

A statistical approach for fracture property realization and macroscopic failure analysis of brittle materials

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To my wife and daughter, my greatest supporters and inspirations.

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Abstract

Lacking the energy dissipative mechanics such as plastic deformation to rebalance localized stresses, similar to their ductile counterparts, brittle material fracture mechanics is associated with catastrophic failure of purely brittle and quasi-brittle materials at immeasurable and measurable deformation scales respectively. This failure, in the form macroscale sharp cracks, is highly dependent on the composition of the material microstructure. Further, the complexity of this relationship and the resulting crack patterns is exacerbated under highly dynamic loading conditions. A robust brittle material model must account for the multiscale inhomogeneity as well as the probabilistic distribution of the constituents which cause material heterogeneity and influence the complex mechanisms of dynamic fracture responses of the material. Continuum-based homogenization is carried out via finite element-based micromechanical analysis of a material neighbor which gives is geometrically described as a sampling windows (*i.e.*, statistical volume elements). These volume elements are well-defined such that they are representative of the material while propagating material randomness from the inherent microscale defects. Homogenization yields spatially defined elastic and fracture related effective properties, utilized to statistically characterize the material in terms of these properties. This spatial characterization is made possible by performing homogenization at prescribed spatial locations which collectively comprise a non-uniform spatial grid which allows the mapping of each effective material properties to an associated spatial location. Through stochastic decomposition of the derived empirical covariance of the sampled effective material property, the *Karhunen-Loève* method is used to generate realizations of a continuous and spatially-correlated random field approximation that preserve the statistics of the material from which it is derived. Aspects of modeling both isotropic and anisotropic brittle materials, from a statistical viewpoint, are investigated to determine how

each influences the macroscale fracture response of these materials under highly dynamic conditions. The effects of modeling a material both *explicitly* by representations of discrete multiscale constituents and/or *implicitly* by continuum representation of material properties is studied to determine how each model influences the resulting material fracture response. For the implicit material representations, both a statistical “white noise” (*i.e.*, Weibull-based spatially-uncorrelated) and “colored noise” (*i.e.*, Karhunen-Loève spatially-correlated model) random fields are employed herein.

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Chapter 1

Introduction

Before introducing any detailed discussions, note figure 1.1 which presents the overall logic of the research content flow and how the focal subjects of each Chapter are connected. The main objective of this research is to develop a computational “black-box” framework which utilizes micromechanics-based approaches to statistically model the affects of stochastic microstructure heterogeneity on the dynamic responses of any general (quasi-)brittle material. There is a novelty behind any method that exploits the general advantage of micromechanics of materials. The practical yet fundamental aim of any self-consistent method is the capacity to perform a myriad of virtual simulations which would otherwise have a substantial associated cost when performed experimentally. Therefore, a reliable method should compensate for the bottle-neck of having to perform a large number of experimental trials to determine the statistical characteristics of a non-deterministic inhomogeneous or composite material.

Chapters 2-3 focus on approaches that link a general material microstructure to quantities by which it can be statistically characterized; this characterization is based on the distribution of a local effective constitutive property dependent of the material composition. Analyzing (quasi-)brittle materials on a constituent level begins with an appropriate mathematical description of the material microscale topology. Chapter 2 introduces the discussion on the various stochastic geometrical spatial attributes of the constituents that constitute a inhomogeneous material model. Accordingly, these fundamental descriptions serve as the basis for **multiscale microstructure models** which can then be used to analyze explicit (*regular* or *random*) heterogeneity. However, since real material microstructure composition is non-deterministic we then consider means of accounting for local effect of a neighborhood of constituents about a material point rather than individual constituent responses. This continuum mechanics approach produces statistically averaged effective material property by exploiting the thermodynamically consistent Representative Volume Element (RVE). Focus is now shifted onto implicit modeling of heterogeneity as a continuum wherein spatially defined stochastic fields are derived from micromechanics-based homogenization approaches. To ensure that the spatial variability is propagated from the random microstructure to the macroscale responses, a derivative of the RVEs known as **Stochastic Volume Elements** (SVEs) are used within the homogenization approaches

of this work. This Chapter is concluded by introducing quantities computed to statistically characterize the previously mentioned stochastic fields; these quantities define aspects such as spatially correlation of the fields between two domain locations as well as relative likelihood of attaining some value of the field from sampling a random process.

Based on the statistical data of Chapters 2-3, Chapters 4-5 discuss continuum-based approaches taken to model “**realistic**” **materials** by representing the random microstructure as random fields sampled from a (non)Gaussian process (GP). Again it can be noted that these continuously approximated random fields preserve the probability structure of the respective microstructures of Chapter 2 from which these are derived. Also presented are the theories regarding discretization of these random fields as well as commonly used methods to obtain the fields; generally this discretization is handled directly by employing stochastic finite element methods (SFEM) to solve the underlying material-dependent stochastic partial differential equations (SPDE). The specific SFEM of interest implemented in this work as the **SPDE Solver** is the non-intrusive kernel expansion method or the *Karhunen-Loève* Expansion method; this Chapter is primarily dedicated to the focus of this random field generation method. An important concept also discussed in this Chapter is the correlation length of the covariance kernel whose eigen decomposition makes this series expansion approximation of the random field possible; the relationship between this correlation length and the spatial fluctuation of the discretized random field is examined.

Finally macroscale **sharp crack** simulations are executed wherein the spatially discretized random field meshes introduced in Chapter 4 serve as the microstructure of a given heterogeneous material. Since this implementation of randomness is non-intrusive, the solid mechanics model benefits from this **dual meshing** of the finite element computation domain and the material domain. To capture the realistic and possibly complex patterns of the highly transient dynamic brittle fracture, a mesh **adaptive** spacetime discontinuous Galerkin (**SDGFEM**) numerical solver is utilized in order to investigate the influence of microscopic and mesoscopic material uncertainties on macroscale fracture dynamics. Although introduced and elaborated upon in Chapters 2 and 4 respectively, the concept of brittle material *size-effect* is investigated from a macroscale fracture standpoint. By employing the random continuum microstructures, derived from various SVEs length-scales

tending to the RVE limit, dynamic fracture responses are investigated for fracture strength realization ranging from highly inhomogeneous strength distribution to realization tending to a homogeneous distribution.

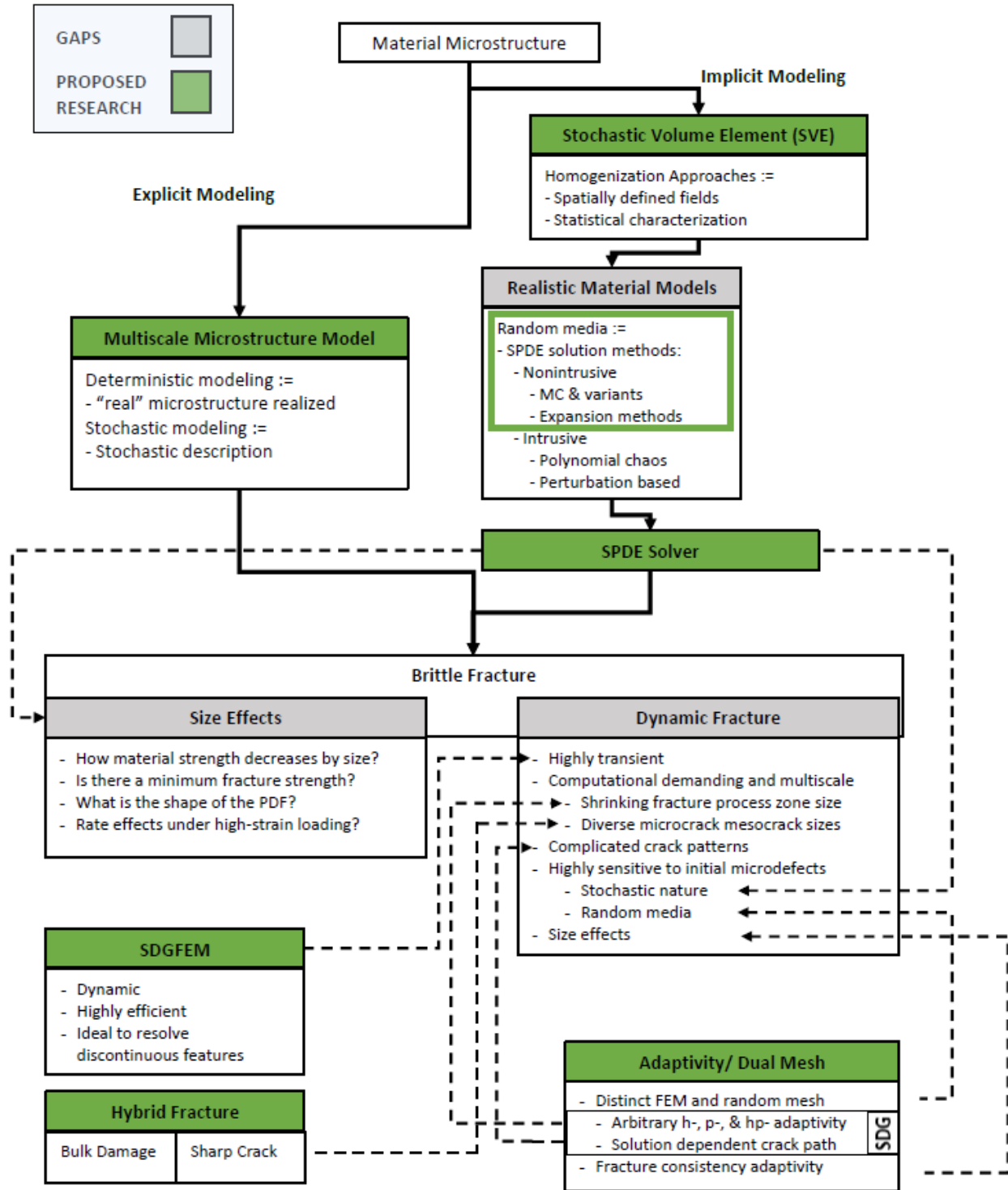


Figure 1.1: Flowchart illustrating logical sequence of proposed algorithm.

Chapter 2

Material micro-structure characterizations

2.1 Introduction

2.1.1 Objectives

This chapter details a continuum-based framework implemented to homogenize the effects of the random and heterogeneous microstructure of a general (quasi-)brittle material. By performing volume element sampling on a structured spatial grid, material domains of random microstructure realizations are spatially characterized in terms of some constitutive material property. Point-wise statistics of the material property are also determined which are used to study phenomenon such as the well-known material “size-effect”. The point-wise statistics will subsequently be used to derive spatially correlated and continuous random field approximations based on the material’s underlying microstructure rather than phenomenology.

2.1.2 Background and motivation

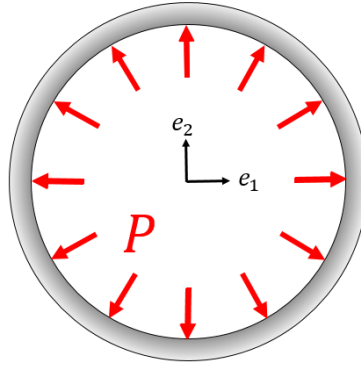
Recent literature have shown that a common-placed concern regarding the modeling of (quasi-)brittle materials is the incorporation of microstructural uncertainty in the mechanical behavior of these ubiquitous materials. An assortment of both numerical and experimental evidence supports the notion that the fracture response of these materials cannot be represented deterministically and must be considered from a probabilistic standpoint. As stated in [50], an attribute of every real material is its inherent heterogeneity; this is especially pertinent when analyzing the responses of (quasi-)brittle materials from a continuum fracture mechanics viewpoint. Unlike ductile materials, brittle materials lack the energy dissipative mechanisms associated with plastic deformation, which would otherwise allow the re-balancing of generated stress. Although quasi-brittle materials admit measurable deformation, they too experience catastrophic failure on a smaller deformation scale relative to ductile materials. This failure (fracturing) is a trademark dissipative mechanism for brittle material, and has been shown to be highly influenced by the underlying microscale constituents of the material(*cf.* [207]). The significance of brittle fracture mechanisms are also evident, when studying the brittle-to-ductile response transition for materials exposed

to conditions such as low temperatures and high rate loading [182].

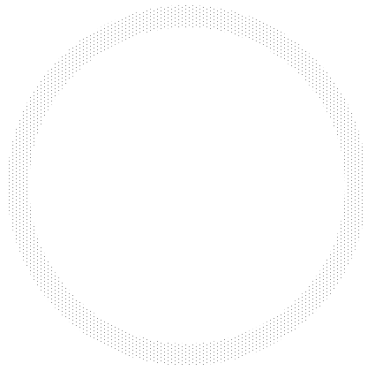
Before considering experimental investigations from literature, general concepts of *Linear Elastic Fracture Mechanics* (LEFM) can support the importance of incorporating, at minimum, *regular* inhomogeneity into the modeling of brittle fracture. Figure 2.1a illustrates a circular ring subject to some initial internal uniform boundary loading consistent with generated uniform stresses throughout the material domain. LEFM dictates theoretically that the stress throughout the domain is governed by some relationship $\sigma(\mathbf{x}) = f(K_c, \sigma_u, \sigma_{applied})$, where K_c , σ_u , and $\sigma_{applied}$ are material fracture toughness, ultimate strength and general applied load respectively. If modeled as a homogeneous (uniform strength) material (as seen in Figure 2.1b), theory infers that every point within the ring should not only achieve ultimate strength simultaneously but should fail instantaneously. This response is highly unrealistic and not experienced in any practical material. However, modeling the material inhomogeneously (as seen in Figure 2.1c) results in weaker material points throughout the domain which act as nucleation sites for fractures. This shields the surrounding regions from generated high stresses and subsequent failure. The averaging of inhomogeneous material properties is a sound approach when considering quantities such as averaged strain and average stress but this averaging is not appropriate for local stress quantities which influence brittle fracture behavior. Further, it is evident that these local stresses are influenced by the local microstructure effects and randomness of the material [26].

Considering experimental studies of brittle fracture, the importance of the material *random* inhomogeneity is well established in their inelastic behavior. The concept of spatial randomness in a real brittle media is investigated by [20] wherein the fracture response is depicted for geometrically identical samples, of the same material, subject to the same loading. Each of the “identical” specimens exhibited non-unique fracture initiation sites that not only support the concept of regular heterogeneity of the material, but also distinctly different fracture patterns (refer to Figure 2.2) supporting random heterogeneity.

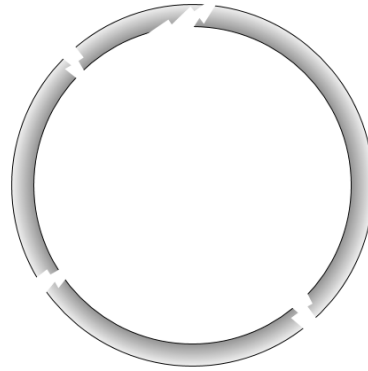
The studies of [123] also showed that this notion can be extended to study the influence of the specimen size on the overall inelastic response of the material. Beyond the linear (elastic) region of the stress-strain plot shown in Figure 2.3, there is an obvious trend of



(a) Problem schematic.



(b) Homogeneous material.



(c) Heterogeneous material.

Figure 2.1: Schematic of brittle material fracture for material modeled as homogeneous and heterogeneous medium in terms of fracture strength distribution.

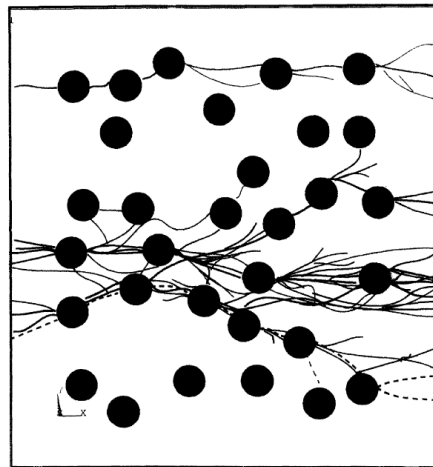


Figure 2.2: Experimentally obtained crack patterns in seven identical material epoxy specimens of with identical distribution of holes and subject to a vertical uniaxial tensile loading [20].

statistical variation of the ultimate strength of the material, as well as the post-ultimate (non-linear) material response.

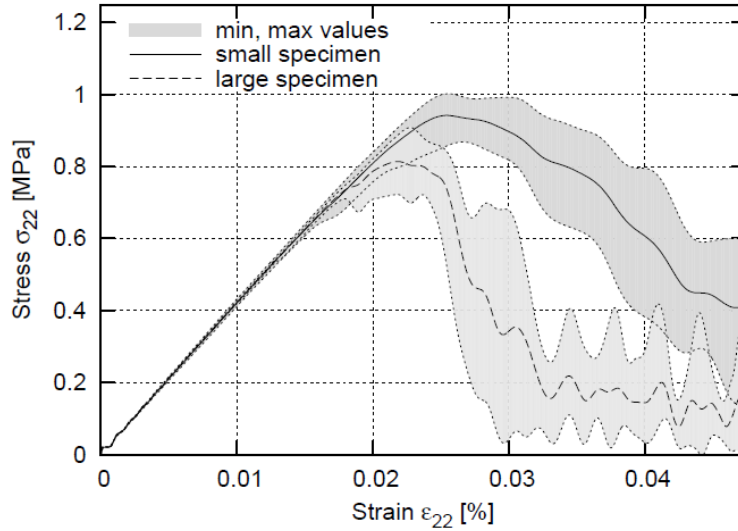


Figure 2.3: Deterministic size effect for 2D concrete specimens subject to uniaxial loading [123].

A more overt depiction of this size influence is taken from [80] and illustrated in Figure 2.4; these studies focus on the ultimate strength of quasi-brittle structures. Analysis of this class of material shows that as the specimen size increases, the specimen becomes weaker with little statistical variation in the measured material strength. This trend is exactly captured in Figure 2.4 and is known as the *size-effect*. The size-effect phenomena is of particular importance when considering probability based models which utilize some scaling law. A more detailed review of this concept can be found in the works of [215, 216, 30], wherein the discussion of size-effect is directed from the viewpoint of Weibull based brittle material failure models.

Each of the previously mentioned brittle material responses demonstrates a high dependency on the randomness of the material microstructure and its constituent distribution. Hence, the natural course of action is to employ a framework that incorporates microscale or mesoscale randomness into the mathematical description of the brittle material in numerical studies.

Modeling random media requires an appropriate characterization of the material randomness. Approaches that explicitly simulate material uncertainty rely on a statistical

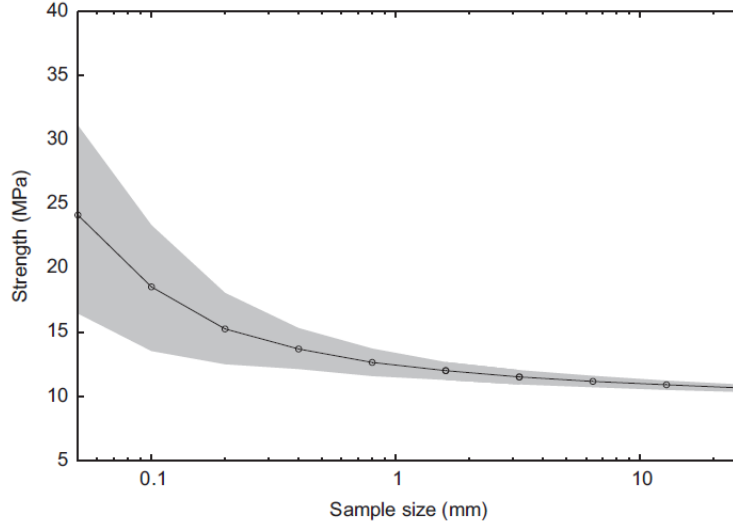


Figure 2.4: Strength of quasi-brittle cellular ceramic structures as a function of specimen size [80].

definition of the explicit features of the microstructure, specifically in terms of geometry and/or aggregate distribution. Ubiquitous models which describe the microstructure as a composition of one simple feature type (*e.g.*, rectilinear microcracks in Figure 2.5b, circular inclusions in Figure 2.5a or granular features in Figure 2.5c) often describe their distribution in terms some probability density. These features are defined by their spatial and angular orientation, characteristic length distribution, spatial density distribution, and other geometry based quantities [163, 61, 190, 32, 219, 76, 38, 225, 191]. Often time the probability structure is assumed in an *ad hoc* fashion; however, studies such as [27, 76, 142] were able to obtain significantly reliable information from microstructure image processing that can be used for statistical characterization. Furthermore, studies modeling the highly aggregate structure of cementitious materials include a greater level of microstructure complexity. These aggregate models incorporate constituents with angular dependency and irregular shapes [104, 218] or model granular features by utilizing Interfacial Transition Zones (ITZ) [214]. Although offering insight on how geometrical aspects of the material microscale features affects its (in)elastic responses, explicit approaches are limited in their application. It is practically impossible to have reliable deterministic representation of a real microstructure which can model the virtually infinite number of microstructure details. Even a “close” numerical representation of a finite number of discrete features can become

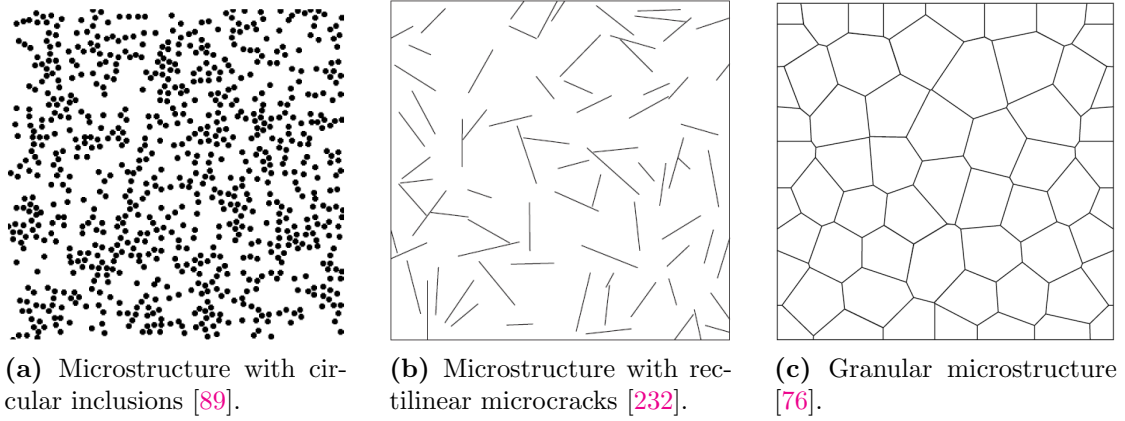


Figure 2.5: Realizations of material microstructures defined by probability structure.

computational costly. Rather, implicit approaches seek to define relationships between local material properties and the local effects of microstructure which are inherently non-deterministic. In this sense, purely brittle material fracture is commonly described by a "weakest-link" approach wherein random fracture strength is defined by a Weibull probability structure. However, works such as [163] have shown that this assumption, albeit valid for purely brittle materials, does not always hold for quasi-brittle materials. This discrepancy is due to size variability of the micro-defects within quasi-brittle materials as well as the material's complex fracture mechanisms. Approximation of random fields in this manner also neglects the concept of spatial-dependency and spatial-correlation. This oversight yields random fields that are heuristic and whose spatial variation is known as statistical "white noise". This supports the notion that "real" material based implicit schemes should account for the effects of the material microstructure when deriving random field definitions. When characterizing randomness, microstructure-based implicit approaches borrow from continuum mechanics and homogenization theory to derive a continuous approximation of heterogeneous material properties. These properties are based on the averaged effects of a neighborhood of micro-defects about a material point. The basis of homogenization schemes is the thermodynamically consistent concept of the *Representative volume element* (RVE). An RVE, which is well defined in [160], permits the continuum representation of a heterogeneous material following the caveats that 1) the RVE is defined as a unit cell in a periodic microstructure, and/or 2) the RVE contains a large number of microstructure

constituents that statistically represents the overall material domain. Essentially, an RVE is the smallest subdomain of a material which contains the same constituent volume fraction and statistical characteristics of the overall large scale material and also behaves identically when subject to homogeneous Dirichlet or Neumann boundary conditions [160, 105]. Although classical homogenization schemes allow the effects of the microstructure within an RVE to be averaged into a local effective material property, the spatial variability does not propagate from the microscale to the effective property. To preserve spatial variability, homogenization is performed at a smaller spatial resolution utilizing a *stochastic (statistical) volume element* (SVE). An SVE is essentially an RVE which is not well-defined but may still allow for the continuum representation of the heterogeneous material. The characterization of material randomness associated with SVEs was studied as it relates to such concepts as microstructure feature clustering and position [190], applied boundary conditions during homogenization [110] and variations in the volume element geometric description [26, 210]. Interesting homogenization studies have been performed which employ non-conventional SVEs; it was shown that these classes of SVEs may yield better estimations of averaged material properties when compared to the more conventional definitions. An example of such a non-conventional SVE is used in the works of [17] wherein SVEs, as seen in Figure 2.6b, are constructed using Voronoi tessellation in a material matrix of non overlapping circular inclusions.

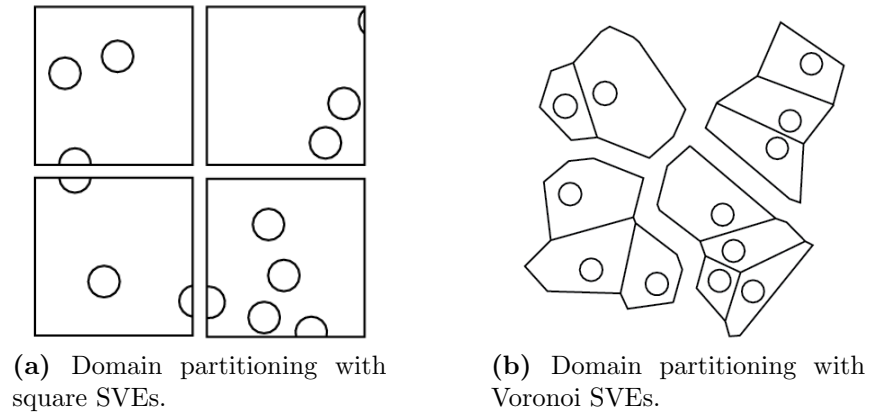


Figure 2.6: Depictions of the partitioning of a material domain with uniformly distribution circular inclusions using conventional square type and non-conventional Voronoi polygon type stochastic volume elements (SVE)s [17].

