A $J$-integral-based arc-length solver for brittle and ductile crack propagation in finite deformation-finite strain hyperelastic solids with an application to graphene kirigami

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Highlights

- We present a new path-following method for crack propagation in hyperelastic media.
- It provides an explicit formula of the $J$-integral for different propagation angles.
- It reconciles with the theory of configurational forces and Griffith’s balance.
- This arc-length can handle very sharp snap-back paths in the equilibrium curve.
- We present an example to fracture in large strains of graphene kirigami sheets.

Abstract

Arc-length methods based on Newton–Raphson (NR) iterative numerical solvers are indispensable in non-linear mechanics to trace the equilibrium curves of systems with snap-back or snap-through behaviours. An example is a crack propagating in a rubber-like solid, which can generate extremely sharp snap-backs when the elastic energy is released.

A standard arc-length solver satisfies the arc-length constraint which only limits the increment in displacements and in load level to a fixed amount. Thus, it cannot guarantee the satisfaction of the energy balance in the rate form. This work proposes an arc-length based on the $J$-integral, and assumes the Griffith balance as a constraint equation.

Firstly, a fracture criterion (critical load and direction of crack increment) is formulated, consistent with the thermodynamic principle of maximum dissipation: a crack propagates in the direction of the maximum strain energy release rate. For this purpose, this paper provides an explicit and simple expression of the $J$-integral for varying angles. This fracture criterion does not require the computation of mixed mode Stress Intensity Factors, or asymptotic solutions or derivatives of the tangent stiffness matrix. By doing so, it is shown that the proposed method easily reconciles with the theory of Configurational Forces.

Secondly, because of the explicit expression of $J$ provided in this paper, it is easy to linearize the discretized equations of motions consistently.

The method proves able to handle very sudden snap-backs occurring under large strains, and both brittle and ductile crack propagation. A particular example of such behaviour is kirigami (paper-cuts) structures made of graphene. The proposed arc-length can capture, for these structures, the transitions from brittle to ductile crack propagation for the same crack patterns, but different pre-crack lengths.

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1. Introduction

The response of a dynamical system (not necessarily mechanical) is given by a set of non-linear first order Ordinary Differential Equations (ODEs). The functional expression of these ODEs might contain several (structural) parameters, and it is often of interest to compute the susceptibility of the static response to such parameters. In static conditions, the initial system of ODEs reduces to a non-linear system of algebraic equations. The roots of this system constitute its equilibrium curves, and the techniques to obtain these curves fall under the name of numerical continuation. Numerical continuation is a well-established branch of the theory of dynamical systems, and a vast literature exists on this topic. The interested reader can refer to the following cardinal textbooks for an introduction and more detailed references [1–3].

In mechanics, the equilibrium is, from a dynamical systems perspective, a single-parameter non-linear problem, with the parameter being a proportional scaling factor of the external forces [4]. The equilibrium curves of a mechanical system are, for this reason, often displayed as force–displacement diagrams. Equilibrium curves in mechanical systems permit, for example, the computation of the maximum sustainable force, and the detection of critical points of instability and bifurcations. To track the equilibrium curves, one could increase the load level (load-control) by small increments; nonetheless, this approach would fail for systems with force–displacement constitutive law. Thus, for these cases, a better option would be to apply displacements, instead of forces, (displacement-control): however, this approach would fail for a non-monotonic displacement in the force–displacement constitutive law. These situations are known as snap-backs (Fig. 1). Riks [5,6] was the first to propose an arc-length method able to trace snap-backs. The idea in the Riks’ method is to add a constraint equation to the nonlinear system, which would limit both the variations in load level and displacements (Fig. 1). Several variants were proposed to the original algorithm: to name just a few, we mention the line-search [7], local arc-length [8], local arc-length for strain softening [9,10], orthogonal methods [11], asymptotic-numerical methods based on Pade approximants [12–14], dissipation-based arc-length [15–18] and kinetic damping [19].

Recent novel contributions to the field include parallelization [20], gluing of multiple Partial Differential Equations (PDEs) into a single numerical continuation framework [21] and gradient-constrained methods [22]. It is also worth mentioning the availability of free Matlab software [23] for continuation and bifurcation in 2D elliptic systems.

When considering fracture of hyperelastic media in finite deformation, the application of the standard Riks’ arc-length would result in overestimating the equilibrium force required to satisfy the Griffith criterion [24]. This will be illustrated with a numerical example in Section 7.3. The reason is that a standard arc-length method only limits the increments in load and displacement, disregarding the energy balance. The dissipation-based arc-length proposed in [15,16] does instead limit the increments in dissipated energy. We discuss the differences between our method and the dissipation-based arc-length more in detail in Section 4.2. For example, [16] applied their method to geometrically non-linear models coupled with plasticity and cohesive zone elements. Instead, in this work we propose a framework with non-linearities for both, geometry and material (hyperelasticity), combined with an explicit treatment of strong discontinuities based on a meshfree discretization. Building on the merits of the idea of an energy-release control method, we anticipate that a $J$-integral based approach provides a more direct way to the satisfaction of the Griffith criterion, on the rate (in the fracture mechanics’ sense) of the energy release.

Moreover, the arc-length proposed in this paper allows simultaneously the incorporation of a criterion for the crack direction. Strictly speaking the non-linear problem becomes a two-parameters numerical continuation (the load level $\lambda$ and the crack orientation $\theta$), as shown in Section 4.3. However, it is shown that it can be transformed into a single-parameter continuation, thanks to an explicit expression of the $J$-integral as a function of $\theta$. This approach allows our method to reconcile with the framework of configurational forces for fracture in finite deformation, contained in a series of seminal works [25–30].

To conclude, Section 7 presents several numerical examples. Firstly, the numerical $J$-integral is validated against an analytical solution of (Section 7.1) from [31–33]; then, the hypothesis behind the fracture criterion is verified by
Fig. 1. Spherical arc-length scheme: \((d_0, \lambda_0)\) is the previously converged state, \((d, \lambda)\) is the next solution on the path. \((\Delta d_k, \Delta \lambda_k)\) is the increment at the \(k\)th iteration. \((\delta d_k, \delta \lambda_k)\) is the iterative step to the increment.

introducing small kinked cracks at the tips of an inclined centred larger crack (Section 7.2); subsequently the proposed method is compared to a standard arc-length, and it is shown its ability to verify the Griffith balance (Section 7.3); next, the propagation of two aligned and misaligned edge-notched cracks (Section 7.4) is studied, with comparisons with the maximum hoop stress criterion in the limits of infinitesimal deformations (Section 7.5). Finally, the arc-length is tested for a type of graphene kirigami structure that contains multiple cracks (Section 7.6).

2. Governing equations

2.1. Variational formulation

In this section, the adopted continuum formulation is Total Lagrangian, with \(B_0 \subset \mathbb{R}^k\), \(k = 2, 3\) being the reference configuration at initial time \(t_0\), and \(B_t\) the deformed configuration at a generic time \(t\). In the following, \(X\) denote the material coordinates and \(x\) the deformation. The deformation is given by the admissible mapping

\[
x = \varphi(X, t) \quad \varphi : (B_0 \setminus \Gamma_0^0) \times [t_0, t_f] \mapsto B_t \setminus \Gamma_c^0 \quad k = 2, 3
\]

with \(t_f\) being the final time and \(\Gamma_c^0\) the image of the current configuration of \(\Gamma_c^0\). We assume that the mapping is bijective everywhere on \(B_0\) with the exception of \(\Gamma_0^0\)

\[
\Gamma_c^0 = \bigcup_{i=1}^{n_c} \Gamma_{c_i}^0 \quad \Gamma_{c_i}^0 \subset \mathbb{R}^{k-1}
\]

with \(\Gamma_{c_i}^0\) being the \(i\)th crack surface and \(n_c\) the number of crack surfaces. It is assumed in the proceeding, that each \(\Gamma_{c_i}^0\) can be a piecewise set of segments for two-dimensional problems, or polygonal flat surfaces for three-dimensional problems. In 2D, for example, for a straight crack,

\[
\Gamma_{c_i}^0 = \left\{ X \in B_0 : X \neq X_{c_i}^0 \right\} \quad X_{c_i}^0 : [s_0, s_f] \in \mathbb{R} \mapsto \mathbb{R}^{k-1} \quad X_{c_i}^0(s) = X_0(1-s) + X_1s
\]

with \(s\) being the parameter, \(s_0\) and \(s_f\) being respectively the initial and the final value at time \(t_0\) and \(t_f\), and \(X_0\) and \(X_1\) the crack-tips. If \(X_0, X_1 \in B_0 \setminus \partial B_0\), then the crack is internal, otherwise, if any of the two tips are on the boundary or outside, the crack is named edge crack.

