Asymptotic analysis of microscopic impenetrability constraints for atomistic systems

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Abstract

We analyze systems of atomistic interactions on a triangular lattice allowing for fracture under a geometric condition on the triangles corresponding to a microscopic impenetrability constraint. Such systems can be thought as a computational simulation of materials undergoing brittle fracture. We show that in the small-deformation regime such approximation can be validated analytically in the framework of variational models of fracture. Conversely, in a finite-deformation regime various pathologies show that the continuum approximation of such a system differs from the usual variational representations of fracture and either needs new types of formulations on the continuum, or a proper interpretation of the atomistic constraints limiting their range and adapting them to a dynamical framework.

Keywords: computational mechanics, variational theory of Fracture, discrete-to-continuum analysis, Γ-convergence, Lennard-Jones potentials,

Introduction

In this paper we analyze a problem related to Computational Mechanics formulated on energies defined on a two-dimensional triangular grid (see for instance [5], [28], [27], [29], and [18]). The class of energies we consider have two main features:

• they allow for *macroscopic fracture*. At the lattice level this is modeled by having solutions with very elongated triangles in the deformed configuration, corresponding to triangles approximating a linear crack in the reference configuration;

• they mimic a *impenetrability constraint*. Indeed, at the lattice level such energies are finite only on configurations that maintain the same ordering of the vertices of the triangles in the reference and deformed configurations.

Many of our considerations will remain valid also for analogous problems in a three-dimensional setting, but the corresponding lattice formulations in that case are more involved.

A simple such model for the energies we have in mind consists in a collection of central interactions between nearest neighbours with Lennard-

Jones potentials, to which the impenetrability constraint is added as a topological adherence to a crystalline reference configuration. We may suppose that the coefficients of the Lennard-Jones potentials are tuned so that the energies are minimized on the reference triangular grid (i.e., on the identity on the triangular lattice). We then expect that their behaviour can be approximated by a continuum description with some energy for which again the identity is a minimizer. In a small-strain regime for deformations close to the identity, the expected approximation is that either we have an approximately linear behaviour for the strain, or brittle fracture arises governed by a Griffith-type energy. The effect of the impenetrability constraint is translated on constraints on the fracture; e.g., that we may only have 'opening fracture'. Our analysis aims on one hand at validating such a heuristic suggestion for small deformations and on the other hand to understand the implication of this microscopic model beyond the small-strain regime.

Another standpoint for this analysis is the general problem of the passage from discrete theories to continuum theories. In order to have a manageable passage to the limit, a balance is required between considering large number of interactions and complex multi-body potentials, and a modeling simplification that enables to diminish the number of variables involved thanks to geometrical or topological constraints. The microscopic impenetrability condition described above is one such constraint, and is often used when only few interactions (e.g., nearest neighbours) are taken into account, since without any additional constraint this simplification often may introduce un-physical spurious states such as everted configurations.

In analytical terms, the problem we have in mind is the question of the validity of a *variational principle* underlying fracture phenomena; i.e., the statement that a discrete problem involving a large number of nodes can be approximately described by a continuum problem involving an energy similar to that of the variational theory of Griffith brittle fracture, which is then described separately by a bulk and a fracture energy function. This can be exemplified by looking at lattice problems where we minimize our discrete energy prescribing the displacement on a portion of the boundary of the sample. Accordingly, the discrete system will be deformed producing a configuration depending on the grid size, which we denote by ε. For ε small, we conjecture that such a configuration is approximately a discretization of the solution to a continuum minimization problem defined by the corresponding boundary displacement. This approximating continuum problem is defined through an energy independent of the boundary conditions, which is then regarded as describing a (approximate) continuum brittle medium.

The suggestion that the approximating problem could be linked to a (possibly anisotropic) Griffith energy, such as those recently considered to study crack growth by Francfort, Marigo et al. [20, 6], can be explained by referring to the description of the effective cohesive behaviour of layers of interatomic planes for atomistic systems described by Lennard-Jones interactions by Braides, Lew and Ortiz [11], which is a (much simpler) one-dimensional analog of the model under examination. That one-dimensional problem depends on a scalar function u describing

the displacement in the direction orthogonal to a system of parallel planes. In the hypothesis of small boundary displacement then the behaviour of $v = u - \mathrm{id}$ (suitably scaled) is described by a one-dimensional Griffith energy. The microscopic impenetrability condition translates in u being increasing, and hence on a simple opening condition for v on the crack sites: $v^+ - v^- > 0$, where v^+, v^- denote the value of the left-/right-hand side of the crack, respectively. That analysis also highlights a *decoupling principle* (already noticed in the earlier paper by Truskinovsky [31]); i.e., that volume and surface effects can be analyzed separately, the first one by looking only at deformations that do not develop fracture through a linearization procedure close to the identity, and the latter by scaling discontinuous deformations at fracture sites so that in the limit only (discontinuous) piecewise-affine functions have to be taken into account (*brittle rigid behaviour*). These two analyses correspond to the characterization of the behaviour of the same microscopic energy after two different scalings. The derivation of linearly elastic energies from atomistic interactions is a classical computation going back to the work of Cauchy, and in recent times has been reinterpreted in terms of a rigorous variational principle (see [14] and successive generalizations, e.g., in [30]). Note that the microscopic constraint does not influence the form of the continuum linear elastic approximation, but ensures that the passage to the limit is analytically well posed by the use of the rigidity estimates by Friesecke, James and Müller [25].

In this paper we will concentrate on the *surface scaling*, which can be thought as examining samples close to the fracture site in the reference configuration, so that bulk effects are negligible. At a microscopic level this amounts to looking at the response of the system when a macroscopic fracture is obtained by the application of forced displacements. The response depends on the orientation of the sample and of the fracture opening, and can be analyzed by computing minimum problems with *hard device* boundary conditions. In a regime of small displacements such boundary conditions can be thought to be the identity and a translation of the identity by a vector b, respectively, on opposite sides of a unit square (in the units of the continuum model), as represented in Fig. 1. This square is triangulated using a triangular lattice $\varepsilon\mathbb{T}$ of lattice spacing ε obtained by scaling a fixed triangular lattice $\mathbb{T}$.

If the displacement b is in the same direction of the sample orientation ν (in other words, it is orthogonal to the fracture site) then, under some hypotheses on the atomistic interactions, an optimal configuration is obtained by elongating a minimum amount of triangles in the direction b. The corresponding minimal energy only depends on ν and its computation reduces to the problem of counting such triangles. Note that, since we think of this behaviour as representing a typical sample close to the fracture site, we have to impose periodic boundary conditions in the direction orthogonal to ν in order that this optimal configuration be compatible with neighbouring lattice arrangements. As a technical remark, this can be easily imposed if ν is a "rational" lattice direction (i.e., it is a multiple of a vector in the lattice), while it needs some approximation argument if ν is not rational, since in that case periodic boundary conditions can be exactly satisfied only in the limit as $\varepsilon \to 0$. The computation of this

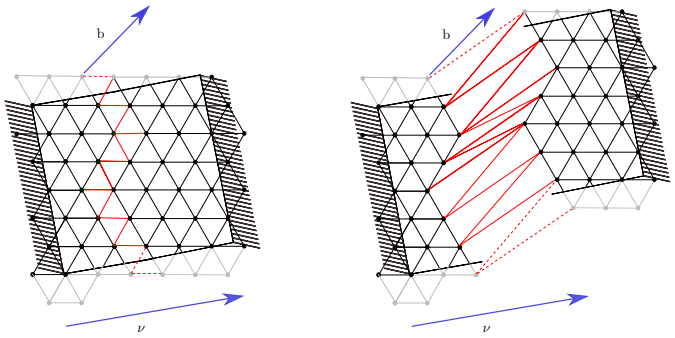

Figure 1: A hard-device microscopic test in the reference and deformed configuration

minimum problem highlights an anisotropic behaviour of the energy $\varphi(\nu)$ necessary to produce a macroscopic fracture in a given direction ν per unit length due to the underlying lattice symmetries, and gives a candidate for the fracture energy density in the variational principle stated above.