Once a full description of the SVE is determined, the material domain can be characterized spatially via effective material properties at a finite number of discrete spatial locations. Such analysis within each SVE is typically carried out via analytic and numerical micromechanics-based simulations of heterogeneous materials; a comprehensive review of these approaches can be found in the [48, 83, 170]. An example of a numerical micromechanics method implemented for spatial sampling (homogenization) is the moving-window generalized method of cells (MW-GMC) [88, 162]; this scheme was developed for the modeling of complex unit cell microstructure and has valid (in)elastic stress-strain relations under multiaxial loading. Methods such as the numerical MW-GMC scheme and their treatment of rectilinear microcracks inspired the general method of spatial sampling used within this research work; however, rather than utilizing uniform domain partitions, a non-uniform sample grid definition is used to define the spatial sampling locations (*cf.* 2.2). Overall, methods of spatial sampling in conjunction with some method of microstructure homogenization provide the framework to determine one- and two-point statistics such as the statistical moments (*i.e.*, mean, variance, skewness, kurtosis), cumulative distribution function (CDF) and probability density function (PDF), as well correlation functions of the sampled discrete data set. Knowledge of these statistical quantities is generally sufficient and usually all that is available in practice when representing a random heterogeneous material by a continuous field. The derivation of the continuous random field approximations is detailed in chapter 4.

2.1.3 Methods of validation

Verification of qualitative size-effect: Spatial sampling was performed utilizing SVEs of prescribed sizes. For the collection of constructed SVE of each respective size, a discrete set of spatially defined random strengths were computed. The first and second statistical moments (*i.e.*, mean and variance) of the complete random fracture strength data set demonstrated that as the SVE characteristic length increased, tending to the RVE limit, both the mean and the variance of the data set monotonically decreased (10.4). This behavior was further confirmed by the empirical PDF of the data set. As the SVE size increased, the PDF peak shifted to a lower fracture strength value, and

the PDF curve exhibited a decrease in probable value span tending to a Dirac delta type function(5.6). This trend of decreasing strength mean and variance as SVE size increased mimics the size-effect and is in good agreement with experimental findings.

2.1.4 Intellectual merit

- The research within this chapter provides a consistent framework for the spatial and statistical characterization of a general microstructure realization by a discrete set of computed fracture strength and elastic modulus random field(s). Utilizing a general descriptions of stochastic representative volume elements, general sampling and homogenization approaches conducted on a functionally-graded spatial (Cartesian/Spherical) grid are investigated.
 - The proposed algorithm can efficiently employ SVEs ranging in sizes from microscale to macroscale characteristic lengths; this allows comprehensive comparative studies of the size-effect for various classes of SVEs and microstructure compositions.
 - The scheme provides the determination of one- and two-point statistics of an arbitrary non-Gaussian data set; the statistics of the corresponding Gaussian data set is simultaneously computed for practical use.
 - Implementation of the non-uniform grid definition make it capable of capturing the statistics associated with the clustering of microstructure constituents; this definition also ensures the interpolation of smoothly continuous covariance point-wise functions.

2.1.5 Research contributions

Main contributions:

- [MATLAB scripted.] Generation of explicit granular microstructure FEM mesh based on Voronoi tessellation partitioning of an initial computational domain.

Spatial distribution and number of the partitions are based on Poisson point process.

- [C++ scripted.] Utilizing $L_x \times L_y$ sized sampling windows, Implemented tool to traverse arbitrary domain microstructure R_i and spatially characterized into set of M discrete effective material properties $\{\Theta(\mathbf{x}^j)\}_{R_i}; j = 1, \dots, M$. At each sampling grid point $\mathbf{x}^j$ a sample window is constructed to isolate a subdomain which is then handled independently by general “black-box” homogenization approach (**NB**: Limited implementation to domain consisting of microcracks).
 - Implementation of sampling grid which is handled by a non-uniform functional grid increment-spacing module; grid spacing is only constrained by a maximum and minimum allowable spacing size.
 - Linking of in-house code to ANSYS finite element analysis software to discretize and determine effective elastic properties (stiffness tensor C , Poisson’s ratio ν , etc...) of isolated subdomain.
 - Computation of fracture strength values by LEFM-based homogenization algorithm; Computations are performed iteratively for each microcrack within subdomains to determine maximum effective strength values.
- [C++ & MATLAB scripted.] Implemented tool to compute point-wise statistics of discrete data for ensemble of N microstructure realizations ($\{\Theta(\mathbf{x}^j)\}_{R_i}; i = 1, \dots, N; j = 1, \dots, M$):
 - Capable of computing K^{th} statistical moments of discrete data (*i.e.*, 1^{st} :mean, 2^{nd} :variance, 3^{rd} :skewness, 4^{th} :kurtosis, etc...)
 - Capable of computing Probability density function (PDF) and cumulative distribution function (CDF) for ensemble of input data.
 - Capable of computing auto-correlation and cross-correlation function data (*i.e.*, covariance) for discrete input data in form of tensor fields. Pointwise covariance functions are cast to admissible analytical forms whose structure is an input parameter.

- Inverse transformed method implemented to dynamically change between original discrete data probability structure and desired arbitrary probability structure; Computation of statistics is carried out for both original and of transformed data simultaneously.

Secondary contributions:

- [MATLAB scripted.] Generation of initial explicit microstructure FEM mesh; meshes may consist of probability described microcracks (size, orientation, placement, etc...), irregular polygonal and circular voids, and/or inclusions of arbitrary geometry.

2.2 Influence of SVE description and Sampling Space Definition

2.2.1 Spatial sampling grid definition: utilizing conventional SVE geometry

Upon employing a "moving-window" type approach, preliminary studies regarding the statistical characterization of heterogeneous materials revealed the importance of an appropriately structured grid description for SVE sampling. Utilizing a square material domain, of length 40m (as seen in Figure 2.7 where $L_{x_1} = L_{x_2} = 40\text{m}$) populated with microcracks of random geometry and orientation, the following solutions motivated the need for nonuniform sampling grid spacing. This grid structure not only preserves the accuracy of the computed statistical characteristics while employing fewer spatial sampling points, but allows for a smooth representation of the statistical data which can be fitted to a useful analytic form.

With the original sampling approach, a spatial grid was constructed (Figure 2.7) by partitioning of a material domain into rectangular sections defined by grid points $\mathbf{x}$. Each consecutive grid point was spaced Δ_{x_1} and Δ_{x_2} meters apart in directions x_1 and x_2 respectively. These grid points comprise a discrete set of N_{total} spatial points

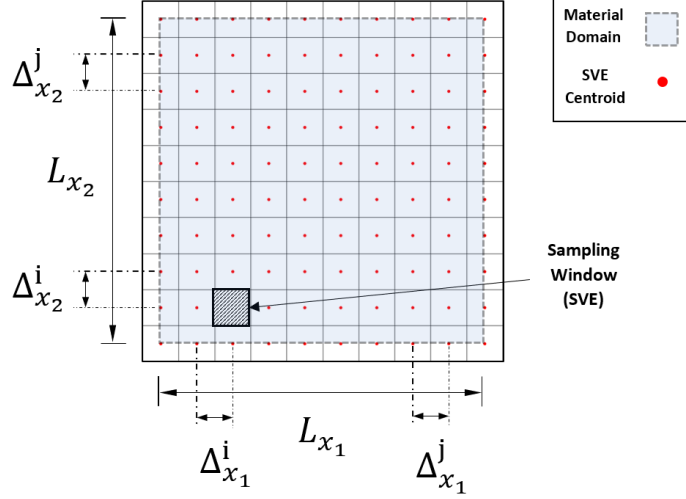


Figure 2.7: Schematic of material domain partitioning for (non-overlapping) SVE sampling employing spatially uniform grid.

$\{\mathbf{x}^k | k = 1, \dots, N_{total}\}$, per random microstructure realization, at which homogenization can be performed. Since the grid is uniform, it is obvious that $\Delta_k^i = \Delta_k^j, i, j = 1, \dots, N_k$, where N_k is the number of grid points defined in direction x_k (*i.e.*, for a given spatial direction, all successive grid points are equally spaced). For simplicity, the increment spacing in all directions were made equal (*i.e.*, $\Delta_{x_1} = \Delta_{x_2}$). Conventional rectangular SVEs of size $\Delta_{x_1} \times \Delta_{x_2}$ were then constructed, as demonstrated in Figure 2.7, such that their centroids coincided with each defined grid point. This allows homogenization to be carried out within an SVE centered at each grid point and the complete discrete set of computed effective material property to be spatially defined by their respective grid point location $\mathbf{x}^k$. Within each SVE, an independent microstructure sub-domain was considered for homogenization; an example of this sub-domain is illustrated in Figure 2.8.

Each sub-domain was then spatially discretized and exported into the ANSYS simulation software; utilizing a finite element approach, each SVE sub-domain was subject to Dirichlet boundary conditions to determine the effective elasticity tensor $\mathcal{C}(\mathbf{x})$ of the material within the sub-domain centered at sampling grid point $\mathbf{x}$. Examples of Von-Mises stress solutions can be seen in Figures 2.9a and 2.9b, where displacement components $[u_{xx}, u_{yy}] = [\epsilon_{xx}x, 0.0]$ and $[u_{xx}, u_{yy}] = [2\epsilon_{xx}y, 0.0]$ are used to prescribe the boundary conditions for normal strain and simple shear strain problem (coordinate convention is $\{x_1, x_2\} = \{x, y\}$). By

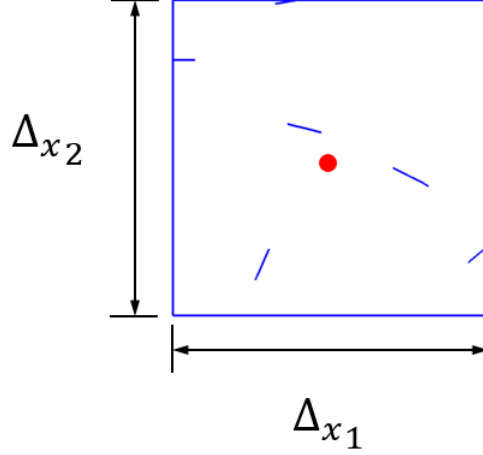
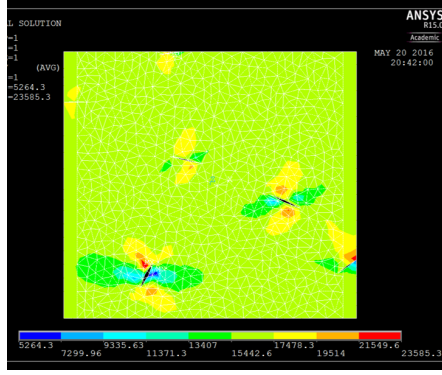


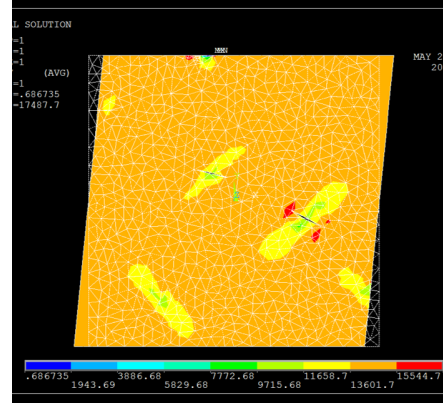
Figure 2.8: Realization of conventional SVE sub-domain containing microcracks.

averaging components of the stress tensor inside the domain for three Dirichlet boundary conditions corresponding to nonzero values for ϵ_{xx} , ϵ_{yy} , and ϵ_{xy} , elasticity tensor is fully characterized. For completion, Figures 2.9c and 2.9d depict stress intensity for previous normal and simple shear strain cases respectively; the local stress intensity value is defined as $SI = \max\{|\sigma_i - \sigma_j|\}$, where there is no summation on indices i, j and σ_i is the i^{th} principal stress component.

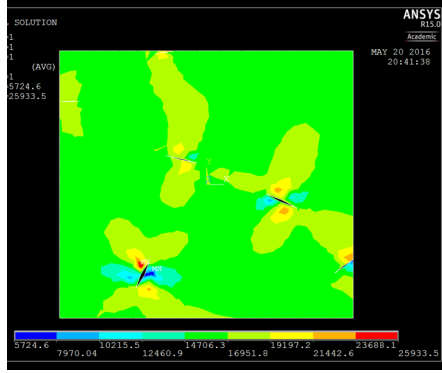
Based on the computed elasticity tensor $\mathcal{C}$, one- and two-point statistics were then determined for the corresponding effective elastic modulus $E(\mathbf{x})$ normalized by the elastic modulus of the pristine material E_0 , and the Poisson ratio $\nu(\mathbf{x})$. Figure 2.10 illustrate the empirical probability density functions (PDF) determined from material domain sampling employing SVEs of size $1\text{m} \times 1\text{m}$ and $4\text{m} \times 4\text{m}$. For convenience, all SVE sizes are of dimension metre (m) unless otherwise specified. From these two cases we can observe a decrease in the PDF span of probable values for both E and ν as each PDF tends to a *dirac* delta type function. This trend makes sense theoretically as larger SVEs tend to the RVE limit; this means that there is a decrease in how much variability is propagated from the random microstructure and consequently a material with spatially homogeneous properties is represented. This preliminary observation of size-effect is further expanded in Section 10.3.1 of chapter 4 which gives a better interpretation in terms of derived linear elastic fracture mechanics (LEFM) based fracture strength values $\bar{s}$.



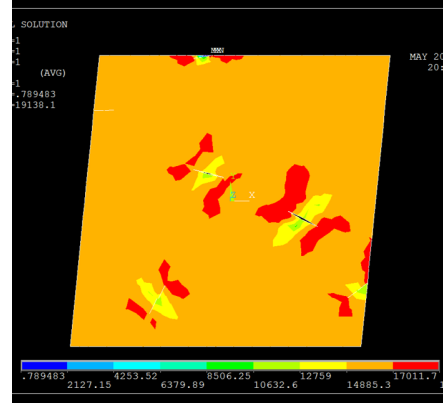
(a) Von-Mises stress solution under applied uniaxial displacement u_{xx} .



(b) Von-Mises stress solution under applied shear displacement u_{xy} .

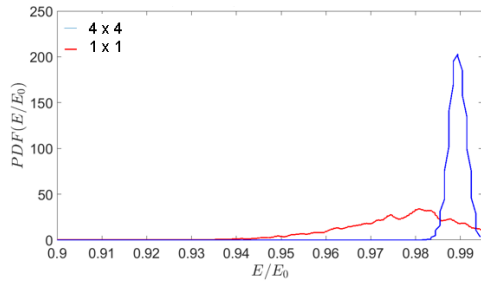


(c) Stress intensity number solution under applied uniaxial displacement u_{xx} .

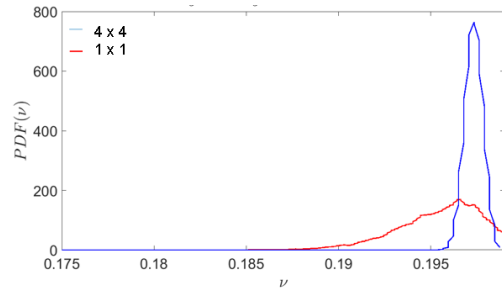


(d) Stress intensity number solution under applied shear displacement u_{xy} .

Figure 2.9: ANSYS analysis of SVE sub-domain 2.8 for the determination of effective material properties (elasticity tensor, $\mathcal{C}$).



(a) Probability density function of normalized elastic modulus.



(b) Probability density function of Poisson's ratio.

Figure 2.10: Empirical one-point statistics of effective elastic properties determined from homogenization using 1×1 and 4×4 SVE sampling.

The covariance function (two-point statistic) was also determined via equation 5.3 in Section 5 and is illustrated for elastic modulus E when SVE size 4×4 was utilized. The stationary isotropic covariance gives quantitative measure of how two quantities at two spatial locations are correlated based on the separation between the two locations. Figure 2.11, demonstrates how discrete points of the covariance point-wise function are then used to perform a "best-fit" operation for defining an analytic form of the covariance function.

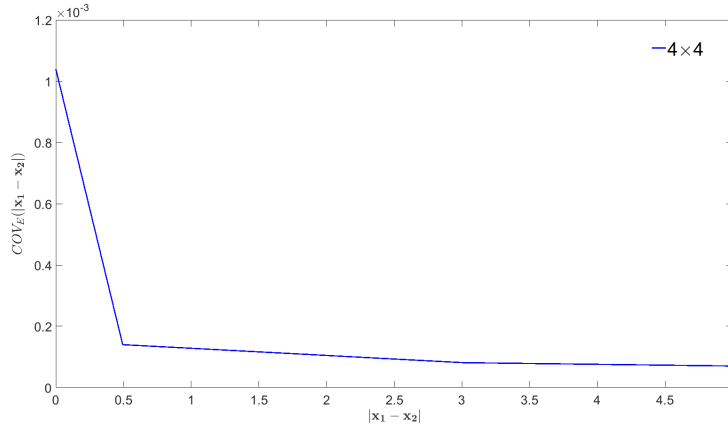


Figure 2.11: Empirical stationary isotropic covariance function of effective elastic modulus determined from homogenization using 4×4 SVE sampling.

A major consideration to be taken, when extrapolating from a discrete data representation of a stationary isotropic covariance function, $COV(|\mathbf{x} - \mathbf{x}'|)$, is how smoothly the covariance function data is captured as the separation distance $|\mathbf{x} - \mathbf{x}'|$ tends to zero(0). Not accurately realizing the larger correlation values of the covariance functions as $|\mathbf{x} - \mathbf{x}'|$ tends to zero(0) can result in a misrepresentation of how variable a quantity of interest is within a particular length scale. Section 5.2.3 of chapter 4 describes the implementation of a non-uniform sampling grid definition that ensures sufficient resolution of the covariance function as separation distance tends to zero. The covariance function derived with this non-uniform grid shows better "goodness of fit" to admissible analytical covariance function forms such as the γ -exponential covariance function. An example of this type of grid can be found in Figure 2.12.

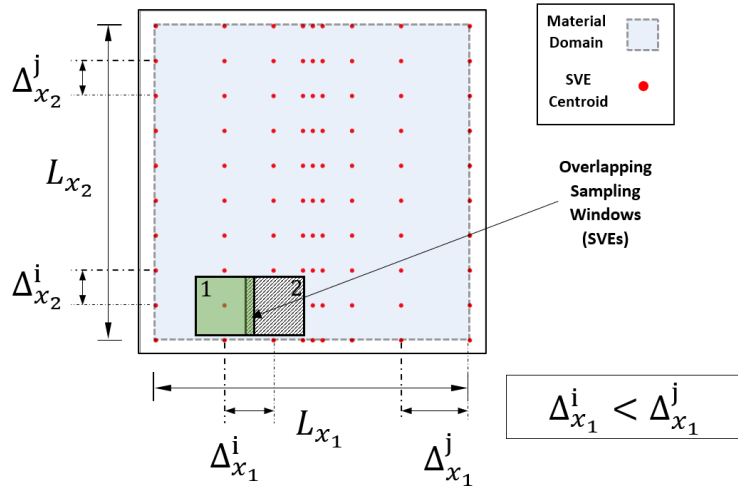


Figure 2.12: Schematic of (overlapping) SVE sampling employing spatially non-uniform grid.

Chapter 3

SVE geometry based on Voronoi Tessellation

An original version of the following article was published in the conference proceedings of International Mechanical Engineering Congress & Exposition 2017 (AMSE IMECE 2017) [14]. The article was originally published under the title “Mesoscale models characterizing material property fields used as a basis for predicting fracture patterns in quasi-brittle materials” but for more comprehensive inclusion into this dissertation, the title was revised to emphasis the concept of interest. Dr. Acton from the College of Engineering, University of St. Thomas, MN, USA and Mr. Bahador Bahmani (PhD student at UTSI) are the main contributor of this manuscript in order, in terms of the analysis of SVEs at the microscale and characterizing their fracture properties. My contributions are minor in the scope of the paper, which focuses on homogenization of Voronoi-based SVEs; I included this manuscript for completeness in terms of homogenizing SVEs, to generating consistent statistics, to macroscopic fracture analysis of a random medium. These are the focus areas of chapters 2 to 4. My contribution to this paper is realization of macroscopic fracture properties that are consistent with the homogenized properties using the Karhunen-Loève method, a topic further discussed in the next chapter. In this publications the SVEs were constructed by Voronoi tessellation partitioning of a material domain of circular inclusions. Statistical data of the random fracture strength obtained SVEs were then used directly in the methods detailed in chapter 4. Interestingly, SVEs of this geometry can provide increased accuracy in the computation of effective elastic properties that would otherwise be lost due to inclusion intersection with SVE boundaries during the domain sampling and homogenization process.

Abstract: To accurately predict fracture patterns in quasi-brittle materials, it is necessary to accurately characterize heterogeneity in the properties of a material microstructure. This heterogeneity influences crack propagation at weaker points. Also, inherent randomness in localized material properties creates variability in crack propagation in a population of nominally identical material samples. In order to account for heterogeneity in the strength properties of a material microstructure, a mesoscale model is developed. A central challenge of characterizing material behavior at a scale below the representative volume element (RVE), is that the stress/strain relationship is dependent upon boundary conditions imposed. To mitigate error associated with boundary condition effects, statistical volume elements (SVE)

are characterized using a Voronoi tessellation based partitioning method. A moving window approach is used in which partitioned Voronoi SVE are analysed using FEA to determine a limiting stress criterion for each window. Results are obtained for hydrostatic, pure and simple shear uniform strain conditions. A method is developed to use superposition of results obtained to approximate SVE behavior under other loading conditions. These results are used to determine a set of strength parameters for mesoscale material property fields. These random fields are then used as a basis for input in to a fracture model to predict fracture patterns in quasi-brittle materials.

Acknowledgments: The authors gratefully acknowledge partial support for this work via the U.S. National Science Foundation (NSF), CMMI - Mechanics of Materials and Structures (MoMS) program grant number 1538332.

3.1 Introduction

Material inhomogeneities at the microstructural scale greatly influence fracture response. Failure initiates locally where stress concentrations are induced in large part by local heterogeneity. Therefore, fracture models that ignore microstructural inhomogeneity, or employ Representative Volume Elements (RVE) to homogenize material properties, may not accurately capture fracture response. The high sensitivity of brittle fracture to material microstructure not only contributes to the form of failure patterns, but also size effects [29, 97, 80] and high response variability for samples with identical geometry and loading specifications [20, 45, 200].

In previous work, the Spacetime Discontinuous Galerkin (SDG) Finite Element Method (FEM) [9] has been employed for the solution of elastodynamic problems. The SDG method has high accuracy from the direct discretization of space and time, and is also efficient in characterizing the local solution properties critical for simulation of fracture in (quasi-) brittle materials by using adaptive operations in spacetime that control discretization errors [10] and track propagating cracks [158].

In this work, a mesoscale modeling technique will be used to characterize mesoscale material property behavior; the model outputs can be used in SDG fracture simulation. The

mesoscale model characterizes behavior of Statistical Volume Elements (SVE) that are below the scale of the RVE. These elements retain a degree of local descriptiveness, which is missing in an RVE-based analysis. Previous work has focused on the use of mesoscale modeling techniques to model composite material behavior [26, 88, 91, 16, 15, 17]. A main advantage of the approach is that it can ultimately be used to create random field representations of local composite properties. This type of mesoscale material characterization can be used as a basis for stochastic simulation, or as a statistical basis for models predicting damage and failure, which is the focus of the current work.

3.2 Mesoscale Material Modeling

A Voronoi tessellation based partitioning scheme is used to model the SVE, in place of a more commonly used square partitioning approach. Voronoi tessellations have been shown to provide closer approximations of material properties because stress concentrations are reduced when inclusions are not allowed to intersect inclusion boundaries [186]. The collection of SVE that partition an RVE are tested using Finite Element Analysis (FEA) to determine material behavior under hydrostatic, pure and simple shear displacement based loading. An SVE failure criterion is defined and superposition is used to determine the approximate failure stress of the SVE when loaded in any direction.

3.2.1 Construction and Loading of SVE

An RVE with randomly placed inclusions is initially partitioned into Voronoi cells using Delaunay triangulation based on center points of inclusions. The cells are grouped into similarly sized SVE by calculating the location of each Voronoi cell centroid with respect to a square grid imposed on the RVE. If a Voronoi cell centroid lies within a given square grid area, the cell is assigned to that SVE grouping. In this work, the RVE is generated with a volume fraction of approximately 10% inclusions; each inclusion diameter has a unit value, the RVE has equal side lengths 100 times the size of the inclusion. Results are given for a material with inclusion to matrix contrast ratio 100 : 1.

Figure 3.1 shows a typical SVE, with grid spacing set to 5 times the inclusion diameter, under the three load cases considered in this work. Displacement conditions on the boundary $\mathbf{u}|_{\partial\Omega}$ are given by:

$$\mathbf{u}|_{\partial\Omega} = \mathcal{E} \cdot \mathbf{x} \rightarrow \langle \epsilon \rangle_{\Omega} = \mathcal{E} \quad (3.1)$$

where hydrostatic, pure shear, and simple shear loading conditions are generated using the three values of $\mathcal{E}$ shown below, respectively.

$$\begin{aligned} \mathcal{E} &= e^H \cdot \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \\ &e^P \cdot \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \\ &e^S \cdot \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \end{aligned} \quad (3.2)$$

Scale factors e^H, e^P and e^S correspond to each of the three cases. Using a superposition approach, any displacement boundary condition can be obtained by linear combination of these three load cases for a planar problem. A stiffness matrix is generated based on the results of these three loading conditions, such that displacement boundary conditions can be related to average nodal stresses on the boundary of the SVE.

