Received: 13 May 2019 | Accepted: 14 June 2019

DOI: 10.1002/pamm.201900151

An FFT-based solver for brittle fracture on heterogeneous microstructures

Felix Ernesti[1,*], **Matti Schneider**[1], and **Thomas Böhlke**[1]

[1] Karlsruhe Institute of Technology (KIT), Institute of Engineering Mechanics (ITM)

The description of material failure as an energy minimization problem, i.e., the Francfort–Marigo model, has been studied widely in recent years. The approximation of the crack surface as a phase field, i.e., smeared interface, enjoys great popularity, as it allows describing fracture as a set of partial differential equations. In numerical homogenization, FFT-based solution methods have been established over the past two decades. Their purpose is to compute the overall response of a heterogeneous microstruture w.r.t. a macroscopic loading and can be applied to a variety of nonlinear materials. The benefits lie in a fast implementation and the possibility to use image data like CT-scans as input without further need for meshing. Based on the results of the master thesis of the first author, we investigate phase field crack propagation on heterogeneous microstructures using FFT-based solvers.

1 Introduction

Sudden failure of material often leads to a collapse of constructive structures and can therefore have immense consequences. Hence, fracture and damage mechanics are of high research interest. The Francfort-Marigo model of brittle fracture, a variational reformulation of Griffith's original fracture theory, enjoys great popularity. Its numerical treatment by smearing the crack path by a phase field has been discussed in many previous works, see for instance [1]. The phase field regularized model is prescribed by finding critical points (u, d) of the energy functional

$$F(u,d) = \int_Y [k_0 + (1-k_0)(1-d)^2]\nabla^s u : \mathbb{C} : \nabla^s u + G_c\left[\frac{d^2}{4\eta} + \eta\|\nabla d\|^2\right] dx. \tag{1}$$

Here, $\nabla^s u$ denotes the symmetrized gradient of the (periodic) displacement field u, d is the (periodic) damage variable, $\mathbb{C}$ is the fourth-order stiffness tensor, k_0 is the remaining stiffness, G_c is the critical energy release rate and η denotes the phase field parameter. In this proceeding, we investigate solving the phase field problem with an FFT-based fast gradient solver on a periodic, heterogeneous microstructure.

2 Solution method

We solve for critical points (u, d) of F using a gradient scheme [2] for each variable, keeping the respective other variable frozen. Assuming the variables u and d are elements of certain Hilbert spaces U and V, the partial gradients $GRAD_u$ and $GRAD_d$ are defined in terms of

$$\begin{aligned}
\langle GRAD_u f(u,d^*), v\rangle_U &= Df(u,d^*)[v],\ u,\ v \in U,\ d^* \text{ fixed},\\
\langle GRAD_d f(u^*,d), s\rangle_V &= Df(u^*,d)[s],\ d,\ s \in V,\ u^* \text{ fixed}.
\end{aligned}$$

We solve for the damage variable by a standard gradient descent scheme and for the displacement field by the heavy ball method, see [3]. The abstract algorithm is given by Algorithm 1. δ is a carefully chosen parameter between 0 and 1 and, h_u and h_d are the associated step sizes for u and d, respectively. The equations where discretized by trigonometric collocation, see [4].

