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MicroFract: An image based code for microstructural crack path prediction

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ABSTRACT

Brittle failure is prevalent in ceramics, fiber composites and metals where the microstructural cracks propagate in the path of least resistance following weak interfaces and grain boundaries. We formulate an image-based methodology for identifying the path of least resistance in the microstructure. In this approach, a user specifies the line direction of the macroscopic crack and a cohesive energy map corresponding to the weak and strong interfaces in the microstructure. The path of least resistance is formulated as a process of minimizing a discretized cost function based on an Ising-type energy model. The main advantage of this algorithm is that it can be exactly solved by the max-flow min-cut theorem. The results are shown via 2D examples from literature and the code and examples are made available to the community.

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Code metadata

Current code version	*MicroFract v1.0*
Permanent link to code/repository used of this code version	http://github.com/ElsevierSoftwareX/SOFTX-D-17-00020
Legal Code License	*FreeBSD license (Clause-2 BSD)*
Code versioning system used	*none*
Software code languages, tools, and services used	*MATLAB*
Compilation requirements, operating environments & dependencies	MATLAB 2010a–2015b, MATLAB Image Processing Toolbox , Multi-label optimization/graph-cut library (gco-v3.0)
If available Link to developer documentation/manual	NA
Support email for questions	veeras@umich.edu

1. Motivation and significance

Detailed simulation of cracks down to the microstructural scale is still difficult due to the computational expense in tracking both microstructural and macroscopic crack trajectory. The problem has been addressed in the past using multiscaling schemes that avoid full mesh resolution. In homogenization models, scale separation is invoked and microstructural failure is separately modeled and the results are homogenized to compute the constitutive response at macroscale material points [1]. However, computing the evolution of complex fracture paths, particularly at the microstructural scale, is a tedious task. Due to the complexity of representing cracks in finite element models, several advanced numerical techniques have been developed in the past. In the context of the finite element method (FEM), these methods are broadly classified into two families, node enrichment FEM (e.g. X-FEM) [2] and elemental enrichment FEM (e.g. E-FEM) [3,4]. Recently, other competing methods for simulation of microstructural cracks have emerged. Instead of introducing discontinuities within the mesh, the fracture paths are directly represented using a phase-field or a level-set [5–7]. The advantage of such methods is that the fracture surfaces are obtained from energy minimization. The primary drawback of these approaches is that the solution may lead to a local minima. Alternatively, in this paper, a discrete version of the energy minimization approach is proposed that leads to a crack path with the global minimum energy.

Microstructural crack trajectory is overall driven by the macroscopic crack direction as shown in Fig. 1(a, b), while microstructure

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resolves the crack along surfaces of low resistances: in effect, the crack follows a zig-zag trajectory following weak microstructural features (Fig. 1(c)). The excess energy to be supplied at the microstructural scale to form a crack of area A is taken as [8],

$$\varepsilon(A) = \int_A (\Gamma - \varphi) dA. \quad (1)$$

where Γ is the cohesive energy along the crack path and φ is the supplied macroscopic energy that acts against cohesion. We define the crack path to be the area A that minimizes this energy. In effect, we are searching for a path of least resistance that has both high stresses and low interfacial strength, and is thus amenable for fracture. Among all possible crack paths of equal area, the fracture follows a path where the overall cohesive energy Γ is the lowest when the macroscopic energy (φ) supplied is uniform [9]. However, in physical models, the macroscopic energy is not uniform and is localized taking the highest value along the macroscopic crack trajectory. Such a distribution of macroscopic energy ensures that the crack follows the macroscopic crack line in the absence of microstructure (ie. if Γ were constant).

The rate of decay of the value of φ away from the crack line determines the banded region across the macroscopic crack line within which a microstructural crack path that minimizes the difference in cohesive energy and supplied energy can be found. Because of the length scale differences between the macro and micro scales, a linearization of energy φ away from crack line is a reasonable assumption (Fig. 1(c)). While φ could be found from elastic energy obtained from a macroscopic simulation, one could also consider using a purely geometric representation by allowing the user to adjust the relative magnitude of φ versus Γ. If φ is made more critical than Γ, the crack path will be closer to the macroscopic crack line. If Γ is made more important, then the crack path could deviate more from the macroscopic crack line.

The problem of finding the crack area A that minimizes $\varepsilon(A)$ is an exercise in functional minimization. Computationally, the solution typically involves solution of a partial differential equation that tracks fracture surface evolution using gradient descent schemes, phase field parameters or level sets as demonstrated in [6,7]. As explained previously, the primary drawback of these approaches are that the solution may lead to a local minima and there is no guarantee of global minimum energy path. Further, these methods have issues in handling non manifold geometries such as microstructures with voids. The primary purpose of this letter is to introduce the use of *graph cuts* method to minimize $\varepsilon(A)$. While this method is popular in image processing [11], there are no precedents for the use of this technique in the mechanics community. Here, the path of least resistance is formulated as a process of minimizing a discretized cost function based on an Ising-type Hamiltonian. The main advantage of this approach is that it can be exactly solved (to get global minimum) by the max-flow min-cut theorem [12,13]. The results are shown via 2D examples from literature and the code and examples are made available to users [14].