3.2.2 Failure Criterion

The mesoscale approach is fully elastic, with failure assumed when a threshold value of stress occurs in the matrix. In particular, stresses are calculated at the matrix/inclusion interface, within the matrix material only, in the direction normal to the inclusion boundary. The “path” function in the finite element program ABAQUS is used to determine the stresses in the matrix surrounding the inclusion, as shown in Fig. 3.2.

A uniaxial tensile, or simple shear loading direction may be assumed. By superposition, the stress at a position $\mathbf{x}$ on the boundary of any inclusion, in the direction normal to the

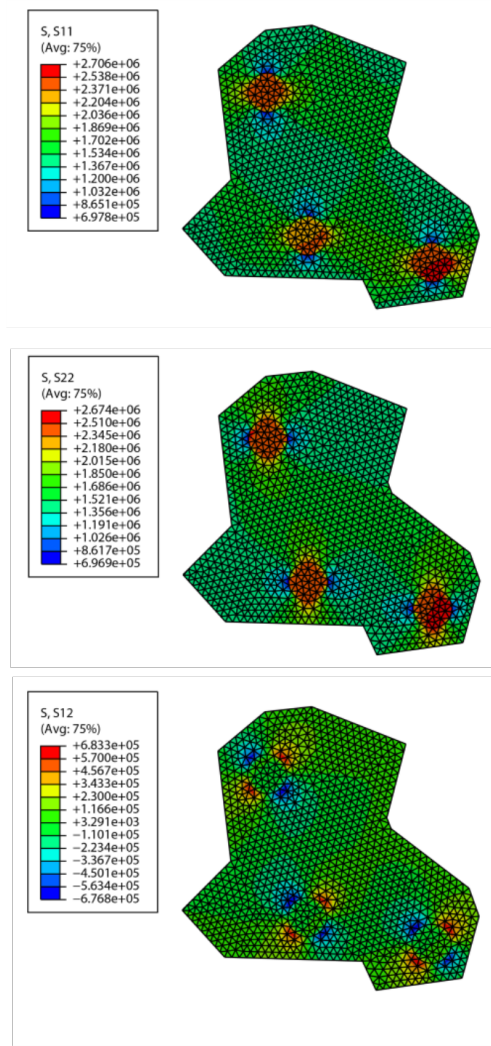


Figure 3.1: Loading of Voronoi Tessellation based sve by (a) hydrostatic (b) pure shear and (c) simple shear displacement boundary conditions.

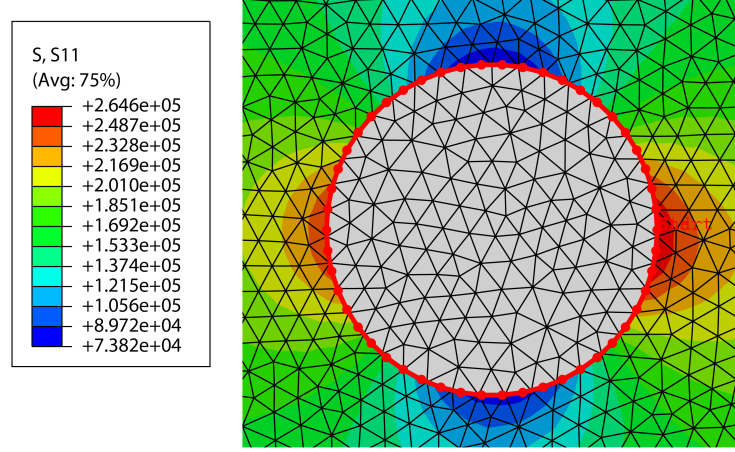


Figure 3.2: Circular path around the inclusion, location where matrix material stresses are determined.

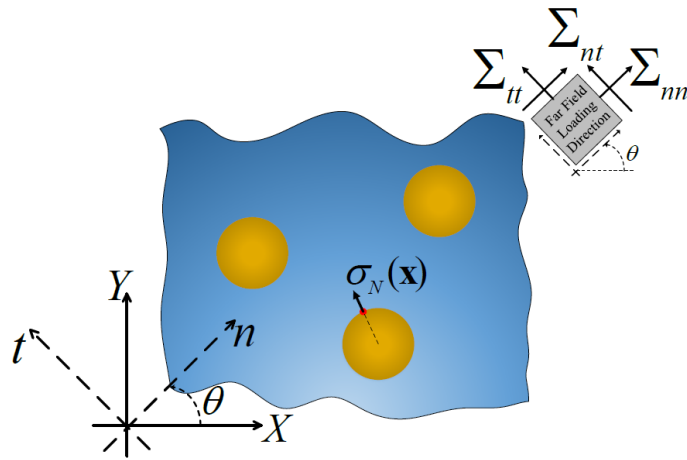


Figure 3.3: Schematic of an SVE and the n, t axes for far-field loading relative to global x, y axes.

inclusion as shown in Fig. 3.3, is given by:

$$\sigma_N(\mathbf{x}) = e^H \sigma_N^H(\mathbf{x}) + e^P \sigma_N^P(\mathbf{x}) + e^S \sigma_N^S(\mathbf{x}) \quad (3.3)$$

where each of the three load cases (hydrostatic, pure shear and simple shear) are denoted by superscripts (H, P and S, respectively).

Using the stiffness matrix developed as described in the previous section, scale factors e^H , e^P and e^S are determined such that superposition of H, P, and S strain loadings generate far field (SVE averaged) stress loading Σ_{nn} , Σ_{nt} , Σ_{tt} , *cf.* Fig. 3.3. The unit magnitude normal and tangential stress loading at an angle θ are realized by having the only nonzero stress components of $\Sigma_{nn} = 1$ and $\Sigma_{nt} = 1$, for normal and shear modes respectively.

Macroscopic failure threshold of SVE is associated with far field stress loadings that makes the maximum of interfacial stress over all points, $\max_{\mathbf{x}}(\sigma_N(\mathbf{x}))$, equal to a predetermined debonding threshold σ^{TH} . Accordingly, normal $\tilde{s}_n(\theta)$ and tangential $\tilde{s}_t(\theta)$ strengths for far field loadings at angle θ are equal to load factors s ,

$$s = \frac{\sigma^{TH}}{\max_{\mathbf{x}}(\sigma_N(\mathbf{x}))} \quad (3.4)$$

that scale unit magnitude normal and tangential far field loadings and cause matrix stress at the inclusion boundary, normal to the inclusion, to reach the threshold value σ^{TH} . While $\tilde{s}_n(\theta)$ and $\tilde{s}_t(\theta)$ correspond to stress values, at angle θ , for which the SVE response starts to significantly deviate from linear elasticity they are very close to the ultimate stress, *i.e.*, strength, of the SVE for quasi-brittle materials. The proximity of linear elasticity stress limit and strength is demonstrated in various works, see for example [80, 155], and is due to the lack of significant bulk energy dissipative mechanisms for quasi-brittle materials.

3.3 Results

Results given in Fig. 3.4 and 3.5 show the strength of a given SVE as a function of the angle of the applied load for uniaxial tensile load $\tilde{s}_n$ and simple shear load $\tilde{s}_t$, respectively, where a threshold value of failure in the matrix is normalized to a unit value. These results show

the SVE reaching failure significantly below this threshold value, for most loading directions, because of the effects of stress concentrations around the inclusion boundaries. Results are given in Fig. 3.4 and 3.5 for a single SVE, with dimensions approximately 5 times the inclusion diameter, taken from a set of approximately 400 SVE that partition an RVE with side length approximately 100 times the inclusion diameter.

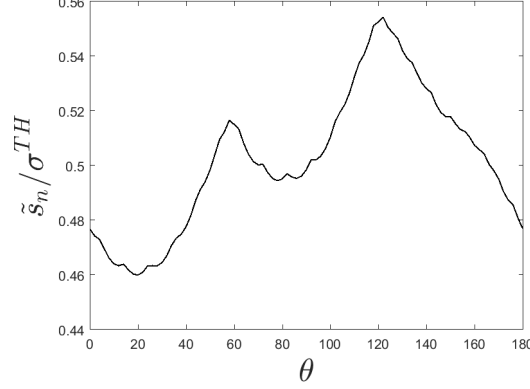


Figure 3.4: Tensile strength of an sve as a function of boundary condition loading direction θ .

To visualize the variability among the population of SVE that partition the RVE, Fig. 3.6 shows the minimum strength value under tensile loading at any load angle for a set of approximately 400 SVE. Based on this data, the probability density function (PDF) in Fig. 3.7 is generated.

Another way to approach the data is to determine the mean value of strength of a given SVE under loadings at all angles (*e.g.*, averaging the results shown in Fig. 3.4). Calculating the average value of tensile strength for the set of all SVE produces the PDF shown in Fig. 3.8.

Finally, the maximum value of strength of a given SVE under loading at all angles may be calculated; the PDF showing these results for tensile strength is given in Fig. 3.9.

The PDF of minimum values of $\tilde{s}_n$ from Fig. 3.7 and the spatial covariance function, computed by the moving window approach [26], are used in the Karhunen-Loève (KL) method [82] to generate random field realizations for $\tilde{s}_n$. The random field realization shown in Fig. 3.10, normalized by σ^{TH} , is subsequently used for the fracture analysis of the domain

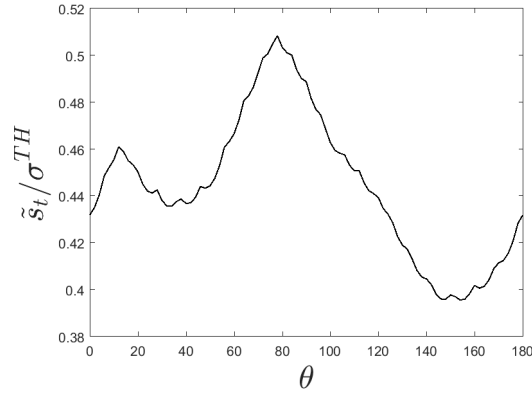


Figure 3.5: Shear strength of an sve as a function of boundary condition loading direction θ .

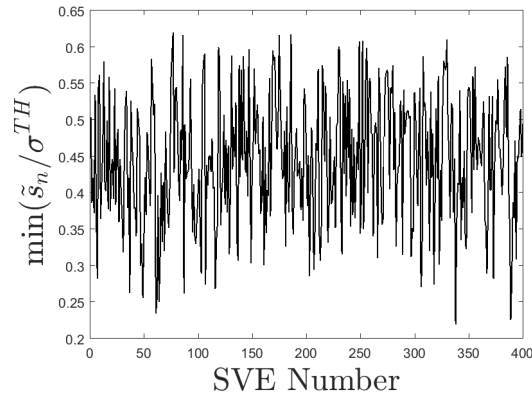


Figure 3.6: Minimum strength value at any loading direction for a set of SVE.

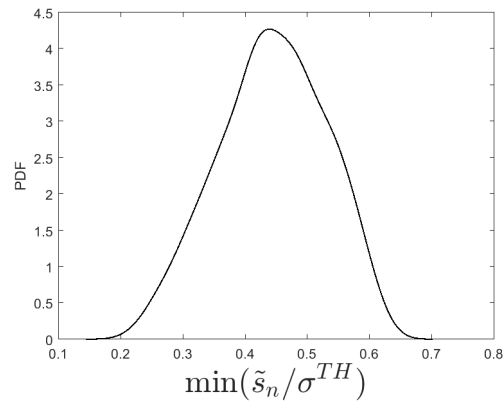


Figure 3.7: PDF of minimum strength value based on SVE data set.

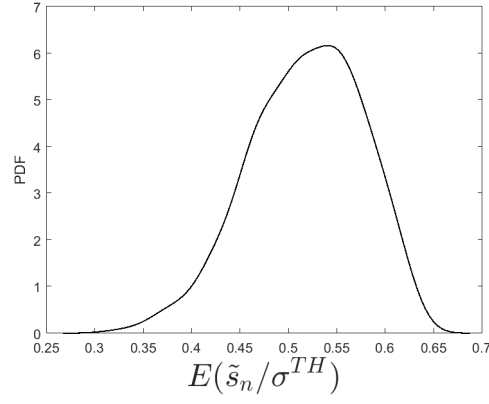


Figure 3.8: PDF of mean strength value based on SVE data set.

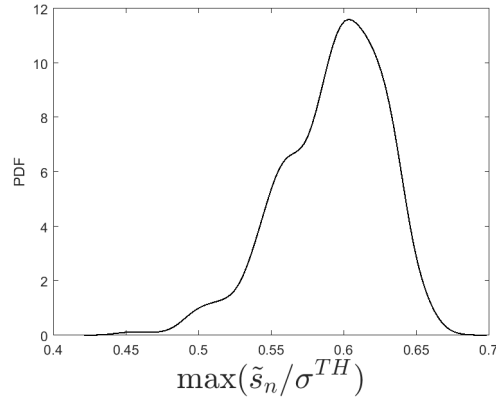


Figure 3.9: PDF of maximum strength value based on SVE data set.

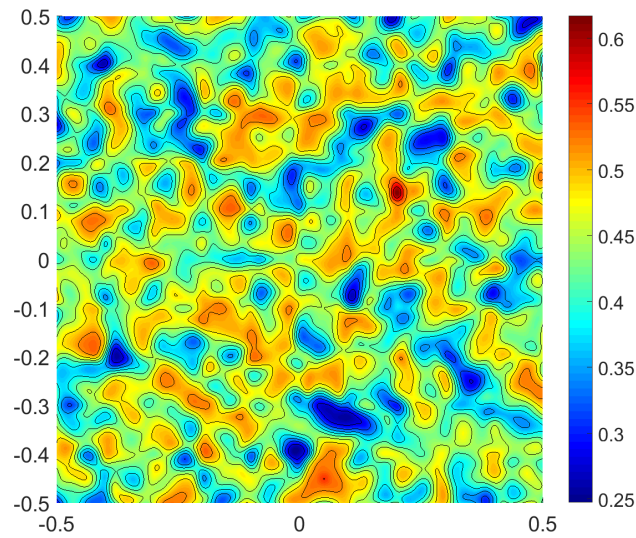


Figure 3.10: A realization of random field for $\tilde{s}_n$ using the Karhunen-Loève method.

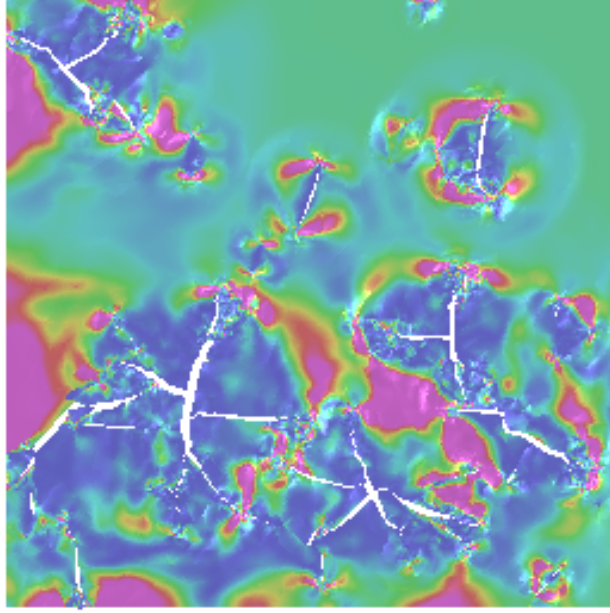


Figure 3.11: Fracture simulation of a domain with nonuniform $\tilde{s}_n$ by the SDG method.

under a spatially uniform (before any crack generation) and temporally increasing stress field. Figure 3.11 shows the final fracture pattern, where as expected fractures have mostly occurred in low failure strength regions. The details of generation of random field for $\tilde{\sigma}_n$ by the KL method and the SDG method used for the fracture simulation can be found in [53, 158].

3.4 Conclusions

Based on this work, a method to capture variability in microstructural material strength has been demonstrated. This characterization includes minimum, mean and maximum values of strength as a function of the angle of loading of a given SVE. It is then possible to generate PDFs of the minimum, mean, and maximum strength values of the population of SVE that partition an RVE. The use of a Voronoi tessellation based partitioning method increases the accuracy of the predicted SVE response by eliminating spurious stress concentrations that arise when inclusions intersect RVE boundaries. The use of a superposition approach when loading each individual SVE allows for determination of SVE behavior at any loading angle based on combination of a set of hydrostatic, pure and simple shear loading conditions.

This work provides a method for generating realistic stochastic fields and as shown it can be used as a basis for fracture modeling. It is critical to accurately model material heterogeneity at the microstructural scale to identify the influence of weaker points in the initiation and propagation of cracking. Future work will investigate the influence of microstructure on statistical properties of fracture strength and subsequently their effect on macroscopic fracture patterns.

Chapter 4

Random field(s) determination based on microstructure statistics

4.1 Introduction

4.1.1 Objectives

This Chapter details a self-consistent algorithm used for the generation of a spatially correlated (non)Gaussian random field. Employing the point-wise statistics, discussed in Chapter 2, a Galerkin finite element method is implemented to solve a generalized eigenvalue problem (EVP) (*i.e.*, Fredholm’s equation with a covariance kernel). The eigen-pair solutions of the EVP allow a continuous random field approximation to be constructed via *Karhunen-Loève* expansion of the field. An insightful relationship between the covariance kernel correlation length-scale and the length scale of spatial variability of the corresponding random field realization is verified. The realized random field will preserve the probability structure imposed by the point-wise statistics, consequently propagating the material uncertainty from the underlying microstructure to the approximated random field. These random field realizations are constructed for use in macroscale dynamic brittle fracture simulations which are discussed in the subsequent Chapter 6.

4.1.2 Background and motivation

A robust representation of the physical responses of heterogeneous materials stems from accurate and reliable solutions to *stochastic* partial differential equations (SPDEs); this class of equations are the direct consequence of accounting for material randomness as a stochastic (random) field in the mathematical description of the problem’s physics. A number of *stochastic* finite element methods (SFEMs) have been developed for this purpose. Moreover, the stochastic field discretization approach utilized must balance 1) computational tractability, 2) mesh-dependent computational cost, and 3) achievable field representation quality. All of the aforementioned aspects collectively affect the properties of the discretized stochastic field and the SFEM’s overall practicality. Unlike its deterministic counterpart, whose discretization construct typically depends on domain geometry and stress gradients,

the SFEMs employ discretizations which are highly dependent on the correlations length-scale¹ of the field being realized [144]. Additionally, the method’s usability depends on the probability structure of the discrete random variables used to define the stochastic field.

The methods deemed most ”exact” in terms of sampling from a random process and determining their statistical characteristics are those based on the *Monte Carlo* (MC) method. Although the MC methods are typically the most tractable in all applications, it can be computationally costly, since the relatively large sample space needed results in slow $\mathcal{O}(N^{-\frac{1}{2}})$ convergence rate for achieving accurate stochastic field mean value. Works such as [36, 99, 178, 62, 96, 180] illustrate this issue as being of particular importance for fracture analysis and structural reliability. Particular studies of this nature would therefore benefit from the use of more efficient MC methods such as [112, 28] which attempt to remedy, to an extent, the method’s shortcomings. Beyond the niche of the MC method, other discretization methods can be employed wherein the burden of computational cost is mitigated while preserving reliable stochastic field representations comparable to MC output. Works such as [185, 183] employ ”linear methods” [144] such as the Kriging technique (optimum linear estimation) exploiting the linearity of the original discrete field to construct the stochastic fields as simple linear functionals of the original field. Having the random mesh discretized independently of the deterministic FEM mesh, this method can be characterized as non-intrusive wherein the structure of the deterministic FEM is not altered. However, if the quantity of interest is non-Gaussian or is a deterministic quantity that is a non-linear function of random variables having unknown or nontrivial covariance function, the Kriging method and others alike are not directly applicable and widespread use is hindered. In practice, when modeling the random characteristics of a given material, the probability structure may not actually be Gaussian; therefore, its treatment should be handled in an unbiased fashion.

Series expansion methods are more appropriate choices as they naturally handle the discretization of non-Gaussian stochastic fields or non-linear deterministic functionals of stochastic fields. Perturbation based SFEMs, utilized in [117, 184] for example, discretize the solution in probability space via 1st and 2nd order Taylor series expansions of the solution

¹*i.e.*, the spatial variability of the stochastic field with respect to a particular length-scale

to solve the SPDEs. A considerable drawback of this method is that its application may be restricted in the highest order of expansion that can be used. Higher order expansion of the large number of terms needed to represent a stochastic field not only results in a larger coefficient of variation but induces numerical round-off error even if a smaller coefficient of variation is used. This limitation commonly impedes application of this method to 1st order perturbation analysis, particularly for nonlinear stochastics, which still shows good agreement with and reduced computational time when compared to MC simulations. *Spectral stochastic Galerkin FEMs* (SSGFEM), detailed in [82], perform the discretization of the deterministic spatial domain and the stochastic space via the Galerkin method. An expansion of the solution, being a functional of stochastic processes, results in direct discretization of both the space and stochastic domain consequently modifying the deterministic FEM structure. As a result, methods such as the *polynomial chaos* (PC) are inherently intrusive and results in a system of coupled FEM and stochastic solutions unknown which can impede their widespread application. Albeit more efficient solution schemes for these methods are demonstrated in [220, 71] for example. Exploiting the advantages of the SSGFEMs while remaining non-intrusive, the *kernel expansion method* (*Karhunen-Loève* (KL) *expansion*) utilizes an eigen decomposition of the covariance kernel of a stochastic field of interest to construct a smooth Gaussian approximation of that field. The properties of the eigen solutions permits utilizing a reduced number of stochastic variables needed to represent the KL expanded field; The method also ensures an optimal minimization of the mean square error induced by this reduction. By construction, KL expansion approximation of the stochastic field preserves the probability structure introduced by the covariance kernel.

Within literature, it is common to study the correlation length ² of a spatially correlated stochastic process; works utilizing the KL methods are no exception. For KL methods, the exact definition of the correlation length is dependent on the form of the covariance that is being considered. Although the covariance function can have any form, provided it is admissible based caveats detailed in [179], the most common form of covariance that is observed in literature is an exponentially decaying function. These exponential covariances

²correlation length is the length scale association with the spatial variation of a random field

are typically isotropic (*i.e.*, $f(\mathbf{x}_1, \mathbf{x}_2)$) and/or stationary (*i.e.*, $f(|\mathbf{x}_1 - \mathbf{x}_2|)$) wherein the correlation length generally appears as a power of the exponent's denominator.

Considering an extensively used exponential covariance function form, [82] shows that as microscopic correlation length decreases there is a slower convergence of the eigenvalue solutions to zero(0) and a greater number of eigenvalues are needed within the KL expansion series for an accurate approximation of the random field. This trend is seen in Figure 4.1 where the correlation length is denoted as b .

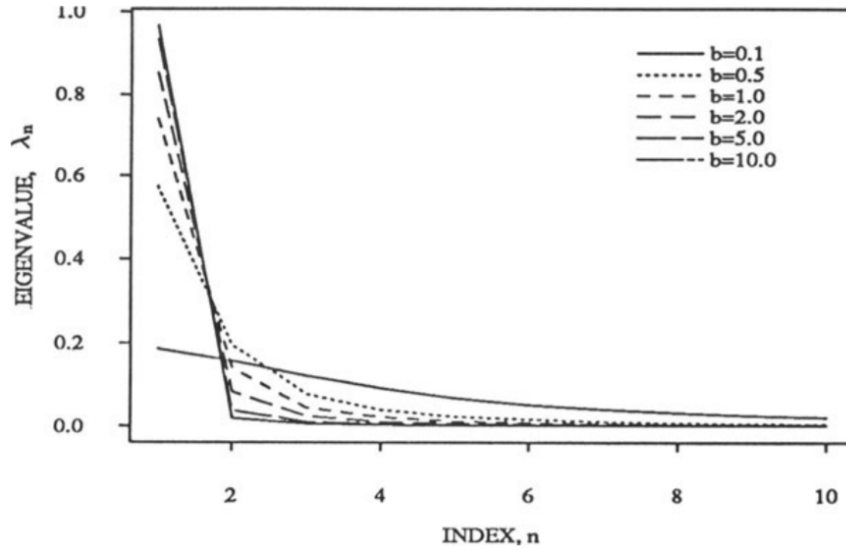


Figure 4.1: Eigenvalue solution relationship with correlation length of γ -exponential ($\gamma = 1$) covariance kernel [82].

A greater number of eigenvalues results in the need for a greater number of eigenfunction solutions. Illustrating the solutions of 1D eigenfunctions, Figure 4.2 demonstrates how the order of mode shapes increases as additional eigenfunctions are realized. Since the generated KL approximations are essentially a superposition of eigenfunctions scaled by both corresponding eigenvalues and Gaussian random variables, it can then be deduced based on these higher mode shapes as to why the use of a smaller correlation length and consequently a greater number of eigen-pair (eigenvalues/eigenfunctions) solutions yields random field realizations with greater variation.

Stemming from these seminal studies, works such as [220] illustrate this concept in a 2-dimensional setting by demonstrating how the use of various covariance functions forms and correlation lengths can effect the spatially variation of a KL realized elastic modulus field.

