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Computing the effective crack energy of microstructures via quadratic cone solvers

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Recently, mathematically well-defined homogenization results for the Francfort-Marigo fracture model were established. To solve the resulting cell formula, efficient computational methods were developed and improvements on solver and discretization techniques were investigated.

We discuss an approach for solving the governing cell formula based on a rewriting as a second order cone problem, a specific normal form for optimization problems. For such a formulation, potent high-accuracy optimization solvers are available. We demonstrate our approach on heterogeneous two-dimensional microstructures.

1 Introduction

Homogenization methods enable to compute the mechanical behavior of heterogeneous materials. Recent theoretical works established a homogenization result [1–3] for the Francfort-Marigo [4] model of brittle fracture. For a fixed time discretization, the heterogeneous model converges to the effective model

$$FM_{\text{eff}}(u, S) = \frac{1}{2} \int_\Omega \nabla^s u : \mathbb{C}_{\text{eff}} : \nabla^s u \, dx + \int_S \gamma_{\text{eff}}(n) \, dA, \tag{1}$$

where $\mathbb{C}_{\text{eff}}$ denotes the effective stiffness and $\gamma_{\text{eff}}(n)$ refers to the effective crack energy, depending on the crack normal n. For the effective quantities, individual and decoupled cell formulae are available. The cell formula for the effective crack energy is based on a $\gamma-$weighted minimal surface. Early contributions in the two-dimensional case have been proposed by Jeulin [5]. To compute this minimal surface efficiently, Schneider [6] suggests a reformulation of the original cell problem relying on Strangs [7] minimum cut - maximum flow duality. The resulting maximum flow cell formula is a convex optimization problem and therefore admits a unique minimum value. For this formulation, novel discretization and solver techniques were established [8], as well as an extension to anisotropic problems was introduced [9].

2 Numerical approach based on a reformulation of the minimization problem

Consider a given rectangular domain $Y \subset \mathbb{R}^d$ and a picewise constant (periodic) field of crack resistances $\gamma : Y \to \mathbb{R}_{>0}$. Following Schneider [6], we may compute the effective crack energy for a prescribed crack normal $\bar{\xi}$ by solving the minimum cut problem for the periodic variable $\phi : Y \to \mathbb{R}$

$$\gamma_{\text{eff}}(\bar{\xi}) = \min_\phi \frac{1}{|Y|} \int_Y \gamma(x) \| \bar{\xi} + \nabla \phi \| \, dx. \tag{2}$$

This optimization problem, which has a non-differentiable objective function, may be transformed into its formal dual problem, the maximum flow problem for the (periodic) flow field $v : Y \to \mathbb{R}^d$

$$\gamma_{\text{eff}}(\bar{\xi}) = \max_{\operatorname{div} v = 0, \, \|v\|^2 \leq \gamma^2} \frac{1}{|Y|} \int_Y \bar{\xi} \cdot v \, dx, \tag{3}$$

which is a constrained optimization problem. To treat (3) numerically, a discretization and a solver need to be selected. Couprie et al. [10] introduced the combinatorial continuous maximum flow (CCMF) discretization for this kind of problem. For $d = 2$ we fix an $N \times N$ voxel grid. The finite dimensional optimization problem reads

$$-\frac{1}{N^2} \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} \bar{\xi} \cdot v[i,j] \longrightarrow \min_{\substack{v_x[i+1,j] - v_x[i,j] + v_y[i,j+1] - v_y[i,j] = 0, \\ v_x[i+1,j]^2 + v_x[i,j]^2 + v_y[i,j+1]^2 + v_y[i,j]^2 \leq 2\,\gamma[i,j]^2}}, \tag{4}$$

where the boundary is treated in a periodic fashion. Thus, we encounter a linear optimization problem of dimension $2N^2$ with N^2 linear equality constraints and N^2 second order cone-type inequality constraints. The python package *CVXPY* [11]

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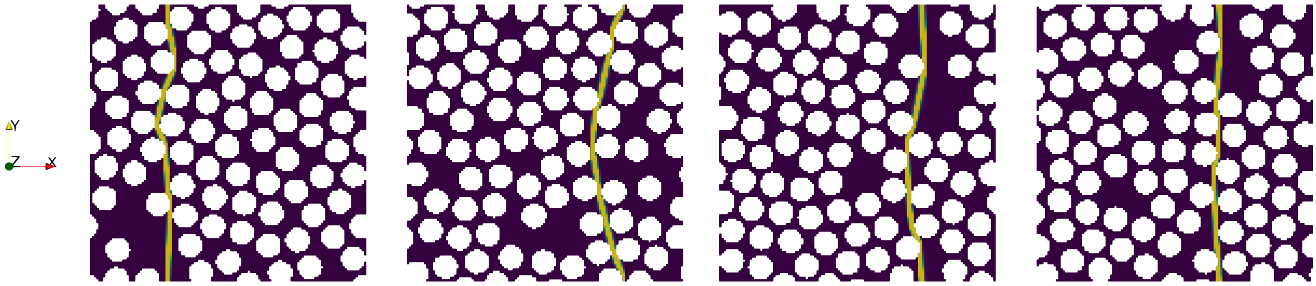
provides a number of efficient solvers for such kind of problems, including the powerful ECOS solver [12]. In addition to the flow field v and the effective crack energy, which corresponds to the negative minimum value of the problem, the solver computes the dual variable ϕ associated to the incompressibility constraint. In order to visualize the crack path cutting the structure we plot the norm of the cut-field $\xi = \bar{\xi} + \nabla\phi$.

3 Computational examples

We consider four different periodic microstructures, each containing 80 spherical inclusions with 50% area fraction in total. The crack resistance of the matrix is given by γ, the inclusions show a crack resistance of $10\,\gamma$. The microstructures are discretized with 128^2 voxels, resulting in $32\,768$ degrees of freedom. The tolerance of the ECOS solver is set to 10^{-8}.
Fig. 1 shows the different microstructures as well as the computed crack paths for macroscopic crack normal $\bar{\xi} = e_x$. As the inclusions show a higher crack resistance, the crack avoids them and forms a shortest path around them. The effective crack energy is increased by $0.6 - 3.7\%$ compared to the matrix crack resistance, depending on the inclusion arrangement. The crack path in Fig. 1(b) shows the longest path with distinct curvature, resulting in the largest effective crack energy. The crack in Fig. 1(d) forms an almost straight line, resulting in the lowest effective crack energy.
The ECOS solver [12] takes about 30s for each computation. Roughly 4s are effectively spent on solving, the high-accuracy tolerance is reached after more or less 23 iterations in each case. The remaining time is spent on problem assembly, solver preparation and preconditioning.



(a) $\gamma_{\text{eff}} = 1.024\,\gamma$ **(b)** $\gamma_{\text{eff}} = 1.037\,\gamma$ **(c)** $\gamma_{\text{eff}} = 1.020\,\gamma$ **(d)** $\gamma_{\text{eff}} = 1.006\,\gamma$

Fig. 1: Crack path for $\bar{\xi} = e_x$ through four different microstructures

4 Conclusion

We provided a method for computing the effective crack energy of two-dimensional microstructures. Reformulating the problem at hand in terms of a second-order cone problem permits to integrate it into existing packages for the python programming language in a simple and straightforward way. The available solvers allow for highly accurate solutions for two-dimensional problems. Several extensions to this approach, such as for instance an anisotropic crack resistance [9], may be integrated in this context as well.

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