The deformation gradient \(F\) is readily obtained as

\[
F = \nabla_0 \varphi(X, t) \quad J = \det(F) > 0 \quad X \in B_0 \setminus \Gamma_c^0
\]

where the subscript \(0\) refers to the material coordinates. We then define the following functionals: the internal energy \(W\)

\[
W[\varphi] = \int_{B_0} w(F) dV
\]
with \( w \) being the strain energy function of the hyperelastic constitutive model; the external work functional (in the absence of body forces)

\[
\mathcal{P} [\varphi] = \lambda \int_{\Gamma_0^p} \dot{\mathbf{u}}^T \mathbf{u} \, dS + \lambda \int_{\Gamma_0^u} \gamma (\mathbf{u} - \bar{\mathbf{u}})^T (\mathbf{u} - \bar{\mathbf{u}}) \, dS
\]

where \( \mathbf{u} \) is the displacement field \( \mathbf{u} = \varphi(\mathbf{X}) - \mathbf{X} \), and \( \lambda \) is the load level (the continuation parameter); the boundary \( \Gamma_0^p \subset \partial B_0 \) is where the traction \( \lambda \mathbf{t}_0 \) is prescribed, with \( \mathbf{t}_0 \) being a unit vector and \( \lambda \) the load level; \( \Gamma_0^u \subset \partial B_0 \) is the boundary where the displacement \( \bar{\mathbf{u}} \) is prescribed, and \( \gamma \) is a penalty factor. Finally, we introduce the potential energy functional as

\[
\Pi [\varphi] = \mathcal{W} [\varphi] - \mathcal{P} [\varphi].
\]

Fig. 2 show \( \mathcal{W}, \mathcal{P} \) and \( \Pi \) in a simplified one-dimensional example. The problem is then formulated as: find the motion \( \varphi \) or the displacement field \( \mathbf{u} \) such that

\[
\varphi = \text{arg} \min_{\varphi \in \mathcal{H}^1(B_0)} \Pi [\varphi]
\]

where \( \mathcal{H}^1(B_0) \) is the space of vectorial functions in \( L^2(B_0) \) that are square-integrable along with their first derivatives. Since we are interested in equilibrium conditions, the kinetic energy functional is not considered here. However, for the sake of an iterative numerical scheme, it is appropriate to define the rate quantities and the variations of the functionals in Eqs. (5)–(7).

\[
\dot{\mathcal{W}}[\dot{\varphi}, \varphi] = \int_{B_0} \dot{\mathbf{w}}(\mathbf{F}) dV = \int_{B_0} \frac{\partial w}{\partial \mathbf{C}} : \dot{\mathbf{C}} \, dV = \int_{B_0} \frac{1}{2} \mathbf{S} : 2\dot{\mathbf{E}} \, dV = \int_{B_0} \mathbf{S} : \dot{\mathbf{E}} \, dV
\]

where \( \mathbf{C} \) is the Right Cauchy–Green tensor, \( \mathbf{E} \) is the Green–Lagrange strain tensor, \( \mathbf{S} \) is the Second Piola–Kirchhoff stress tensor

\[
\mathbf{C} = \mathbf{F}^T \mathbf{F} \quad \mathbf{E} = \frac{1}{2} (\mathbf{C} - \mathbf{I}) \quad \mathbf{S} = 2 \frac{\partial w}{\partial \mathbf{C}}
\]

and the corresponding variation is

\[
\delta \mathcal{W}[\delta \varphi, \varphi] = \int_{B_0} \mathbf{S} : \delta \mathbf{E} \, dV.
\]

The rate of the external work is

\[
\dot{\mathcal{P}}[\dot{\varphi}, \varphi] = \lambda \int_{\Gamma_0^p} \dot{\mathbf{u}}^T \mathbf{u} \, dS + \lambda \int_{\Gamma_0^u} \gamma \dot{\mathbf{u}}^T (\mathbf{u} - \bar{\mathbf{u}}) \, dS
\]

with the corresponding variation

\[
\delta \mathcal{P}[\delta \varphi, \varphi] = \lambda \int_{\Gamma_0^p} \delta \mathbf{u}^T \dot{\mathbf{u}} \, dS + \lambda \int_{\Gamma_0^u} \gamma \delta \mathbf{u}^T (\mathbf{u} - \bar{\mathbf{u}}) \, dS.
\]

Eq. (8) can be reformulated as

\[
\delta \Pi [\delta \varphi, \varphi] = \delta \Pi [\delta \mathbf{u}, \mathbf{u}] = 0
\]

that is

\[
\int_{B_0} \delta \mathbf{E} : \mathbf{S} dV - \int_{\Gamma_0^p} \delta \mathbf{u}^T \lambda \mathbf{t}_0 \, dS - \gamma \int_{\Gamma_0^u} \delta \mathbf{u}^T (\mathbf{u} - \bar{\mathbf{u}}) \, dS = 0.
\]

Another rate of interest is the strain energy release rate \( G \).

\[
G[\varphi_a] = -\frac{\partial \Pi[\varphi_a]}{\partial A} = \frac{\partial \mathcal{P}[\varphi_a]}{\partial A} - \frac{\partial \mathcal{W}[\varphi_a]}{\partial A} = \frac{1}{2B} \lim_{\Delta a \to 0} \frac{\Pi[\varphi_a + \Delta a] - \Pi[\varphi_a]}{\Delta a}
\]
where \( A = 2B a \) is the crack surface area, where \( B \) is the thickness of the body (in 2D), and \( a \) is the crack length.

\[
a = \int_{\Gamma_0} ds. \tag{17}
\]

The subscript \( a \) in Eq. (16) indicates the motion of the body \( B_0 \) containing cracks \( \Gamma_0^a \) of measure \( a \). The term rate is intended in the fracture mechanics’ sense, meaning with respect to the fracture area, and not with respect to time.

2.2. Discretized equations of motion

Because of the ease of introducing discrete cracks without remeshing, we will use a meshfree setting, namely the Reproducing Kernel Particle Method (RKPM) [34]. For the explicit treatment of cracks, we follow the intrinsic enrichment presented in [35–37].

Let us first define the functional spaces for the test and the trial functions. We adopt a Bubnov–Galerkin method, for which test \( \delta u(X) \) and trial \( u(X) \) vectorial functions are chosen in affine spaces. For the test functions, we select the following Sobolev space \( V \) defined as:

\[
\delta u(X) \in V = \left\{ \delta u(X) \in H^1(B_0) \mid \delta u(X) = 0 \in \Gamma_u \right\} \tag{18}
\]

whilst for the trial functions, we select the Sobolev space \( S \)

\[
u(X) \in S = \left\{ u(X) \in H^1(B_0) \right\}. \tag{19}
\]

In the definition (19) we purposely left out the constraints imposed by the essential boundary conditions since the RKPM approximation used in the weak form does not satisfy the Kronecker condition. Therefore, essential boundary conditions will be enforced through penalty conditions. Furthermore, we pose no restrictions on the continuity of these functions, since we are seeking a discontinuous approximation.

2.3. RKPM approximation

We discretize the body \( B_0 \) with a cover of \( N \) overlapping spheres \( Q_I \subset B_0 \) of variable radii \( r_I \), \( I = 1, \ldots, N_I \), such that \( B_0 \subset \bigcup_{I=1}^{N} Q_I \). We call nodes the centres of these spheres \( X_I \), and we consider \( h \) as an average measure of the distance between two neighbouring nodes. Because of the overlap, \( h < r_I \), \( I = 1, \ldots, N \).

We can then define the finite dimensional subspaces \( V^h \subset V \) and \( S^h \subset S \) of approximating functions

\[
S^h = \left\{ u^h \in H^1(B_0) \mid u^h \in R^1(B_0) \right\} \tag{20}
\]

where \( R^1 \) is the functional space of the RKPM functions, with reproducibility up to the first order. Conversely to finite element functional spaces, functions in \( R^1 \) are defined globally over the body \( B_0 \); the local character is maintained because the shape functions are compact support functions, that is they are null beyond the radius \( r_I \). Furthermore, functions in \( R^1 \) remain in this space even if they are discontinuous.