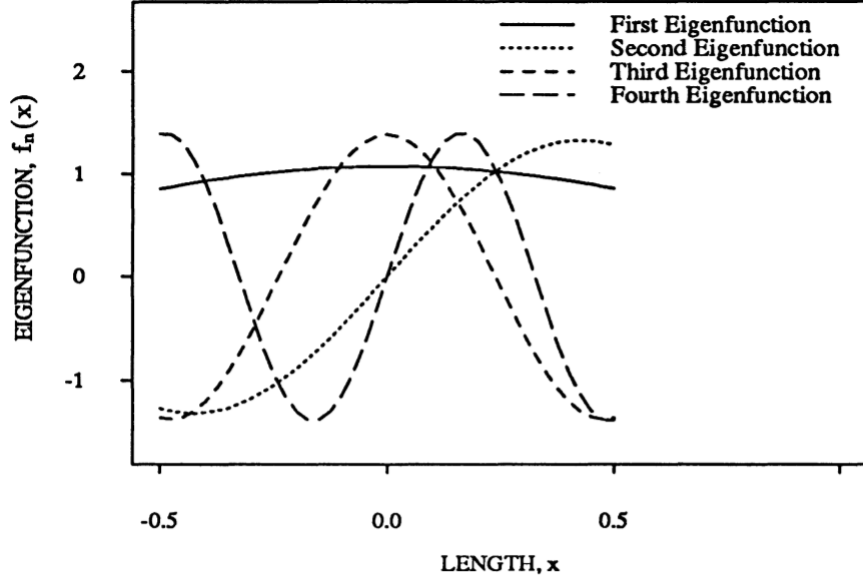


Figure 4.2: 1D eigenfunction solutions utilizing γ -exponential ($\gamma = 1$) covariance kernel [82].

Figure 4.3 depicts the covariance functions and an arbitrary realization of the discretized elastic modulus corresponding to each covariance function.

Moreover, works such as [67] utilized a consistent 2-dimensional covariance definition to show a more comprehensive inversely proportional relationship between the elastic modulus spatial changes and corresponding correlation length; this analysis is seen in Figure 4.4.

Although very insightful, the covariance function parameters (*e.g.*, correlation length,...) are commonly chosen in an *ad hoc* fashion which consequently produce random field approximations that are more phenomenological than material microstructure based. Albeit the KL theory in this Chapter is generally consistent with previous works, one of the main novelties of this work is the utilization of statistics that are more adherent to material microstructures. Therefore, the realizations of random fields are more consistent with a “real” (quasi)brittle-like material as the microstructure is more representative of a (quasi)brittle-like material.

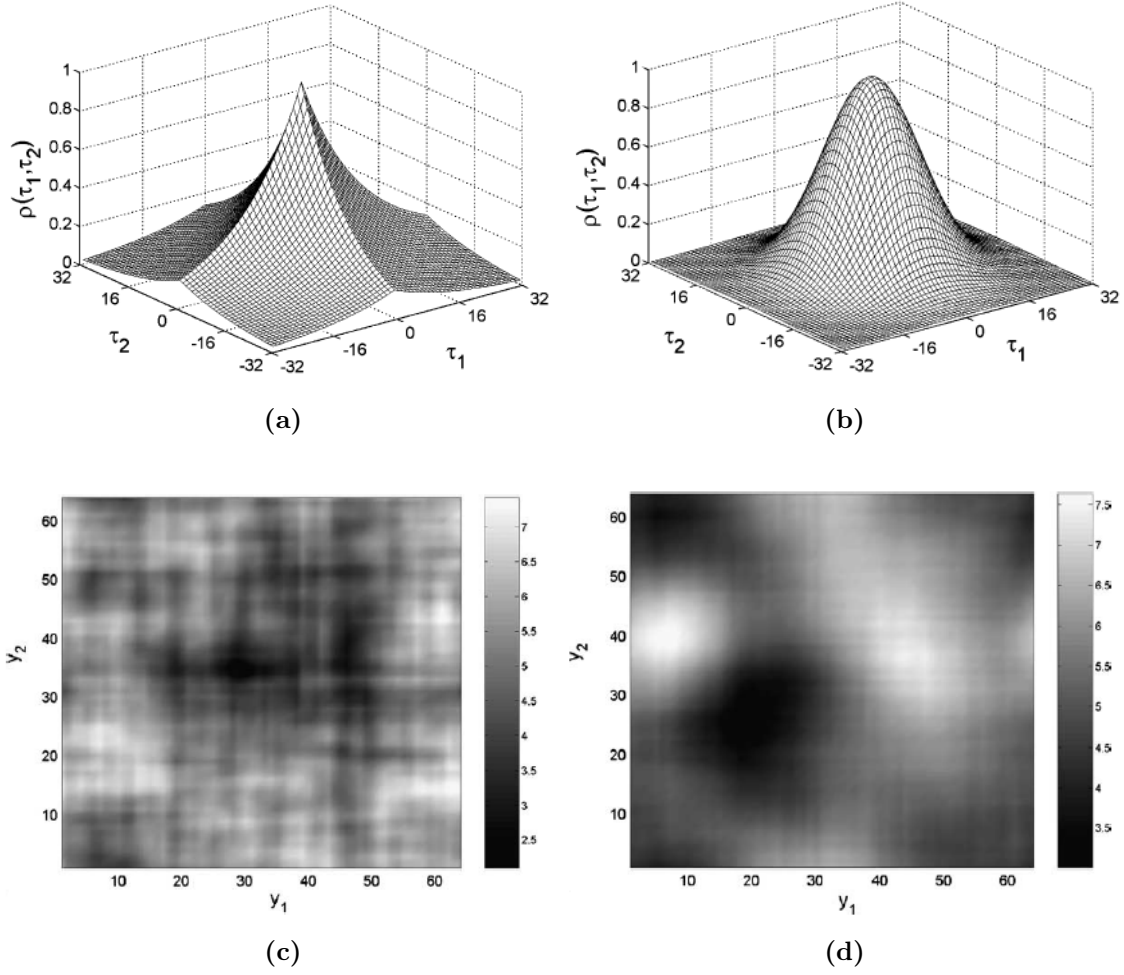


Figure 4.3: Comparison of elastic modulus KL 2D realization generated from two stationary covariance functions having different correlations lengths [220].

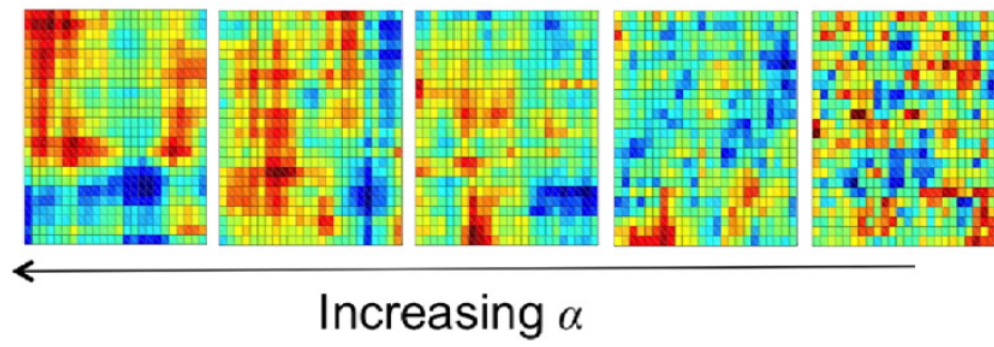


Figure 4.4: Elastic modulus KL realization comparison for increasing correlation length α [67].

4.1.3 Methods of validation

Verification of Fredholm equation (Generalized EVP) solver: To validate the accuracy of the numerical method implemented for generation of the (non)Gaussian random fields it is sufficient to validate the generalized Eigenvalue problem Galerkin solver. An attempt was made to recapture the exact analytical and numerical solutions to an accepted problem within literature. The derivation of the analytical solution is detailed in the works of [220, 82] employing the following covariance kernels since these solutions can be obtained analytically:

$$COV(\mathbf{x}^1, \mathbf{x}^2) = \exp\left(-\frac{|\mathbf{x}^1 - \mathbf{x}^2|}{16}\right) \quad (4.1)$$

where $\mathbf{x}^1$ and $\mathbf{x}^2$ are spatial separation distances.

When considering the numerical eigenvalue solutions, Figure 4.5 shows that the implemented Galerkin solver solutions were in good agreement with those derived in the literature.

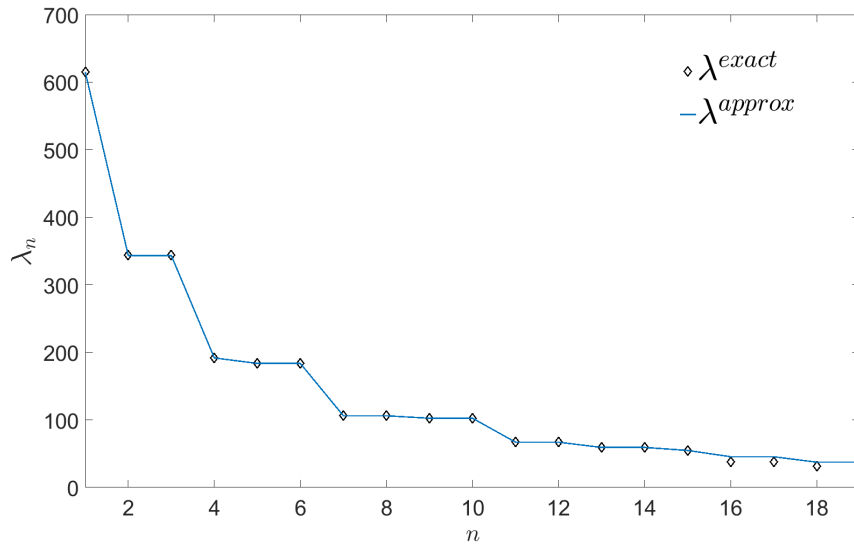


Figure 4.5: Comparison of analytic and numerical solutions corresponding to covariance kernel equation 4.1.

Figure 4.6 demonstrates qualitatively that the numerically obtained eigenfunctions are in good agreement with the analytic eigenfunction solutions in literature when the covariance kernel equation 4.1 is employed.

4.1.4 Intellectual merit

- The research within this Chapter provides a computational scheme for computing microstructure dependent, spatially correlated, and continuous scalar random field realizations utilizing the Karhunen-Loève (KL) expansion method. These realizations can be used as a non-intrusive means of defining more realistic random material properties into various formulations.
 - The scheme has no restriction on the initial discrete random field data’s probability distribution; provided that the cumulative distribution function (CDF) of the probability density function (PDF) is known for the initial discrete data. The *inverse transform method* provides a natural transformation between the initial arbitrary distribution and the Gaussian distribution needed within the KL method.
 - Discretization of the continuous random field and the generalized eigen-value problem’s eigenfunctions can be performed on a relatively fine spatial mesh which internally produce sparse finite element matrices during solution. The numerically implemented eigen problem solver utilizes sparse matrix data structures and sparse matrix eigen problem solver.

4.1.5 Research contributions

Main contributions:

- [C++ scripted.] Implemented in-house Galerkin FEM based tool to generate N independent realizations of scalar random fields utilizing Karhunen-Loève (KL) expansion. KL meshes are generated only depending on the statistics (covariance & mean) of a discrete random field.

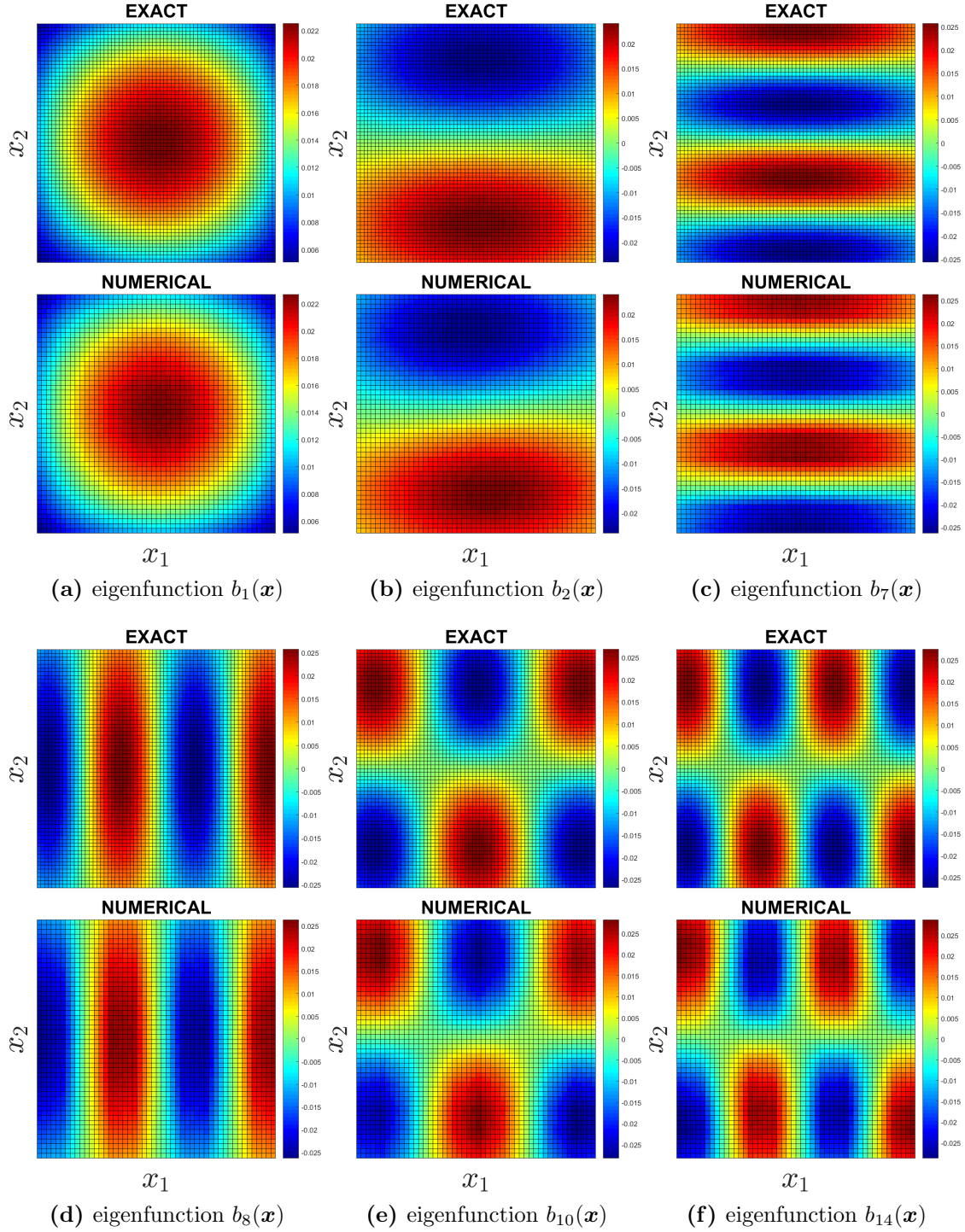


Figure 4.6: Comparison of eigenfunctions 1, 2, 7, 8, 10, and 14 analytic versus numerical solutions.

- Source of the statistics is arbitrary. Generally, the statistics utilized in generating spatially correlated random field realizations are determined in an *ad hoc* fashion and are commonly assumed to be of a Gaussian distribution; some assumptions of the initial data statistics take the form of a prescribed correlation length or an assumed probability structure whose statistical characteristics have known analytic forms. This work’s implementation of generating random fields relies on statistics that are determined from sampling and homogenization of a material microstructure; alleviating the need for assuming statistics which may lead to more phenomenological random field realizations.
- Capable of solving generalized eigenvalue problem, having sparse global matrices, without burdening computational resources. This allows for high resolution of the spatial mesh when discretizing the random field which is ultimately used as a material property input for elastic, fracture, and other general problems solved by the adaptive solver discussed in Chapter 6.
- Capable of generating non-Gaussian random field solutions utilizing the inverse transform method provided a pointwise/analytic CDF of the original field is known.

Miscellaneous contributions:

- [MATLAB scripted.] Tools for data processing and visualization of the generated 2D KL random field meshes.

Chapter 5

Formulation of random field statistics and spatial realizations

An original version of the following article was published in the conference proceedings of the 51th US Rock Mechanics/Geomechanics Symposium (ARMA 2017) [53]. The article was originally published under the title “Fracture modeling of rocks based on random field generation and simulation of inhomogeneous domains” but for more comprehensive inclusion into this dissertation, the title was revised to emphasis the concept of interest. This section aims to present an in depth discussion on the theory and implementation of the general Karhunen-Loève expansion method which is used extensively throughout this research. We also present preliminary investigations on the effects of inhomogeneous media within fracture mechanics, specifically within fluid-pressure driven crack propagation. Randomness was implicitly incorporated into the model via inhomogeneous representation of the material fracture strength. These fracture strength realizations were generated using the a kernel expansion of a covariance function. This covariance and other statistical information was derived from spatial sampling and LEFM based homogenization (utilizing sample windows sizes ranging from microscale to macroscale) of a domain with random distribution of microcracks. This works introduces the observations of size-effect; we are also introduced to the effects of sample window size and correlation length on the spatial variation of the continuous fracture strength values. The statistical quantities and their derivations were introduced in the previous chapter 2; however, this article serves as a further elaboration on these concepts. Since the aim of this section is to present the concepts related to random field generation, a more comprehensive study on the effects of spatial random homogeneity will be presented in the following chapter 4 as it relates to macroscale fracturing.

Abstract: Realistic fracture simulations in rock as a heterogeneous brittle material with significant inherent randomness, require the use of models that incorporate its inhomogeneities and statistical variability. Since brittle materials do not match ductile materials in dissipating energy in the bulk, their fracture response is highly dependent on the stochastic microscale distribution and strength of defects. The high dependence of their fracture progress on microstructural defects results in wide scatter in their ultimate strength and the so-called size effect. Our approach for incorporating randomness in rocks is based on the modeling of stochastic volume elements (SVEs). Although representative volume

elements (RVEs) are more commonly used in solid mechanics, SVEs are more appropriate for fracture analysis since they ensure that the material randomness is maintained. They still average microscale features similar to RVEs, and provide a more economical solution approach than those methods that explicitly model all microcracks in rock. To create a random field for macroscopic fracture strength field, we first generate several realizations of rock with a prescribed crack density and distribution. SVEs are then constructed with their centers at known spatial position on these random realizations. Next, by using a moving window approach, where the SVE traverses the known positions in these random realizations, we obtain first and second moments of the target random field. Point-wise probability distribution function and spatial covariance function are derived and used to generate consistent realizations of random fields based on the Karhunen-Loève (KL) method. Finally, such realizations will be used for the analysis of dynamic stimulation of a wellbore in a tight formation. A powerful and mesh adaptive spacetime discontinuous Galerkin finite element method is used for dynamic fracture simulations.

Acknowledgments: The authors gratefully acknowledge partial support for this work via the U.S. National Science Foundation (NSF), CMMI - Mechanics of Materials and Structures (MoMS) program grant number 1538332.

5.1 Introduction

Rocks, having highly random solid aggregates structure, are inhomogeneous at various scales. At microscale, heterogeneity is due to the presence of microcracks, granular microstructures which can include a large number of randomly oriented zones of potential failure in the form of grain boundaries. At macroscale, inherent homogeneity is the results of the matrix containing different rock types, and weak features such as faults and fracture networks. Rock inhomogeneities are crucial as they affect the continuum level mechanical characteristics such as strength, toughness, and elasticity properties of the material. These heterogeneities imposed by the rocks microstructure greatly influence the material peak and post-instability responses [224]. This is most evident in (quasi)brittle materials as they lack energy dissipative mechanisms to re-balance stresses induced by microscale stress concentrations. Another key

aspect of brittle fracture, related to its dependence on material microstructure, is that for the same geometry and loading condition various crack patterns, ultimate loads, and absorbed energies can be experienced [20, 45, 200, 61]. These observations emphasize the importance of including randomness in material properties of rock in its fracture analysis.

Rock fracturing studies can *explicitly* or *implicitly* incorporate heterogeneities and/or discontinuous features within material models or computational approaches. Models derived from *explicit* approaches directly consolidate defects, microcracks, and other inhomogeneities into the scheme. Studies such as lattice models contain features making them favorable candidates to explicitly model material inhomogeneities. In that respect, a lattice of elements representative of a particle network are connected with springs [188] and heterogeneity is accounted for by varying strength and size of lattice particles [131]. However, the applications of explicit schemes are at times limited to small space and time scales because of the need to directly resolve existing microstructures.

An example of an implicit model is the probabilistic Weibull model. [215, 216]. The Weibull model provides physical insight by accurately modeling size-effect (*i.e.*, the decrease of failure strength as a specimen size increases) in brittle materials. Continuum fracture models calibrated based on a material’s microstructure, such as the damage models of [208, 107, 194, 138], are other examples of implicit approaches.

Furthermore, it is possible to derive macroscopic effective constitutive quantities with a homogenization approach wherein the elemental problem is solved in a *Volume Element* (VE). There are two commonly used classes of VEs known as *Representative Volume Element* (RVE) (which also is referred to as *Representative Elementary Volume* (REV) in rock mechanics), and its counterpart *Stochastic Volume Elements* (SVEs), *cf. e.g.*, [26, 210, 190, 122]. A compilation of RVE definitions can be found in [166] but generally states that for an RVE to be valid it must: 1) be sufficiently smaller than the macroscale structure and sufficiently larger than microscale, 2) must contain a large number of micro-heterogeneities for the statistical homogeneous and ergodic properties to ensure proper representation of the macro response, and 3) have a response which is independent of the boundary condition type. When the size of a VE decreases, or the average microscopic feature size increases, the VE approaches the SVE regime which [72] deems as a more accurate

averaging scheme than RVEs. The advantages of SVEs are that they can preserve material spatial heterogeneities and model stochastic fracture response from one sample to another one with exactly the same geometry and loading. The random fields that can be realized from SVEs by means of methods such as Karhunen-Loève (KL) expansion, used in works [220, 192], can be very effective and efficient for fracture analysis of brittle and quasi brittle materials as they preserve microstructure variability, but average it to a larger and more manageable length scale.

The authors have successfully used the Weibull model in the context of a spacetime discontinuous Galerkin finite element method [12] and demonstrated that having spatial inhomogeneity in fracture strength, through using a random crack nucleation model, can greatly improve predicted dynamic fracture patterns. In the present work, we want to derive the statistics of fracture strength field at the continuum macroscale based on the statistics of cracks in rock at microscale. Finally, a tight reservoir with a generated stochastic fracture random field is simulated in section 5.3.

5.2 Formulation

In this section the formulation is outlined for a scheme which allows the derivation of an analytical representation of correlated physics fields based on a material's microstructure, specifically for this work microcrack distribution in rocks. Section one presents a more formal definition of an SVE and how it is characterized. Section two presents the concept of the (non)Gaussian Karhunen-Loève expansion, the probability assumptions that accompany its derivation, and brief description on how it is solved numerically with finite element methods. Section three discusses the spatial sampling algorithm and spatial grid structure used to determine Cumulative Distribution Function (CDF) of a non-Gaussian random field and covariance of a Gaussian random field needed for implementation into the KL expansion. Section four introduces the equations used to determine fracture strength which are extrapolated by employing the spatial sampling method. Finally, section five presents a dynamic stimulation of a wellbore where rock fracture strength is realized by the aforementioned stochastic approach.

5.2.1 Random Microstructure Characterization

Practically, it is not possible to fully determine the real microstructure of rock at every point in a large region such as a reservoir. These properties are supposed to be subsequently used for mechanical and fracture analysis. In lieu of using a deterministic approach where properties are provided at every point, the characterization of rock microstructure and obtaining of effective material properties are handled by statistical averaging in a continuum mechanics viewpoint, specifically by using Stochastic Volume Elements (SVE). To elaborate on the concept of SVEs, let us define the macroscale domain length L_M , microscale heterogeneity average length l_m and the SVE characteristic size L_{VE} seen in figure 5.1.

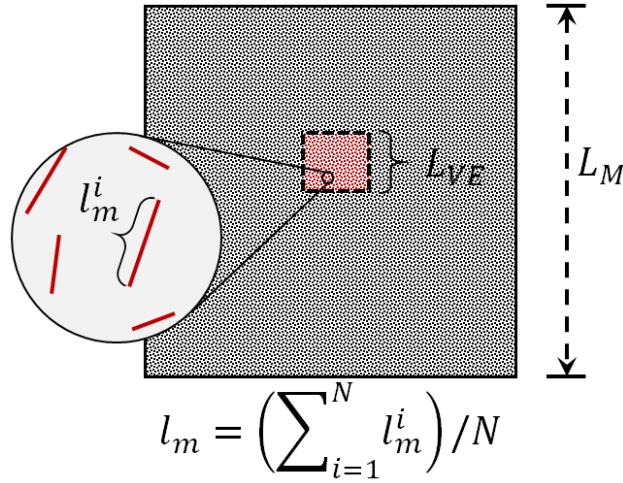


Figure 5.1: Macro- to Micro-scale length scales relevant to SVE homogenization.

The size of the SVE is affected by the characteristic length scale of the domain and the average length of microscale fractures. Assuming that the SVE is much smaller than the domain of interest ($L_{VE} \ll L_M$), the relative size of SVE to the contained microstructures is characterized through the ratio $\beta = L_{VE}/l_m$. As $\beta \rightarrow \infty$ the SVE approaches the RVE limit and randomness is lost given RVEs homogenize material properties and yield constant values from point to point for a macroscopically homogeneous material. A more detailed discussion on the relative sizes of an SVE to the domain and characteristic microstructure sizes is given in [72]; as discussed therein, in many cases of homogenization it is assumed that the RVE limit is reached (without verifying this condition in many cases). Roughly speaking and in practice, for RVEs β is often greater than 10 to 100, with higher values required when

microstructural features are more complex, distinct from the bulk, or at higher densities. As discussed in the introduction, we specifically prefer to use SVEs to maintain spatial variability within one realization and sample to sample variations across realizations. For SVEs, the size L_{VE} is chosen below the RVE limit to preserve randomness while observing the caveats that: 1) L_{VE} is larger than the microstructure length scale l_m and much smaller than the macroscopic length scale L_M , and 2) the SVE must contain a sufficient number of micro-heterogeneities to provide a comprehensive representation of the domain.