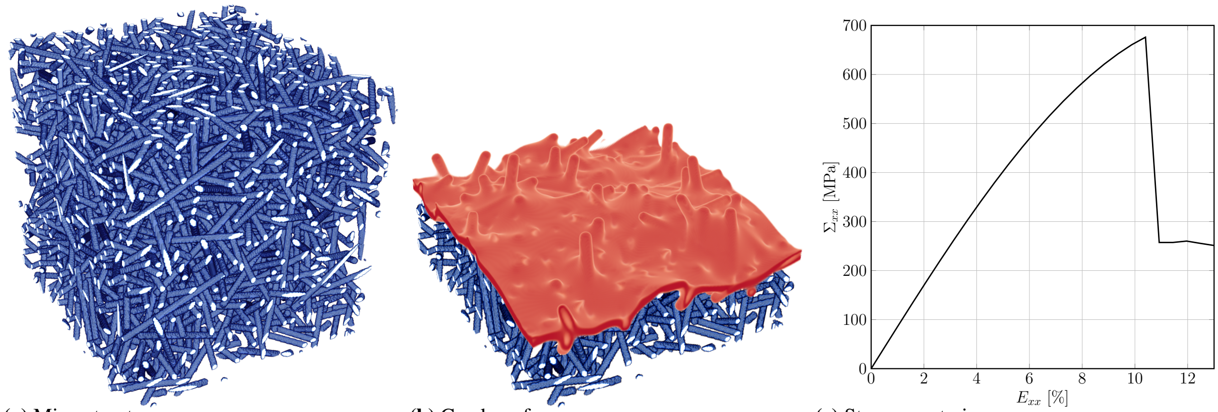
* Corresponding author: e-mail felix.ernesti@kit.edu, phone +49 721 608 48133, fax +49 721 608 44187

Algorithm 1 Coupled heavy ball method

Fix initial guess (u^0, d^0)
$n \leftarrow 0$, $k \leftarrow 0$, $u^{-1} = u^0$
while u not converged **do**
  while d not converged **do**
    $d^{k+1} = d^k - h_d GRAD_d F(u^n, d^k)$
    $k \leftarrow k + 1$
  end while
  $u^{n+1} = u^n - h_u^n GRAD_u F(u^n, d^k) + \delta^n (u^n - u^{n-1})$
  $n \leftarrow n + 1$
end while
return (u^n, d^k)

3 Numerical Results

We apply the model to a fiber reinforced composite with a fiber volume percentage of 10, see Fig. 1(a). The microstructure was generated using a sequential addition and migration algorithm, see [5] and discretized by 256^3 voxels. The fibers are of equal length with aspect ratio 20 and isotropic orientation distribution. We assume the matrix material to behave according to the phase field model with elastic constants $E = 3.45\text{GPa}, \nu = 0.39$ and critical energy release rate $G_c = 3.19\text{N/mm}$, whereas the fibers behave purely elastic with $E = 72\text{GPa}$ and $\nu = 0.22$. We apply a load in x-direction by increasing the mean value $E = E_{xx} e_x \otimes e_x$ of the strain field $\nabla^s u$ linearly. The macroscopic stress vs strain relation is shown in Fig. 1(c). The stress increases monotonically until a critical value. Then it is reduced within one computational step to a value depending on the remaining stiffness k_0. The resulting crack surface is shown in Fig. 1(b). It is on average perpendicular to the tensile direction, taking locally a shortest path around the fibers. Effects like fiber pullout and matrix failure are visible.



(a) Microstructure **(b)** Crack surface **(c)** Stress vs. strain

Fig. 1: Microstructure, crack surface and stress strain relation for fiber reinforced composite

4 Conclusion

We presented an accelerated gradient descent scheme to solve the phase field fracture problem on a heterogeneous microstructure. The fully coupled, implicit implementation ensures the handling of a large NDOF within reasonable computation time.

Acknowledgements The authors thank W. Dörfler from the faculty of mathematics at KIT for co-supervising F. Ernesti's master thesis and the German Research Foundation (DFG) for partial financial support within the GRK 2078.

References

[1] C. Miehe, M. Hofacker, and F. Welschinger, CMAME **199**, 2765–2778 (2010).
[2] M.Schneider, CMAME **315**, 846–866 (2017).
[3] B. Polyak, USSR Comp. Math. Math. Phys **4**, 1–17, (1964)
[4] H. Moulinec and P. Suquet, CMAME **157**, 69–94 (1998).
[5] M. Schneider, Comp. Mech. **59**, 247–263 (2017).