The functions \( u^h \in S^h \) (and similarly \( \delta u^h \in V^h \)) are expressed as a linear combination

\[
u^h(X, t) = \sum_{I=1}^{N_I} \phi_I(X) \ d_I(t) \tag{21}
\]

\[
\delta u^h_T(X) = \sum_{I=1}^{N_I} \delta d_I^T \phi_I(X) \tag{22}
\]

where \( d_I(t) \) are nodal coefficients (not nodal values) and \( \phi_I(X) \) shape functions centred in \( X_I \)

\[
d_I^T = \begin{bmatrix} U_I^T & V_I^T & W_I^T \end{bmatrix}. \tag{23}
\]
The shape functions are computed as
\[ \phi_I(X) = \omega(X_I, X)P(X)^T M^{-1}(X) P(X_I) \] (24)
where the weighting function is defined as
\[ \omega(X_I, X) = \Delta V_I w \left( \frac{|X_I - X|}{r_I} \right) \] (25)
with \( \Delta V_I \) a measure of the sphere of radius \( r_I \) centred in \( X_I \), \( P(X) \) denotes a complete basis of the subspace of polynomials of degree \( k \), \( P(X) = \{ p_0(X), p_1(X), \ldots, p_k(X) \} \), and \( M \) is the moment matrix
\[ M(X) = \sum_{I \in S_X} \omega(X_I, X)P(X_I)P(X_I)^T \] (26)
where the index set \( S_X \)
\[ S_X = \{ J \in \{1, 2, \ldots, N\} \ | \ ||X - X_I|| \leq r_I \}. \] (27)
The moment matrix \( M \) can also be viewed as a Gram matrix defined with a discrete scalar product
\[ (u, v)_X = \sum_{I \in S_X} \omega(X_I, X)u(X_I)v(X_I) \] (28)
and, from a numerical point of view, it is convenient to work with a centred and scaled version to enhance the condition number of the system of normal equations. This correction implies that the following definition of \( M \) is adopted here
\[ M(X) = \sum_{I \in S_X} \omega(X_I, X)P \left( \frac{X_I - X}{r} \right) P^T \left( \frac{X_I - X}{r} \right) \] (29)
where \( r \) denotes the average of all the compact support radii. The matrix \( M \) can be inverted quickly using an iterative algorithm based on the Sherman–Morrison formula [38] which provides explicit equations for \( M^{-1} \) and proved to reduce sensibly the computational costs associated with Eqs. (29) and (24).

The continuity properties of the RKPM shape functions are clearly linked to the continuity properties of the function \( w \) in Eq. (25), which is usually referred to as the kernel of the approximation. This work considers the so-called \( 2k \)th order spline, which is the \( C^{k-1} \) function given by
\[ w(\xi) = \begin{cases} (1 - \xi^2)^k & 0 \leq \xi \leq 1 \\ 0 & \xi > 1. \end{cases} \] (30)
The reproducibility is given by using as nodal coefficients the polynomial basis \( P \) computed in the nodes \( x_I \):
\[ u^h(X) = \sum_{I=1}^{N_i} \phi_I(X)P(X_I)^T = P(X)^T M^{-1}(X) \sum_{I=1}^{N_i} \omega(X_I, X)P(X_I)P(X_I)^T = P(X)^T M^{-1}(X)M(X) = P(X)^T \] (31)
meaning that the approximation \( u_h(X) \) is interpolative to all the functions in the basis \( P \). To impose the discontinuity introduced by the presence of a crack, we use an intrinsic enrichment, where the RKPM shape functions (24) are rendered simultaneously discontinuous over the crack segments, and continuous around the crack tips. For a more complete description, the reader is invited to refer to [35,36,39] for curved cracks described by Non-Uniform Rational B-Spline (NURBS) parametrizations.

2.4. Discrete balance equations

Following [40], using Eq. (21), the discretized variation of the deformation gradient becomes
\[ \delta F^h = \delta d B_0^T \] (32)
with
\[ \mathbb{B}_0^T = \begin{bmatrix} \frac{\partial \phi^T}{\partial X_1} & \frac{\partial \phi^T}{\partial X_2} \end{bmatrix} \]  
(33)

and the following holds
\[ \delta \mathbf{F} : \mathbf{P} = \delta \mathbf{E} : \mathbf{S}. \]  
(34)

Replacing (21) into (15), the following equilibrium equations are obtained
\[ \mathbf{F}^{(i)}(\mathbf{d}) - \lambda \mathbf{F}^{(e)} = 0 \]  
(35)

where \( \lambda \) is the load level, \( \mathbf{F}^{(e)} \) is the external forces vector
\[ \mathbf{F}^{(e)} = \int_{\Gamma_u} \begin{bmatrix} \phi^T & 0 \\ 0 & \phi^T \end{bmatrix} \mathbf{i}_0 d\Gamma_u. \]  
(36)

\( \mathbf{F}^{(i)} \) is the internal forces vector that depends on the constitutive model of the material
\[ \delta \mathbf{d}^T \mathbf{F}^{(i)}(\mathbf{d}) = \int_{\mathcal{B}_0} \delta \mathbf{E} : \mathbf{S}^h \, dV = \int_{\mathcal{B}_0} \delta \mathbf{F} : \mathbf{P}^h \, dV = \delta \mathbf{d}^T \int_{\mathcal{B}_0} \begin{bmatrix} \frac{\partial \phi}{\partial X_1} P_{11}^h(\mathbf{d}) + \frac{\partial \phi}{\partial X_2} P_{21}^h(\mathbf{d}) \\ \frac{\partial \phi}{\partial X_1} P_{12}^h(\mathbf{d}) + \frac{\partial \phi}{\partial X_2} P_{22}^h(\mathbf{d}) \end{bmatrix} \, dV \]  
(37)

hence
\[ \mathbf{F}^{(i)} = \int_{\mathcal{B}_0} \begin{bmatrix} \frac{\partial \phi}{\partial X_1} P_{11}^h(\mathbf{d}) + \frac{\partial \phi}{\partial X_2} P_{21}^h(\mathbf{d}) \\ \frac{\partial \phi}{\partial X_1} P_{12}^h(\mathbf{d}) + \frac{\partial \phi}{\partial X_2} P_{22}^h(\mathbf{d}) \end{bmatrix} \, dV. \]  
(38)

2.5. Tangent stiffness matrix

For each iteration, it is necessary to compute the tangent stiffness matrix \( \mathbf{K}_T \) of the internal forces. It can be shown that
\[ \mathbf{K}_T = \frac{\partial \mathbf{F}^{(i)}}{\partial \mathbf{d}} = \mathbf{K}_T^g + \mathbf{K}_T^m \]  
(39)

where superscript \((\cdot)^g\) stands for geometric part, which takes into account geometrical nonlinearities
\[ \mathbf{K}_T^g = \int_{\mathcal{B}_0} \mathbb{B}_0^T \mathbf{S}^h(\mathbf{u}^h) \mathbb{B}_0 \, dV \]  
(40)

where \( \mathbf{S} \) is in Voigt notation. Instead, \((\cdot)^m\) stands for the material part, which takes into account material nonlinearities
\[ \mathbf{K}_T^m = \int_{\Omega_0} \mathbf{B}^h(\mathbf{u}^h) \mathbf{A}^{SE}(\mathbf{u}^h) \mathbf{B}^h(\mathbf{u}^h) \, dV \]  
(41)

where
\[ \mathbf{B}^h(\mathbf{d}) = \begin{bmatrix} \frac{\partial \phi}{\partial X_1} & \frac{\partial \phi}{\partial X_2} \\ \frac{\partial \phi}{\partial X_1} & \frac{\partial \phi}{\partial X_2} \\ \frac{\partial \phi}{\partial X_1} & \frac{\partial \phi}{\partial X_2} \end{bmatrix} \]  
(42)
and $A^{SE}$ is the *Second Elasticity Tensor* in Voigt form, defined, in tensorial form, as

$$A^{(2)} = \frac{\partial S}{\partial E}. \quad (43)$$

### 2.6. The constitutive model

In all the following examples, we will assume *plane stress* and *incompressible* Neo-Hookean material. In this case, the pressure $p$ can be explicitly determined. Indeed, following [41], the strain energy density function $w$ is

$$w(C) = \frac{1}{2} \mu_0 (I_1 - 3) \quad (44)$$

where $\mu_0$ is the *initial* shear modulus, $I_1$ is the first invariant of the Right Cauchy–Green tensor.

The corresponding *Second Piola–Kirchhoff Stress* is

$$S = \mu_0 I - p C^{-1}. \quad (45)$$

The pressure is given by

$$p = \frac{1}{\det(C)} \bar{C}^{-1} \quad (46)$$

where the bar indicates the $2 \times 2$ in-plane components of the tensor.

The second elasticity tensor is

$$A^{(2)} = 2\mu \frac{1}{\det(C)} \left( \bar{C}^{-1} \otimes \bar{C}^{-1} + I \right) \quad (47)$$

where

$$I = \frac{\partial \bar{C}^{-1}}{\partial \bar{C}^{-1}}. \quad (48)$$

### 3. Crack propagation criterion

The Griffith criterion [24] states that for a crack of initial length $a$ to grow, the following condition needs to verify

$$G[\varphi_a] - G_c(a) = 0 \quad (49)$$

where $G_c$ is the *critical strain energy release rate* of the material, and $G$ is defined in Eq. (16). For brittle fracture, $G_c$ is independent of the crack length $a$, for ductile fracture instead, $G_c = G_c(a)$. The functional $P$ (in Eq. (6)) for a discretized medium, becomes, for deformation-independent loads

$$P\left[\varphi^h_a\right] = \lambda F(e)^T d = F(i)^T d \quad (50)$$

where the last step used Eq. (35).