5.2.2 Karhunen-Loève (KL) Expansion

For a given domain $\bar{D}$ at an arbitrary location $\mathbf{x}$ a spatially-dependent correlated random field value $\eta(\mathbf{x})$ is to be determined. The value of this random field is derived based on a random variable ω which is of a probability structure known *a priori* (*i.e.*, $\eta = \eta(\mathbf{x}, \omega)$). In practice, it is not common to have an analytical representation of the random field or impossible to know its value at every discrete point within the domain but rather it is more likely that the values of the random field's expected value $\mathbb{E}(\eta(\mathbf{x})) = \mu_\eta(\mathbf{x})$ and covariance $COV_\eta(\mathbf{x}^1, \mathbf{x}^2)$ are known at a finite number of locations within the domain. Having these quantities (at all points), it is possible to derive a simple formula which approximates the mean and covariance of the known random variable distribution; a common method for producing such a formula is the Karhunen-Loève (KL) expansion of the random field $\eta = \eta(\mathbf{x}, \omega)$. The truncated KL expansion of the random field yields the following representation of the field,

$$\eta(\mathbf{x}, \omega) = \mu_\eta(\mathbf{x}) + \sum_{i=1}^{n_{KL}} \sqrt{\lambda_i} b_i(\mathbf{x}) Y_i(\omega)$$

where $\{\lambda_i, b_i(\mathbf{x})\}_{i=1}^{n_{KL}}$ are eigen-pairs determined from the covariance of the random field and $Y_i(\omega)$ are centered, uncorrelated random variables¹ which derive the probability distribution of the random field. Since the values of Y_i s are independent if and only if they have spherical Gaussian (normal) distribution, in practice KL method is used for fields with point-wise Gaussian distribution. This, enables independent generation of random variables Y_i . Thus, we need to transfer a general random field to one with point-wise Gaussian distribution before

¹ $\mathbb{E}(Y_i(\omega)) = 0$, and $\mathbb{E}(Y_i(\omega)Y_j(\omega)) = 0$

using the KL method. This point is further elaborated when discussing (5.2) below. Thus, we assume that the KL expansion is carried out for a Gaussian random field $\eta(\mathbf{x}, \omega) \sim N(\mu_\eta, \sigma_\eta)$ (where σ_η is random field standard deviation),

$$\eta(\mathbf{x}, \omega) = \mu_\eta(\mathbf{x}) + \sum_{i=1}^{n_{KL}} \sqrt{\lambda_i} b_i(\mathbf{x}) y_i. \quad (5.1)$$

The aforementioned eigen-pairs are obtained by solving the generalized eigenvalue problem (EVP),

$$\int_{\bar{D}} COV_\eta(\mathbf{x}^1, \mathbf{x}^2) b(\mathbf{x}^2) d\mathbf{x}^2 = \lambda b(\mathbf{x}^1).$$

It is beneficial to note that due to the positive and symmetric nature of the covariance the eigenfunctions $b_i(\mathbf{x})$ are real and orthogonal ². It is also important to note that all the eigenvalues λ_i are non-negative real values. The generalized eigenvalue problem is solved using a conventional Galerkin finite element method (CFEM) which allows the eigenfunction to be discretized over the spatial domain. The integral form of the EVP reduces to a generalized algebraic eigenvalue problem [82],

$$\mathbf{C}\mathbf{D} = \mathbf{\Lambda}\mathbf{B}\mathbf{D}.$$

The N -dimension symmetric positive definite matrices $\mathbf{C}$, $\mathbf{B}$, and The N -dimension matrices $\mathbf{\Lambda}$ and $\mathbf{D}$ are defined as,

$$\begin{aligned} \mathbf{C}_{ij} &= COV(\mathbf{x}^i, \mathbf{x}^j), \\ \mathbf{B}_{ij} &= \int_{\bar{D}} h_i(\mathbf{x}) h_j(\mathbf{x}) d\mathbf{x}, \\ \mathbf{\Lambda}_{ij} &= \delta_{ij} \lambda_i, \\ \mathbf{D}_{ij} &= d_i^{(j)}, \end{aligned}$$

where $\mathbf{x}^i$ and $\mathbf{x}^j$ are i -th and j -th finite element nodal degrees of freedom respectively for which covariance matrix term $\mathbf{C}_{ij}$ is evaluated. The above algebraic equation is solved for

² $\int_{\bar{D}} b_i(\mathbf{x}) b_j(\mathbf{x}) d\mathbf{x} = \delta_{ij}$

$\mathbf{\Lambda}$ and $\mathbf{D}$ (where the columns of $\mathbf{D}$ are the eigenvectors at each node of a prescribed FEM mesh) with $h_i(\mathbf{x})$ being the complete set of finite element shape functions.

In practice, the random field being approximated may in fact not be Gaussian; however, we can map a non-Gaussian $\xi(\mathbf{x}, \omega)$ to a Gaussian random field $\eta(\mathbf{x}, \omega)$ by using the CDF-inverse relation,

$$\eta(\mathbf{x}, \omega) = F_\eta^{-1}(F_\xi(\xi(\mathbf{x}, \omega))), \quad (5.2)$$

where F_ξ and F_η are the Cumulative Density Functions (CDF) of the non-Gaussian and Gaussian random fields, respectively. Subsequently, the KL method is used to generate random field realizations for the Gaussian field $\eta(\mathbf{x}, \omega)$ given that in (5.1) random variables y_i are independent, making their random generation practical. Finally, we can transfer the random field generated for the Gaussian field $\eta(\mathbf{x}, \omega)$ back to $\xi(\mathbf{x}, \omega)$ using the inverse of (5.2), *i.e.*, $\xi(\mathbf{x}, \omega) = F_\xi^{-1}(F_\eta(\eta(\mathbf{x}, \omega)))$.

5.2.3 Statistics of Random Microstructure: Spatial Sampling

Since the above KL expansion derivation requires the knowledge of covariance function $COV_\eta(\mathbf{x}^1, \mathbf{x}^2)$ and mean value of the random field $\eta(\mathbf{x}, \omega)$, we employ a spatial sampling method to extrapolate values for both field quantities utilizing stochastic volume elements (SVEs). Representative Volume Elements (RVEs) are frequently used to homogenized mechanical properties of materials; however, since for quasi-brittle materials spatial inhomogeneity, *i.e.*, microstructural variations, plays an important role in their fracture response, we employ SVEs to homogenize rock properties.

To statistically characterize a heterogeneous material we consider a finite set $D = \{\bar{D}_n; n \in [1, 2, \dots, N]\}$ of N realizations $\bar{D}_n$. Each realization has a distribution of microscale fractures based on a prescribed probability structure and crack density. All realization domains are bounded by a boundary/surface Γ_D (*i.e.*, $\Gamma_D = \Gamma_{\bar{D}_1}, \dots, \Gamma_{\bar{D}_N}$) and use the same (un)structured sampling grid of K points $\mathbf{x}^k = (x_1^k, \dots, x_M^k); k \in [1, K]$. The sampling points define the center points of SVEs considered. This concept is shown in figure 5.2 for a 2 dimensional domain.

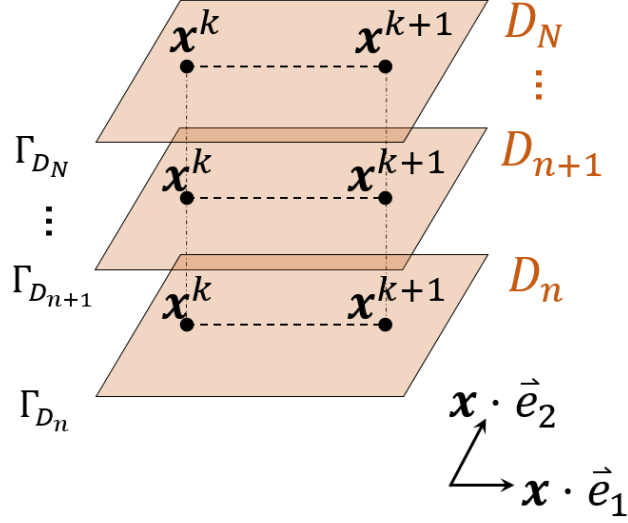


Figure 5.2: Spatial positions of sampled points inside each N realizations.

By forming SVEs centered at the grid points, a statistically averaged value of the material property considered is computed for each of these points based on its corresponding values across all N realizations. To have a better characterization of covariance function, we use a nonuniform sampling scheme where more SVEs are sampled close to the SVE in the center of the domain; that is, the incremental distance between two successive points is not uniform wherein it increases as the points are farther away from the domain center and closer to the boundary $\Gamma_{\bar{D}}$; this is seen in figure 5.3. This higher resolution about the domain center enables computing the covariance function more accurately, given that the values of the function tend to zero quickly as the distance of the two points increases.

By having the considered material property computed at all SVEs, *i.e.*, all sampled points across all SVEs, we can compute various statistical quantities for the given homogenized property, including its point-wise probability density function (PDF) and two-point covariance function. Let $\Theta(^n\mathbf{x}^k)$ be a property value extrapolated by an SVE within realization n at grid point k . The covariance function between points $\mathbf{x}^p$ and $\mathbf{x}^q$ is computed as,

$$\begin{aligned}
& COV(\Theta(\mathbf{x}^p), \Theta(\mathbf{x}^q)) \\
&= \mathbb{E}(\Theta(\mathbf{x}^p)\Theta(\mathbf{x}^q)) - \mathbb{E}(\Theta(\mathbf{x}^p))\mathbb{E}(\Theta(\mathbf{x}^q)) \\
&= \sum_{n=1}^N \frac{(\Theta(\mathbf{x}_n^p) - \mathbb{E}(\Theta(\mathbf{x}^p)))(\Theta(\mathbf{x}_n^q) - \mathbb{E}(\Theta(\mathbf{x}^q)))}{N},
\end{aligned} \tag{5.3}$$

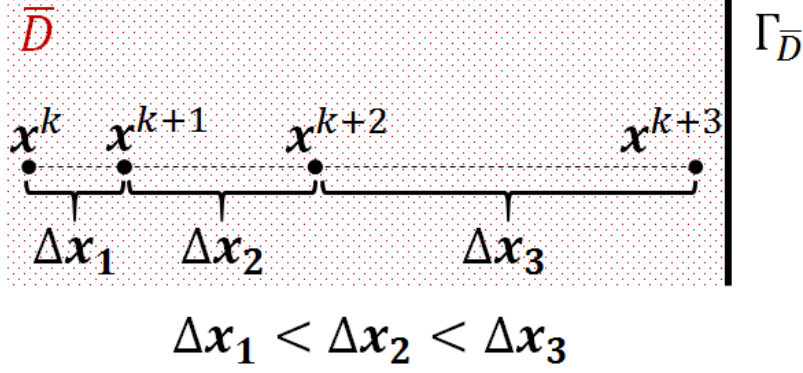


Figure 5.3: A nonuniform grid is used for better characterization of covariance function near zero.

where $p, q \in [1, \dots, K]$. Considering that the values of the cumulative distribution function (CDF) $F(\theta)$ and probability density function (PDF) $P(\theta)$ are mutually dependent through the following relationship, it is sufficient to define only one of the two,

$$F(z) = \int_{-\infty}^z P(\chi) d\chi \quad (5.4a)$$

$$P(z) = \frac{\partial F(z)}{\partial z} \quad (5.4b)$$

Having a data set of $n_t = KN$ discrete values $\Theta(\mathbf{x}_n^p)$ ($1 \leq p \leq K, 1 \leq n \leq N$) with minimum Θ_{min}^s and maximum Θ_{max}^s values, the empirical cumulative distribution function is given as,

$$\forall \theta \quad \Theta_{min}^s \leq \theta \leq \Theta_{max}^s : \quad \tilde{F}(\theta) = \frac{1}{n_t} \sum_{i=1}^{n_t} \mathbf{1}_{\chi_i \leq \theta},$$

where $\mathbf{1}_A$ is the indicator of event A .

5.2.4 Computation of fracture strength for an SVE

In this section we describe how a fracture strength value is computed and assigned to an SVE. Figure 5.4 shows a sample SVE in domain $\bar{D}$. Beside the cracks that are inside the SVE, those that intersect its boundaries are also considered in deriving an effective strength for the SVE. The fracture strength is computed by finding the minimum unidirectional tensile stress, along all directions in $[0, 2\pi]$, such that at least for one of the crack tips in the SVE,

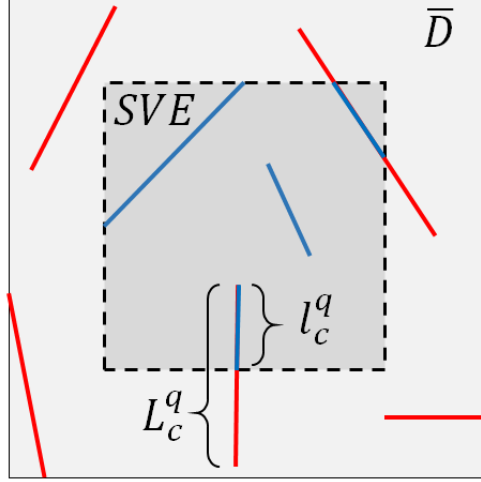


Figure 5.4: Cracks considered for computation of effective strength for an SVE: (blue line: considered crack segments internal to SVE, red line: neglected crack segments external to SVE)

$K = K_c$ where K is the stress intensity factor (SIF) at the crack tip and K_c is the fracture toughness of rock.

Underlying to this definition of fracture strength is that the propagation of microcracks is governed by linear elastic fracture mechanics (LEFM) theory and that upon the propagation of the first microcrack the SVE basically can be considered as completely failed. The second assumption is justifiable as many results in the literature, see for example [155], demonstrate that for quasi-brittle RVEs and SVEs with microcracks and microdefects the load at which material response starts to deviate from linear elasticity is very close to the volume element's failure strength. This is due to the lack of considerable plastic deformation or other bulk energy dissipating mechanisms. In the context of our model for rock, wherein microcracks are randomly distributed, the point of major departure from linear elasticity is when the SIF for the most critical crack in the SVE reaches the fracture toughness. Finally, instead of doing a full FE analysis, we assume that the SIF of each crack can be approximated by that of a crack in an infinite domain. Clearly, this crude approximation ignores crack interactions, but is expected to provide relatively accurate representation for the macroscopic fracture strength field.

Let L_c and l_c be the full length and length of the q th microcrack within the SVE, respectively. The critical stress for this specific q th microcrack within the SVE is given

by the equation

$$\bar{s}^q = \left(\frac{L_c^q}{l_c^q} \right)^\alpha \frac{K_c}{\sqrt{\pi L_c^q/2}},$$

where as mentioned K_c is the fracture toughness and α is a constant value coefficient. If $\alpha = 0$ we have $\bar{s}^q = K_c/\sqrt{\pi L_c^q/2}$ which is the critical tensile stress for a crack of length L^q in an infinite domain with fracture toughness K_c . On the other hand, if $\alpha = \frac{1}{2}$ we obtain $\bar{s}^q = K_c/\sqrt{\pi l_c^q/2}$, *i.e.*, critical tensile stress for a crack of length l_c^q . Obviously, for cracks that are inside the domain, the value of α is irrelevant. However for those that intersect it, from the discussion above a value $\alpha = \frac{1}{2}$ only considers the part of the crack that is inside the SVE and $\alpha = 0$ models it as a full crack in the SVE. Given that the critical stress for such crack is clearly larger than the latter and should be considered lower than the former in deriving an effective critical stress for this crack in relation to the given SVE (considering that only a small fraction of the crack can be inside the SVE), we propose to use the intermediate value of $\alpha = \frac{1}{4}$. As discussed in section 5.4 with more physics-based approached we can obtain more realistic values for $\bar{s}^q$.

Once we compute critical stresses $\bar{s}^q$ for all cracks $q \in Q$ inside or intersecting a given SVE, the strength of the SVE $\bar{s}$ is defined as,

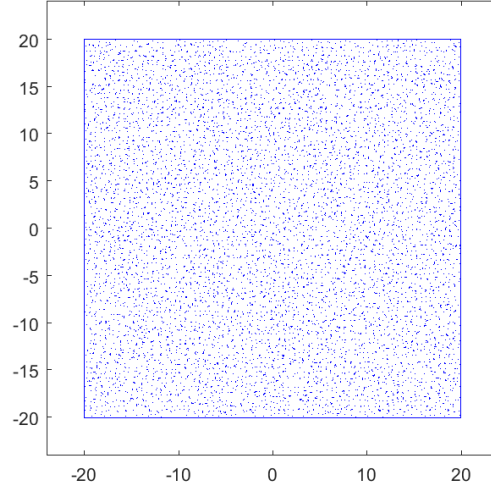
$$\bar{s} = \min_{q \in Q} \{\bar{s}^q\}.$$

With this definition, a fracture strength is assigned to all SVEs, *i.e.*, for all spatial positions and for all random realizations. These values are in turn used to compute PDF and covariance function from (5.4b) and (5.3), respectively. Finally, the KL method from section 5.2.2 is used to generate random fields whose statistics are consistent with the underlying microstructure (in this case rock with embedded microcracks).

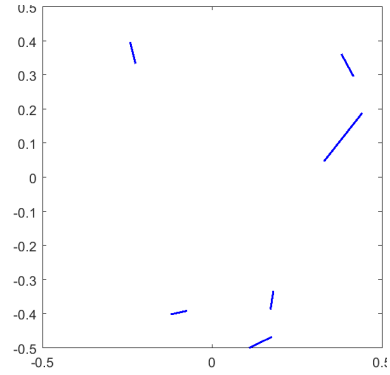
5.2.5 Spacetime discontinuous Galerkin method

We use an h -adaptive spacetime discontinuous Galerkin (SDG) finite element method [9, 10] for our analyses of dynamic stimulation of a wellbore. This method uses basis functions which are discontinuous across all element boundaries. The SDG method directly discretizes

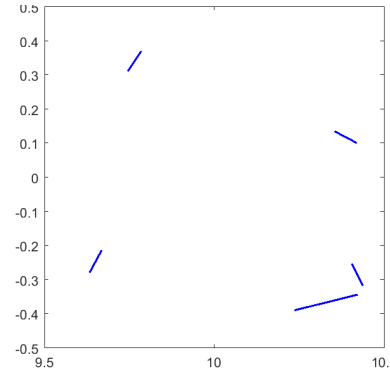
spacetime using nonuniform grids that satisfy a special causality constraint [3]. This is contrary to conventional time marching schemes used for advancing the solution in time. These features yield unique properties such as local and asynchronous solution scheme, arbitrarily high and local temporal order of accuracy, and linear solution scaling with number of elements. Utilizing advanced adaptive operations in spacetime, and the local and asynchronous solution features of the SDG method, we can very accurately and efficiently capture complex fracture patterns by a *crack tracking* adaptive scheme [1, 158]. The solution is mesh independent and accommodates crack propagation in any desired direction, a feature similar to the popular XFEM and GFEM methods, but removes the need to enrich element basis functions. All these features make the SDG method ideal for dynamic rock fracture simulations reported in section 5.3.4.



(a) Example of realization $\bar{D}$ with random microstructure architecture.



(b) SVE sample from figure 5.5a centered at $\mathbf{x} = (0, 0)$.



(c) SVE sample from figure 5.5a centered at $\mathbf{x} = (120, 0)$.

Figure 5.5: A 40×40 domain and two sampled SVEs.

5.3 Numerical Results

The spatial domain $\bar{D}$ used for generating the following statistical data is a simple rectangular domain centered at the Cartesian position $\mathbf{x}_{\text{center}} = (0, 0)$ and spanning 40 meters in both $\vec{e}_1$ and $\vec{e}_2$ directions (*i.e.*, $\mathbf{x} \in \bar{D} = [-20, 20] \times [-20, 20]$). An example of a realization containing the above spatial specifications is seen in figure 5.5a.

To generate rock domain realizations with microcracks, we need to assume a certain statistics for the microcracks; for the numerical results reported herein, we assume that the microcrack length follow a Weibull distribution [215, 216] and its angle is uniformly distributed between $[0, 2\pi]$ (that is there is no angular bias, as for example for rocks with bedding planes). Furthermore, the average and standard deviation of microcrack length are 20cm and 3.5cm, respectively. Finally, we use a take-and-place algorithm to distribute generated cracks in a domain of edge size $L_{\bar{D}} = 40\text{m}$. A sample realization is shown in figure 5.5a. It can clearly be seen that the average length lengths are smaller than the SVE size and the SVE size is much smaller than the domain size, conditions that were discussed in section 5.2.3. As discussed in section 5.2.3, the center points of sampled SVEs form a nonuniform grid. Two sample SVEs generated from the domain in figure 5.5a are shown in figures 5.5b and 5.5c.

5.3.1 The effect of the SVE size on random field statistics

The size of the SVE directly influences the statistics of the random field characterized. To study the relation between the SVE size and the fracture strength random field statistics, square SVEs with edge sizes of 1, 2, and 4 were considered. The PDFs of the fracture strength field in figure 5.6 are accordingly labeled by $\text{SVE}1 \times 1$, $\text{SVE}2 \times 2$, and $\text{SVE}4 \times 4$. Since the distribution of the fracture strength is assumed to have log-normal structure, there is no advantage of determining empirical PDF data as opposed to directly utilizing analytic forms of the log-normal PDF; determination of the empirical point-wise PDF using this works algorithms is done for consistency to ensure that they can be captured accurately. As the SVE size becomes larger and tends to the RVE size limit, the peak of the PDF curve

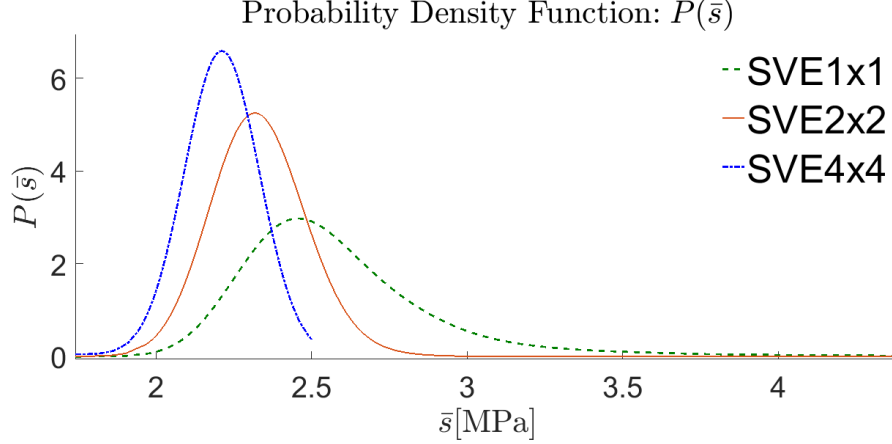


Figure 5.6: The effect of the SVE size on random fracture strength field statistics.

shifts to the left, that is a weaker material is represented. This is the well-known size effect for (quasi-)brittle materials; as the size of the domain increases there is a larger likelihood that a more critical crack or defect exists in it. That is why larger samples tend to have lower fracture strength. In fact, domain size calibrated Weibull model and many other stochastic models in the literature attempt to represent this phenomenon.

Another observation is that as the window size decreases, the sampled fracture strength values are more likely to have wider variations. The reason is that at small sizes, the SVE may land in a region with long crack(s) or a short one, thus yielding a low or a high fracture strength, respectively. This is demonstrated by higher standard deviations for smaller SVE window sizes in figure 5.6. On the contrary, as the SVE window size tends to the RVE limit size, the PDF tends to a Dirac delta function centered at the constant statistically averaged value. In this case, no matter where the volume element is sampled and which realization is considered, the crack ensemble represents macroscopically homogeneous value.³ Clearly, the sizes considered herein are intentionally small (*i.e.*, the volume elements are SVEs) to capture rock strength variability. The following numerical results assume spatial sampling with an SVE length of one (*i.e.*, $\text{SVE}1m \times 1m$) as this size offered greater variability in fracture strength values but is large enough to not violate the requirements of the SVE containing a sufficient number of heterogeneities.

³For the RVE limit and the independence of fracture strength from the volume element center point, we are assuming a limiting strength exists as the volume element size tends to infinity and that rock is macroscopically homogeneous for fracture strength. Obviously, these assumptions can be relaxed and are not related to the SVE homogenization approach presented in this manuscript.

5.3.2 KL random fields

The KL random field meshes were generated based on two assumptions,

1. The material modeled was isotropic with a rotationally invariant scalar fracture strength, and the covariance function depending only on distance between two arbitrary points.
2. The sampled fracture strength values have log-normal probability distribution and covariance is calculated for strength values transformed to a standard normal distribution.

Assumption two means that instead of using CDF inverse approach, we used a log normal best fit for the PDFs in figure 5.6. Given the good level of fit we observed, this assumption is well-justified. Moreover, the covariance function for fracture strength, cast in the standard normal form (*cf.* section 5.2.2), is interpolated by the exponentially decaying function,

$$COV(\bar{s}(\mathbf{x}^1), \bar{s}(\mathbf{x}^2)) = e^{-\left(\frac{|\mathbf{x}^1 - \mathbf{x}^2|}{d_c}\right)^2},$$

where d_c is a characteristic correlation length scale implied by the form of the function.⁴ Again, there was no hindrance in using the actual point-wise covariance function obtained by (5.3). However, the very good fit between the function form above, with $d_c \approx 0.386$, and the actual discrete covariance function was the rationale in using the analytical form for the function, which is shown in figure 5.7.

Solving the algebraic generalized eigenvalue problem with a Galerkin finite element method, the values for eigenvalues λ_n and eigenfunctions $b_n(\mathbf{x})$ were determined. The continuous and smoothly decreasing eigenvalues can be seen in figure 5.8.

For brevity only the corresponding eigenfunctions for $n = 1, 2, 4$, and 21 are shown in figure 5.9.

⁴Covariance function takes the value of one at zero relative distance, *i.e.*, $COV(\bar{s}(\mathbf{x}^1), \bar{s}(\mathbf{x}^1)) = 1$, because fracture strength field is first mapped to a standard normal distribution which has a point-wise covariance value of unity.