2. Software description

The image is modeled as an Ising lattice with each pixel modeled as a lattice site. The interactions between the pixels can be seen as 'edges' on the lattice (see Fig. 2). We have a finite set of pixels P and a finite set of labels L. A labeling is assignments of labels in L to pixels in P. The individual pixels are referred with small letters p and q, label of pixel p is denoted by l_p.

The total energy can be written as the following sum:

$$\varepsilon = \sum_{p,q} V_{pq}(l_p, l_q) + \sum_p D_p(l_p) \quad (2)$$

where D_p is the cost of assigning the label l_p to pixel p, V_{pq} is the cost for assigning labels l_p and l_q to neighboring pixels p and q. In the context of modeling a crack line, a binary labeling scheme $l_p \in \{0, 1\}$ is used. Once the energy is minimized, the microstructural crack is given by the interface between the regions labeled zero and one, with the label being one on the positive side of the crack and zero on the negative side of the crack as shown in Fig. 2(left). The first term relates to the cohesive energy of pixels p and q. The second term in Eq. (2) relates to the macroscopic energy term φ and a linear variation is used. For a pixel p on the positive side of macroscopic crack line, we use $D_p(0) = \lambda \|p\| / p_+$ and $D_p(1) = 0$ where $\|p\|$ is the distance of pixel p from the macroscopic crack line, p_+ is the distance of the pixel located farthest from the crack line on the positive side of the crack, and λ is a constant. The above definition of D_p ensures that the label 1 (with lower D_p) is highly preferred on the positive side of the crack during energy minimization. For a pixel p on the negative side of macroscopic crack line, we use $D_p(1) = \lambda \|p\| / p_-$ and $D_p(0) = 0$ where p_- is the distance of the pixel located farthest from the crack line on the negative side of the crack. This definition of D_p ensures that the label 0 is highly preferred on the negative side of the crack. As we reach pixels closer to the crack line, the distance $\|p\|$ tends to zero and label 1 also becomes increasingly feasible on the negative side of the crack. In other words, there is a band around the macroscopic crack line where both labels are feasible and the final choice of the microstructural crack is made by also weighting the cohesive energy contribution in the first term of Eq. (2).

The cohesive energies of pixels (Γ_p) are read in by the user in the form of a color image. The energies are binned into N discrete levels and the level number (0,…,N-1) is used to describe a discrete cohesive energy $\widehat{\Gamma}_p$. If adjoining pixels have different labels, that means the microstructural crack passes through the pixels and an averaged value of $\widehat{\Gamma}$ is used to model the cohesive energy for that edge. This energy is taken to be zero if the adjoining pixels have the same label. Mathematically, this is defined using the first term in Eq. (2) as: $V_{pq}(l_p, l_q) = 0 \text{if} l_p = l_q$, and $V_{pq}(l_p, l_q) = mean(\widehat{\Gamma}_p, \widehat{\Gamma}_q) \text{if} l_p \neq l_q$. When minimizing the energy expression (2), the first term tends to draw the microstructural crack towards a path along which the cohesive energy is minimum. The second term ensures that this path is chosen close to the macroscopic crack trajectory. Thus, this approach solves a discrete version of the continuum energy minimization problem in Eq. (1). The constant λ adjusts the relative magnitude of first and second terms in the energy expression (2). If λ is higher, then the microstructural crack path will be closer to the macroscopic crack line. From our numerical experiments, a value of $\lambda = N/2$ was found to be optimal.

The advantage of the discrete energy form of Eq. (2) is that it can be exactly solved by the max-flow min-cut theorem [11–13,15]. The theorem states that in a flow network, the maximum amount of flow passing from the source to the sink is equal to the total weight of the edges in the minimum cut, i.e. the smallest total weight of the edges which if removed would disconnect the source (label 0) from the sink (label 1). By an image analogy of the flow network, this cut corresponds to the microstructural crack path in our formulation. Boykov–Kolmogorov algorithm is an efficient way to compute the max-flow and is used in our code, more details can be found in [11–13,15,16].