The rate of the internal energy, in Eq. (9), becomes

$$\dot{W}\left[\varphi^h_a, \varphi^h_a\right] = F^{(i)}^T \dot{d}. \quad (51)$$

For large displacements and small strains, there is a linear relation between the Green–Lagrange Strain $E$ and the *Second Piola–Kirchhoff stress* $S$. Therefore, $W$ can be simply written as

$$W\left[\varphi^h_a\right] = \frac{1}{2} \int_{\Omega_0} S : E \, dV = \frac{1}{2} F^{(i)}^T d = \frac{1}{2} P. \quad (52)$$
Fig. 2. Definition of strain energy release rate between two equilibrium states: $G = -\frac{\partial \Pi}{\partial A}$, with $A$ being the crack surface area.

For geometrically non-linear constitutive material models, with both displacements and strains being large, Eq. (52) is not valid. Integrating by parts Eq. (51)

$$
\mathcal{W} \left[ \varphi^h_a \right] = \int_0^d F^{(i)} \, d \, d = F^{(i)} \, d - \int_0^d \left( \frac{\partial F^{(i)}}{\partial d} \right)^T \, d \, d = P - \int_0^d d^T K T \, d = \int_0^d d^T d F^{(i)}
$$

(53)

where in the last step we used the definition of tangent stiffness matrix. Therefore,

$$
- \Pi \left[ \varphi^h_a \right] = \mathcal{P} \left[ \varphi^h_a \right] - \mathcal{W} \left[ \varphi^h_a \right] = \int_0^d d^T d F^{(i)} = \int_0^d d F^{(i)} \, d
$$

(54)
Fig. 3 depicts the proposed fracture criterion. The initial crack of length $a_0$ will propagate in the direction $\theta_{\text{max}}$ of maximum strain energy release rate $G$. This criterion is commonly adopted in fracture mechanics [26,27]. The assumption in this paper is that the $G$ at crack $a_0 + \delta a$ is computed before the crack is actually introduced, that is, at crack length $a_0$. In fact, we hypothesize that the initial crack grows with an infinitesimal virtual kink $\delta a$, much smaller than the original length. In this case, the stress states at $a_0$ and $a_0 + \delta a$ are not substantially different. Therefore, $G$ at $a_0 + \delta a$ can be computed by rotating of an angle $\theta$ the relevant quantities (stress and displacement gradients) at $a_0$. This variation of the $J$-integral with the angle has an explicit expression, as explained in the proceeding of the section. This means that $J$ at any angle $\theta$ can be computed from the fields in the original frame $X = [X_1, X_2]$ (see Fig. 3). This explicit expression turns out to be a simple trigonometric function, easy to maximize. The hypothesis behind the criterion is verified in an example in Section 7.2.

The $J$-integral for finite deformation can be written as

$$J = [1 0] \int_{D_\rho} \left( \nabla_0^* u^* T P^* - w I \right) \nabla_0^* q dS$$

where the domain $D_\rho$ is a circle around the crack-tip of radius $\rho$, $P$ is the First Piola–Kirchhoff stress, $w$ is the strain energy density function and $q$ is a weight function

$$q : D_\rho \subset B_0 \mapsto [0, 1] \quad q(X) = \begin{cases} 0 & X \in \partial D_\rho \\ 1 & X \text{ is a crack-tip.} \end{cases}$$

The tensors in Eq. (56) need to be rotated in the local reference frame, indicated by the superscript *. The quantities in Eq. (56) transform according to the following laws:

$$\nabla_0^* u^* = R(\theta)^T \nabla_0 u R(\theta)$$

because the displacement gradient transforms as a second-order tensor, with rotation tensor $R$

$$R(\theta) = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}$$

$$\nabla_0^* q = R(\theta)^T \nabla_0 q.$$
On the basis of an infinitesimal crack kink, the \( J \)-integral at a propagating crack tip can be expressed in a rotated coordinate system as

\[
J \left[ \varphi_h \right] = J(\mathbf{d}, \theta) = [1 \; 0] \int_{D_p} \left( (\mathbf{R}(\theta)^T \nabla_0 \mathbf{u}^h \mathbf{R}(\theta))^T (\mathbf{R}(\theta)^T \mathbf{P}^h) - w^h \mathbf{I} \right) \mathbf{R}(\theta)^T \nabla_0 q \; dS
\]

that can be rearranged as

\[
J(\mathbf{d}, \theta) = [1 \; 0] \int_{D_p} \mathbf{R}(\theta)^T \left( \nabla_0 \mathbf{u}^h \mathbf{R}(\theta)^T - w^h \mathbf{I} \right) \mathbf{R}(\theta)^T \nabla_0 q \; dS
\]

where the term in the round brackets depends on \( \mathbf{d} \).

Expanding Eq. (63), it is possible to obtain

\[
J(\mathbf{d}, \theta) = J_1(\mathbf{d}) \cos(\theta) + J_2(\mathbf{d}) \sin(\theta) = \mathbf{j}^h(\mathbf{d}) \cdot \mathbf{e}
\]

where \( \mathbf{e} = (\cos(\theta), \sin(\theta)) \) is the unit vector of the direction of propagation of the crack, and \( \mathbf{j}^h = \mathbf{j}^h(\mathbf{d}) = [J_1(\mathbf{d}), J_2(\mathbf{d})] \).

\[
J_1(\mathbf{d}) = \int_S \frac{\partial q}{\partial X_1} \left( \frac{\partial u_1}{\partial X_1} P_{11} + \frac{\partial u_2}{\partial X_1} P_{21} - W \right) + \frac{\partial q}{\partial X_2} \left( \frac{\partial u_1}{\partial X_2} P_{12} + \frac{\partial u_2}{\partial X_2} P_{22} \right) \; dS
\]

\[
J_2(\mathbf{d}) = \int_S \frac{\partial q}{\partial X_1} \left( \frac{\partial u_1}{\partial X_2} P_{11} + \frac{\partial u_2}{\partial X_2} P_{21} \right) + \frac{\partial q}{\partial X_2} \left( \frac{\partial u_1}{\partial X_2} P_{12} + \frac{\partial u_2}{\partial X_2} P_{22} \right) \; dS.
\]

It must be noted that the notation used is the same as \([26,27]\), and our findings reconcile with their results (see Section 5).

Differentiating \( J \) with respect to \( \mathbf{d} \) requires more effort. Indeed,

\[
\frac{\partial J}{\partial \mathbf{d}} = \frac{\partial J_1}{\partial \mathbf{d}} \cos(\theta) + \frac{\partial J_2}{\partial \mathbf{d}} \sin(\theta).
\]

Considering that \( \mathbf{d} = d_i I, \; i = 1, 2 \; I = 1, \ldots, N, \) with \( N \) the number of nodes and that

\[
u_i = \phi_I d_i I
\]

then

\[
\frac{\partial \mathbf{u}}{\partial X} = \frac{\partial u_i}{\partial X_j} = \frac{\partial \phi_I}{\partial X_j} d_i I
\]

hence

\[
\frac{\partial}{\partial \mathbf{d}} \frac{\partial \mathbf{u}}{\partial X} = \frac{\partial}{\partial d_i I} \frac{\partial u_i}{\partial X_j} = \frac{\partial \phi_I}{\partial X_j} d_i I = \frac{\partial \phi_I}{\partial X_j} \delta_{ik}
\]

\[
\frac{\partial W}{\partial \mathbf{d}} = \frac{\partial W}{\partial \mathbf{F}} \frac{\partial \mathbf{F}}{\partial \mathbf{d}} = \mathbf{P} \frac{\partial \mathbf{F}}{\partial \mathbf{d}} = \mathbf{P} \frac{\partial \mathbf{u}}{\partial \mathbf{d}} = P_{ij} \frac{\partial \phi_I}{\partial X_j} \delta_{ik}
\]

\[
\frac{\partial \mathbf{P}}{\partial \mathbf{d}} = \frac{\partial \mathbf{P}}{\partial \mathbf{F}} \frac{\partial \mathbf{F}}{\partial \mathbf{d}} = \mathcal{A}^{(1)} \frac{\partial \mathbf{u}}{\partial \mathbf{d}} \frac{\partial \mathbf{u}}{\partial \mathbf{d}}
\]

where \( \mathcal{A}^{(1)} \) is the First Elasticity Tensor (a fourth order tensor). Eq. (72) in index notation is