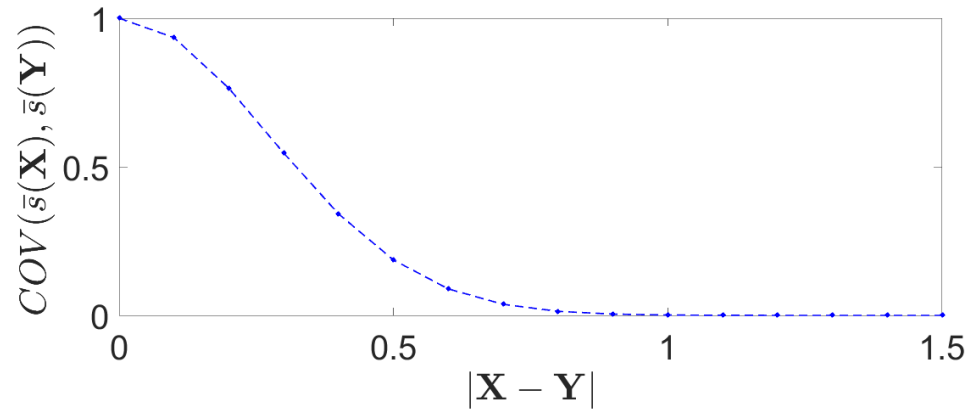


Figure 5.7: One-dimensional covariance function based on $SVE1 \times 1$ results.

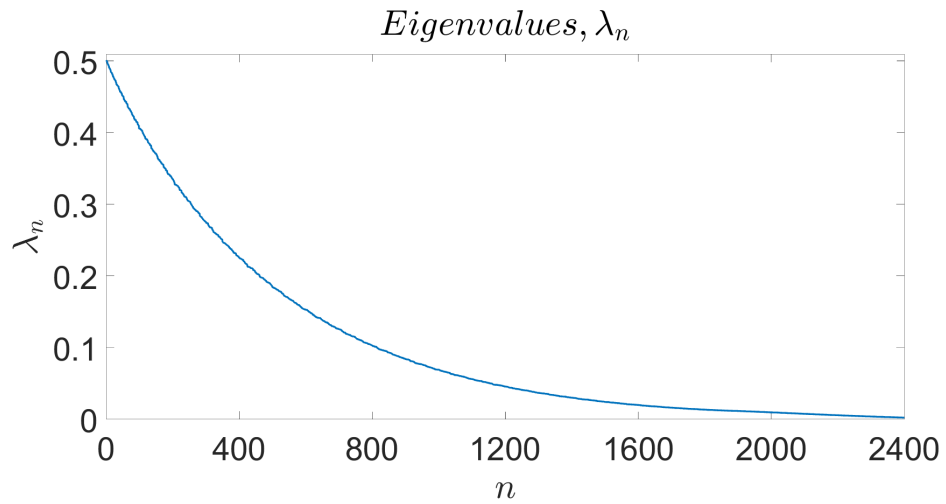


Figure 5.8: Eigenvalues λ_n for $COV(\bar{s}(\mathbf{x}^1), \bar{s}(\mathbf{x}^2)) \approx e^{-((|\mathbf{x}^1 - \mathbf{x}^2|)/0.386)^2}$, corresponding to $SVE1 \times 1$ results.

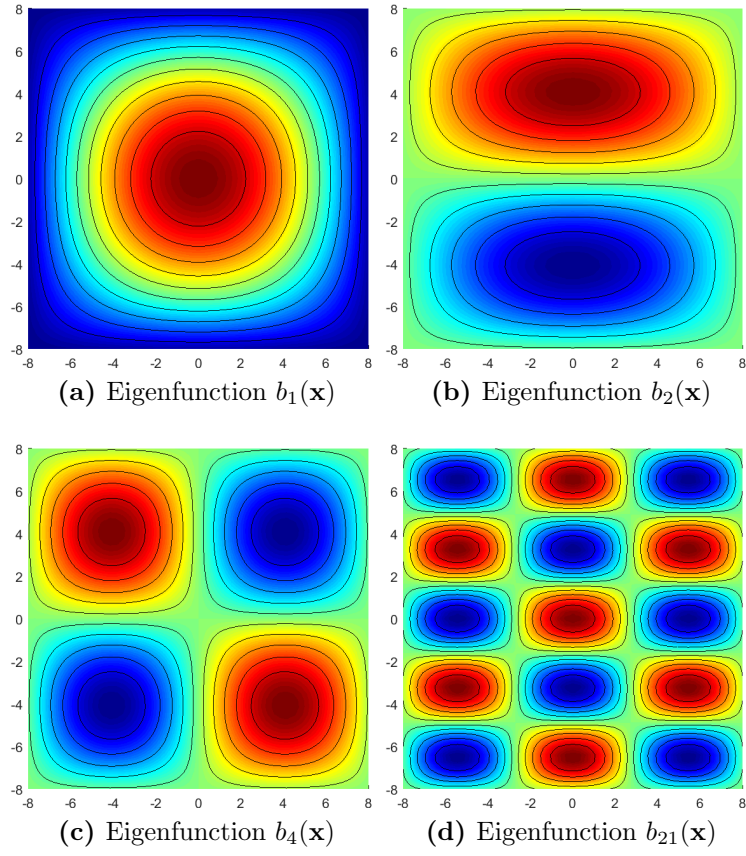


Figure 5.9: Eigenfunctions for $n = 1, 2, 4$, and 21 corresponding to eigenvalues in figure 5.8.

5.3.3 Discrete grids for fracture strength and FEM solution

A key feature of the random field discretization, using the Karhunen-Loève (KL) expansion method, is that the discrete mesh for fracture strength can be realized independent of the solid mechanics finite element mesh. Accordingly, finite element method discretization and mesh adaptive operations, *e.g.*, refinement and coarsening in spacetime [10, 158], can be performed without having to re-evaluate random fields which otherwise could lead to inaccurate and inconsistent random field values. For fracture simulations in section 5.3.4 a $16\text{m} \times 16\text{m}$ domain is considered. Accordingly, a structured 2D mesh of dimensions $[-8, 8] \times [-8, 8]$ is used for KL expansion method. For this grid, 2D quadrilateral elements (100×100 elements) of equal element size are used for solving the eigenvalue problem and generating random field realizations. The KL discrete mesh is shown in figure 5.10.

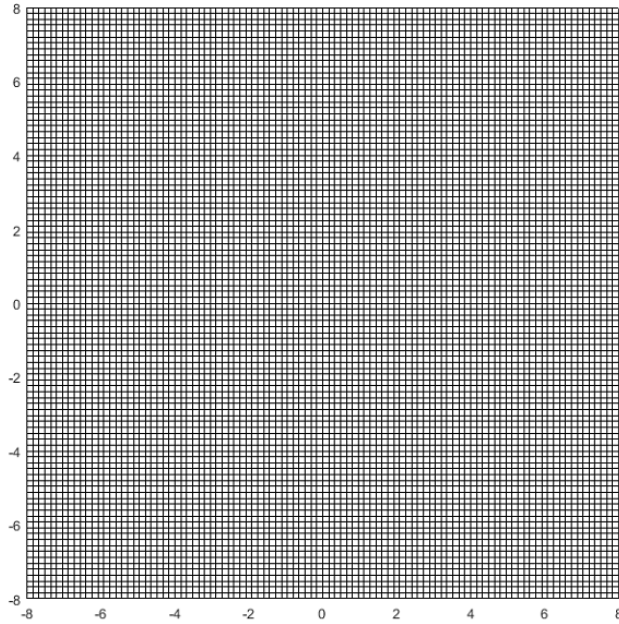


Figure 5.10: Structured spatial mesh for discretization of KL eigenvalue problem and random field realizations.

As mentioned in section 5.2.3 it is possible to transform a Gaussian random field $\eta(\mathbf{x})$ to a non-Gaussian $\xi(\mathbf{x})$ knowing the cumulative distribution function of both reference and target field distribution. With the assumption that the original sampled fracture strength

has a log normal distribution this transformation simplifies to the form,

$$\xi(\mathbf{x}) = e^{\mu_\eta + (\eta(\mathbf{x})\sigma_\eta)},$$

where μ_η and σ_η are the mean and standard deviation of the Gaussian random field which in this case can be determined from the known mean μ_ξ and standard deviation σ_ξ of the log-normal field by the following equation,

$$\sigma_\eta = \sqrt{\ln \left(1 + \frac{\sigma_\xi^2}{\mu_\xi^2} \right)}.$$

$$\mu_\eta = \ln \left(\frac{\mu_\xi}{\sqrt{1 + \frac{\sigma_\xi^2}{\mu_\xi^2}}} \right).$$

The effective non-Gaussian random field $\xi_{eff}(\mathbf{x}) = \bar{s}(\mathbf{x})$ that is used in rock fracture simulations is $\bar{s}(\mathbf{x}) = \bar{s}_{min} + \xi(\mathbf{x})$ where $\bar{s}_{min}$ is the minimum value obtained during the SVE sampling algorithm. Figure 5.11a is a visualization of the random field realization number one for correlation length $d_c \approx 0.386\text{m}$. This random field for fracture strength is used for the reference dynamic rock fracture simulation in section 5.3.4.

Before presenting dynamic fracture results, the effect of covariance function correlation length d_c on the KL random field solution is discussed. Figure 5.11 depicts random field solutions for correlation length scales $d_c \approx 0.386\text{m}$, and $d_c = 0.5\text{m}, 1.0\text{m}, 2.0\text{m}$. As the correlation lengths tend to zero there is a faster decline in the correlation of values between two points as the points become farther apart relative to the given correlation length scale d_c . The correlation decreases result in high variability of random field values within an arbitrarily small area. Smaller correlation lengths could potentially be obtained from sampling of a rock formation with higher variability in the location and strength of defects and using smaller SVE window sizes.

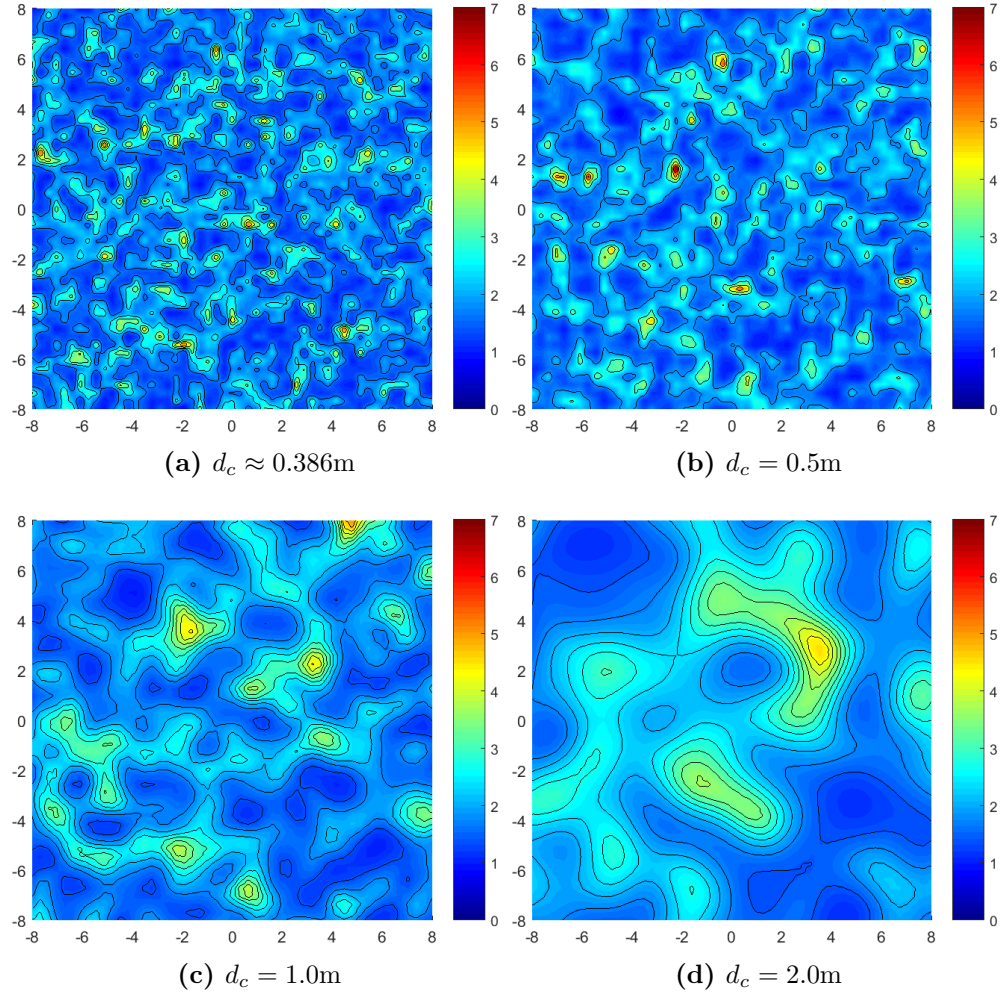


Figure 5.11: The first realization of KL-generated grids for fracture strength of different correlation lengths, $d_c \approx 0.386\text{m}$ and $d_c = 0.5\text{m}, 1.0\text{m}, 2.0\text{m}$.

5.3.4 Dynamic simulation of a wellbore with random fracture strength

Herein, we demonstrate the use of generated random fracture fields for the analyses of dynamic simulation of a wellbore in a tight reservoir. We choose a hybrid propellant method where loading is applied at highly dynamic rates [101, 159], but similar to hydraulic fracturing the pressure is applied through perforations on the sides of the wellbore. Figure 5.12 shows the set-up of the problem where a circular wellbore, subjected to confinement pressure $\sigma_h = \sigma_H = 2.425$ MPa, is located in the center of a $16\text{m} \times 16\text{m}$ rectangular domain. The wellbore is perforated at four distinct angular locations, *i.e.*, 0 rad, $\pi/2$ rad, π rad, and $3\pi/2$ rad, which upon loading promotes propagation in those directions. The dynamic pressure load, applied on the perforation surfaces, ramps up from ambient pressure to a maximum value of 23.0MPa in 10 ms. The bulk material properties are: Young's Modulus $E = 20$ GPa, mass density $\rho = 2500$ kg/m³, and Poisson's ratio $\nu = 0.20$.

The values of fracture strength $\bar{s}(\mathbf{x})$ are extracted from the independent KL random field solution discretization. The fracture strength equation parameters used in the SVE sampling algorithm are fracture toughness $K_c = 1.13\text{MPa}\sqrt{m}$ and coefficient $\alpha = \frac{1}{4}$. For 1×1 SVE sampling size, this resulted in mean value, standard deviation, and minimum value of fracture strength equal to $\mathbb{E}(\bar{s}) = 2.2$ MPa and $\sigma_{\bar{s}} = 455$ kPa, and $\bar{s}_{\min} = 1.34$ MPa, respectively.

Figure 5.13 shows a sequence of visualization of the problem with SVE 1×1 fracture strength random field values. The first realization shown in fig 5.11a is used for this simulation. Figures 5.13a and 5.13b show stages right before and after the main cracks bifurcate, respectively. In figure 5.13c, cracks start to bifurcate and induce microcracking more frequently because the cracks are accelerating and the applied pressure load on crack surfaces is still ramping up. Finally, in figure 5.13d the existence of regions of high kinetic and strain energy densities, mapped to height and color fields respectively, corresponds to a highly transient crack propagation regime. Crack path oscillation, microcracking, and crack bifurcation are all mechanisms in which quasi-brittle materials such as rocks dissipate high input energy power.

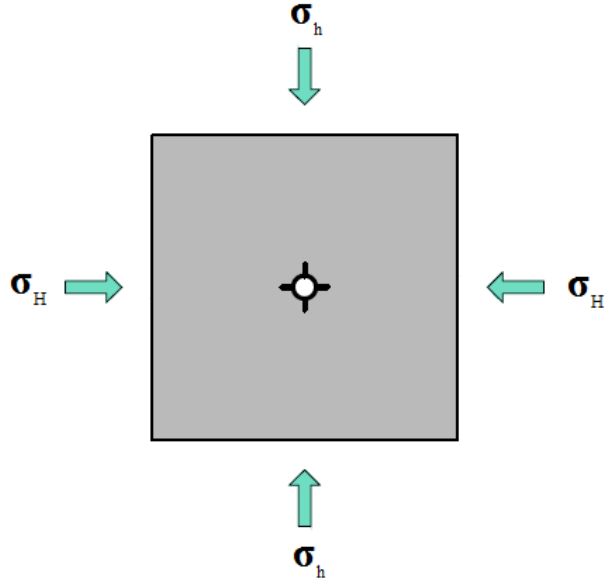


Figure 5.12: Problem sketch for dynamic stimulation of a wellbore.

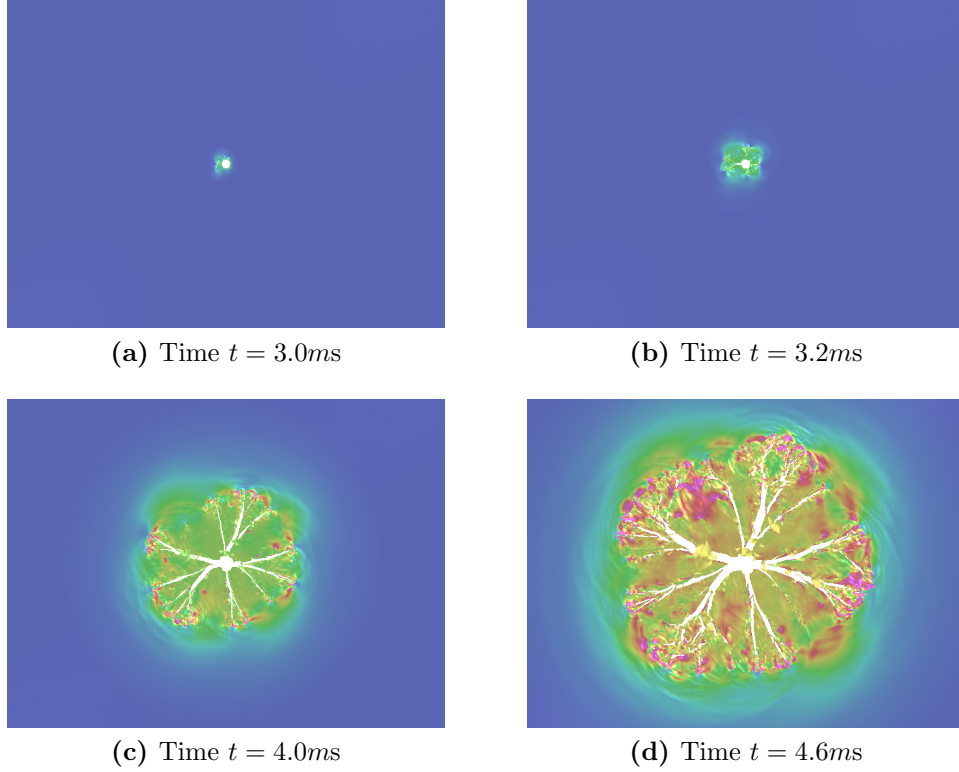
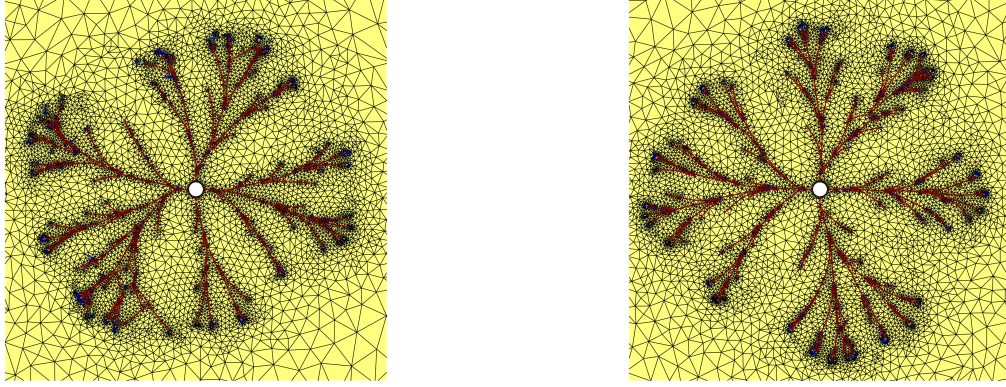


Figure 5.13: A series of solution visualization of dynamic wellbore stimulation. Fracture strength values are based on the KL mesh in figure 5.11a for $SVE1 \times 1$. Strain energy and height fields are mapped to color and height fields respectively.



(a) Variable fracture strength for $d_c \approx 0.386\text{m}$.

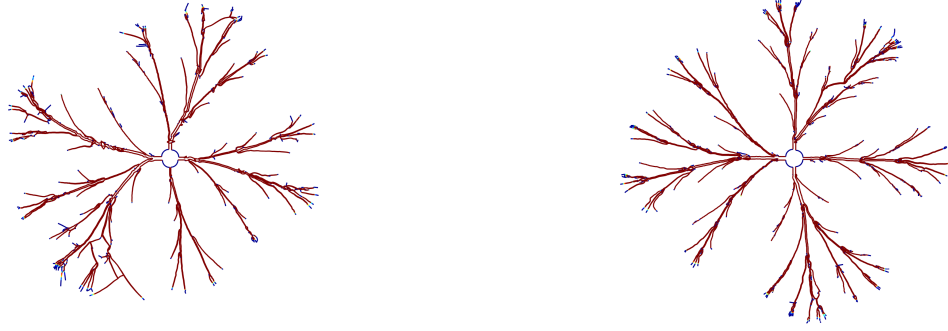
(b) Constant fracture strength $\bar{s} = 2.2 \text{ MPa}$.

Figure 5.14: Comparison of finite element space mesh for random and nonrandom fracture strength, at time $t = 4.2\text{ms}$.

By using the KL random field solutions seen in figures 5.11a, and a domain of homogeneous fracture strength we wanted to investigate the effect of incorporating variability in fracture strength field on fracture response. In figures 5.14 and 5.15 finite element space front and deformed shaped of fracture network are compared for solutions obtained with KL random field solution with correlation length $d_c \approx 0.386\text{m}$, and spatially homogeneous fracture strength $\bar{s} = 2.2 \text{ MPa}$ (which matched the mean value of the mesh generated by $\text{SVE}1 \times 1$) at time $t = 4.2\text{ms}$.

Figure 5.14 is better suited to observe high levels of mesh refinement around moving crack tips, while the fracture patterns can more clearly be seen in figure 5.15. Herein, we use the interfacial damage model from [1] to represent processes of surface debonding on a fracture interface. In both figures, damage value is mapped to color with the range blue to red denoting zero to full interfacial damage. As we observe, in all cases except in fracture process zones right in the wake of crack tips, the rest of crack segments experience full damage. That is, as expected regions that are supposed to be physically debonded have a damage value of one.

Fracture patterns for random fracture strength are shown in figures 5.14(a) and 5.15(a). With the results for the homogeneous fracture strength, *cf.* figures 5.14(b) and 5.15(b), we observe some distinctions between these results and those obtained with KL random field



(a) Variable fracture strength for $d_c \approx 0.386\text{m}$.

(b) Constant fracture strength $\bar{s} = 2.2 \text{ MPa}$.

Figure 5.15: Comparison of deformed shape for random and nonrandom fracture strength, at time $t = 4.2\text{ms}$.

solutions. Specifically, incorporating fracture strength randomness, in lieu of a homogeneous value, results in fracture patterns with slightly fewer microcracks and crack branching. Also, the fracture patterns obtained with variable fracture strength are less symmetric with respect to horizontal and vertical lines passing through the center of the wellbore. We attribute this to local variations in fracture strength that can further break the symmetries implied by the geometry and loading for this problem.

5.4 Conclusions

By using stochastic volume elements, and by assuming that at the microscale defects in the form of microcracks populate rock, we used a stochastic approach to generate random fields for fracture strength of rocks. A set of rock domain realizations were spatially sampled using nonuniform grids wherein an SVE was constructed at each grid point. By using an approximate equation, which ignored the interaction of individual cracks, we assigned a fracture strength value to each SVE. Thereafter, distribution statistics (*i.e.*, probability density, cumulative distribution, covariance) based on a non-Gaussian probability structure were determined. By solving an algebraic generalized eigenvalue problem with finite element method we determined eigenvalue and eigenfunction pairs used in the Karhunen-Loève

expansion of a Gaussian random field. The KL random field was subsequently transformed to reflect the probability structure of the originally sampled non-Gaussian random field through a simple cumulative density function relationship. This obtained non-Gaussian random field randomizes fracture strength values for fracture analysis of rocks.

In this work we assumed a certain statistics for in-situ microcracks in rock. In future works we aim to use actual microcrack statistics such as those reported in [156] and employ more robust approaches for generation of microcracked domains as in [90, 108]. We also ignored the interaction of microcracks in the computation of stress intensity factors. For each SVE by solving a few simple boundary loading conditions using finite element methods, we can calculate stress intensity factors for each crack for any macroscopic direction of applied tension. This enables the derivation of more accurate, and angular-dependent fracture strengths at the SVE level. In turn, this would better demonstrate the differences in fracture response obtained by a stochastic model for fracture strength, consistent with underlying microcrack distribution, and the models that assume a spatially uniform fracture strength. Although treating fracture strength as a random field appears to be more important than elastic moduli, we plan to determine their individual statistics as well as mutual cross-correlations. Since these quantities are not expected to be mutually independent, we also intend to generalize the presented work and simultaneously generate random fields for more than one scalar field.

Chapter 6

Macro-scale simulations

6.1 Introduction

6.1.1 Objectives

Via macroscale simulations, this chapter seeks to outline some of the effects of material heterogeneity on brittle dynamic fracture responses. All studies are performed by incorporating various forms of microstructure-dependent material uncertainty. Material stochastics are modeled either explicitly by employing randomly generated micro-/meso-scale microstructures, implicitly by employing random (in)elastic material properties, or a combination of both approaches. These combinations allow for a better understanding of what can be considered sufficient in modeling a more “realistic” random material. In addition to elasto-dynamic problems, the effects of material inhomogeneity are also studied for hydro-elastic problems. Hydraulic fracture simulations are solved aided by a complex data structure to model fluid flow, fluid transition, and interactions between hydraulic fractures and randomly distribution natural fractures. Further, the complex fracture patterns common to dynamic brittle fracturing are more accurately captured by the mesh-independent crack path solutions; This is performed via mesh adaptive operations within a space-time discontinuous Galerkin finite element solver (SDGFEM).