3. Illustrative examples

The first example shows formation of transverse cracks under tension normal to fibers in a polymer matrix composite [17]. The process involves initial fiber–matrix de-bonding followed by coalescence into larger cracks (Fig. 3(a)). This type of cracking is seen in carbon-fiber reinforced polymer composites under both monotonic and cyclic loading, and the cracking is brittle and unstable in

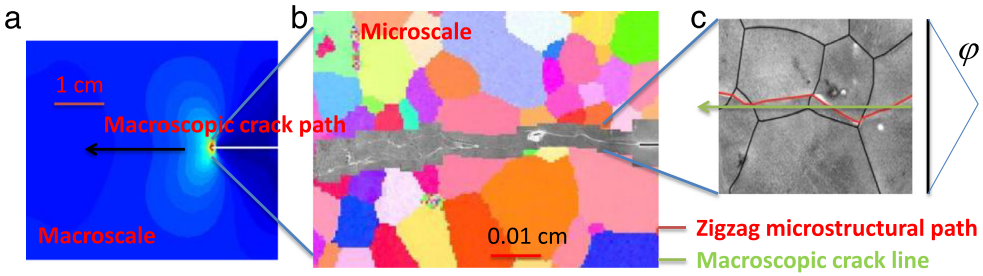

Fig. 1. Multiscale nature of fracture: (a). Stress field and crack direction predicted by macroscopic simulation (b). The microstructural crack trajectory largely follows the macroscopic crack path [10] (c). The crack follows a zig-zag trajectory following weak microstructural features. φ is the supplied macroscopic energy and is taken to peak along the macroscopic crack line.

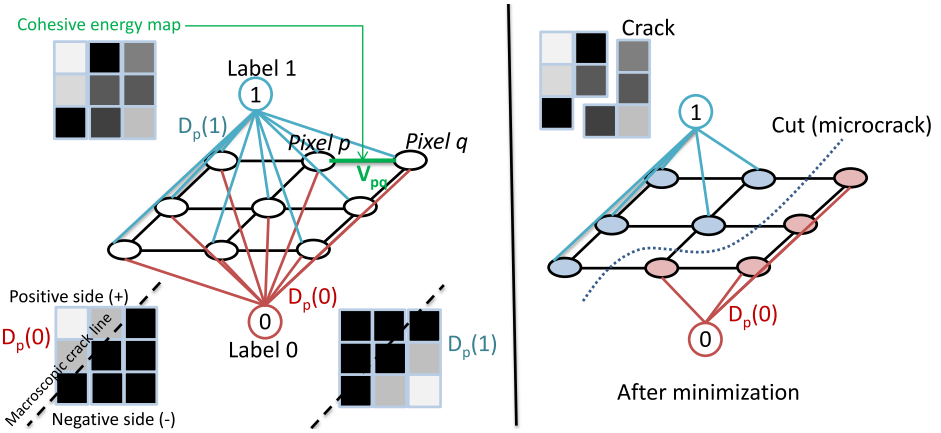

Fig. 2. (left) The graph cut problem setup. The cohesive energies are used to build the interactions between pixels. The label cost D_p (shown as images) gives the interaction of nodes with labels. (right) Energy minimization leads to a cut that separates regions with labels 0 and 1.

nature. In the graph cuts approach, four levels of cohesive energies were chosen ($N = 4$) with the weakest level (lowest cohesive energy) being the fiber matrix interface and the highest value in the interior of the fiber. The coloring of the cohesive energy is the grayscale image in Fig. 3(c). The white line in Fig. 3(c) shows the macroscopic crack direction imposed in the code. This direction was chosen based on the initial and final locations of the crack as seen in the micrograph. The green line indicates the computed crack trajectory and is very close to the experimentally observed crack path. The main difference arises in the topmost fiber where the crack emerges on the left side, however, this crack is arrested and does not propagate further. The propagating contiguous crack is correctly identified in our approach.

The second example shows intergranular stress corrosion cracking of Inconel [18]. Stress corrosion cracking (SCC) involves the presence of a corrosive medium, in this case, an alkaline environment in the heat exchanger, in addition to applied stresses. This results in loss of the protective oxide layer and depletion of chromium leading to failure along the grain boundaries in a brittle mode as seen in Fig. 3(b). The white line in Fig. 3(d) shows the macroscopic crack direction imposed in the code. This direction was chosen based on the initial and final locations of the crack as seen in the micrograph. The grain boundary is given the lowest cohesive energy followed by the matrix as seen in the grayscale image shown in Fig. 3(d), and four levels ($N = 4$) of cohesive energy were used. The crack path (shown in green) is well captured except for a grain at the bottom where the crack is seen to bifurcate whereas a path to the left is preferred by the graph cuts approach. While this approach produces reasonable primary fractures, it does not create multiple fracture paths or crack bifurcation, for these purposes multi-graph cuts algorithm will be used in the future releases. Another aspect of this approach is that anisotropic behavior at the microstructural scale is not fully taken into account. Cohesive energies depend on the direction of cleavage, for example, the $\langle 111 \rangle$ cleavage direction in copper has a lower energy than a $\langle 110 \rangle$ direction. Future work will be focused on improved modeling of this anisotropy.