\[
\frac{\partial P_{ij}}{\partial d_k I} = \mathcal{A}^{(1)}_{ijkl} \frac{\partial \phi_I}{\partial X_l}
\]

\[
\frac{\partial A_1}{\partial \mathbf{d}} = \int_S \left( \frac{\partial}{\partial \mathbf{d}} \frac{\partial u_1}{\partial X_1} P_{11} + \frac{\partial u_1}{\partial X_1} \frac{\partial P_{11}}{\partial \mathbf{d}} \frac{\partial}{\partial \mathbf{d}} \frac{\partial u_1}{\partial X_1} \frac{\partial P_{11}}{\partial \mathbf{d}} \right) \; dS
\]

\[
+ \frac{\partial}{\partial \mathbf{d}} \left( \frac{\partial u_1}{\partial X_2} P_{21} + \frac{\partial u_1}{\partial X_2} \frac{\partial P_{21}}{\partial \mathbf{d}} \frac{\partial}{\partial \mathbf{d}} \frac{\partial u_1}{\partial X_2} \frac{\partial P_{21}}{\partial \mathbf{d}} \right) \; dS
\]

\[
+ \frac{\partial}{\partial \mathbf{d}} \left( \frac{\partial u_2}{\partial X_1} P_{12} + \frac{\partial u_2}{\partial X_1} \frac{\partial P_{12}}{\partial \mathbf{d}} \frac{\partial}{\partial \mathbf{d}} \frac{\partial u_2}{\partial X_1} \frac{\partial P_{12}}{\partial \mathbf{d}} \right) \; dS
\]

\[
+ \frac{\partial}{\partial \mathbf{d}} \left( \frac{\partial u_2}{\partial X_2} P_{22} + \frac{\partial u_2}{\partial X_2} \frac{\partial P_{22}}{\partial \mathbf{d}} \frac{\partial}{\partial \mathbf{d}} \frac{\partial u_2}{\partial X_2} \frac{\partial P_{22}}{\partial \mathbf{d}} \right) \; dS
\]
\[ \frac{\partial A_2}{\partial d} = \int_S \frac{\partial q}{\partial X_1} \left( \frac{\partial}{\partial d} \frac{\partial u_1}{\partial X_2} P_{11} + \frac{\partial u_1}{\partial X_2} \frac{\partial P_{11}}{\partial d} + \frac{\partial}{\partial d} \frac{\partial u_2}{\partial X_2} P_{21} + \frac{\partial u_2}{\partial X_2} \frac{\partial P_{21}}{\partial d} \right) \]
\[ + \frac{\partial q}{\partial X_2} \left( \frac{\partial}{\partial d} \frac{\partial u_1}{\partial X_2} P_{12} + \frac{\partial u_1}{\partial X_2} \frac{\partial P_{12}}{\partial d} + \frac{\partial}{\partial d} \frac{\partial u_2}{\partial X_2} P_{22} + \frac{\partial u_2}{\partial X_2} \frac{\partial P_{22}}{\partial d} \right) \]
\[ - \frac{\partial W}{\partial d} \right) dS. \]

(75)

To facilitate the reproducibility of the results by the reader, the Appendix reports the complete expanded expressions for the derivatives in Eqs. (75) and (74).

4. The J-integral based arc-length solver

4.1. The standard arc-length method

A classical arc-length solver seeks the solution \((d, \lambda)\) for the discretized equation of equilibrium

\[ \Psi(d, \lambda) = F^{(i)}(d) - \lambda F^{(e)} = 0 \]

(76)

with \(F^{(i)}(d)\) being the internal force vector, \(P\) is the external force vector and \(\lambda\) is the load level. Eq. (76) is a non-linear system of \(2N\) equations in \(2N + 1\) unknowns. Hence, it is necessary to add an equation, normally called the spherical arc-length constraint

\[ g(d, \lambda) = \Delta d^T \Delta d + \psi^2 \Delta \lambda^2 F^{(e)\top} F^{(e)} - l^2 = 0 \]

(77)

where \(l\) is the arc-length parameter, and \(\Delta d = d - d_0\), where \(d_0\) is a previously converged state, \(\psi\) is a parameter that is inserted to balance the contributions from both the displacement and the load levels \([42]\). Fig. 1 depicts the scheme in a simplified one-dimensional example with \(\psi \neq 0\) in Eq. (77). With \(\psi = 0\), Eq. (77) is known as cylindrical arc-length constraint.

In an iterative scheme, the increment \(\Delta d\) towards the next converged state \((d, \lambda)\) is given by

\[ \Delta d_{k+1} = \Delta d_k + \delta d_k \quad \Delta \lambda_{k+1} = \Delta \lambda_k + \delta \lambda_k \]

(78)

where

\[ \delta \lambda_k = -\frac{1}{\kappa} (h^T d_\Psi + g_k) \]

(79)

\[ \delta d_k = d_\Psi + \delta \lambda_k d_e \]

(80)

where

\[ \kappa = w + h^T d_e \]

(81)

\[ h = \left( \frac{\partial g}{\partial d} \right)_k \]

(82)

\[ w = \left( \frac{\partial g}{\partial \lambda} \right)_k \]

(83)

\[ g_k = \Delta d_k^T \Delta d_k + \psi^2 \Delta \lambda_k^2 F^{(e)\top} F^{(e)} - l^2 \]

(84)

\[ d_e = K_T^{-1} F^{(e)} \]

(85)

where \(K_T\) is the tangent stiffness matrix

\[ K_T = \left( \frac{\partial F^{(i)}}{\partial d} \right)_k \]

(86)

\[ d_\Psi = -K_T^{-1} \Psi_k \]

(87)

where

\[ \Psi_k = F^{(i)}(d_0 + \Delta d_k) - (\lambda_0 + \Delta \lambda_k) F^{(e)}. \]

(88)
4.2. Dissipation-based arc-length

Gutierrez [15] and Verhoosel et al. [16] proposed an energy release control for failure in brittle and ductile solids. The arc-length constraint is

$$g = \Delta G - \tau$$

(89)

where \(\tau\) is size of the step, and \(G\) is the proper strain energy release rate, defined as time derivative of energetic quantities

$$G = \dot{P} - \dot{W}$$

(90)

where \(\dot{P}\) is the power of the external forces and \(\dot{W}\) the rate of the strain energy. It must be remarked that in fracture mechanics, \(G\) can also be expressed as a change in fracture surface area cf. Eq. (55). Particularly, they presented a scheme for geometrical non-linear constitutive models, that is with large displacements and small strains. In these assumptions, Eq. (52) is valid. Instead, in this paper we present a full large strain–large displacement model.

To retain the advantageous and clever idea of a dissipation-based arc-length, in this work we propose to compute the strain energy release rate from the J-integral, and modify the arc-length constraint to reflect a fracture criterion commonly adopted in fracture mechanics, that is the critical load for crack initiation is such that

$$G = G_c$$

(91)

where \(G_c\) is the critical strain energy release rate, often referred in the literature as fracture energy. In addition to the arc-length proposed by Gutierrez [15] and Verhoosel et al. [16], the one proposed in this paper incorporates a criterion for the direction of crack propagation. In addition, the proposed solver operates on actual rates (in the fracture mechanics sense) of energy, rather than increments of energy.

4.3. The proposed J-integral arc-length constraint

The scheme in Section 4.1 will not necessarily enforce the Griffith energy balance (49) in the presence of a propagating crack, as the numerical example in Section 7.3 demonstrates. Therefore, the constraint in Eq. (77) is replaced by

$$g = J(d, \theta_{\text{max}}) - G_c$$

(92)

where \(G = J\) was exploited. In addition, \(J\) depends on the orientation of the crack increment. It is reasonable to accept that the crack will propagate in the direction \(\theta_{\text{max}}\) of maximum strain energy release rate

$$\theta_{\text{max}} = \arg \max_{\theta \in [0, 2\pi]} J(d, \theta).$$

(93)

To summarize, the scheme becomes a two parameters arc-length continuation, in \(\theta\) and \(\lambda\). For simplicity, only one crack-tip is assumed, but similar arguments can be made for multiple crack tips.

$$\begin{cases}
F^{(i)}(d) - \lambda F^{(e)} = \Psi(d, \lambda) = 0 \\
J(d, \theta_{\text{max}}) - G_c = g(d, \theta) = 0 \\
\theta - \theta_{\text{max}} = f(d, \theta) = 0.
\end{cases}$$

(94)

Hence, in an iterative perspective, the following Newton–Rahpson step is required:

$$\begin{bmatrix}
\delta d_{k+1} \\
\delta \lambda_{k+1} \\
\delta \theta_{k+1}
\end{bmatrix} =
\begin{bmatrix}
K_T & -F^{(e)} & 0 \\
0 & \frac{\partial J}{\partial \theta} & -g_k \\
0 & \frac{\partial f}{\partial \theta} & -f_k
\end{bmatrix}
\begin{bmatrix}
-\Psi_k \\
-g_k \\
-f_k
\end{bmatrix}.$$  

(95)

However, the two-parameters continuation in Eq. (94) can be re-formulated as a standard continuation as in Section 4.1. Indeed, Eq. (93) can be solved analytically as later reported in Eq. (102), as it consists in finding the
maximum of function $J(d, \theta)$ as in Eq. (64). It must be remarked that $J(d, \theta)$ can physically only be non-negative, and that it is a continuous periodic function in $\theta$, as $J(d, 0) = J(d, 2\pi)$. Hence, a local maximum can be easily obtained, as it will be shown in Section 5.