We will focus on two issues.

• analysis for infinitesimal displacements. In this case we will show that the macroscopic description as a brittle Griffith material with an opening condition on the fracture holds;

• analysis for finite displacements. In this case the surface energy cannot be determined by a simple analysis of the minimal number of elongated triangles. We will see that more complex (and less physical) configurations will appear, forced by the microscopic constraint.

These analyses will be performed in the framework or the variational theory of fracture, which requires some concepts of Geometric Measure Theory. To that end we will include some technical definitions and outline the main points of the proofs, whose details can be found in [10].

1 The analytical setting

1.1 Lattice sets and functions

At this moment, we have to be more specific about the discrete energies that we are going to consider, even though many of our arguments will rely on geometric considerations only. We will denote by $\mathbb{T}$ the triangular lattice in $\mathbb{R}^2$ generated by the vectors $\eta^1 = (1, 0)$, $\eta^2 = (1/2, \sqrt{3}/2)$. We introduce also the following notation

$$\eta^3 = \eta^1 - \eta^2, \qquad \mathrm{S} = \{\pm\eta^1, \pm\eta^2, \pm\eta^3\}.$$

Note that S is the set of unitary vectors in the lattice $\mathbb{T}$ and for each $\mathtt{i} \in \mathbb{T}$ $\mathtt{i} + \mathrm{S}$ is the set of its nearest neighbours in $\mathbb{T}$.

We define also the set D of *coordinate directions* as

$$\mathrm{D} = \{\eta^\perp \,:\, \eta \in \mathrm{S}\};$$

i.e., directions orthogonal to some vector η^k.

Given a reference configuration Ω and a lattice spacing ε which is thought to be very small (eventually, tending to 0 in the analytical approximation), we will consider the collection $\mathcal{T}_\varepsilon(\Omega)$ of all triangles with vertices in $\varepsilon\mathbb{T}$ and contained in Ω. For any $T \in \mathcal{T}_\varepsilon(\Omega)$ we will consider a triple (i_1^T, i_2^T, i_3^T) composed of its vertices labelled clockwise. Our admissible displacements are functions

$$u : \varepsilon\mathbb{T} \cap \Omega \to \mathbb{R}^2, \qquad i \mapsto u(i)$$

with the property that for all $T \in \mathcal{T}_\varepsilon(\Omega)$ the triple $(u(i_1^T), u(i_2^T), u(i_3^T))$ defines the vertices of a *non-degenerate triangle, which in this way are still ordered clockwise.* This requirement can be translated in a functional condition on the affine function defined on the triangle T interpolating the discrete values at the vertices i_j^T, which we may still denote $u : T \to \mathbb{R}^2$; namely, that

$$\det \nabla u > 0.$$

Patching up this definition of u on each such T we simply have a positive-determinant constraint on the piecewise-affine interpolation of u on $\varepsilon\mathbb{T}\cap\Omega$.

1.2 Lattice energies

The simplest way to define the energy of such a lattice function u on Ω will be through summation of three-point interactions as

$$F_\varepsilon(u) = F_\varepsilon(u, \Omega) = \sum_T \varepsilon\, f\Big(\frac{u(i_1^T)}{\varepsilon}, \frac{u(i_2^T)}{\varepsilon}, \frac{u(i_3^T)}{\varepsilon}\Big),$$

the summation being performed on $\mathcal{T}_\varepsilon(\Omega)$.

The value $f\big(\frac{u(i_1^T)}{\varepsilon}, \frac{u(i_2^T)}{\varepsilon}, \frac{u(i_3^T)}{\varepsilon}\big)$ can be regarded as the energy necessary to deform the reference triangle T with vertices (i_1^T, i_2^T, i_3^T). We suppose this energy to be of order 1 for large deformations of the triangle; i.e., when one (actually, necessarily at least two) of the deformed sides has length much larger than ε, that is,

$$|u(i_j^T) - u(i_k^T)| >> \varepsilon \text{ for some } j, k.$$

Since the linear dimension of each T is of order ε, in order to generate a macroscopic crack we will have a number of deformed triangles of order $1/\varepsilon$, which explains the scaling by ε in the definition of F_ε.

Note that this energy may be regarded as defined on functions $v : \mathbb{T} \to \mathbb{R}^2$ by setting

$$v(i) = \frac{1}{\varepsilon} u(\varepsilon i), \text{ so that } F_\varepsilon(u, \Omega) = \varepsilon \sum_T f((v(i_1^T), v(i_2^T), v(i_3^T)),$$

with the summation now on triangles in $\mathcal{T}_1\big(\frac{1}{\varepsilon}\Omega\big)$ with unit side length. This observation may be handy in computations where we can simplify the notation by parameterizing functions v on the fixed unit lattice.

The assumptions on f are as follows. We suppose that

• $f(u,v,w)$ is independent of permutations of the vertices which keep the clockwise ordering (i.e., $f(u,v,w) = f(v,w,u) = f(w,u,v)$), so that indeed it depends on the deformation of the triangle T;

• (*frame indifference*) f is invariant by rigid motions; i.e.,

$$f(Ru+q, Rv+q, Rw+q) = f(u,v,w)$$

for all R rotations and $q \in \mathbb{R}^2$;

• (*minimization on rigid motions*) the minimum of f is achieved exactly on clockwise-ordered vertices of equilateral triangles with unit side length, so that ground states are exactly images of the lattice $\mathbb{T}$ by rigid motions. We normalize the minimum of f setting it to 0;

• (*non-degeneracy of minimum points*) f is C^2 on its domain, and we have

$$f(u,v,w) \geq C((|u-v|-1)^2 + (|u-w|-1)^2)$$

on a neighbourhood of the minimizers of f, for some positive constant C.

• (*possibility of fracture*) there exists a positive constant C_0 which gives the optimal value of $f(u,v,w)$ as at least two side lengths of the deformed triangle tend to $+\infty$. We make the simplifying assumption that C_0 is achieved when two sides tend to infinity and the other one has length 1.

Remark 1.1 (surface relaxation effects)**.** The last simplifying assumption is indeed a restriction, since it implies that, as triangles neighbouring elongated triangles producing a macroscopic crack are concerned, triangles with minimal energy are still of equal scaled side-lengths 1, thus neglecting surface relaxation and boundary-layer effects. We are then supposing that we may neglect those (however fundamental) effects in this model (see however Remark 2.6 below).

Remark 1.2 (Lennard-Jones interactions)**.** As an example, we may consider f as the summation of independent central interactions such as Lennard-Jones ones; i.e., after normalizing,

$$f(u,v,w) = J(|u-v|) + J(|v-w|) + J(|w-u|) - 3\min J,$$

where

$$J(r) = \frac{C}{r^{12}} - \frac{2C}{r^6},$$

for which $C_0 = 2J(\infty) + J(1) - 3\min J = 2C$. In our setting we could also consider more general energies, taking into account next-to-nearest neighbour or longer-range interactions, as long as the geometry of minimizers remains the same, but we prefer to stick to this simpler formulation.

