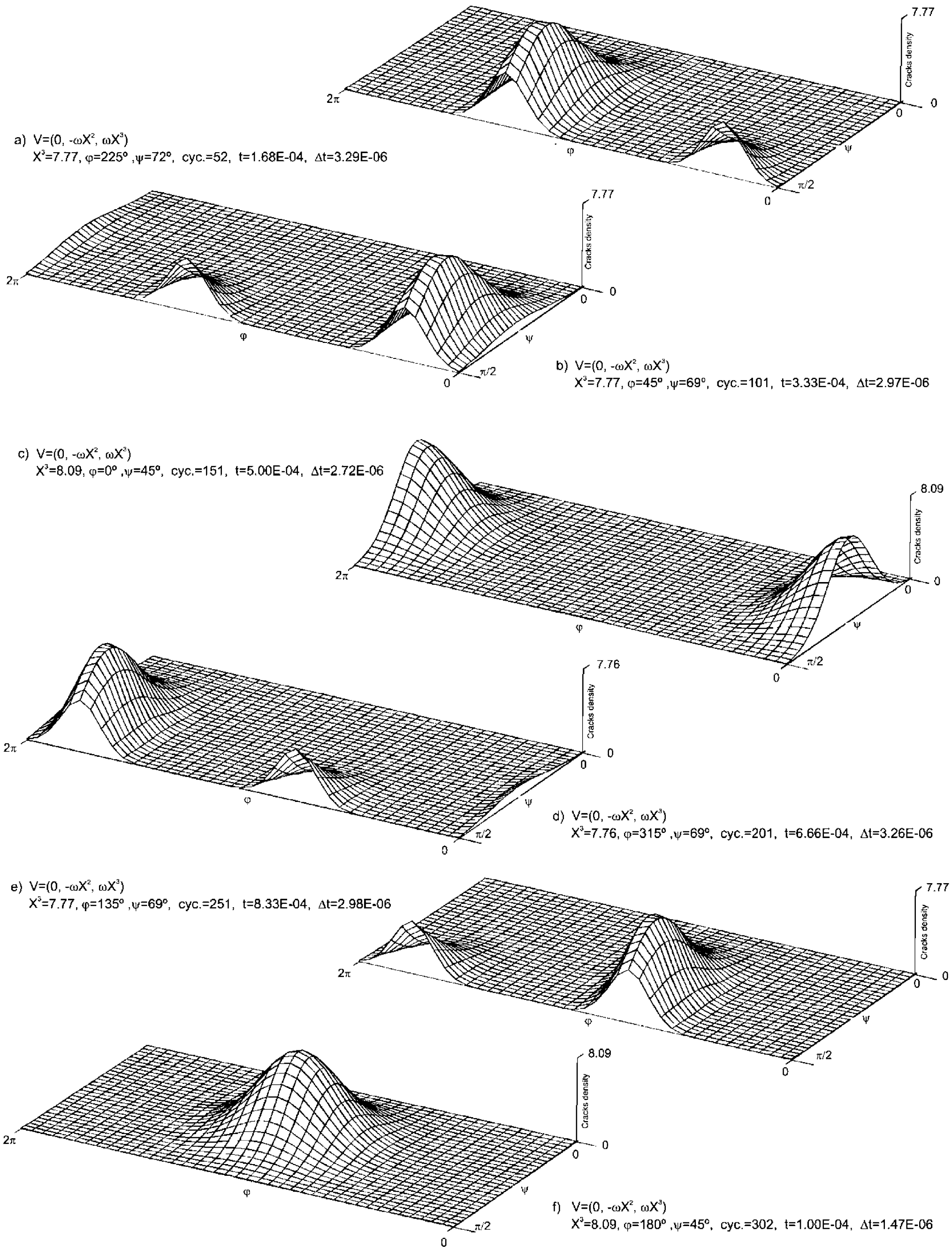

Fig. 6. Microcracks distributions for rotations about the X^1-axis. Rotation angles: 60°, 120°, 180°, 240°, 300° and 360°.

If these fields do not match, the behaviour routines need to provide a new guess, starting an iteration process.

Some of the most important routines in MBR form the CRACKING package. This set of routines produce at each time step, and each iteration cycle, the crack strain fields, an update of the microcrack density function $N(t, \mathbf{n})$, and the crack density or damage tensor (Kachanov, 1987).

In order to learn about the state of damage of our material at time t, we need an update of the density function that we obtain approximately solving problem (21) using the described algorithm.

Several codes have been written to accomplish this goal. They have been included in the Fortran program CAL. The main features of CAL are described in Section A.2.

Although it is quite clear how CAL should be embodied in the general program, this has not been done yet, and as a consequence, users must specify to CAL the motion of the microcracks population and any other information inputs required by the different codes.

A.2. Description of the program CAL

The Fortran program CAL updates at each time step of the pure convection evolution process, the density of microcracks population in the microcracked brittle material.

The code starts reading the elements of matrix A, the constant coefficients of the approximated system (29), which need to be evaluated only once throughout the whole process using the technique developed in Section 4.3.

After that, the truncation level of the spherical harmonics series is declared (in detail we fix M, the said level $2M$ cannot exceed 10). In a realistic application of this method, the computational cost would probably require smaller truncation levels.

The next data we feed into the program is the definition of the initial distribution of microcracks. The code contemplates three different options:

- A microcracks population with a uniform orientation distribution.
- A microcracks population with one prevailing orientation characterised by a bidimensional normal distribution, which is approximated by a linear combination of spherical harmonics. The Fourier coefficients of this expansion are evaluated using a Gauss–Legendre numerical integration method.
  A 10th order approximation of an initial binormal distribution is represented in Fig. 5.
- To continue with the computation when the input data is a final distribution of microcracks, a result of previous steps.

Once the knowledge of the initial conditions of the Cauchy problem is completed, the motion of the body that will produce the evolution under study should be given. In a general simulation program, this information will be provided by the CLP.

After the motion is specified, the gradient and the divergence of $\mathbf{v}$ are evaluated. With this information, the process of integration of the approximating system (29) starts.

We have equipped our code with two integration routines, an embedded Runge–Kutta method (Calvo et al., 1990) for non-stiff problem (Hairer et al., 1991) and a variable step size BDF for stiff problem (Hairer et al., 1981). We decide which one should be used by analysing the R–K step size evolution versus stability and accuracy, that will show us the degree of stiffness of the system. The time integration of Eq. (29) can be done as part of the time step integration scheme of the general finite element program. At the end of each computation, the code graphically displays the microcracks distribution approximation at time t or after a prescribed number of time steps. The corresponding illustration represents for a particle X a picture (at time t) of the density (number of cracks per unit volume per unit of solid angle) of the distribution in orientation of the population. It also prints out the time evolution of several of the most representative quantities in the microcracks distribution. All the details related to these routines are given in Vega Miguel (1996).

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