Therefore, assuming that $\theta_{\text{max}}$ is readily obtainable at each iteration, the continuation (94) becomes

$$\begin{aligned}
\{ F^{(i)}(d) - \lambda F^{(e)} &= \Psi(d, \lambda) = 0 \\
J(d, \theta_{\text{max}}) - G_c = g(d) &= 0
\end{aligned}$$

which represents the polar equation of a straight line, as reported in equation 7.18 of [27]. In addition, because of Eq. (99) it is possible to compute explicitly the Frank diagram of $J$.

5. Link with a constitutive theory based on configurational forces [27]

Indeed, with the positions $J_1 = |j| \cos(\beta)$, $J_2 = |j| \sin(\beta)$. Eq. (64) can be arranged as

$$J(d, \theta) = |j| (\cos(\beta) \cos(\theta) + \sin(\beta) \sin(\theta)) = |j| \cos(\beta - \theta).$$

Therefore, the maximum of $J(d, \theta)$ is given by the angle $\theta$ satisfying

$$\frac{\partial J}{\partial \theta} = 0 \quad \frac{\partial^2 J}{\partial \theta^2} < 0$$

which means

$$\frac{\partial J}{\partial \theta} = -|j| \sin(\beta - \theta) \quad \frac{\partial^2 J}{\partial \theta^2} = -|j| \cos(\beta - \theta).$$

Eqs. (101) are simultaneously satisfied by

$$\theta_{\text{max}} = \beta = \arctan(J_2, J_1)$$

which means that the crack propagation direction (for a constitutively isotropic material) $e$ points in the same direction as the vector $j$

$$e = \frac{j}{|j|}$$

which is the same result found in [27] (equation 8.11 of their paper). In addition, because of Eq. (99) it is possible to compute explicitly the Frank diagram of $J$.

The Frank diagram of a function $\varphi(\theta)$ describing a curve in polar form $r = \varphi(\theta)$ is defined as

$$\text{Frank}(\varphi) = \left\{(r, \theta) : r = \frac{1}{\varphi(\theta)} \right\}.$$

Therefore,

$$\text{Frank}(J) = \left\{(r, \theta) : r = \frac{1}{|j| \cos(\beta - \theta)} \right\}$$

which represents the polar equation of a straight line, as reported in equation 7.18 of [27]. In addition, for isotropic crack-tips with fracture energy $G_c$ independent of the orientation $\theta$, there is at most one possible kinking angle $\theta$, which correspond to $\theta_{\text{max}}$ in Eq. (103). Our finding is then in agreement with this corollary of their Criticality Theorem.
6. Strategies for continuation

6.1. Line search

When \( \det (K_T) \) is close to zero, the step from Eqs. (79) and (80) can become larger than the radius of convergence of a Newton–Rahpson (NR) scheme. In this case, the residual might increase, while it should, instead, decrease. To recover a descent in the norm of a residual, it is opportune to combine a Newton–Rahpson scheme with a Line-Search (LS) algorithm [7]. The idea of a LS is to search for an adequate decrease of the norm of the residual. The problem in Eq. (96) is re-formulated as

\[
(d, \lambda) = \arg \min_{(d, \lambda)} F(d, \lambda) \quad F(d, \lambda) = \frac{1}{2} \Psi(d, \lambda)^T \Psi(d, \lambda) + \frac{1}{2} g(d)^2.
\]  

(106)

Since \( F \) is a non-negative function in \((d, \lambda)\), its minimum is also a zero. Hence, Eqs. (106) and (96) have the same solutions.

Instead of taking the full NR step, LS seeks for a fraction \( \eta \)

\[
\Delta d_{k+1} = \Delta d_k + \eta \delta d_k \quad \Delta \lambda_{k+1} = \Delta \lambda_k + \eta \delta \lambda_k
\]

such that

\[
F(d_{k+1}, \lambda_{k+1}) \leq F(d_k, \lambda_k) + \eta \frac{\partial F}{\partial \Delta d} \Delta d_k + \eta \frac{\partial F}{\partial \Delta \lambda} \Delta \lambda_k.
\]  

(108)

The value of \( \eta \) is given by the minimum of the function \( f(\eta) = F(d_k + \eta \Delta d_k, \lambda_k + \eta \Delta \lambda_k) \). Since the actual function \( f(\eta) \) is not known \textit{a priori}, it is assumed quadratic or cubic

\[
f(\eta) \approx \left( f(1) - f(0) - \frac{df}{d\eta}(0) \right) \eta^2 + \frac{df}{d\eta}(0) \eta + f(0)
\]  

(109)

with

\[
\frac{df}{d\eta}(0) = \frac{\partial F}{\partial \Delta d} \Delta d_k + \frac{\partial F}{\partial \Delta \lambda} \Delta \lambda_k = \left( \Psi^T K_T + g \chi \right) \Delta d_k + (-F^{(e)T} \Psi) \Delta \lambda_k.
\]  

(110)

6.2. Pseudo J-integral arc-length for the pre-propagation stage

Fig. 4 shows a typical snap-back in a force–displacement curve occurring for a crack propagating in an elastic solid. The phase \( OF \) is the response for an initial crack of length \( a_0 \), then at point \( F \) the crack starts growing, at which \( G = G_c \). All the points in \( OF \) are characterized by a value of the strain energy release rate inferior to the critical one. To get to the point \( F \) from an initial position \( 0 \), one could follow the spherical arc-length (Fig. 4(a)) and then switch to a \( J\)-integral arc-length. This is because applying the \( J\)-integral arc-length from point \( O \), would result in getting straight to the point \( F \). It would appear then that the \( J\)-integral does not capture the intermediate states. In addition, it is sometimes required to proceed through intermediate steps, especially if the displacement at point \( F \) is quite large. In fact, this could avoid excessive distortions during each iteration, which could lead to negative Jacobian.

Nonetheless, the proposed arc-length can be easily modified to capture the intermediate states in \( OF \). Indeed, it suffices to replace \( G_c \) in Eq. (92) with a value \( G_0 < G_c \), and increase it after each converged step until it reaches the critical value \( G_c \). The increment \( \Delta G \) can be decided, for example, by the number of desired iterations \( k_d \) and the number of the actual corrector iterations \( k_c \) achieved at the previous state. For example, the following law provides a balanced increment in \( G \):

\[
G_{0,\text{new}} = \min \left( G_{0,\text{old}} + \Delta G_{\text{new}}, G_c \right) \quad \Delta G_{\text{new}} = \Delta G_{\text{old}} \left( \frac{k_d}{k_c} \right)^{0.5}.
\]  

(111)

In this paper, we only considered one crack tip, the one with the maximum value of the \( J\)-integral. It is possible, in principle, to apply it for each crack-tip and have separate increments of \( \Delta G \).
7. Numerical examples

Unless stated otherwise, the examples in this section assume an incompressible Neo-Hookean material model in plane stress (44), with \( \mu = 0.4225 \text{ MPa} \) and \( G_c = 10 \text{ kJ/m}^2 \), values typical of natural rubber.

7.1. Comparison of the J-integral with an analytical solution

Firstly, the accuracy of the numerical J-integral (Eq. (63)) is verified through comparison with an analytical expression [31]. The test is shown in Fig. 5, where, for a Neo-Hookean incompressible solid in plane stress

\[
J = \mu h_0 \left( \alpha - \frac{1}{\alpha} \right)
\]

where the stretch \( \alpha \) results from

\[
\alpha = 1 + \frac{\bar{v}}{h_0}
\]

where \( \bar{v} \) is an applied displacement. To mimic an infinitely long strip, the domain of study is rectangular, with height being \( 2h_0 \) and length \( 40h_0 \), with \( h_0 = 0.025 \text{ m} \). The mesh size \( \Delta h \) used is 0.01 m, and the domain \( D_\rho \) for the J-integral had radius \( \rho = h_0 \). It was seen path-independence for relatively small values of \( \rho/h \). Fig. 6 shows a comparison between computed values of J-integral and Eq. (112). The curves are almost overlapping, with an error of at most 1%.