1.3 Approximate continuum parameters

We now consider the problem of characterizing the space of continuum functions u on which approximations of discrete functions u_ε for ε small can be parameterized, under the hypothesis of $F_\varepsilon(u_\varepsilon)$ be equi-bounded. We have already noticed that such u_ε may be interpreted as piecewise-affine functions and justified the scaling of the energy so that fracture

is allowed in the limit. For ε small we will then have the possibility of having a set of triangles that are deformed into very elongated triangles and can be considered a crack in the limit reference configuration. The equiboundedness of the energies also implies that ∇u_ε must be close to a rotation for most of the triangles T which do not contribute to the limit crack. We will see that the limit parameter is characterized as being a piecewise-rigid motion outside a crack set. In order to properly define this set of functions u we recall some definitions that are common in the modern variational theory of Fracture [6]. The key idea in the definition of a correct functional-analytic framework is to consider possibly discontinuous functions and identify cracks with the discontinuity sets of such functions. In such a context Griffith-type fracture energies are well defined and a number of boundary-value problems have solutions. The definition of such functions (special functions of bounded variation [4]) requires some Geometric Measure Theory concepts in order to define in a proper way the length of a crack (in three dimensions this would be the surface area of a crack) in the reference configuration and its orientation. This is done by considering the *one-dimensional Hausdorff measure* as measuring the length, and a *measure-theoretical normal* at almost every point of the crack site. The latter can be characterized by a blow-up argument: if we "zoom in" close to a point of the crack site, the crack site tends to appear as a straight line with a well-defined orientation, except for some exceptional points (crack tip, bifurcation points, corners). Besides a technical definition, we will try to maintain the analytical details to a minimum.

In the surface scaling, the sample will behave as a brittle rigid material; i.e., the continuum reference configuration will be subdivided into regions where the deformation is approximately a constant rigid motion. The crack site; i.e., the boundaries of such regions, will have finite total length (more precisely, finite one dimensional Hausdorff measure) and will be regular enough as to have a normal at almost every point of its (suitably defined) boundary in the sense hinted at above. The precise analytical definition that we will use is the following.

Definition 1.3 (sets of finite perimeter)**.** *We say that a set $E \subset \Omega$ is a* set of finite perimeter *in Ω if there exists a sequence of polyhedral sets $\{P_j\}$ whose boundaries have equibounded lengths such that the symmetric difference has infinitesimal Lebesgue measure $|E \triangle P_j|$ as $j \to +\infty$. If E is a set of finite perimeter then there exists a set ∂E (the* (approximate) boundary *of E) of finite $\mathcal{H}^1$ measure and a unit vector ν (the* internal unit normal *to E) such that the distributional derivative of the characteristic function of E is a measure concentrated on ∂E with density ν with respect to $\mathcal{H}^1$.*

Despite its technical appearance this definition simply states that sets of finite perimeter can be regarded as sets with piecewise C^1 boundary with finite length. Similarly, special functions of bounded variation u can be regarded as C^1 functions outside a piecewise-C^1 crack set $S(u)$ (see [4] for a rigorous definition and their properties, which will only be used as a technical tool in the proof of Theorem 1.5).

We can now define the space of continuum parameters as those func-

tions whose gradient is a constant rotation on each sets of finite perimeter of an underlying partition.

Definition 1.4 (piecewise rigid deformations)**.** *A function $u : \Omega \to \mathbb{R}^2$ will be called a* piecewise rigid deformation *if there exists a partition $\{E_h\}$ of Ω into sets of finite perimeter, vectors b_h and rotations $A_h \in SO(2)$ such that*

$$u(x) = b_h + A_h x \text{ almost everywhere on } E_h,$$

and the set

$$S_u = \bigcup_h \partial E_h$$

has finite $\mathcal{H}^1$ measure.

We may show that (a subset of) the space of piecewise-rigid deformations is the correct functional setting of our continuum description, as stated in the following theorem.

Theorem 1.5 (piecewise-rigid deformations as continuum parameters)**.** *Let u_ε be functions with $F_\varepsilon(u_\varepsilon) \leq C < +\infty$ and $\|u_\varepsilon\|_\infty \leq C < +\infty$ regarded as piecewise-affine functions. Then, up to extraction of subsequences, such functions converge in $L^1(\Omega;\mathbb{R}^2)$ to a piecewise-rigid deformation on Ω.*

This theorem states that functions u_ε equibounded in energies, which we also suppose to be pointwise equibounded in order to avoid that u_ε tend to infinity on a portion of Ω (which is perfectly allowed in Fracture theory), are approximated by piecewise-rigid deformations.

Proof. We fix a positive constant C and consider the functions $\overline{u}_\varepsilon$ defined as the piecewise-affine interpolation of u_ε on triangles where $f \leq C$ and an arbitrary vector, e.g., 0, elsewhere. We can picture these sets as obtained by removing from the domain triangles undergoing a large deformation. The number of those triangles is at most of order $1/\varepsilon$ and their total measure is then at most of order ε, and hence negligible. Describing the limits of u_ε is then equivalent to describing the limits of $\overline{u}_\varepsilon$. Since the gradients $\nabla\overline{u}_\varepsilon$ are equibounded, and the total lengths of their crack sites are also bounded, their limit is a special function of bounded variation, denoted by u, whose crack site $S(u)$ has with finite $\mathcal{H}^1$ measure. It remains to note that the hypotheses of frame indifference and non-degeneracy of minimum points for f imply that the gradients $\nabla\overline{u}_\varepsilon$ are close to some rotations, that may vary from triangle to triangle, although the sum of the contributions of their distance from the sets of rotation is globally going to 0. As $\nabla\overline{u}_\varepsilon$ tends to ∇u only weakly, we use a lower semicontinuity argument and the classical rigidity result to infer that $\nabla u \in SO(2)$ almost everywhere and its crack site has finite $\mathcal{H}^1$ measure. A rigidity theorem for special functions with bounded variation [16] allows us to conclude the claim. □

2 The small-displacement regime

We now consider small displacements from the identity function, which is by assumption an absolute minimizer of our energies. This amounts to

making the assumption that

$$u_\varepsilon = \mathrm{id} + \delta\, v_\varepsilon, \text{ with } \varepsilon << \delta << 1, \tag{2.1}$$

with v_ε equibounded; i.e., $\|v_\varepsilon\|_\infty \leq C < +\infty$. Analytically, we first consider the limit as $\varepsilon \to 0$ and then as $\delta \to 0$.

A first application of Theorem 1.5 gives that u_ε can be approximately described by a limit u^δ, which is a piecewise-rigid deformation with underlying partition $\{E_h^\delta\}$. As a consequence, also v_ε can be approximately described by a function v^δ, so that, on each element E_h^δ, we have

$$\nabla u^\delta = R_h^\delta = \mathrm{id} + \delta A_h^\delta,$$

where A_h^δ is the constant value of ∇v^δ on E_h^δ. Passing to the limit as $\delta \to 0$ we eventually obtain an underlying partition of sets E_h, and the corresponding function v with $\nabla v = A_h$ on E_h. Since the tangent space to $SO(2)$ at the identity are skew-symmetric matrices and

$$A_h = \lim_{\delta \to 0^+} \frac{R_h^\delta - \mathrm{id}}{\delta}$$

we obtain that A_h is a skew-symmetric matrix; i.e., it is an *infinitesimal rotation*.

Summarizing, in the small-displacement regime, the continuum parameter will be a *piecewise infinitesimal rotation* v, with an underlying partition of Ω into sets of finite perimeter $\{E_h\}$, on each of which ∇v is a constant skew-symmetric matrix.

2.1 Computation of a candidate Griffith-fracture energy density

We now turn our attention to the description of the asymptotic behaviour of sequences of energies $F_\varepsilon(u_\varepsilon)$ under assumption (2.1) as $\varepsilon \to 0$ and $\delta \to 0$. This can be done using the formalism of Γ-convergence, which consists in estimating a lower and an upper bound energy separately. Both lower and upper bounds are defined on the limit parameters v; if these bounds coincide, then their common value F is called the Γ-limit. The reason why it is important to compute a Γ-limit is that its definition is equivalent to the validity of the variation principle that minimum problems for the Γ-limit F approximate those for F_ε.

We first focus on the lower bound.