4. Impact

There are no codes publicly available for computing fracture path at a microstructural level. The present code provides a simple image-based interface in the popular language MATLAB for computing fracture trajectories. The only input to the code is an image of the cohesive energy distribution and the user should graphically input the macroscopic crack line. By comparing against experimental observations, the user may use the results to interpret fracture mechanisms at the microstructural scales. Beyond a post-fracture method, it is possible to use the code to identify possible fracture paths during in-situ testing when using strain localization images from methods such as digital image correlation as input. The appendix to the paper explains the key inputs to the code.

5. Conclusions

The code (MicroFract) and the examples here are available for download [14] and provides a valuable image-based tool for material scientists interested in identifying weak chain in a microstructure. The technique will be extended to 3D microstructures in a future release.

Acknowledgment

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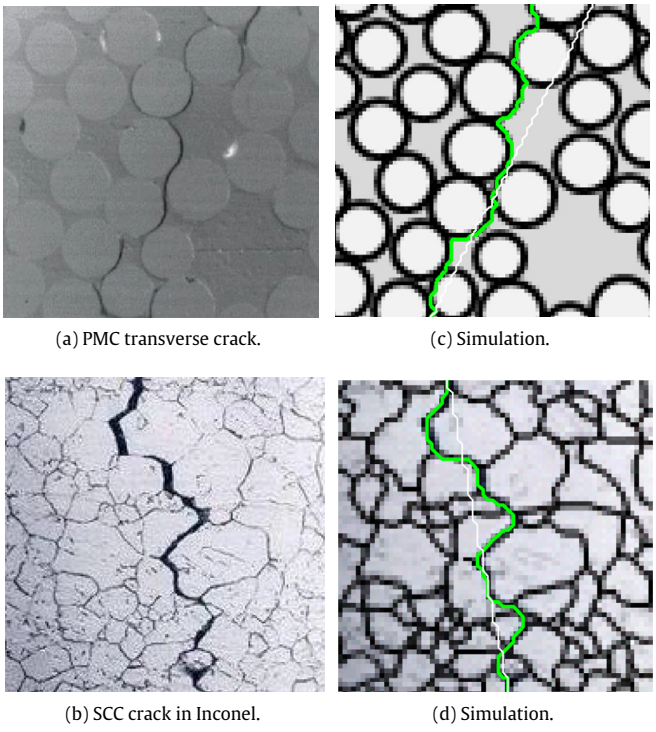

(a) PMC transverse crack. (c) Simulation.

(b) SCC crack in Inconel. (d) Simulation.

Fig. 3. (a,b). transverse cracks under tension normal to fibers in a polymer matrix composite and intergranular stress corrosion cracking of Inconel (c,d) Graph cuts solution: green line indicates the computed crack trajectory and white line indicates the macroscopic crack line. The image in (c,d) is colored according to the cohesive energies used before binning to four levels. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Appendix A. MicroFract code input description

A brief discussion on how to give inputs to the code 'MicroFract.m' is presented below:

Comment 1: The code reads in the cohesive energy image in BMP, JPEG or GIF formats. For computational speed, the image (IMG) is resampled to a 64 × 64 *grayscale matrix named 'bond'. This size (underlined below) can be adjusted by the user.*

IMG = imread('polycrystal.bmp'); ….

mag = 64/imgsz; bond = rgb2gray(imresize(IMG, mag));

Comment 2: 'bond' matrix is normalized from zero to one and then binned to 4 *integer levels. Variable 'maxlevels' can be adjusted by the user to specify the number of bins.*

maxlevels = 4;….

bond = uint8(bond * maxlevels);

Guidance to generate the cohesive energy image and identify energy levels: For examples in Fig. 3(c) and (d), we used image processing software (GIMP) to manually redraw the boundaries over the experimental image using a thicker black line (grayscale 0). In the case of Fig. 3(d), the original image in grayscale was kept as the background. For the composite in Fig. 3(c), the interior of the fibers were recolored white and the exterior was colored gray. The levels of cohesive energy in the code can be changed using variable 'maxlevels' as explained in comment 2 above. We suggest use of the number of levels tailored to the problem at hand. For the composite case, four levels of cohesive energy were chosen to bin the fiber, matrix, interface and the transition region from the interface to matrix/fiber separately. The problem can also be run with higher bin levels. For the case of 5 levels, the results still compare well with experiments although problem complexity is higher.

Appendix B. Supplementary data

Supplementary material related to this article can be found online at http://dx.doi.org/10.1016/j.softx.2017.04.002.

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