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A diffusive dynamic brittle fracture model for heterogeneous solids and porous materials with implementation using a user-element subroutine

Udit Pillai[b,1], Yousef Heider[a,*,1], Bernd Markert[a]

[a] Institute of General Mechanics, RWTH Aachen University, Templergraben 64, 52062 Aachen, Germany
[b] Centre for Structural Engineering and Informatics, Faculty of Engineering, University of Nottingham, Nottingham NG7 2RD, UK

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ABSTRACT

This paper addresses brittle fracture simulation using the phase-field modelling (PFM) as an effective and prominent method to predict crack onset and topology in heterogeneous solids and porous materials. This includes the study of the significant crack behaviour change due to the inhomogeneous nature of the materials, where the Weibull distribution is used for creating spatial variations of the material properties. The permanent changes in the permeability and volume fractions of the individual constituents in the cracked porous domain are appropriately accounted for. The present work combines the well-established macroscopic Theory of Porous Media (TPM) and the PFM by means of a user element (UEL) in the software ABAQUS. The coupled system of TPM and PFM equations is then solved in a monolithic fashion for both homogeneous and heterogeneous cases. Numerical examples present a comparative study demonstrating the difference in fracture patterns between homogeneous and heterogeneous solids and porous cases.

1. Introduction

Prediction of failure mechanisms involving crack initiation and propagation is of prime importance in many engineering fields, which are related to production and safety assessment. One of the prominent applications is hydraulic fracturing, applied in enhanced geothermal systems (EGS) through injection of high-pressure water into deep rock layers in order to enhance the rock's low permeability. Another important application, is hydraulic fracturing process (fracking) prevalent in oil and gas industries to extract unconventional natural resources, like shale gas, petroleum and brine from deep rock formations. Hydraulic fracturing also has applications in geomechanics to study the stability of dams. In the underlying research work, the phase-field modelling (PFM) is employed for fracture modelling, which is an energy-based diffusive crack approach scheme with an internal length-scale parameter that controls the amount of diffusion. The PFM uses a scalar phase-field variable, which indicates the cracked state of a material. Moreover, the PFM has proved its relevance in predicting brittle fractures by simulating complex crack patterns including crack initiation, branching and merging. Several studies have been conducted in the past to establish a complete theoretical and numerical framework and to gain more understanding and control of fracturing processes in pure solids and in porous materials.

In the early developments for depicting brittle solid fractures, Griffith [28] treated crack propagation with an elastic energy-based approach and related it to a critical energy release rate, which marked the foundation of the classical theory of brittle fracture. Irwin [32] further extended the classical theory by proposing a new criterion for crack initiation and established a relationship between factors, like the strain energy release rate or the fracture work rate, and the elastic stresses and strains near the leading edge of brittle cracks. In earlier works based on discrete crack models, a crack was incorporated as a geometrical entity and the crack path was constrained only to the element edges. For complex crack patterns and coarser meshes, this lead to a significant overestimation of the fracture energy when the true crack path deviated from the predicted crack path (Msekh et al.[51]). An important milestone in the crack initiation and propagation modelling was achieved with the development of the extended finite element methods (XFEM) by Belytschko and Black [6], Moës and Belytschko [50]. XFEM, based on the generalised finite element method, enables a local enrichment of the approximation space via the partition of unity method, which equips it with huge flexibility in predicting the true stress behaviour and resolving stress singularities at the crack tip. However, XFEM requires a pair of level set functions to be defined for each individual crack segment and faces serious computational challenges in cases of complex models with additional degrees of freedom

* Corresponding author.
E-mail address: heider@iam.rwth-aachen.de (Y. Heider).
[1] These authors contributed equally to this work.

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and for the case of closing cracks, where contact formulations have to be included.

Phase-field modelling of fracture, which relies on a variational model of crack evolution, was first proposed in the work of Francfort and Marigo [27] in the late 1990s to get rid of the constraints posed by classical Griffith's theory, like pre-existing and well-defined crack paths. This approach was later implemented numerically by Bourdin et al. [12]. Important contributions were made by Miehe et al. [42], Kuhn and Müller [33] within the variational framework by simulating multi-dimensional fractures involving mixed-modes with dynamic effects. In Aldakheel et al. [4], an important extension towards ductile fracture using Gurson-type plasticity at finite strain can be found. Additional applications and PFM-related solution schemes can be also found in, e.g., Ambati et al. [5], Patil et al. [52], Ehlers and Luo [25], Weinberg and Hesch [59], Cajuhi et al. [16], Miehe et al. [44,41] among others. Msekh et al. [51] implemented the PFM for homogeneous brittle solid fractures combining UEL and UMAT subroutines in the commercial FEM software ABAQUS and highlighted the implementation details. Later, Liu et al. [36] solved the coupled PFM problem using ABAQUS by monolithic and sequentially staggered schemes and compared the two methods on scales of accuracy, computational efficiency and sensitivity to mesh sizes.

