Computational fracture mechanics with scattered data approximations

1 Background

Crack propagation is a fundamental aspect of fracture mechanics and appears in various engineering applications ranging from aerospace, civil engineering, and material science to biomechanics. Fast and accurate computational techniques are essential for predicting crack trajectories, assessing structural integrity, and preventing catastrophic failures. The study of crack propagation is particularly crucial in brittle materials, where failure often occurs through the initiation and propagation of cracks. Brittle materials, characterized by limited plastic deformation, exhibit a sudden and catastrophic failure once a critical crack size is reached. Understanding how cracks propagate in these materials, constructing theoretical models, and developing numerical algorithms to simulate them are essential for designing structures with improved fracture resistance and reliability. Due to emerging technologies centered around hydrogen, structural integrity is paramount once the material is exposed to hydrogen. This exposure leads to hydrogen embrittlement, a phenomenon where the presence of hydrogen in a material leads to reduced ductility and increased susceptibility to cracking [1,5,11].

2 Project description

For numerical simulation of crack propagation within classical continuum theory, at least two potential approaches exist. The first approach considers the fracture as a sharp entity wherein the displacement field is permitted to be discontinuous across the crack path. To capture this entity with standard finite element method (FEM), the computational mesh needs to match the geometry of fracture by remeshing the domain as the crack propagates. The governing equation (with no body force) reads as

\[ \nabla \cdot \sigma = 0, \quad \text{in } \Omega_C \]  (2.1)

where \( \Omega_C = \Omega \setminus \Gamma_C \) with \( \Omega \) the whole body and \( \Gamma_C \) the crack surface. The displacement and traction boundary conditions are also imposed on the Dirichlet and Neumann parts of the boundary, and \( \sigma \cdot n = 0 \) is imposed on \( \Gamma_C^+ \cup \Gamma_C^- \) where \( \Gamma_C^+ \) and \( \Gamma_C^- \) are opposite surfaces of crack \( \Gamma_C \). Here, it is assumed that the crack surfaces do not come to contact. The stress tensor \( \sigma \) is given by the constitutive equation \( \sigma = \frac{\partial \psi_e}{\partial \varepsilon} \) where \( \varepsilon \) is the strain tensor and \( \psi_e \) is the elastic energy density. The displacement field is discontinuous across \( \Gamma_C \) and the stress is (theoretically) singular at the crack tip [13]. In the eXtended Finite Element Method (XFEM) (or Generalized FEM), the standard discretization space is enriched by adding discontinuous functions in elements across the crack, and near-tip asymptotic functions in elements around the tip [3]. By using this approach, the problem of remeshing is avoided because the crack geometry is modelled independent of the underlying mesh. However, the discontinuous approach and the use of XFEM present some limitations for crack simulations. From a practical point of view, crack-tip enrichment is not straightforward and it is still a challenging problem to model complex crack problems where crack initiation, branching and coalescence are of physical importance [15]. The second approach uses a continuous or a phase field model and involves a reformulation of the problem in the context of energy minimization [2]. In this approach (so-called variational) the sharp interfaces representing the cracks are approximated by a smooth diffusive field \( \phi \) and the Euler–Lagrange equation

\[ -\ell^2 \Delta \phi + \phi = \frac{2\ell}{G} (1 - \phi) H^+(\varepsilon), \quad \text{in } \Omega \]  (2.2)

is coupled with equilibrium equation (2.1). The phase-field dependent stress tensor \( \sigma \) is defined as \( \sigma = g(\phi) \frac{\partial \psi_e(\varepsilon)}{\partial \varepsilon} \) where \( g \) is a degrading function which is defined, for example, as \( g(\phi) = (1 - \phi)^2 \) for \( \psi_e^+ \geq \psi_e^- \) and
$g(\phi) = 1$ otherwise. Here, $\psi^+_e$ and $\psi^-_e$ are tensile and compressive parts of the strain energy decomposition

$$\psi_e(\varepsilon) = \psi^+_e(\varepsilon) + \psi^-_e(\varepsilon).$$  \hfill (2.3)