Definition 2.1 (lower bound)**.** *We say that F is a* lower bound *for F_ε if whenever u_ε is of the form* (2.1) *with $v_\varepsilon \to v$ as $\varepsilon \to 0$ and $\delta \to 0$, then we have*

$$F_\varepsilon(u_\varepsilon) \geq F(v) + o(1)$$

as $\varepsilon \to 0$ and $\delta \to 0$.

Our aim is to define a lower bound that depends only on the underlying partition $\{E_h\}$, more precisely on the boundaries of the element of the partition, and not on the traces of the function v on such boundaries. This is in accord with the energies in the Griffith theory of Fracture,

whose energy densities depend on the crack site but not on the fracture opening.

In order to define the energy density corresponding to such a lower bound, we focus on a point x_0 at the crack site with normal ν. Up to a scaling argument (corresponding to the definition of ν as the orientation of the limit normal after blow-up) we may suppose that the crack is approximately straight close to x_0, and estimate the energy due to the appearance of a crack considering a unit square centered in x_0. On the two sides of the crack the function takes approximately the value $\mathrm{id}+\delta v^-(x_0)$ and $\mathrm{id}+\delta v^+(x_0)$; i.e., up to a constant translation of $-v^-(x_0)$, we are driven to considering test problems as described in the Introduction with boundary data the identity and the identity plus b, with

$$b = \delta[v(x_0)] = \delta(v^+(x_0) - v^-(x_0))$$

on opposite sides of the test square.

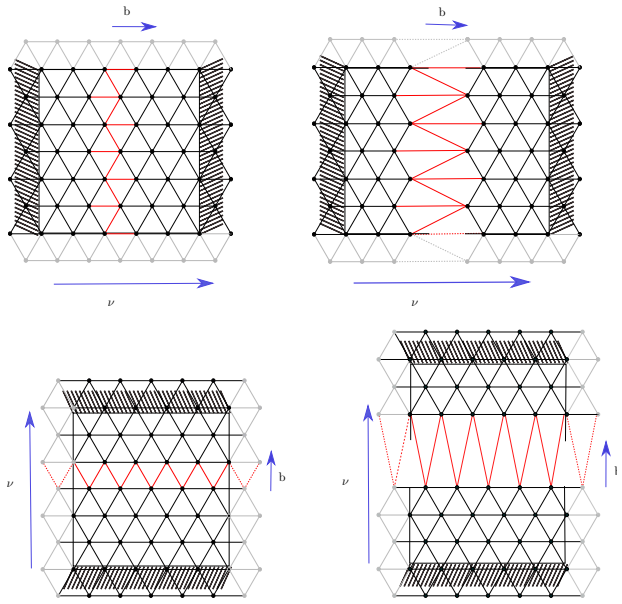

Figure 2: Opening cracks in direction e_1 and e_2

Under these assumptions, if b is a positive multiple of ν (*straight opening-crack regime*), then the minimal energy in the problems in Fig. 1 will be given by εC_0 times the number of triangles with two elongated sides. We note that this number is proportional to $1/\varepsilon$ but may depend on the orientation ν of the fracture site. In Fig. 2 we picture the configurations with minimal energy in two different cases, the first one corresponding to fracture orthogonal to a lattice direction.

The computation in this straight opening regime gives an energy per unit length with a hexagonal symmetry that can be explicitly written in

the form

$$\varphi(\nu) = \frac{2}{\sqrt{3}} C_0 \sum_{k=1}^{3} |\langle \nu, \eta^k \rangle| \tag{2.2}$$

This energy density is minimal when ν is a coordinate direction. The rigorous computation of this energy density can be found in [10].

The energy φ is the candidate for an anisotropic Griffith fracture energy, the anisotropy due to the underlying triangular lattice at a microscopic level. Indeed, we have the following result.

Proposition 2.2 (lower bound)**.** *Let v be a piecewise infinitesimal rotation with underlying partition $\{E_h\}$, and denote $S(v) = \Omega \cap \bigcup_h \partial E_h$. Then a lower bound for F_ε is given by*

$$F(v) = \int_{S(v)} \varphi(\nu_v) d\mathcal{H}^1, \tag{2.3}$$

where ν_v denotes the normal to $S(v)$.

Proof. The proof is obtained by a blow-up argument at each point of $S(v)$. Up to a scaling argument we reduce to a test problem in a unit square and to a limit interface which is orthogonal to ν. Up to the addition of an asymptotically negligible number of triangles, the union of the elongated triangles at the discrete level must contain a set S disconnecting the two sides of the square perpendicular to ν. If we use the function u which coincides with the identity and identity plus ν on the two sets disconnected by S, we obtain a test function for $\varphi(\nu)$ which gives a lower bound. □

The lower bound has been obtained by comparing with test functions for a straight opening fracture, but may be reached also if b is not exactly a multiple of ν. We now show a converse statement; i.e., that we may deduce a constraint on the fracture opening vector b from the validity of the lower bound: If for a given v the corresponding energy density is the $\varphi(\nu)$ described above at some point in $S(v)$, then the (possibly non-straight) *opening-fracture constraint*

$$\langle b, \nu \rangle \geq 0 \tag{2.4}$$

for $b = v^+ - v^-$ must hold, which gives this as a macroscopic counterpart of the microscopic constraint.

Proposition 2.3. *Suppose that the lower bound in Proposition* 2.2 *holds. Then the opening-crack constraint $\langle [v], \nu \rangle \geq 0$ holds at almost all points of $S(v)$.*

Proof. This constraint can be deduced from the fact that when the minimum of the test problems in the unit squares is (approximately) $\varphi(\nu)$ then essentially only one layer of triangles can be elongated and all other ones must remain essentially undeformed. The actual computation is rather sophisticated, so we only give a hint of the proof. It relies on the fact that bounds on the Jacobian determinant of u_ε on the set composed of non-elongated triangles guarantee the convergence of the traces of u_ε on

the boundary of such sets to the traces of its limit (which we have denoted by u^δ) on its jump set S_{u^δ}[3]. From this, one can deduce that $\delta\langle[v^\delta],\nu\rangle = \langle[\mathrm{id}+\delta v^\delta],\nu\rangle = \langle[u^\delta],\nu\rangle \geq o(1)$, so that $\langle[v^\delta],\nu\rangle \geq o(1)$ and eventually $\langle[v],\nu\rangle \geq 0$. □

Proposition 2.3 will allow us to exhibit an upper bound for F_ε according to the following definition.

Definition 2.4 (upper bound)**.** *We say that F is an* upper bound *for F_ε at v if there exist u_ε of the form* (2.1) *with $v_\varepsilon \to v$ as $\varepsilon \to 0$ and $\delta \to 0$, such that*

$$F_\varepsilon(u_\varepsilon) \leq F(v) + o(1) \tag{2.5}$$

as $\varepsilon \to 0$ and $\delta \to 0$.

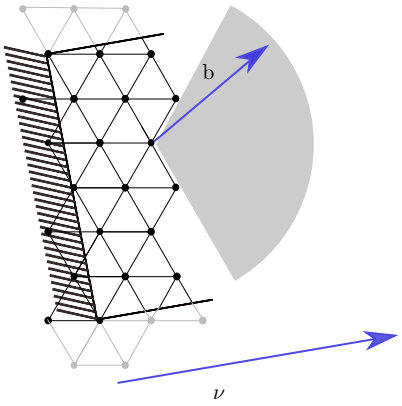

Figure 3: Deformation-free opening angle

Remark 2.5 (deformation-free opening angle)**.** The opening-crack constraint is sharp if ν is a coordinate direction; i.e., if at almost all points of $S(v)$, ν is a coordinate direction (i.e., the cracks follow the directions of the lattice) and $\langle[v],\nu\rangle \geq 0$ then we may find u_ε such that (2.5) holds. Some extra care must be taken when ν is not orthogonal to a lattice direction. Indeed, in this case, the orientation assumption on microscopic triangles gives a constraint on the direction of b in terms of a cone (or, in a two-dimensional terminology, an angle) of possible opening vectors that we obtain without deforming any additional triangle other the ones necessary to open the crack, as represented in Fig. 3.