With reference to porous media, different fundamental theories describing the constitutive behaviour of multiphasic continua have been given in literature. The most prominent amongst those are the approach developed by Biot [7–9] and the Theory of Porous Media (TPM) established by Bowen [13,14], De Boer [20] and Ehlers [22–24]. The TPM considers a macroscopic continuum approach based on the mixture theory, see Truesdell [58] and Bowen [13,14], wherein the overall continuum consists of spatially superimposed solid and liquid phases coupled with each other through interaction terms. Simulation of hydraulic fracturing in porous media poses multiple modelling challenges, including treatment of the solid and liquid phases and their interaction during pre- and post-crack regimes, incorporating changes of permeability and volume fractions during crack propagation. Additionally, the fluid flow needs to be modelled appropriately, accounting for its change from Darcy-type flow in the porous medium to Navier-Stokes-type flow in the cracked medium [30]. One of the first attempts to simulate hydraulic fracturing was done by Boone and Ingraffea [11], where two-dimensional numerical approximations for poroelastic materials were considered. The FEM equations were solved using a partitioned solution procedure for poroelastic problems. Accounting for the continuous topological changes in the porous domain, Schrefler et al. [55] presented a dependency between the crack opening and the permeability in Darcy's flows. Secchi and Schrefler [56] and Cao et al. [17] simulated 3D hydraulic fracturing in fully saturated porous media using a cohesive fracture model. The model did not require a predefined fracture path, but needed a constant updating of mesh near the crack tip to consider geometry evolution. For incompressible viscous fluids, the fluid flow inside the crack was considered laminar and governed by the Poiseuille law as derived by Adler et al. [3]. Adachi et al. [2] added some modifications to the fluid flow equations, like a leak-off sink term, and presented controlling parameters for the crack growth evolution.

Significant contributions in the field of PFM were made by Miehe et al. [43] by relating the crack propagation only to the strain energy, where the evolution of the phase-field was related to a local history variable termed as the crack driving force. Extending this concept, Miehe et al. [46,42], Miehe and Mauthe [45] established a link between the diffusive crack modelling and the hydro-poro-elastic response of porous bulk materials. The energy-based crack driving force was further generalised to the solid effective stresses-based threshold criterion. A recent article by Heider and Markert [30] combined the TPM and PFM models to derive a more realistic hydraulic fracture model accounting for permanent local changes in the permeability and the volume fractions, while adopting the fluid velocity instead of the seepage velocity as a primary variable to confer with the idea of changing flows from Darcy-type to Stokes-type in the cracked region. Additionally, Heideret al. [31] introduced an extended 3D study of the TPM-PFM approach that included a model calibration based on experimental data. Ehlers and Luo [25] have introduced a fully-coupled computational approach to simulate hydraulic fracturing in 2D and 3D settings by including the phase-field variable into the constitutive model for the solid and fluid phases, thus accounting for a direct influence of cracks on the solid deformations and the fluid velocities. Another approach involving PFM for hydraulic fracturing in porous media based on Biot's Theory has been investigated by Mikelić et al. [48,49], Lee et al. [34] allowing them to implement advanced numerical schemes and explore different features of hydraulic fracturing.

The present work focuses on developing a fully-coupled computational framework for simulating dynamic hydraulic fracturing combining the TPM and PFM approaches via ABAQUS[2] UEL and UMAT subroutines. In this, in order to extend the existing fracture methodologies to deal with large-scale practical engineering problems involving a huge number of degrees of freedom, we use the robust multiphysics solving capabilities of ABAQUS involving parallel computing algorithms and automatic time-stepping schemes. Changes in the permeability, the volume fractions and the fluid flow behaviour during crack propagation are incorporated directly into the constitutive porous media model. Moreover, the present work discusses the procedure to model heterogeneities using a Python 2.7.6 script in conjunction with the ABAQUS input file to include initial material property variations based on the Weibull probability distribution, see Chen et al. [18] for details about the methodology. Numerical examples presented at the end of the paper show that the crack paths and fracture energies can significantly be affected when the heterogeneities are incorporated.

2. Theoretical background

2.1. Macroscopic porous media approach

Following the TPM for biphasic porous materials, the fluid and solid constituents are considered immiscible and ideally disarranged over a representative elementary volume (REV). The homogenisation of the REV yields a smeared-out continuum φ with overlapped solid and fluid constituents φ^α {$\alpha = S$ for the porous solid skeleton and $\alpha = F$ for the pore fluid}, viz.

$$\varphi = \bigcup_\alpha \varphi^\alpha = \varphi^S \cup \varphi^F. \tag{1}$$

In view of immiscibility, the volume fractions $n^\alpha := dv^\alpha/dv$ can be defined as the local ratio of partial volume dv^α of constituent φ^α with respect to the total volume dv of the whole mixture φ. Within the context of a fully-saturated medium, no vacant spaces exist inside the matrix. As a direct consequence of this, the saturation relation $\sum_\alpha n^\alpha = n^S + n^F = 1$ also holds true, where n^S is the solidity and n^F is the porosity.

With the help of the volume fractions n^α, two different density functions for each constituent φ^α, the material density (effective or realistic) $\rho^{\alpha R} := dm^\alpha/dv^\alpha$ and partial density $\rho^\alpha := dm^\alpha/dv$ can be formulated, where dm^α and dv^α are the local mass and local volume elements, and dv is the aggregate volume element of the mixture. The fluid and solid effective densities (ρ^{SR}, ρ^{FR}) are assumed to be constant, where a constant temperature is considered. However, the material incompressibility of the individual constituents does not lead to bulk incompressibility, since the partial densities (ρ^S, ρ^F) and the overall mixture density can change due to altered volume fractions (n^S, n^F). Based on the TPM, the solid and fluid volume fractions should lie between 0 and 1, i.e. $0 < n^\alpha < 1$, and the fluid flow in interconnected pores is governed by Darcy or Forchheimer filter laws, see, e.g., [37].

[2] ABAQUS version 6.14 on Linux86 64.