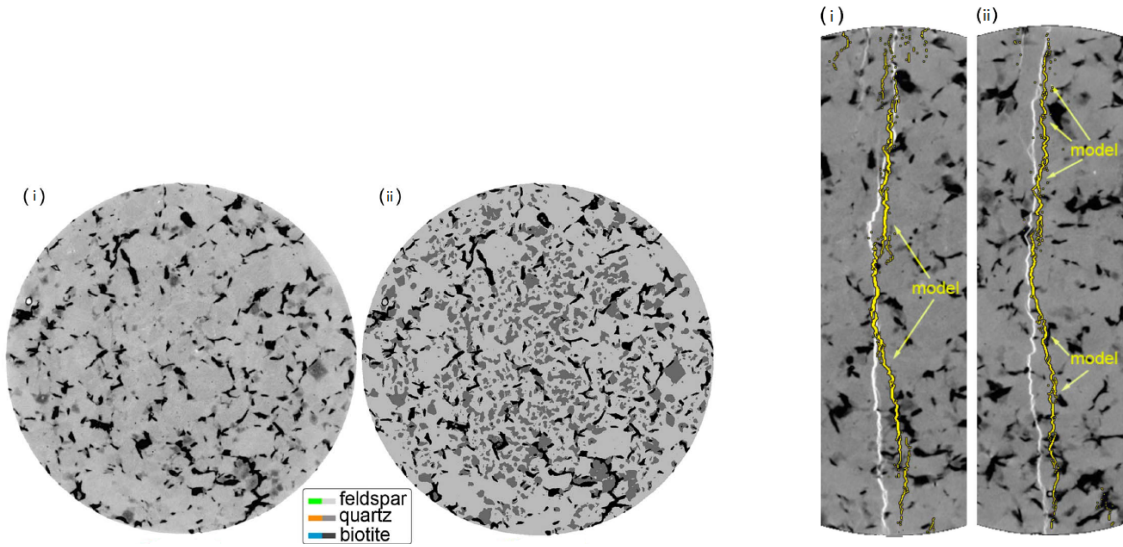
6.1.2 Background and motivation

Unlike ductile materials whose failure is preceded by measurable deformation, brittle materials lack dissipative mechanisms associated with plastic deformation; beyond their ultimate load these materials experience catastrophic failure in the form of fractures with little to no measurable precursory deformation. The onset of growth of brittle fractures is governed by the interaction and coalescence of microscopic discontinuities (*e.g.*, inclusions, voids, granular boundaries, surface and interior flaws) which like every real brittle material is inherently heterogeneous and random [50]. Various approaches have been utilized to investigate this multiscale problem of incorporating random heterogeneity into fracture models. This is done in an attempt to better understand and model real brittle material’s post ultimate load behavior.

We can first consider baseline investigations wherein the inhomogeneity of a material is modeled in a deterministic fashion. The approaches utilized therein explicitly model the materials constituents, on various scales, based on *in-situ* knowledge of the material structure’s geometry and properties on appropriate scales (*cf.* [76, 142]). Figure 6.1 illustrates two instances of this type of modeling approach which explicitly model the granular features of poly-crystalline (commonly studied class of quasi-brittle) materials on both a macroscale (6.1a,6.1b) and microscale (6.1c,6.1d). Each of the aforementioned, and studies alike, utilizes image processes to obtain the geometry of the detectable features of the underlying structure upon magnification.

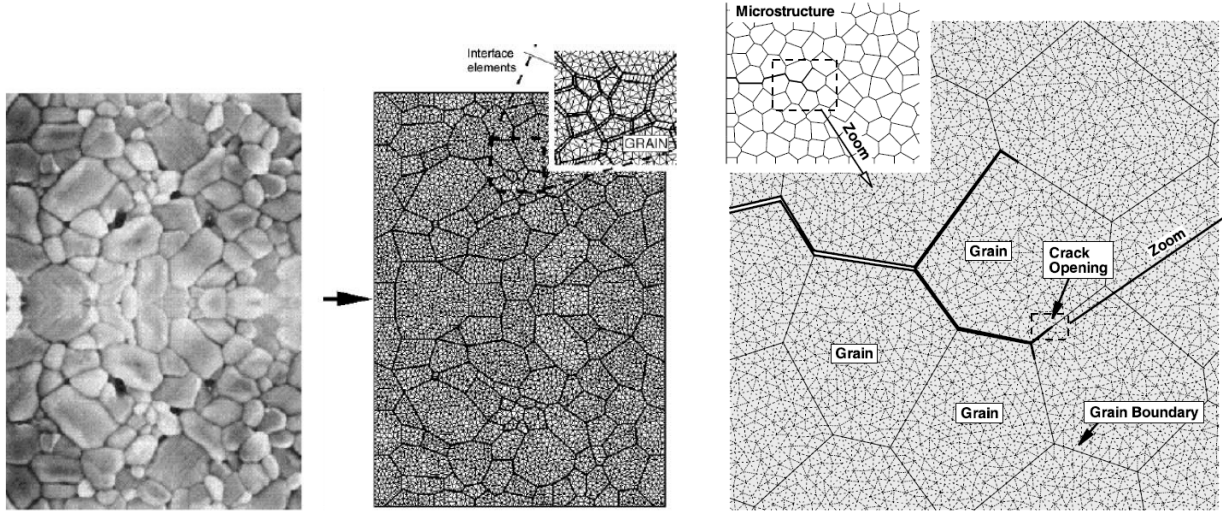
Although the numerical solutions of inelastic responses and fracture behaviors captured by these models are in good agreement with real experimental results, they exhibit nontrivial disadvantages. One such shortcoming is evident particularly when (meso-)macro-scale deterministic material models are employed. There may exist an underestimation of the inhomogeneity of the material as a consequence of neglecting uncertainties that would otherwise propagate from the lower length scales (6.1c,6.1d). Another disadvantage of these approaches is the availability of real microstructure specifications. Models of higher spatial dimension may require an internal description of the real sample microstructure which may not be readily available for simulations at relatively large scales such as geomechanical problems. Furthermore, the main disadvantages of deterministic approaches is that for a given material, an arbitrary specimen in an ensemble of samples cannot reliably reproduce fracture patterns that are unique to the overall material. This sample-to-sample uncertainty motivated fracture studies that investigate the effects of describing different aspects of brittle material features (*e.g.*, shape, size, orientation, etc...) but based on some probability structure.

The effects of randomness in microstructure size and various geometric features have been studied for numerous material compositions such as composites containing voids and inclusion (*cf.* [20, 116, 219, 200, 175, 58, 44, 209, 69, 61, 145, 103, 202]), crystalline materials (*cf.* [76, 134, 225, 56, 132, 38, 75, 85, 84, 226, 191, 124]) and in some cases an initial distribution of microcracks and defects (*cf.* [18, 234, 235]). Further, some



(a) (i) Material mesoscale image used to generate (i) explicit material model [142].

(b) Superimposed experimental and numerical fracture results for two material samples (i-ii) [142].



(c) (left) High resolution image of poly-crystal material microstructure used to capture interfaces of polygonal granular features for (right) generation of FEM mesh for explicit material modeling [76].

(d) Schematic of microcracking at grain boundaries [76].

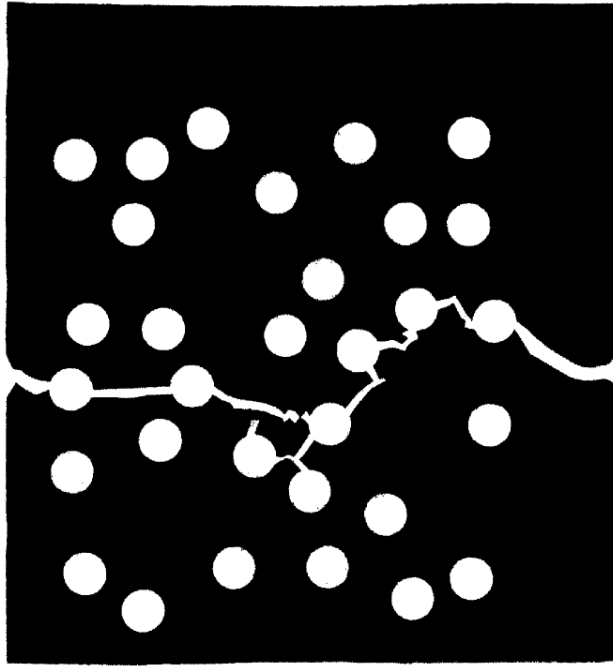
Figure 6.1: Explicit deterministic modeling of poly-crystalline brittle material structure generated from image processing at varying scales.

studies that involve the modeling of random microcrack distribution investigate the effects of microcrack distribution on the stability and propagation of a dominant crack (*cf.* [78, 47, 109, 151, 115, 51, 37, 41, 206, 139, 140, 137]). Figure 6.2 illustrates examples of fracture solutions obtained for a few cases wherein the previously mentioned random microstructures were used.

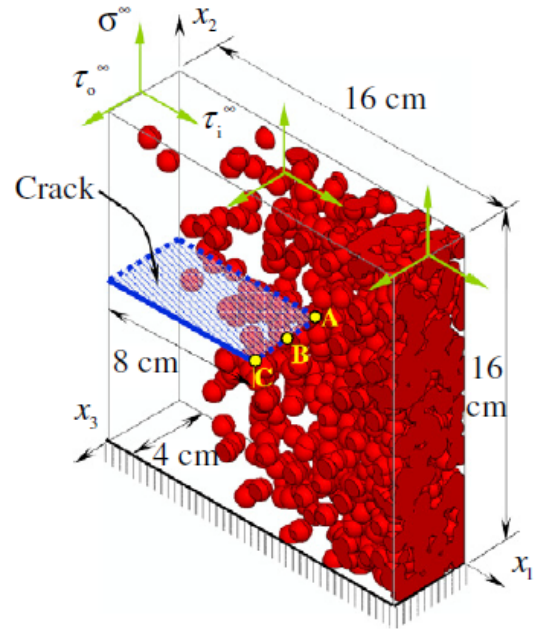
Apart from the issue that certain microstructure models may over simplify the aggregate composition of some inhomogeneous materials (*e.g.*, cementitious materials), random microstructure models are prohibited by computation resources. Attempting to resolve a large number of discrete microdefects can make these models less computationally tractable as the number of realized defects increases. To remedy this issue, some studies implicitly resolve the material microstructure by spatially defined, continuum-based random material properties; these are either influenced by individual (or sets of) microdefects or derived from an *ad hoc* probability structure.

Employing homogenization schemes and other implicit approaches, randomness is considered when defining various (in)elastic material properties (*cf.* [59, 67, 142, 45, 125, 121, 98, 234, 233, 187, 128, 93, 60, 193]). The solutions from one such study is seen in figure 6.3b wherein the elastic modulus is modeled as a spatially correlated Gaussian process. The approaches in [67] investigated the effects of inhomogeneous elasticity on crack arresting and stress distribution during macrocrack propagation. For completion, the details on how these and similar random fields are derived can be found in the discussions of Chapter 4.

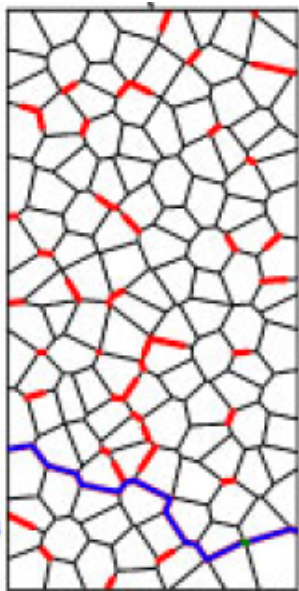
On the macroscopic scale, sharp crack models are used to resolve brittle fractures. The stability of these macrocracks is highly dependent on the underlying microstructure which can be modeled explicitly or implicitly as previously mentioned. In addition, brittle material fracture responses become much more complicated under dynamic loading. Several studies have demonstrated the significant effects of material microscale randomness on dynamic fracture responses (*cf.* [61, 234, 235]). The results of these studies further motivate the need for accounting for microscopic randomness in macroscopic brittle fracture modeling. Consequently, highly dynamic loading conditions yield complex fracture patterns consisting of path oscillation, side microcrack growth and main crack branching (*cf.* [195, 196]). From the viewpoint of finite element discretization, The reliability of brittle fracture path



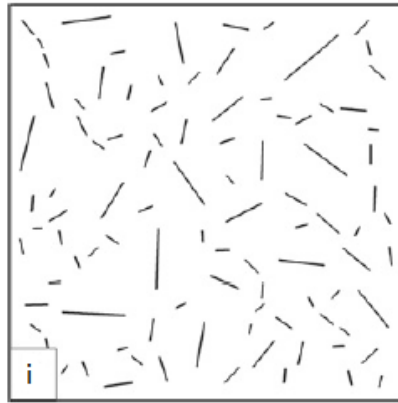
(a) Domain with randomly distributed voids [20].



(b) Domain with randomly distributed particulate inclusions [175].



(c) Domain with randomly distributed granular features [191].



(d) Domain with randomly distributed rectilinear microcracks [61].

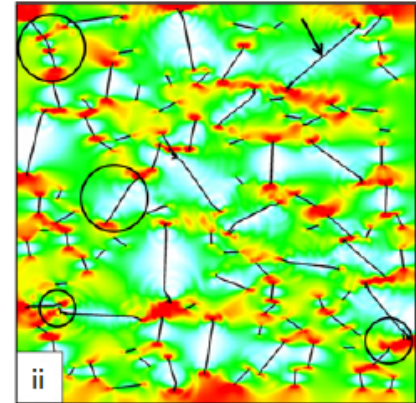
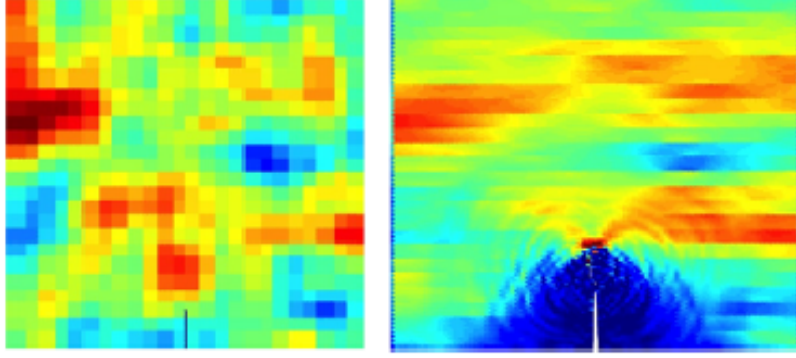
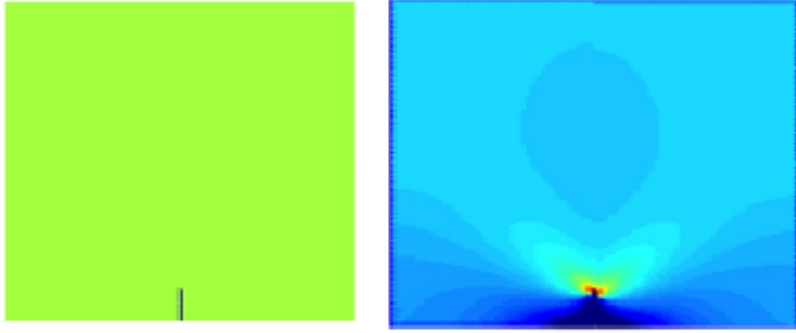


Figure 6.2: Examples of fracture simulations utilizing materials microstructure of random feature shape and geometry.



(a) (left) Inhomogeneous elastic stiffness; (right) intermittent fracture solution and stress distribution for random heterogeneous material [67].



(b) (left) Homogeneous elastic stiffness; (right) intermittent fracture solution and stress distribution for homogeneous material [67].

Figure 6.3: Comparison of initial computation domain and fracture solutions generated for materials modeled with homogeneous and random inhomogeneous (spatially correlated) elastic stiffness.

solutions is dependent on how accurately the spatial mesh can produce these complex fracture topology.

Figure 6.4 illustrates common approaches used for crack tracking in finite element methods.

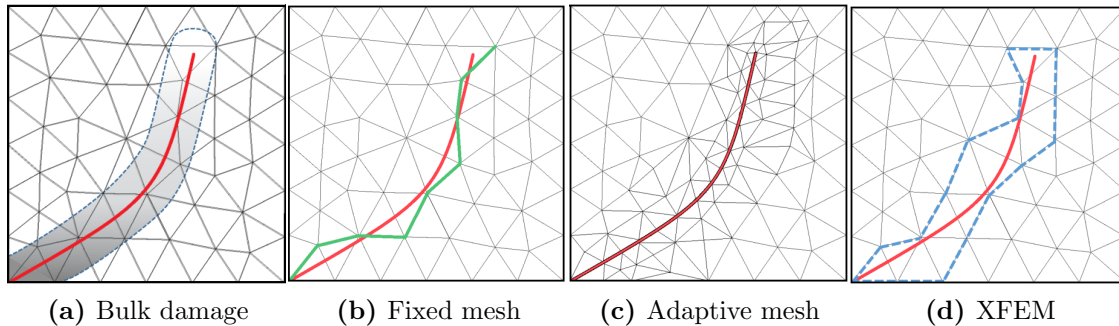


Figure 6.4: Discretization schemes for tracking cracks in the Finite Element Method

Continuum damage models are particularly useful when describing material degradation in a non-discrete setting. By averaging the effects of a discrete microstructure into a single variable, these models can produce and track localized crack paths by employing appropriate mesh sizes in the damaged region. Cracks from these models are realized as smeared regions in the material bulk (*cf.* 6.4a); therefore, physical crack faces are not modeled. Consequently, the use of these models is limited, when sharp crack interfaces are necessary such as is the case with hydraulic fracture simulations where the interaction of fluid and physical crack interfaces is significant. Another approach for sharp crack modeling utilizes a fixed mesh discretization where the predefined mesh element interfaces serve as the only possible paths for crack propagation (*cf.* 6.4b). Common use of this approach can be seen in the modeling of inter-granular fracture for poly-crystalline brittle materials. Unfortunately, for non-trivial loading conditions where the crack path is not intuitive or simple, the dynamic responses of these cracks are not dependable. To overcome this restriction, adaptive meshing approaches can be used to model arbitrary and complex crack patterns(*cf.* 6.4c) by aligning the element boundaries with solution-dependent crack paths [177, 176]. Tracking discontinuous crack propagation using adaptive meshing with classical FEM is difficult due to the continuously changing domain topology. Additional issues arise from the continuity constraints on the interpolated solutions of adjoining elements; this continuity is by continuous basis functions. Another method which overcomes the fixed mesh restrictions while allowing arbitrary,

solution-dependent, crack paths is the eXtended FEM (XFEM) method (*cf.* 6.4d). This method models cracks as they propagate within the enriched finite elements without the need for re-meshes. The XFEM methods remedy the issues which arise from modeling cracks via classical FEMs; however, modeling increasingly complex dynamic fracture patterns is computationally daunting because of the need for additional enrichment functions within the elements. All of the numerical results presented in this document were generated employing a variant of the adaptive meshing approach. The discontinuous Galerkin finite element method (DGFEM) utilizes adaptive mesh operations to track arbitrary crack paths. This is performed at a reduced computational cost owing to the method’s ability to more easily capture discontinuous features with discontinuous FEM basis functions. Using a novel and highly adaptive space-time DGFEM [11] to model macroscopic dynamic fracturing, the effects of explicit and implicit material microstructure heterogeneity are investigated in the proceeding sections of this chapter.

6.1.3 Methods of validation

Validation of the hydraulic fracturing implementation: The highly dynamic hydraulic loading in the following section demonstrate the framework’s capability to capture complex fracture patterns; however, the capability of the method capturing fracture behavior expected of hydraulic fracturing simulations needs to be verified. The solutions obtained by simulations employing real-life process parameters were validated based on their agreement with what is observed in real-time or is at least accepted in literature. A particular hydraulic reorientation problem, which has been studied experimentally and numerically, served as the basis of validation; the results obtained reproducing this study were compared to that of [70] and can be found in Section 7.3.1. Essentially, a vertically oriented hydraulically loaded crack was allowed to propagate into a material bulk subject to anisotropic *in-situ* pressures. The effects of the confinement pressure anisotropy and hydraulic loading rate are studied as to how they influence the divergence of the growing path away from alignment with the initial hydraulic fracture orientation. Good agreement between solutions can be found

in this Section 7.3.1 as well as particular fundamental method comparisons presented for clarity.

Validation of Christoffel equation computation for hyperbolic PDE wavespeed:

For general anisotropic solids fracture problems, the computation of the wavespeed becomes more complicated as the level of anisotropy increases. Materials which exhibit some degree of directional symmetry benefit from a reduction in the number of elastic constants needed to define their stiffness tensors; consequently, their wavespeeds can be computed analytically from the Christoffel equation. When analytical solutions are not feasible, numerical solvers are necessary to compute these wavespeeds. To validate the Christoffel equation numerical solver, implemented to determined bulk wavespeeds from a full anisotropic stiffness tensor, the solutions are compared to that of a material for which a closed form equation can be obtained for the wavespeed solutions. A detailed presentation of these verification cases can be found in Section 6.2.2 for both isotropic materials and an anisotropic material with cubic symmetry.

6.1.4 Intellectual merit

- The novelty of the methods detailed in this chapter is the micro-mechanical approach of a non-intrusive linking of microstructure randomness to macroscopic fracture responses.
 - Explicit and Implicit representations of the microstructure demonstrate how dynamic loading conditions influence the modeling of material heterogeneity for two classes of problems: i) Hydro-elastic problems simulating hydraulic fracture (HF) in an explicitly inhomogeneous bulk material matrix, ii) elasto-dynamic simulation of crack initiation and propagation in inhomogeneous material subject to various far-field and thermal loading conditions.
 - * HF simulations are made possible by a complex data structure which can track connectivity within independently (un)loaded sets of fracture networks allowing fluid-flow and fluid-transfer to be modeled.
 - * Instantaneous fluid transfer and pressure application upon crack intersection is mitigated by an algorithm to regularize the applications of the hydraulic

load; this allows the newly loading crack to gradually feel the affects of the fluid pressure.

- The complexity of the fracture patterns is not hindered by a FEM mesh dependency but is influenced by admissible solution-based crack propagation directions as well as the spatial variation and composition of the heterogeneous materials.
- Beyond the loading rate at which the “weakest-link” approach is appropriate, a implicit continuum random field representation of the inhomogeneous material comprehensively demonstrates how fracture dynamics is influenced by the size-effect and degree of spatial variation of fields.

6.1.5 Research contributions

Main contributions:

- [C++ scripted.] Implemented a simplicial complex based data structure in conjunction with disjoint set theory to track crack network development. This data structure is employed to track explicit crack network geometry, connectivity and overall network parameters to enable fluid flow, fluid transfer and hydraulic loading in fracture problems (*i.e.*, enables hydraulic fracture simulations).
- [C++ scripted.] Developed add-on capabilities and redefined code implemented constitutive equations. This enables the spacetime discontinuous Galerkin solver to model solid mechanics of heterogeneous and general anisotropic media, specifically for fracture formulations.
- Developed numerical solver for the solution of the Christoffel equation to compute hyperbolic PDE wavespeeds from the full stiffness tensor of anisotropic media. (NB: These computed (more conservative) wavespeeds can be used to determine accurate Reimann solutions used within discontinuous Galerkin FEM jump conditions [11].)

Secondary contributions:

- Implemented aperture based criteria to regulate and smoothen fluid transfer to an unloaded crack upon intersection with a hydraulically loaded fracture. Otherwise instantaneous fluid transfer leads to high stress gradients, and unrealistic fluid flow and hydraulic fracture propagation behavior.

Miscellaneous contributions:

- Increased the efficiency and usability of a spatial mesh solution visualization tool as well as added post-processing and analytical tools which enable:
 - Fracture visualizations with deformation solutions,
 - Arbitrary data comparison plotting (*e.g.*, pressure fraction versus solution time, strain energy versus total network crack length),
 - Energy dissipative studies to determine how system energies behave as fracture network grow and material domain deforms.

6.2 Courant-Friedrichs-Lewy (CFL) condition for hyperbolic problem: wavespeed for general anisotropic material

6.2.1 Christoffel equation: phase velocity

An important aspect of the space-time discontinuous Galerkin FEM solver utilized in the previous fracture studies is its ability to construct nonconforming meshes by direct discretization in the spatial and temporal domain. This feature, which allows locality of the solution during time advancement, is highly dependent on the hyperbolic PDE concept of causality. This concept essentially relates how fast the wave solution can propagate through a given media [11] based on a given wavespeed. This wavespeed c can be computed as a function of the mass density ρ as well as the stiffness tensor of a material. The stiffness tensor can be represented in 3-dimensional space by either a 4th order tensor of 81 components or a 2nd order 6×6 symmetric tensor containing the 21 independent components (elastic constants) of the corresponding 4th order tensor. For isotropic media, the wavespeed c is simply defined as $c = \sqrt{E/\rho}$ where E is the elastic modulus; this definition is possible because the stiffness tensor of isotropic materials is rotational invariant and therefore c attains the same value in all spatial directions. For more anisotropic media, whose tensors are not rotational invariant and wavespeeds are dependent on spatial direction, this simple definition of c may not be sufficient. Although there exist analytical definitions of wave-velocities based on special cases of anisotropic material, a numerical solver is generally needed for the case of a material which is defined by all 21 independent elastic constants [65, 126]. By solving the reduced form of the Christoffel equation [79, 114] in terms of the elastic constants, one can determine the necessary wave velocities of a general anisotropic media,

$$\sum_{ij} [M_{ij} - v^2 \delta_{ij}] s_j = 0 \quad (6.1)$$

where v is the monochromatic plane wave in polarization direction $\hat{\mathbf{s}}$ and $\mathbf{M}$ is the symmetric positive-definite Christoffel matrix defined for direction $\mathbf{q}$ as

$$M_{ij} = \sum_n q_n \frac{C_{inmj}}{\rho} q_m. \quad (6.2)$$

It is typical to have the stiffness tensor written as the 6×6 matrix C_{IJ}

$$\begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{pmatrix} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ - & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ - & - & c_{33} & c_{34} & c_{35} & c_{36} \\ - & - & - & c_{44} & c_{45} & c_{46} \\ - & - & - & - & c_{55} & c_{56} \\ - & - & - & - & - & c_{66} \end{pmatrix} \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ 2\epsilon_4 \\ 2\epsilon_5 \\ 2\epsilon_6 \end{pmatrix} \quad (6.3)$$

which is contracted from the tensor C_{ijkl} through Voigt notation seen in Table 6.1.