7.2. Verification of the fracture criterion

After having verified the accuracy of the numerical J-integral, we proceed in testing the validity of the assumption at the basis of the fracture criterion in Section 3 and Fig. 3. The idea is recalled and further explained in Fig. 7 for.
Fig. 6. Validation against the analytical solution in Eq. (112): continuous line: numerical; dashed line: analytical. The error is within 1%.

Fig. 7. Verification of the maximum dissipation assumption: a sample with an inclined central crack of length $2a_0$, $a_0 = 0.1L$ and initial angle $\beta$ is stretched (with $\alpha$ being the stretch) uni-axially in displacement control. Given these conditions, two crack kinks (red lines) of inclination $\theta$ are added asymmetrically to simulate a crack growth scenario. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

An inclined central crack of a sample stretched uni-axially under displacement control: the value of the $J$-integral at the tip of a kinked crack $\Delta a$ inclined of $\theta$ from an initial crack $a_0$ inclined of $\beta$ is the same as the value of the $J$-integral for the initial crack $a_0$ without the kinks, obtained by simply rotating of $\theta$ the relevant fields. Two values of the stretch $\alpha$ are considered, namely $\alpha = 1.2$ and $\alpha = 1.4$, where the stretch $\alpha$ is computed according to Eq. (113). For simplicity, the same value is applied before and after introducing the kinks. Therefore, the value of $J$ after the kinks, will be inevitably higher (Figs. 8(a) and 9(a)). Hence, for a better comparison, the values after the kinks are normalized with respect to the maximum value (Figs. 8(b) and 9(b)). For the loading conditions in Fig. 7, it is known that the crack will tend to kink and propagate in a direction orthogonal to the loading ($\theta = 0$). In fact, Figs. 8 and 9 show a maximum at $\theta = 0$, and the shapes of the normalized curves are indeed very similar, with minor discrepancies due to the finiteness of the kinks, whose minimum length is limited by the mesh size $\Delta h$. In fact, in principle the kinks $\Delta a$ should be chosen as small as possible, to be consistent with the infinitesimal assumption of the virtual kinks; but, in practice, $\Delta a$ needs to be sufficiently larger than the value of the radius $\rho$ in $D_\rho$, which guarantees an accurate and
Fig. 8. Variation of $J$ with the inclination $\theta$ of the kink for an inclined central crack of $\beta = 30^\circ$ under tensile stretch $\alpha = 1.2$: continuous line, Eq. (64) used at initial crack $a_0$; dots, numerical values with explicit cracks $a_0 + \Delta a$.

path-independent value of the $J$-integral. This value of $\rho$ is dictated, in turn, by the mesh size $\Delta h$, according to the findings of Section 7.1. In this example, the value of $\Delta h$ is 5 mm, whilst $\Delta a = 15$ mm.

7.3. Crack propagation with the cylindrical, spherical and proposed arc-length

After having verified the fracture criterion, we proceed next to show that a cylindrical or a spherical arc-length criterion (Eq. (77)) does not necessarily satisfy the onset of the Griffith criterion (Eq. (49)), hence cannot be used in tracing equilibrium curves. The geometry and the boundary conditions are shown in Fig. 10. Fig. 11 shows the equilibrium curves obtained with a cylindrical arc-length (Eq. (77) with $\psi = 0$) and a spherical arc-length (Eq. (77) with $\psi = 1$). The value of the $J$-integral (Fig. 11(b)) exceeds the critical value $G_c$. Even if they satisfy the Griffith inequality $G \geq G_c$, they do not provide correct information on the onset of crack propagation for various crack lengths. Instead, Fig. 12(b) illustrates that the value of $J$ remains fixed at $G_c$ for all the subsequent steps. In addition, the equilibrium curve in Fig. 12(a) interestingly shows a double snap-back behaviour. The related deformations to critical points 1–4, with the crack openings, are shown in Fig. 13.
7.4. Double Edge Notched Tensile (DENT)

In this section we consider the crack propagation and interaction of two edge cracks in a specimen under displacement control conditions. In these conditions, the arc-length parameter is the stretch $\alpha$, and the nominal traction $\lambda$ is computed as a reaction force. The two cracks are separated by a distance $h$, symmetrically positioned with respect to the mid-plane of the sample ($y = 0$). Different values of $h$ are considered, including the collinear case with $h = 0$. For collinear cracks, both cracks will propagate in a straight direction, until they merge (Fig. 15).

For $h > 0$, the cracks tend to bend anti-symmetrically, to form a lenticular fragment: Fig. 16 shows the equilibrium curve for $h/L = 0.3$ with the relative deformed configurations. The curving of the cracks brings considerable additional stretchability to the structure: for example, with $h/L = 0.3$, the final stretch at complete fracture is higher than the case with $h = 0$, as it can also be seen from the equilibrium curves (Fig. 17).

The misalignment length $h$ has a minor effect on the overall strength, but a major non-proportional influence on the stretch at fracture. On one hand increasing $h$ can bring the cracks too far apart to intersect (Fig. 18); on the other
Fig. 10. Numerical example for the cylindrical, spherical and the proposed arc-length method: $L = 1$ m, $a = 0.1 L$, $\beta = 30^\circ$.

hand, decreasing $h$ can lead the crack path to intersect too soon (for example $h/L = 0.05$) leading to a more ductile behaviour, but lower stretch at fracture.

A trend seems to appear, towards an optimal value of $h$ that maximizes the stretch at fracture. For such value, the two cracks intersect in a point that is, at the same time, located on the boundary: for this reason, we will refer to this intersection as a triple point.

The value of $h/L = 0.14$ provides this condition, and it seems to be an optimal value for the maximum stretch at fracture (Fig. 19).

Finally, it must be noted that for relatively high values of $h/L$, counter-intuitively, the top crack tends to curve downwards. This is a consequence of the large deformations and strains, and it is an effect not predictable by the linear theories. Indeed, for Linear Elastic Fracture Mechanics (LEFM), the path of the crack at the top for $h/L = 0.8$ should have initially curved upwards, and then steadily proceed horizontally. This effect is explained more in detail in the next section.

7.5. Comparison with the maximum hoop stress criterion for Linear Elastic Fracture Mechanics (LEFM)

To fit the assumptions of the LEFM, the proposed arc-length method was tested for a ceramic material (Alumina), which exhibits high Young Modulus (corresponding to a shear Modulus $\mu = 165$ GPa), but very low fracture energy $G_c = 60$ J/m$^2$, or, in terms of fracture toughness, $K_c = 5$ MPa$\sqrt{m}$. The test in Fig. 14 was carried out for $h/L = 0.6$ with two different solvers: (i) the fully non-linear finite deformation with an hyperelastic constitutive model, with the $J$-integral-based arc-length and the fracture criterion proposed in this paper, (ii) a linear elastic solver with a maximum hoop stress criterion [43]. The proposed arc-length returns the same results of the maximum hoop stress criterion, in terms of crack paths (Fig. 20) and equilibrium curve (Fig. 21). In addition, Fig. 21 shows that the maximum strain at fracture is around 0.18%, which is consistent with the assumptions of the linear theories.

As anticipated at the end of Section 7.4, the path for the crack at the top predicted by the LEFM, tends to slightly curve upwards, and then propagate orthogonally to the loading direction: instead, for a material with high toughness, the same crack tends to curve downwards, as a result of the large deformations.

7.6. Graphene kirigami structures

The previous example shown that it is possible for transition from a brittle to a ductile fracture just by changing the positions of the cracks. Kirigami (from the Japanese kiru = to cut, kami = paper) is the ancient Japanese art of paper sculptures, and it consists in cutting and stretching a single sheet of paper. The stretch causes the cracks to open, and display the artistic pattern, as shown in Fig. 22. Recently, many authors attempted to design flexible structures following this idea [44–50], and notably [51–53] applied the kirigami idea to graphene materials. The novelty of
Fig. 11. Failure of the cylindrical and spherical arc-length in capturing snap back and the correct values of $G_c$ for a growing crack; dotted black line is the cylindrical arc-length, blue thin line is the spherical arc-length with $\psi = 1$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

This paper is that the proposed arc-length method, combined with the ability of introducing cracks, can predict the maximum stretch at fracture and strength of graphene kirigami sheets. As an example, Fig. 23 depicts a kirigami-style structure, with an alternating pattern of cracks, along the lines of the example in Section 7.4. A sophisticated constitutive model for finite deformation of graphene can be found in [54]: however, for the sake of simplicity, a compressible Neo-Hookean model is used, with energy function

$$W = \frac{1}{2} \mu_0 (I_1 - 3) + \lambda_0 \frac{1}{2} (\log J)^2 - \mu_0 \log J$$

(114)

where $\mu_0$ is the initial shear modulus, $\lambda_0$ the initial bulk modulus. For graphene, the following values are used [54]: $E = 1.030$ TPa and $\nu = 0.231$, while the fracture energy $G_c = 15.9$ J/m$^2$ [55]. With reference to Fig. 23, $D = 100$ Å, and $L = 340$ Å. Fig. 24 shows two equilibrium curves for the same type of kirigami structures (same pre-crack patterns): the spacing $d$ between the cuts is the same, but the cuts have different length. It is interesting to see that the structure with shorter cracks has higher strength, but brittle behaviour and lower stretch-at-fracture; instead, the one
with the longer cracks, exhibits a ductile behaviour, with much higher stretch at fracture, albeit with lower strength. Fig. 25 shows all the crack propagation steps for various points on the curve. Ideally, one could use the arc-length in this paper to optimize the design of the cuts such that both high strength and high toughness are achieved.