If we denote by ν^+ and ν^- the two directions closest to ν orthogonal to the lattice vectors such that ν lies in the arc (ν^-,ν^+), then we have the constraints

$$\langle b,\nu^+\rangle \geq 0 \text{ and } \langle b,\nu^-\rangle \geq 0. \tag{2.6}$$

Note that these constraints can be regarded as a homogenization of the single constraint $\langle b,\nu\rangle \geq 0$ when we restrict to $\nu \in D$; i.e., when we

consider only cracks with normal ν being a coordinate direction, at almost every point of $S(v)$.

This defines a *deformation-free opening angle*. This angle is a straight angle centered in ν only when ν is a coordinate direction, in which case the constraint is (2.4), and otherwise it describes an angle of 120 degrees containing ν in its interior.

Remark 2.6. When listing the assumptions on the function f as the possibility of fracture is concerned, we have made the simplifying assumption that triangles with two (very) elongated sides have minimal energy when the third side has length ε (i.e., it is "undeformed"). For general energies, we do not expect this to hold, and the minimal energy will be achieved when the third side has length approximately $a\varepsilon$ for some $a > 0$. This would influence the width of the deformation-free opening angle, and the constraint (2.6), but the deformation-free opening angle always contains the normal ν itself and for opening cracks the correction to φ only gives a constant addition to $\varphi(\nu)$ due to the boundary-layer effect of the rearrangements of the triangles on both sides of the crack.

For functions v for which $b = [v]$ satisfies the constraint (2.6) the description in terms of the fracture energy density φ is sharp.

Theorem 2.7 (asymptotic description)**.** *Let $\{E_h\}$ be a partition of Ω composed of Lipschitz sets with piecewise C^1-boundaries, and let v be a piecewise infinitesimal rigid motion with underlying partition $\{E_h\}$ such that* (2.6) *holds at almost all points in $S(v)$ with $b = [v]$ and $\nu = \nu_v$. Then the fracture energy F defined in* (2.3) *is the Γ-limit of F_ε at v; i.e., F is both an upper and a lower bound for F_ε.*

Proof. Since the lower bound holds for all v, we only have to prove the upper bound. By an approximation argument, we can suppose that all E_h are polygons with normals coordinate directions at almost every point, and that at most three such sets meet at a single point. Note that condition (2.6) ensures that an approximation by polygons satisfies (2.4). A recovery sequence for the upper bound is then obtained simply by taking u_ε as the discretization of $\mathrm{id}+\delta v$. □

It must be noted that the regularity of the boundaries of $\{E_h\}$ is required only for technical reasons. Its necessity is due to the lack of approximation theorems for functions satisfying an opening-crack constraint when the underlying partition is not regular. From Theorem 2.7 we deduce that the same result holds for a set of admissible deformations $\mathcal{D}(\Omega)$ abstractly defined as the set of piecewise infinitesimal rigid motions v with underlying partitions $\{E_h\}$ that can be approximated by functions v_j satisfying the hypotheses of Theorem 2.7 and such that $F(v_j) \to F(v)$.

We note that there is a gap between the necessary condition obtained in Proposition 2.3 and the more strict condition (2.6) for which we prove the upper bound in Theorem 2.7. We conjecture that indeed Proposition 2.3 can be improved to prove the necessity of condition (2.6).

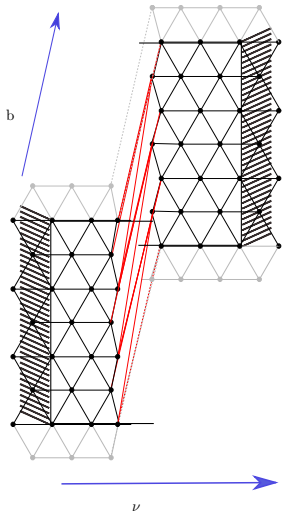

Figure 4: Surface relaxation for directions external to the deformation-free angle

Remark 2.8 (geometric surface relaxation)**.** The domain of the Γ-limit is larger than the one described in Theorem 2.7, or its abstract completion $\mathcal{D}(\Omega)$. Indeed, we can exhibit a finite upper bound under the sole condition $\langle [v], \nu \rangle \geq 0$, and still obtained by elongating only one row of triangles. It this case, though, we have to deform also some boundary triangles, which justifies the terminology "deformation-free" introduced above. In order to explain this fact, we consider the test problems on squares for opening vectors b satisfying the larger constraint (2.4) but not (2.6). The minimum value in the test problem is still finite, but cannot be achieved by only elongating one layer of triangles while keeping all others undeformed. It is necessary instead to deform the boundary triangles on either side of the elongated layer, in order to accommodate the triangles to satisfy the orientation constraint. This is a sort of *geometric surface relaxation*. We use this term in order to distinguish this rearrangement of boundary triangles from the energetic surface relaxation due to the unbalance of interactions close to the fracture site. That type of relaxation is typical to systems with next-to-nearest neighbour interactions, which generate a boundary layer in the direction orthogonal to the fracture site to accommodate missing interactions, as observed by Charlotte and Truskinovsky [17]. Here, the overall effect is felt only when b does not lay in the "deformation-free" angle.

Note that this last remark suggests that a complete Γ-limit should be expressed through an energy density of the form $\varphi([v], \nu)$, where this function is finite only when $\langle [v], \nu \rangle \geq 0$ and it coincides with $\varphi(\nu)$ if ν is a coordinate direction, or $[v]$ and ν satisfy (2.6). This addition to the classic Griffith theory does not seem unreasonable, since a rearrangement of

atomistic position is necessary at a microscopic level for fracture openings (almost) orthogonal to ν, when ν itself is not orthogonal to the lattice directions. However, since in general we expect fracture to follow the lattice direction, this more precise value of the energy density may have little impact on the actual computational issues, while it seems to be a challenging analytical problem.

These considerations and Theorem 2.7 validate the use of this discrete model as a finite-element approximation of an (anisotropic) Griffith fracture model with a linearized opening constraint $\langle [u], \nu \rangle \geq 0$ on the fracture site in the hypothesis of small-opening fracture.

3 The finite-deformation regime

In the case of finite deformations we are not restricted to small perturbation of the identity, and absolute minimizers of the discrete energies are all (discretizations of) rigid motions. The macroscopic description for elastic deformations subjected to the positive-determinant constraint is a long-standing challenging analytical problem. Our scaling allows to concentrate on surface effects.

Theorem 1.5 ensures that the limit energies will be finite only on piecewise rigid motions. We now consider the question whether the microscopic fracture-opening mechanism can be described macroscopically by a Griffith energy density with an opening constraint also in the finite-deformation regime.

For the sake of simplicity in the sequel we assume that the three-point interaction density $f(u, v, w)$ be as in Remark 1.2, where we choose the constant C in the Lennard-Jones potential to be equal to $C_0/2$, in order that f satisfy the hypotheses of Section 1.2.

3.1 Validity of the lower bound

As a first step in our analysis we show that the anisotropic Griffith-fracture energy $F(u)$ defined in (2.3) provides a lower bound for the energies $F_\epsilon(u_\epsilon)$ also for general sequences of deformations u_ϵ, not necessarily small perturbations of rigid motions, extending thus the result stated in Proposition 2.2 for straight-opening-crack deformations and valid more generally in the small-displacements regime.