The same holds for definition of the local strain energy history variable $H^+$ to eliminate the compressive part and ensure the irreversibility of the crack [6]. The constant $G$ is the material fracture energy. Both equilibrium equations are defined on the whole $\Omega$ (including the diffuse crack region) and the boundary condition on $\phi$ is $\nabla \phi \cdot n = 0$ on $\Gamma$. The new system leads to a smooth but rapid transition between the unbroken and broken states of the material. Information on the evolution of cracks is incorporated into the field equations (equation (2.2)) and thereby initiation, propagation, branching and coalescence of cracks are handled, automatically [1,6,15]. On the down side, in this approach the computational cost of solving the two-field nonlinearly coupled system of equations is high. In the presence of hydrogen, the material becomes more brittle and its strength decreases. In this case the material fracture energy must be considered as a function of hydrogen concentration, let say $G = G(\theta)$, where $\theta$ is the hydrogen concentration, and a new conservative equation

$$\frac{\partial \theta}{\partial t} + \nabla \cdot J(\theta, \phi, \varepsilon, \sigma) = 0, \quad \text{in } \Omega$$  \hfill (2.4)

for a suitable flux function $J$ together with some Neumann and Dirichlet boundary conditions must be coupled with the phase filed equation (2.2). The elastic energy density $\psi_e$ and therefore the definition of stress tensor $\sigma$ will be updated, accordingly [1].

The aim of this project is to expand the existing theory by exploring potential extensions in both mathematical and mechanical aspects. Reflecting on the introduction above, the theoretical models presented in the literature on mechanics of hydrogen assisted fracture calls for efficient computational schemes. On the computational side, our goal is to replace the current finite element techniques by the scattered data approximation methods, including radial basis functions and moving least squares approximations, to overcome some limitations associated with subspace enrichment strategy in the discontinuous approach, and mesh refinement challenges and low-order accuracy in the continuous phase field techniques. Additionally, our aim is to develop a specialized and stable computational algorithm for effectively solving the mass conservation law (2.4) within the hydrogen-assisted fracture model. On the mechanics side, we will consider and apply other effective strain energy decompositions for different type of cracks (see for example [4]) and look for introducing new decomposition formulas of the form (2.3). Furthermore, benefiting from the computing machine developed, the classical continuum theory will be possibly enhanced with non-classical elements such as strain gradient plasticity, or higher order elasticity theories such as strain gradient elasticity. We will equip the new methods with rigorous mathematical proofs and strong numerical evidence, and implement the new methods as an open-source library.

## 3 Interdisciplinary justification

This project lies at the intersection of mechanics, applied mathematics, and computational science. We will address the mathematical and computational aspects of a broadly applicable problem in solid mechanics and conduct mathematical analysis, numerical implementation, validation, and large-scale computation. From the mechanics side, we will study the effects of strain energy decompositions and hydrogen embrittlement on simulation of the crack propagation. We highlight that the efficient and safe storage of hydrogen is a critical aspect of harnessing its green energy benefits. Therefore, addressing the crack propagation problem in hydrogen storages is vital for ensuring the reliability and safety of hydrogen-based technologies.

## 4 Supervisors

**Davoud Mirzaei** (davoud.mirzaei@it.uu.se), is an associate professor at division of scientific computing (TDB), specializing in numerical methods for partial differential equations. He has a significant contribution
to the scientific computing community by developing some numerical PDE solvers based on scattered data approximations. See for instance [7–10]. He also has a successful track record of completing scientific projects as a principal investigator. This includes receiving six consecutive grants from the School of Mathematics at the Institute for Research in Fundamental Sciences (IPM) between 2016 and 2022, as well as a grant from the Iranian National Science Foundation (INSF) from 2019 to 2021. He has supervised 18 master’s students, 5 PhD students, and 3 postdoctoral researchers at the University of Isfahan between 2013 and 2022. After joining UU since August 2022, he has been supervising a master’s student in computational science, who is enrolled at KTH Royal Institute of Technology.

Mahmoud Mousavi (mahmoud.mousavi@angstrom.uu.se), is an associate professor in Applied Mechanics at UU, leading a research group with the focus on “Architected Materials”, and currently supervising postdoc, PhD and master students. The group has been financially supported primarily by Swedish Research Council, Horizon Europe, Industry grants, and Uppsala University. He has extensive experiences within subjects addressed in this proposal including continuum mechanics, defect mechanics, fracture mechanics, and multi-scale computational simulation [11–14].

Under the guidance of the supervisors, the Ph.D student will formulate physical models and design and implement efficient numerical algorithms for solving the models.

5 Funding

The Ph.D. student will be employed at the Division of Scientific Computing (TDB) at the Department of Information Technology, Uppsala University. The project main costs are the salary of the PhD student. This will be financed by CIM (50%) and TDB (50%).

References