8. Conclusions

This paper proposed a path-following method for tracing the bifurcation diagram of crack propagation in hyperelastic media, which account for both geometrical and material nonlinearities. Unlike other methods available in the literature, the one presented here does not require the computation of mixed-mode Stress Intensity Factors, and, consequently, the knowledge of asymptotic near crack-tip solutions. This approach incorporates the principle of maximum dissipation rate and thus is thermodynamically consistent. The basis of the proposed method is the rate form of the Griffith balance (Eq. (49)), and requires only the computation of the $J$-integral for rotated stress and displacement gradient fields (Eq. (56)). The assumption behind the method (verified in this paper) is that the fields
Deformations of the snap-backs in Fig. 12. Colours show $\sigma_{22}$ (in Pa). There is a double snap-back: even if the crack is larger at point 3, its maximum vertical displacement is slightly higher than point 2. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

The maximum dissipation assumption leads to an explicit formula for $J$ for varying angles of propagation (Eq. (64)). The maximization of such equation allows to reconcile with a constitutive theory for kinking and curving of cracks based on the theory of Configurational Forces [27].

The results show that the proposed arc-length can handle very sharp snap-back paths in the equilibrium curve (for example, Figs. 12, 17 and 24), and for multiple crack problems. In particular, these examples show that misaligned cracks combined with hyperelastic materials can lead to very deformable structures. The idea of non-collinear cracks can be exploited to design extremely stretchable structures, similar to the Japanese art of paper sculpture (kirigami). In combination with the use of high-strength materials, like graphene, it is believed that this could be a pathway to obtain sheets with simultaneous high strength and high toughness.

The examples show the ability of the arc-length solver to predict the large deformations of graphene kirigami sheets, and to capture the transition from brittle to ductile for the same pattern, but with different lengths (Figs. 24 and 25).
Fig. 14. Double edge cracks tensile tests with applied stretch $\alpha$: $W = 0.08$ m, $L = 0.2$ m, $a_0 = 16$ mm.

Fig. 15. Double edge collinear cracks tensile tests with applied stretch $\alpha$: $W = 0.08$ m, $L = 0.2$ m, $a_0 = 16$ mm. Traction-stretch equilibrium curve, along with deformed configurations at dotted points; the star indicates the stretch at complete fracture.

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Appendix. Full expressions of the consistent linearization of the $J$-integral

In the following,

$$\phi^T = \begin{bmatrix} \phi_1(X) & \phi_2(X) & \ldots & \phi_N(X) \end{bmatrix} I = 1, \ldots, N$$

(A.1)
Fig. 16. Double edge non-collinear cracks tensile tests with applied stretch $\alpha$: $W = 0.08 \, \text{m}$, $L = 0.2 \, \text{m}$, $h = 0.06 \, \text{m}$, $h/L = 0.3$, $a_0 = 16 \, \text{mm}$. Traction-stretch equilibrium curve, along with deformed configurations at dotted points; crack paths on the undeformed configuration are shown on the left. The star indicates the stretch at complete fracture.

Fig. 17. Double edge non-collinear cracks tensile tests: comparison of equilibrium curves for increasing $h/L$. The star at the end of each curve indicates the stretch at complete fracture.

\[
\frac{\partial}{\partial d} \frac{\partial u_1}{\partial X_1} = \begin{bmatrix} \frac{\partial \phi}{\partial X_1} \\ 0 \end{bmatrix} \quad (A.2)
\]

\[
\frac{\partial}{\partial d} \frac{\partial u_1}{\partial X_2} = \begin{bmatrix} \frac{\partial \phi}{\partial X_2} \\ 0 \end{bmatrix} \quad (A.3)
\]

\[
\frac{\partial}{\partial d} \frac{\partial u_2}{\partial X_1} = \begin{bmatrix} 0 \\ \frac{\partial \phi}{\partial X_1} \end{bmatrix} \quad (A.4)
\]

\[
\frac{\partial}{\partial d} \frac{\partial u_2}{\partial X_2} = \begin{bmatrix} 0 \\ \frac{\partial \phi}{\partial X_2} \end{bmatrix} \quad (A.5)
\]
Fig. 18. Double edge non-collinear cracks tensile tests: comparison of crack paths in the reference configuration for varying \( h \).

Fig. 19. Double edge non-collinear cracks tensile tests: optimal \( h/L \) for maximum stretch at fracture. The value of \( h/L = 0.14 \) causes the crack paths to join at a triple point. The star at the end of each curve indicates the stretch at complete fracture.

\[
\frac{\partial W}{\partial d} = \begin{bmatrix}
P_{11} \frac{\partial \phi}{\partial X_1} + P_{12} \frac{\partial \phi}{\partial X_2} \\
P_{21} \frac{\partial \phi}{\partial X_1} + P_{22} \frac{\partial \phi}{\partial X_2}
\end{bmatrix}
\]  

(A.6)

\[
\frac{\partial P_{11}}{\partial d} = \begin{bmatrix}
A_{1111}^{(1)} \frac{\partial \phi}{\partial X_1} + A_{1112}^{(1)} \frac{\partial \phi}{\partial X_2} \\
A_{1121}^{(1)} \frac{\partial \phi}{\partial X_1} + A_{1122}^{(1)} \frac{\partial \phi}{\partial X_2}
\end{bmatrix}
\]  

(A.7)
Fig. 20. Double edge non-collinear cracks tensile tests for alumina and for $h/L = 0.6$: comparison of crack paths between the proposed arc-length (red line) and the maximum hoop stress criterion (black line). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 21. Double edge non-collinear cracks tensile tests for alumina and for $h/L = 0.6$: comparison of equilibrium curves between the proposed arc-length (red line) and the maximum hoop stress criterion (black line). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

\[
\frac{\partial P_{12}}{\partial d} = \begin{bmatrix}
A_{1211}^{(1)} \frac{\partial \phi}{\partial X_1} + A_{1212}^{(1)} \frac{\partial \phi}{\partial X_2} \\
A_{1221}^{(1)} \frac{\partial \phi}{\partial X_1} + A_{1222}^{(1)} \frac{\partial \phi}{\partial X_2}
\end{bmatrix}
\tag{A.8}
\]

\[
\frac{\partial P_{21}}{\partial d} = \begin{bmatrix}
A_{2111}^{(1)} \frac{\partial \phi}{\partial X_1} + A_{2112}^{(1)} \frac{\partial \phi}{\partial X_2} \\
A_{2121}^{(1)} \frac{\partial \phi}{\partial X_1} + A_{2122}^{(1)} \frac{\partial \phi}{\partial X_2}
\end{bmatrix}
\tag{A.9}
\]
The First Elasticity Tensor $\mathcal{A}^{(1)}$ can be obtained by the Second Elasticity Tensor $\mathcal{A}^{(2)}$ from

$$\mathcal{A}_{ijkl}^{(1)} = \delta_{ik} \delta_{jl} + F_{in} \mathcal{A}_{nml}^{(2)} F_{km},$$

(A.11)
where $F_{ij}$ is the deformation gradient

$$A^{(2)} = 4 \frac{\partial^2 W}{\partial C \partial C} = 2 \frac{\partial S}{\partial C}.$$  \hspace{1cm} (A.12)

Fig. 24. Equilibrium curve for a tensile test in displacement control of a graphene kirigami structure: red line $d = 36 \, \text{Å}, \ a = 41 \, \text{Å}$; black line $d = 36 \, \text{Å}, \ a = 76 \, \text{Å}$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 25. Graphene kirigami structure with $d = 36 \, \text{Å}, \ a = 41 \, \text{Å}$ (Fig. 23): traction–stretch equilibrium curve, along with deformed configurations at points. Beyond the critical fracture initiation point (indicated by the cross), the crack pattern is stable, such that it allows further stretching. The same pattern, but with shorter cracks, instead propagates in an unstable manner (red line of Fig. 24).

References