Proposition 3.1 (lower bound for finite deformations)**.** *Let u be a piecewise rigid rotation with underlying partition $\{E_h\}$, and denote $S(u) = \Omega \cap \bigcup_h \partial E_h$. Then a lower bound for F_ε is given by*

$$F(u) = \int_{S(u)} \varphi(\nu_u) d\mathcal{H}^1,$$

where ν_u denotes the normal to $S(u)$ and φ is given by (2.2)*.*

Proof. Also in this case one may argue by the blow-up argument quoted in the proof of Proposition 2.2. We may also give an alternative proof based on a direct counting argument of the elongated sides of triangles of

a given sequence u_ϵ approximating u. This can be done regrouping such sides in dependence of their orientation with respect to lattice directions and using a slicing technique. With fixed η_k a lattice direction, the slicing argument allow us to estimate asymptotically the number of elongated sides parallel to η_k as proportional to the quantity $|\langle \nu_u, \eta_k \rangle|$ per unit crack length. In particular, the factor of proportionality is independent of k and coincides with C_0 multiplied by an explicit constant depending only on the geometry of the lattice (see [10] for details). □

3.2 A new type of constraint on the opening fractures

We now analyse the constraint at a point x belonging to the fracture site. Since the analysis for small opening fracture relies mainly on geometrical arguments we can repeat it for finite opening, taking into account that on either side of the fracture site the deformation is a discretization of a rigid motion.

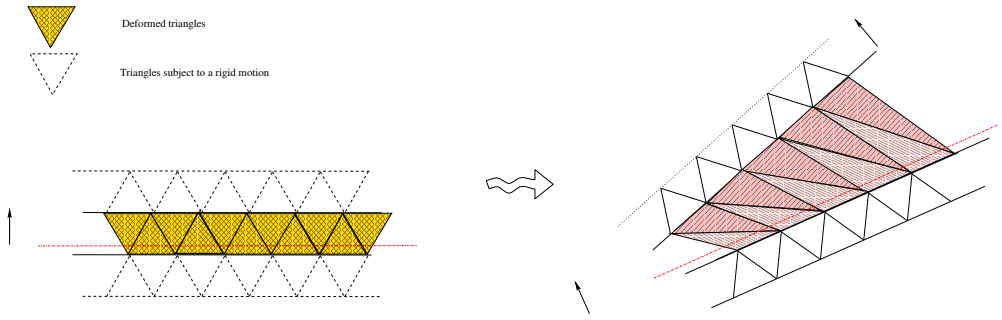

Figure 5: Triangles deformed by the pointwise interpolation

We first consider the simpler case of a fracture with a discontinuity set in a lattice direction. For a pictorial description we refer to Fig. 5.

Note that the image of any deformed triangle, with clockwise oriented vertices (i_1^T, i_2^T, i_3^T) in the reference configuration, is in one case $(u^-(i_1^T), u^+(i_2^T), u^-(i_3^T))$, and, in the other one, $(u^-(i_1^T), u^+(i_2^T), u^+(i_3^T))$. Thus, the orientation-preserving constraint amounts to the new *opening-fracture constraints*

$$\langle u^+ - u^-, R^- \nu \rangle \geq 0,$$

and, exchanging the role of u^+, u^-,

$$\langle u^+ - u^-, R^+ \nu \rangle \geq 0.$$

This new constraint is consistent with the fact that at the points $u^+(x), u^-(x)$, image respectively of the point $x \in S(u)$, $R^+\nu, R^-\nu$ are the new normals, in the deformed configuration, to the crack sites.

We now show that for deformations such that the lower bound in Proposition 3.1 is optimal the new constraint on the fracture opening $[u] = u^+ - u^-$ above holds true.

Proposition 3.2. *Let u be a function in the domain of the continuum limit energy. Let ν be the normal to the fracture site at a point x, and suppose that the fracture energy density at the point x be given by $\varphi(\nu)$. Then, if $R^{\pm} \in SO(2)$ denote the rotations corresponding to u on either sides of the fracture site, we have*

$$\langle [u], R^{\pm}\nu \rangle \geq 0.$$

Proof. At a discrete level, close to x we will have a single layer of deformed triangles; which can be regarded as a stripe between two piecewise-linear curves made by triangle sides. An energetic argument shows that most of the images of the triangles must have boundary segments oriented orthogonally to $R^{\pm}\nu$, on the respective side. The orientation constraint applied on any of those triangles then translates in the desired inequality. □

We now provide a class of deformations for which $F(u)$ is an upper bound.

Contrarily to what happens for small displacements, a relevant condition to ensure the validity of the upper bound for finite deformations is a *strict opening-fracture constraint*, that is

$$\langle [u], R^{\pm}\nu_u \rangle > 0 \tag{3.1}$$

together with the condition that $S(u)$ be a finite union of segments with normal a coordinate direction.

Indeed, if the segments composing $S(u)$ meet at most pairwise, condition (3.1) ensures that a discretization of u, obtained as a pointwise evaluation of u at the lattice points, is orientation preserving and provides a recovery sequence for the upper bound.

We point out that the gap between condition (3.1) and the necessary condition to the validity of the upper bound of Proposition 3.2 cannot be overcome. In fact, in case of a *folded deformation*, that is, $S(u)$ consisting of a line parallel to a lattice direction and $R^{+} = -R^{-}$, it holds $\langle [u], R^{\pm}\nu_u \rangle = 0$, and any discretization of such deformation violates the impenetrability constraint.

When more than two segments meets, in the configurations considered above, more compatibility conditions have to be taken into account. By a density argument a target case to be considered is the case in which we have three segments with coordinate normals meeting at a triple point x_0. In such a case in order to prove the validity of the upper bound we have to add to condition (3.1) along each single segment, the additional hypothesis that, denoted by (A_1, A_2, A_3) a clockwise ordering of the regions delimited by the three segments and by u_i the rigid deformation on the region A_i, then the triangle with vertices $(u_1(x_0), u_2(x_0), u_3(x_0))$ maintains the same ordering. When these conditions are satisfied, then we call x_0 a *positive triple point* for u.

We can now state a result validating the macroscopic description by a Griffith-type anisotropic surface energy of our microscopic lattice model subject to a impenetrability constraint for a class of finite deformations.

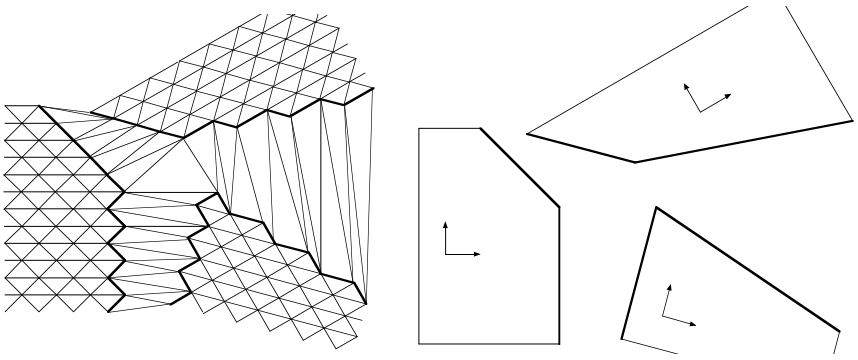

Figure 6: A positive triple point

Theorem 3.3 (asymptotic description)**.** *Let u be a piecewise rigid motion such that its underlying partition of Ω is composed by polygons whose boundaries have coordinate normals, meeting at most at positive triple points and such that condition* (3.1) *holds along the boundaries. Then the fracture energy F defined in* (2.3) *is the Γ-limit of F_ε at u; i.e., F is both an upper and a lower bound for F_ε.*

Proof. Since the lower bound holds for all u, we only have to prove the upper bound. A recovery sequence for the upper bound is then obtained simply by taking u_ε as the discretization of u. Indeed, for such u_ε, the hypothesis on positive triple points ensures that, at level ε, the deformation of the microscopic triangle containing the triple point has positive determinant. □

Remark 3.4. In the case when a piecewise rigid motion u has polygonal underlying partition with normal ν which is not a coordinate direction, then in order for u to be approximated by coordinate polygons with normal orthogonal to a lattice direction and satisfying (3.1), condition

$$\langle [u], R^{\pm}\nu \rangle > 0$$

is not sufficient and must be replaced by the stronger fracture-opening constraint

$$\langle [u], R^{\pm}\nu^{+} \rangle > 0, \qquad \langle [u], R^{\pm}\nu^{-} \rangle > 0,$$

where ν^{-} and ν^{+} are the two minimal normals orthogonal to two consecutive lattice directions generating ν.

Remark 3.5. Theorem 3.3 and in particular condition (3.1) imply that the energy density actually depends on the trace of the rotations $R^{\pm}\nu$ on both sides of the fracture. This can be seen as a dependence on the

tangential derivative of the traces $u^{\pm}$, so that actually we have to take into account energy densities

$$\varphi\Big([u], \frac{\partial u^{\pm}}{\partial \nu^{\perp}}, \nu\Big).$$

This is an unexplored type of energies depending on the deformation of $S(u)$.

3.3 Pathologies for finite deformations

In the previous sections we have computed the Γ-limit of our discrete system when the macroscopic configuration satisfies compatibility conditions on the fracture site and at meeting points of three (or more) fracture sites. Those conditions can be regarded as a *positive-determinant constraint on the fracture*. In this section we will see how all those conditions can be removed. In this way macroscopic configurations "with fracture with negative-determinant" can be obtained from atomistic configurations satisfying a microscopic positive-determinant constraint, at the expense of a strictly greater energy.

3.3.1 Removal of compatibility conditions on the fracture site − multiple microfracture

By introducing more than one layer of deformed microscopic triangles we may remove all constraints on $S(u)$, while the macroscopic energy varies by a factor proportional to the number of additional layers.

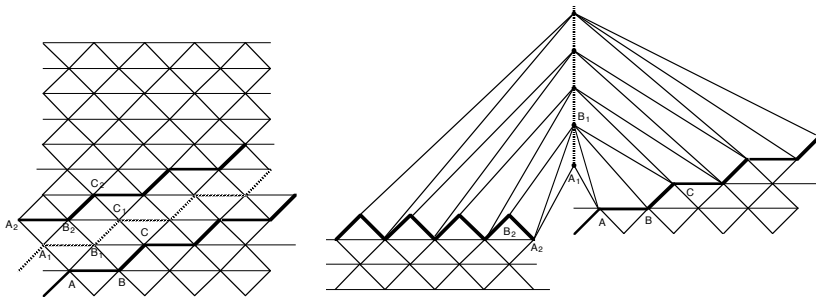

Figure 7: Multiple microscopic fracture

In Fig. 7 the macroscopic deformation on the fracture does not satisfy the conditions

$$\langle u^{+}(x) - u^{-}(x), R^{\pm}\nu_i\rangle \geq 0$$

for the two "microscopic" coordinate normals ν_i. However, the discrete functions in the construction depicted in Fig. 7 all have positive determinant thanks to the introduction of a "fictitious" layer of atoms. In this case the limit energy per length doubles.

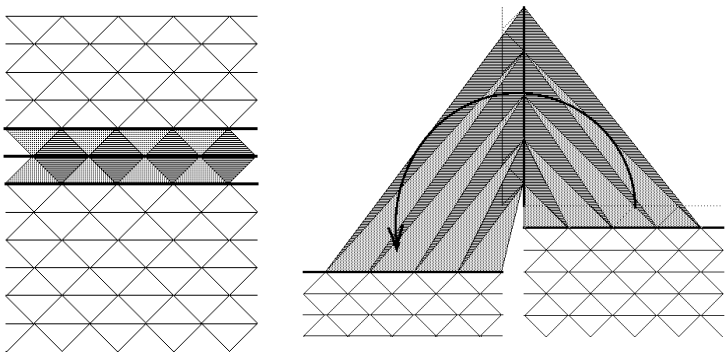

Figure 8: Multiple microscopic fracture - reference and deformed configurations

A variation of this example is given in Fig. 8 and 9 to highlight that the introduction of an extra layer of atomic interactions allows to remove the condition $\langle u^+(x) - u^-(x), R^{\pm}\nu\rangle \geq 0$ even when ν is a coordinate normal. By repeating this process the macroscopic deformation may exhibit a interpenetration phenomenon.

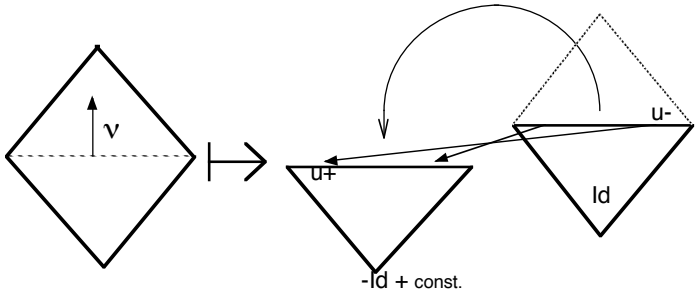

Figure 9: Multiple microscopic fracture - macroscopic configurations

Note that for some deformations surface relaxation may be energetically convenient with respect to multiple-layer fracture. This clearly is the case the situation exemplified in Fig. 4.

3.3.2 Removal of compatibility conditions on "triple points" – micro-deformed fracture

The condition on triple points in the previous section ensures that the deformation of a microscopic triangle at that point is of positive determinant (and hence, being a single triangle, gives a negligible energy contribution). If such a condition does not hold then the use of (small variations of) pointwise interpolations on the different regions of the un-

derlying partition is not possible, since for ε small there will always be a microscopic triangle whose vertices are mapped in three points which fail the positive-determinant constraint. However, it is possible to use a different interpolation by introducing an additional microscopic fracture enclosing small sets where the deformation is not in $SO(2)$. Note that this is possible if such sets have the dimension of an interface.

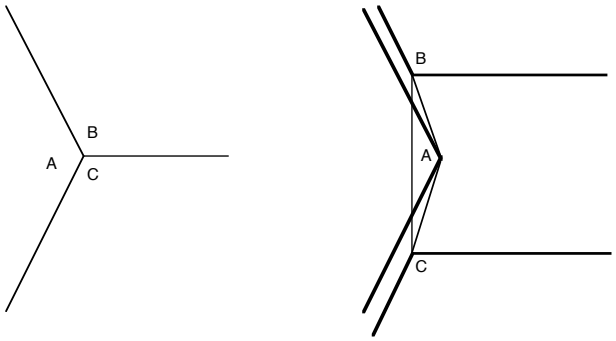

Figure 10: Triple point with "negative determinant" – reference and deformed macroscopic deformation

In Fig. 10 it is represented a deformation with a triple point failing the positive-determinant condition. In this case we introduce a microscopic approximation as represented in Fig. 11.

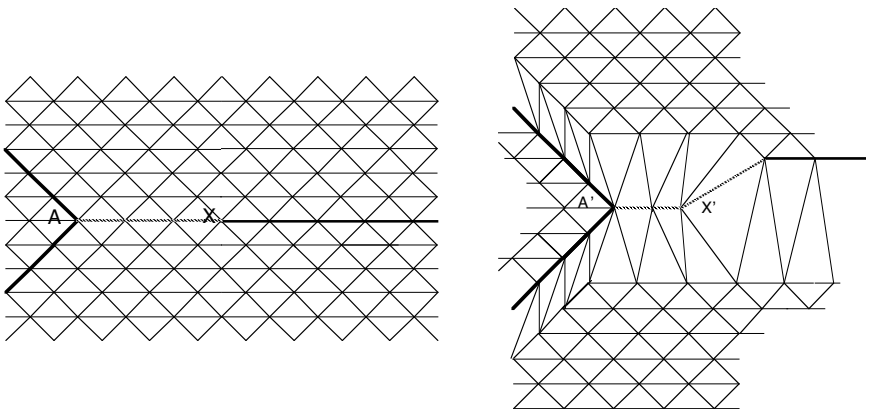

Figure 11: Triple point with "negative determinant" – reference and deformed microscopic deformations

On the fracture site we introduce a segment $[A, X]$ where the point-wise single-layer interpolation of the jump is substituted by a double-layer

approximation. Note that the image $[A', X']$ of this segment undergoes an additional linear deformation. Note that the energy of this approximation provides the additional contribution

$$\Big(\varphi(\nu) + J\Big(\frac{[A', X']}{[A, X]}\Big)\Big)\mathcal{H}^1([A, X]),$$

where the second term is due to the compression of the triangles on the segment $[A, X]$ in the reference configuration. This energy depends on the choice of X and X', which are variables in the construction (satisfying some constraints due to the positive-determinant requirement in the resulting construction). This shows that even in this simple case an optimization problems arises between the introduction of an additional microfracture and a microscopic compression. Of course, more complex constructions with more parameters can also be introduced.

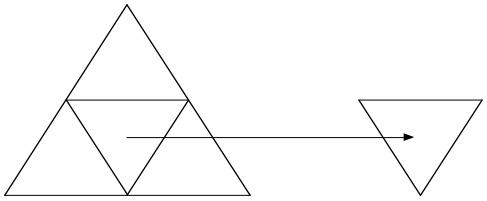

Figure 12: Deformation violating the impenetrability constraint

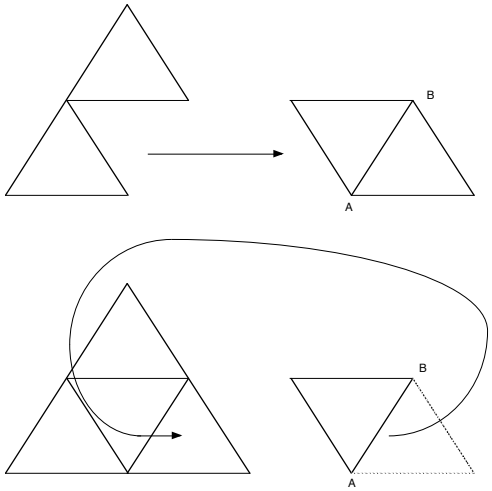

Figure 13: Construction of approximations satisfying the positive-determinant constraint

3.3.3 Global failure of impenetrability constraints – optimal decomposition and healing microfractures

In the constructions illustrated above we were able to exhibit a microscopic recovery sequence by working separately on each fracture site or triple point. In the presence of a complex geometry of the domain, besides a use of those constructions one has also to take into account the possibility of introducing further "fictitious" microscopic interfaces to get around impenetrability constraints. As a simple example, we may consider the deformation in Fig. 12, where the central smaller triangle is removed and translated from its position in the larger triangle. This macroscopic deformation can be approximated by microscopic ones all satisfying the positive-determinant constraint (see Fig. 13). One such approximation can be obtained by translating a rhombus and subsequently composing this translation with a deformation rotating half of this rhombus as described in Section 3.3.1 (see also Fig. 9). Note that this last rotation entails the introduction of one or more microscopic fictitious layers of atoms.

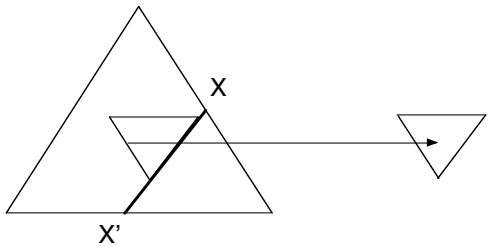

Figure 14: Deformation that can be obtained with auxiliary fractures

Another simple example is depicted in Fig. 14, where the triangle to be removed is strictly contained in the interior of a larger triangle. In this case, in order to proceed as in the previous construction, one has to introduce an "auxiliary fracture" as the segment $[X, X']$ in the figure. The determination of the optimal shape and location of such auxiliary fracture sites is clearly a complex optimization problem. Note that in this case, also the determinant constraint for triple points has to be taken into account.

4 Conclusions

We have examined a two-dimensional atomistic system of nearest-neighbour interactions allowing for macroscopic fracture parameterized on a triangular lattice, with a microscopic positive-determinant constraint which mimics the effect of long-range interactions and limits the ground states to rotations.

In parallel to the one-dimensional case we have focused our attention on the fracture term of the resulting continuum approximation by suitably

scaling the energies. We have thus determined

• a surface energy density $\varphi = \varphi(\nu)$ depending on the orientation of the crack site, this reflecting the triangular symmetries of the underlying lattice;

• conditions on the interface that reflect the positive-determinant constraint.

In the case of small deformations such conditions can be interpreted as an opening-crack constraint and the surface energy density describes precisely the energetic cost of opening a crack, except for some corrections when the crack is not oriented following the lattice directions and for crack opening almost tangential to the crack. As a conclusion, and taking into account the corresponding analysis for the bulk scaling (also analyzed in recent works by Friedrich and Schmidt [22, 23, 24, 21]), we infer that in this case a good continuous approximation is a *Griffith brittle fracture energy with opening constraint on the fracture*.

In the case of finite deformations the analysis is more complex. In particular we have

• the conditions on the interfaces are of a novel type that take into account both the gradient of the deformation on both sides of the fracture and the orientation of the fracture site in the reference configuration. Energies containing interfacial terms considering such quantities have been only partially examined and seem to be a challenging analytical issue [3];

• we also have a positive-determinant constraint on points where more cracks meet (triple points). Failure to satisfy such conditions also at one point give an additional contribution of the order of a finite fracture energy;

• such conditions are not a closed constraint, and can be removed by adding "fictitious" micro-fractures. The optimal location and form of those micro-fractures depends on the corresponding macroscopic deformation, and is a complex optimization problem.

We argue then that in the finite-deformation case, a hyperelastic fracture energy is not a good approximation of the discrete system that we are examining. Conversely, the use of such a system to model fracture phenomena outside the small-deformation regime seems to need some corrections in order to avoid non-local effects highlighted by the analytic description of the corresponding continuum model. In particular

• the fictitious micro-fractures caused by the determinant constraint seem to be completely artificial. In a dynamical test they would be produced when the two sides of a crack are at a finite distance. It seems more reasonable to enforce the determinant constraint only for small distances (e.g., a multiple of the lattice spacing), and to introduce a dynamical criterion for the evolution of fracture, such as the ones studied by Francfort, Marigo and colleagues [20, 6].

• the effect of conditions on triple points seems to be overestimated since the failure of the determinant constraint at a single point results in the creation of a finite crack. A mechanism to avoid this phenomenon could be to substitute a strict determinant constraint with the penalization on the number of triangles which fail to satisfy the positive-determinant condition.

Moreover, we have neglected interactions other than nearest neighbours. In this way the interfacial energy does not reflect the possibility of surface relaxation; i.e., the fact that atomistic interactions are unbalanced close to interfaces. This is an important effect as first highlighted by Charlotte and Truskinovsky [17], especially at the boundary of the domain and in the determination of the location of fractures. It has been partially addressed by Theil [32], and should be included in further investigations on the subject. The one-dimensional analysis by Braides and Solci [13] suggests that considering longer range of interactions (e.g., next-to-nearest neighbours) could be used in the place of the determinant constraint in order to eliminate non-local effects for non-opening cracks, at the expense of introducing internal and external boundary layers, whose precise description in dimension larger than one seems analytically challenging.

Acknowledgments

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