Table 6.1: Convention for indices contraction between tensor and Voigt notation.

Tensor indices	Voigt indices
$i = j = 1$	1
$i = j = 2$	2
$i = j = 3$	3
$i = 2, j = 3$ or $i = 3, j = 2$	4
$i = 1, j = 3$ or $i = 3, j = 1$	5
$i = 1, j = 2$ or $i = 2, j = 1$	6

The solution of equation 6.1 is obtained by solving an eigenvalue problem where the 3 real positive eigenvalues $\{\lambda_i | i = 1, 2, 3\}$ ¹ of $\mathbf{M}$ give the wave *phase* velocities by the relation $\lambda_i = v_i^2$. A sufficient definition for the wavespeed c which is ultimately used in the SDGFEM implementation is $c^2 = \max_{\theta, \phi} \max_i \{\lambda_i(\theta, \phi)\}$, where θ and ϕ are the spherical coordinates which define unit vector $\mathbf{q} = [\cos(\theta)\sin(\phi), \sin(\theta)\sin(\phi), \cos(\phi)]^T$.

¹The three bulk wave velocities computed yield one (pseudo-)longitudinal and two (psuedo-)transversal velocities [114].

6.2.2 Phase velocity solution validation

By considering classes of materials that deconstruct the Christoffel equation into forms that can be handled easily, if not analytically, the Christoffel equation solver in this work can be validated. We first consider an isotropic material defined by lamé λ and shear μ modulus where the stiffness tensor written in Voigt indices is:

$$\begin{pmatrix} \lambda + 2\mu & \lambda & \lambda & 0 & 0 & 0 \\ - & \lambda + 2\mu & \lambda & 0 & 0 & 0 \\ - & - & \lambda + 2\mu & 0 & 0 & 0 \\ - & - & - & \mu & 0 & 0 \\ - & - & - & - & \mu & 0 \\ - & - & - & - & - & \mu \end{pmatrix}. \quad (6.4)$$

When equation 6.4 is implemented into equation 6.1 and factorized, this yields the equation

$$(\mu - \rho v^2)^2(\lambda + 2\mu - \rho v^2) = 0. \quad (6.5)$$

Note that this factorized equation is independent of wave propagation direction which consequently yields bulk wave speed that are independent of direction; this is expected for isotropic media. Equation 6.5 yields unique solution v_L corresponding to longitudinal bulk wave speed and double solution v_T corresponding to transversal bulk wave speed,

$$v_L = \sqrt{\frac{\lambda + 2\mu}{\rho}} \quad (6.6)$$

$$v_T = \sqrt{\frac{\mu}{\rho}}. \quad (6.7)$$

Computing these values for known isotropic material lamé parameters, they can be compared to the bulk wavespeed values determined from the numerical solver. Table 6.2 shows these computed values. We can see that the numerical values are in good agreement with that of the numerical solver values. Since directional dependency is not an aspect of isotropic material, anisotropic materials can be used to ensure that the solver capture and correctly

Table 6.2: Longitudinal (v_L) and transversal (v_T) bulk wave velocities (m/s) for isotropic linear materials. mass density (10^3kg/m^3) and Lamé parameters (10^{10}N/m^2).

Material	ρ	λ	μ	Exact		Numerical	
				v_L	v_T	v_L	v_T
Silica	2.2	1.6	3.1	5954	3754	5954.37	3753.77
Aluminum	2.7	6.4	2.5	6498	3043	6497.86	3042.90
Iron	7.7	11.0	7.9	5900	3203	5899.59	3203.08
Steel	7.8	8.6	7.9	5593	3182	5593.04	3182.48
Nickel	8.9	20.0	7.6	6289	2922	6288.92	2922.20

accounts for the unit vector $\mathbf{q}$. Since a large number of materials have crystal symmetry, consider this class of material where the number of independent elastic constants reduces the stiffness tensor to the following:

$$\begin{pmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ - & c_{11} & c_{12} & 0 & 0 & 0 \\ - & - & c_{11} & 0 & 0 & 0 \\ - & - & - & c_{44} & 0 & 0 \\ - & - & - & - & c_{44} & 0 \\ - & - & - & - & - & c_{44} \end{pmatrix}. \quad (6.8)$$

Borrowing from the analytical solutions of [65], the *slowness surface* for a cubic material (copper) could be compared to the corresponding slowness surface from the implemented solver. With wave (phase) velocity defined as $\mathbf{v} = v\mathbf{q}$, the slowness vector is defined as the inverse of the phase velocity (*i.e.*, $\mathbf{s} = s\mathbf{q} = v^{-1}\mathbf{q}$). The slowness surface consists of any point where the tip of any admissible slowness vector, originating at O , terminates. A comparison of slowness surfaces on a plane of symmetry (*i.e.*, spherical coordinate $\phi = 0$) can be seen in Figure 6.5 for a copper material of values $c_{11} = 1.7$, $c_{12} = 1.2$, $c_{44} = 0.75$, (GPa), and $\rho = 8.9e+3(\text{kg/m}^3)$. We observe that the numerically obtained slowness surface for the corresponding bulk waves are in good agreement with the analytical solutions. Both of the above cases validates the reliability of implemented Christoffel equation solver to a sufficient degree of accuracy.

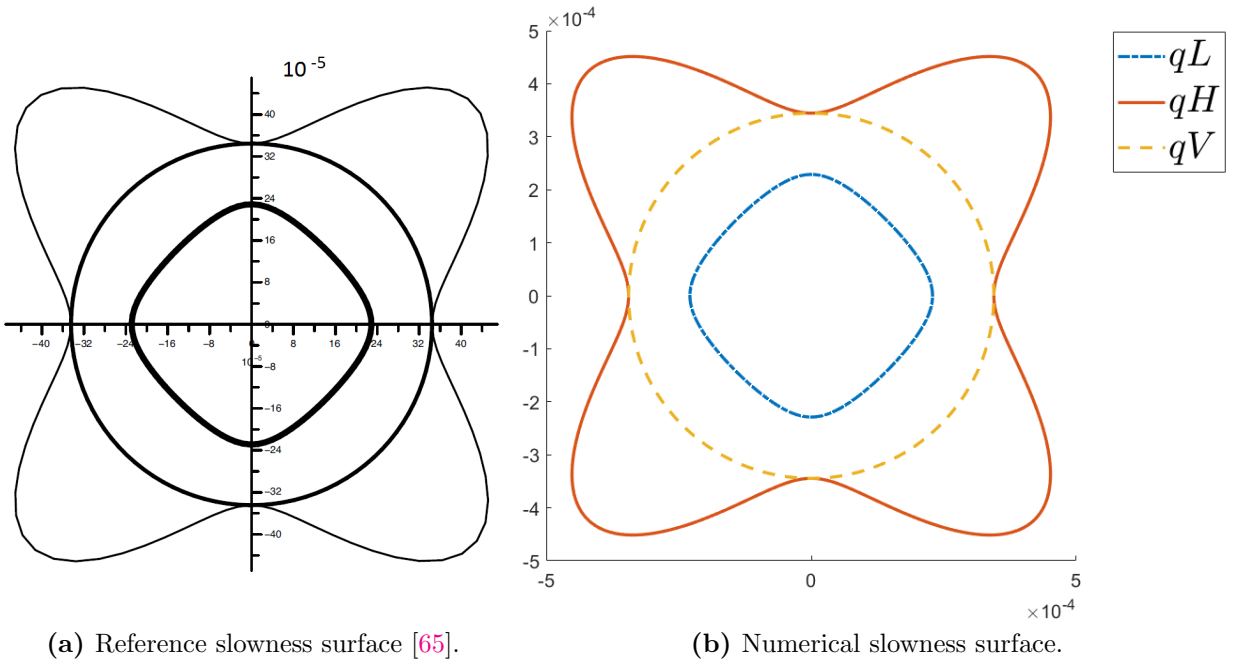


Figure 6.5: Comparison of numerically obtained slowness surface (m/s) versus slowness surface from reference text [65].

Chapter 7

Hydraulic fracturing simulations: An explicit microstructure representation of the initial natural fracture network

An original version of the following article was submitted and is currently under review for publication in the International Journal for Numerical and Analytical Methods in Geomechanics under the same title [52]. This article presents a detailed discussion on the implementation of a data structure that allows the modeling of fluid driven fractures in an explicitly inhomogeneous random media. We were first introduced to hydraulic fracturing in section 5 wherein inhomogeneity was modeled as an implicit fracture strength random field; however, the observations of those studies were merely preliminary and did not give much insight on the effects of material uncertainty on hydraulic fracture patterns. This section aims to fill in those gaps by presenting a framework that models inhomogeneity explicitly and study how this affects the progress of the fracture network. A major topic in hydraulic fracture simulations is the interaction of the hydraulically loaded fracture and the initial distribution of natural fractures that exist as features such as bedding planes. This initial distribution greatly influences the effectiveness of the overall hydraulic fracturing process and product recovery. This section discusses this concept and how simulation factors such as hydraulic loading rate, and crack geometry and orientation affect the formation of the fracture network.

Abstract: We model the connectivity of cells in a finite element domain and in a fracture network by a simplicial complex data structure. The complete adjacency information between cells is determined by one level down facet and one level up cofacet neighborhood information. Combined with a disjoint set data structure, explicit algorithms are derived to efficiently track network connectivity and load transfer between independent fracture sets. We also propose an approach to regularize the application of hydraulic load to newly intersected in-situ cracks to smoothen the transition of pressure on intersected cracks from ambient to hydraulic pressure and to avoid the sudden loading of the entire length of these cracks. Numerical results demonstrate the performance of crack connectivity and load transfer models and the effect of regularization model. The results show that as the angle between an incoming hydraulically loaded crack and an in-situ crack increases, the effect of in-situ crack shifts from slight realignment, to diversion / offsetting of the loaded crack. As the angle difference approaches the normal angle, the loaded crack tends to penetrate through

the in-situ crack. These schemes are also used for transient simulation of 2D reservoirs with multiple perforations surrounded by in-situ cracks with and without any orientation bias. It was shown that from two perforations with angles closer to in-situ cracks at low loading rates to all perforations at higher loading rates are activated. The h -adaptive asynchronous spacetime discontinuous Galerkin (aSDG) method is used to track complex fracture patterns in dynamic fracture simulations.

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7.1 Introduction

Hydraulic fracturing is widely used in the energy oil industry. This treatment enhances the product yield of a low-permeability reservoir through the induction of hydro-fractures into a natural fracture network. Therefore for the efficiency of processes, it is crucial to understand the underlying mechanisms which can have varying degrees of difficulty due to complex fracture networks both natural and induced. Having an accurate representation of fracture network, both induced and in-situ, is helpful in: i) the application of hydraulic loading, ii) the analysis of mechanical integrity of the reservoir, iii) deriving effective properties by homogenizing the effect of (micro)cracks below a certain length scale, and iv) the estimation of the reservoir product yield.

With an appropriate representation of the hydraulic and natural fracture network, it is possible to properly track fluid flow through arbitrary network topology as well as derive hydraulic load transfer algorithms for accurate application of loading on fracture surfaces. The importance of an accurate representation of complex fracture networks is motivated by the complexity of the hydraulic fracturing process wherein geological evidence and *in-situ* experiments confirm that multi-segmentation is common-placed and affects the process physics and efficiency [136]. Knowledge of the inherent natural fracture connectivity is also critical as hydraulic fracture propagation into a distribution of low connectivity results

in more intact rock damage, an increase in fracture intensity, and controlled propagation; propagation into a highly connected distribution results in leak-off and potential growth arrest and poor process efficiency [92]. Various works in literature have demonstrated that with the appropriate representation of both the fracture network and the fluid flow therein, the hydraulic fracture process can be modeled as a fully coupled hydro-mechanical problem [135, 19, 205, 174, 223, 148, 197] or approximately as a uncoupled (constant pressure) phenomenological problem [131, 70, 228, 222, 34].

The intersection of hydraulically loaded microcracks with in-situ faults and macrocracks is another aspect that warrants accurate modeling of crack connectivity in rock. As the propagating crack intersects a fault, it can be arrested or diverted by the fault, penetrate through it, or its path being offset. The intersection of a hydraulically loaded crack with an in-situ crack has been studied extensively in the literature to better understand the physics of hydraulic load transfer and crack intersection and/or analyze the stability of the reservoir; see for example [119, 120, 131, 230, 229, 205, 174]. In more realistic situations, hydraulically loaded fractures may interact and intersect with many macroscopic cracks and faults [157, 197]. Having a robust approach to model crack connectivity is very important in analyzing the stability of reservoir due to hydraulic fracturing.

Moreover, fractures affect various properties of rock such as its permeability and mechanical and thermal properties. Many homogenization theories provide effective properties by analyzing Representative Elementary Volumes (REVs), also known as Representative Volume Elements (RVEs), containing microcracks. In most studies effective properties are expressed in terms of macroscopic properties such as crack density. However, some works show that details of microcrack distribution and connectivity can play as important of a role as microcrack density; for example, [232, 49, 143, 113, 199] demonstrate the effects of microcrack geometry as well as spatial statistics on effective mechanical properties and permeability, and provide discussion therein on the effect of crack connectivity where applicable.

Even if the size of in-situ cracks are not small enough to enable modeling their effect by homogenization theories, their distribution and interaction with other cracks are important aspects in modeling reservoir stimulation; upon the completion of the hydraulic fracturing

treatment, proper multiscale representation of the developed fracture network aides in the determination of the effectiveness of the process by its overall contribution to the growth of the reservoir product yield. It is suggested that around 15% underestimation of the reservoir yield is possible when a computational model neglects the existence and connectivity of microcracking. Although it is not common to study connectivity at a microscale, this information can be used in a continuum view-point to compute flow parameters such as effective permeability; *cf.* [222, 232]. With the more common macroscale fracture networks, fluid flow parameters are correlated to degrees of network connectivity and admissible flow paths, which can aide in developing fluid flow algorithms depending on connectivity.

There are several data structures and computational techniques to model complex fracture networks. These models can be used to represent hydraulic fracture intersections with multiple in-situ fractures or discontinuities. For example, the Distinct Element Code (3DEC) [100] or the combined Finite-discrete element method (FDEM) [141, 92] employ the popular discrete element method (DEM) to represent domains with cracks. These works use fictitious joints to account for network connectivity and explicitly model crack intersections. *Extended Finite Element Methods* (XFEMs), *cf.* [35, 149, 68], use enriched basis functions to permit a crack to propagate through a finite element. Some of the recent XFEM formulations allow crack intersections within an element by using special crack connectivity functions such as T-junctions in [197]. In lieu of a sharp crack approach, [148] simulated the hydraulic process by defining network cracks in terms of a regularized damage phase field; for this approach, the employment of the level set method to represent regularized fracture surfaces directly takes care of tracking connectivity. In the present manuscript, the tracking of network connectivity will be handled by an approach which expands upon concepts of graph theory (*cf.* [63, 161, 212, 81]) and the disjoint set theory.

Networks represented by graph theory are locally and globally efficient while their topology preserves fracture patterns in both micro- and macro-scales; this is due to their “small worlds” property [212] meaning that this class of network may contain high connectivity between neighboring nodes while still preserving short average path lengths between nodes. For example, [223] uses a graph network structure to develop algorithms for updating hydraulic fracture network, within the combined *finite discrete element method*

(FDEM) framework proposed by [153]. This model can capture damage and failure processes in rock, driven by hydraulic pressure. Graph theoretic search algorithms were used by [63] and [161] to characterize admissible flow paths between network locations of interest. Graph theory is also used in [81] to determine the structural integrity of a fracture network while modeling fluid flow on fracture edges.

In this study a hydraulic fracture network is modeled by a *simplicial complex* (SimpComp) data structure which expands upon the fundamentals of graph theoretic approaches. The SimpComp represented network contains a collection of simplices characterized by the dimension of the network cell which they represent. These correspond to vertex, edge, triangle, and tetrahedron for zero to three dimensional objects, respectively. For a 2D spatial network representation, this network fundamentally reduces to a graph-based network with a simple and efficient approach to access neighborhood information. This new convention allows for multidimensional fracture surface representations while borrowing from the multi-graph, adjacency multi-list properties and various path-search methods of graph theory. SimpComp also utilizes the disjoint set theory to reduce the computation burden associated with path search algorithms and increase the efficiency of tracking load transfers and growth of disjoint fracture networks.

We use the *asynchronous spacetime discontinuous Galerkin* (aSDG) finite element method [9] for the solution of the elastodynamics problem. Using mesh adaptive schemes [10, 158, 6] element boundaries are aligned with requested crack extension directions; hence similar to *Generalized finite element methods* (GFEM), cf. [73, 203, 204, 94], and XFEMs no approximation is made in the direction of crack propagation. However, given that crack surfaces do not run through the element, no crack-enrichment functions are needed in our approach. The idea of aligning element boundaries with crack surfaces is also used in formulating *universal meshes* [177, 176]. However, the latter method is primarily used for quasi-static fracture modeling and the formulation of mesh adaptivity is drastically different from that of the aSDG method. Finally, it is noted that on fracture surfaces, contact-stick and contact-slip modes are incorporated into the fracture model by means of an interfacial contact [8] and damage [6] model, as opposed to conventional cohesive models.

The organization of this manuscript is as follows. In §10.2, the two main aspects of formulation, including data structures and algorithms formulated for modeling crack connectivity and load transfer (§7.2.1 and §7.2.2), and a scheme proposed to regularize the transition of pressure to newly intersected in-situ cracks (§7.2.3) are presented. This is followed by a brief review of the aSDG method and an interfacial contact/damage model in §7.2.4. Finally, the numerical results in §8.5 demonstrate the effectiveness of the proposed methods in regularizing the application of hydraulic load and in modeling crack connectivity and load transfer when multiple hydraulically loaded cracks interact with in-situ cracks. Various types of crack interaction (realignment, offsetting and diversion, and penetration) are observed in these problems.

7.2 Formulation

7.2.1 Data structures for representation of fracture network

7.2.1.1 Simplicial Complex / Graph Theoretic

In this section, the *Simplicial Complex* (SimpComp) approach for network representation is presented. SimpComp representation is similar to a graph model in 2D problems, wherein cracks and crack tips act as edges and vertices of a graph; a graph G is constructed by two interconnected sets, *vertices* V and *edges* E (*i.e.*, $G = \{E, V\}$). The finite and non-empty set V consists of 0 dimensional cells and the V -dependent set E is a collection of paired vertices which form 1 dimensional objects. SimpComp extends this concept by employing *simplices*, which by definition are d dimensional “volumes” formed by $d+1$ vertices in an $\mathbb{E}^d$ Euclidean space. In addition to the aforementioned *vertices* and *edges*, the complex can represent features of higher dimension by implementing higher order simplices such as *triangles* and *tetrahedra*. For example, in 2D a two dimensional *triangle*, is comprised of a set of *facets*, *i.e.*, edges. A simplicial complex (SC) representation of a collection of triangles T includes the triangles and all their lower dimension *faces*, $SC = \{T, V, E\}$. In 3D, a tetrahedron is identified by its 2D triangular facets and a simplicial complex representation of a collection of tetrahedra Tt include the tetrahedra and all their lower dimension faces, $SC = \{Tt, T, V, E\}$.

As becomes evident, these collections of lower dimensional faces can be fully determined by only one dimension down neighborhood information. The precise definitions of facet and face are followed below.

Deviating from the graph theoretic approach, a simplicial complex stores connectivity information in a more comprehensive manner. The capability of representing higher dimensional network cells prevents the direct use of elementary graph operations, *e.g.*, *shortest path* search and *transitive closure* based connection checks. This introduces the need to redefine these operations for SimpComp. For a graph structure, connectivity of n vertices and m edges are defined appropriately by either an $n \times n$ *adjacency matrix* A or an $n \times m$ *incidence matrix* B . The connection of two vertices v_i and v_j by an edge is indicated by adjacency component $|A_{ij}| > 0$ and $A_{ij} = 0$ otherwise. An edge e_j having a vertex v_i as one of its paired vertices is indicated by incidence matrix entry $|B_{ij}| > 0$ and $B_{ij} = 0$ otherwise. With connectivity defined in this way, it is obvious that as a fracture network advances, being dense and/or becoming more complex, these matrices become sparse and their storage costly. By employing linked lists, the storage cost of sparse matrices can be greatly reduced; however, incorporating network cells of higher dimensions increases the computational complexity of these linked list because of the increased number of underlying adjacency and incidence matrices. SimpComp employs a more comprehensive and less costly approach for tracking network connectivity between vertices, edges, triangles, and higher order cells wherein each simplex has both knowledge and access to all other simplices it is connected to.

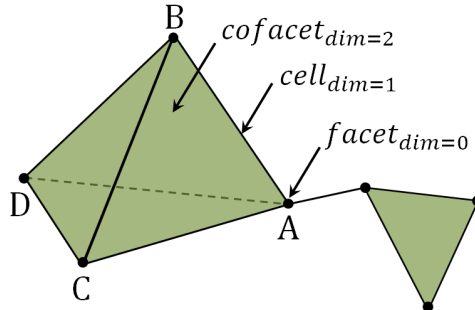


Figure 7.1: Simplicial complex representation of a collection of cells. The facet and cofacet relation between cells is sufficient to determine the adjacency of any two cells in the collection.

The definition of a `SimpComp` is closely related to the notion of a *cell*. A cell refers to a base simplex of arbitrary (spatial) dimension, whose connectivity to all other cells is defined by *facet* and *cofacet* relationships. A reference cell can be the *facet* of any connected cells one dimension higher than itself and/or the *cofacet* of any connected cell one dimension lower than itself; this relationship, depicted in Fig. 7.1, allows duality of access between two connected cells. The facets of facets of a cell, recursively to any lower dimension including vertices, are called *faces* of the cell. For example in the figure, edge AB is a facet of triangle ABC and ABC is a facet of tetrahedron ABCD, hence AB is a face of this tetrahedron. Conversely, ABCD is called a *coface* of AB. For the same reason, vertices A to D are faces of tetrahedron ABCD, and this tetrahedron is their coface. For fracture simulation `SimpComp` is comprised of all crack segments and their lower level faces (including their vertices). One dimension down facet and up cofacet information is sufficient to investigate any type of connectivity between different cells in the fracture network. As will be discussed in §7.2.2, facet and cofacet neighborhood information is a part of cell data members in our design.

7.2.1.2 Disjoint Set Theory

`SimpComp` provides a convenient representation of the connectivity of developing fracture network. The *disjoint set theory* is used in conjunction with `SimpComp` to keep track of which groups of cracks are hydraulically loaded and to what source of loading they are connected. Implemented by a *disjoint set specifier*, the primary aim of the disjoint set theory in this scheme is to track independent subsets of connected cells as well as cells generated during solution. Generally, the disjoint set specifier is tasked with distinguishing the loading states of both the hydraulic loaded and unloading in-situ cracks. It should be noted that both the load transfer mechanisms and fluid flow physics are highly dependent on fracture paths. One of the most immediate benefits of the disjoint set scheme and specifier is that it alleviates the need of performing complex path searches and transitive closure operations, with respect to connectivity checks for example; this greatly reduces computation cost and time. Each cell contains *hydraulic load data members* which consist of information that characterizes specific load states; this load data member is then mapped to specific disjoint sets, which is dynamically updated as the network develops.

The general concept of how the dynamic connectivity of a fracture network is tracked using disjoint set theory is depicted in Fig. 7.2. The initial fracture network, *cf.* Fig. 7.2a, consists of a hydraulically loaded fracture in disjoint set S_1 , and two disconnected, unloaded in-situ cracks in the mutually disjoint sets S_2 and S_3 . The loaded and unloaded crack segments are depicted by solid and dashed lines, respectively. As the loaded fracture in S_1 propagates, it intersects the unloaded fracture in S_2 and effectively transfers the hydraulic load to the in-situ crack; both fractures are now in a loaded state, residing in a new set $S_1 \cup S_2$ with the fracture in S_3 remaining unloaded and disjoint; *cf.* Fig. 7.2b.

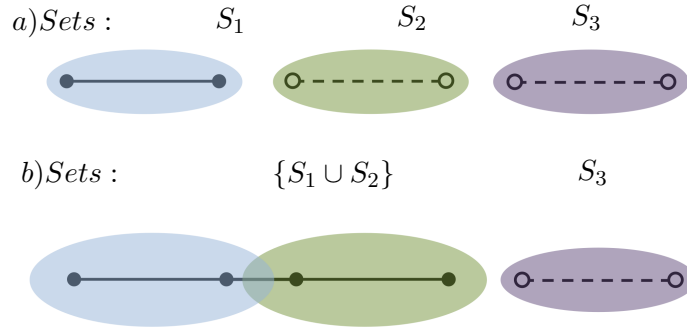


Figure 7.2: Fracture load state and disjoint set update. Loaded and unloaded cracks are depicted by solid and dashed lines, respectively.

7.2.2 Algorithm for network growth and load transfer

Now capable of a full network topology representation employing the SimpComp data structure in collaboration with the disjoint set data structure, an algorithm for network topology growth and dynamic load transfer is demonstrated in Fig. 7.3. Before providing the details of crack nucleation and extension and load transfer algorithms, a brief overview of different types of scenarios encountered in a crack propagation problem is provided. The initial stage of a domain, *e.g.*, a reservoir, is identified by initial perforations such as l_0 in Fig. 7.3a. Unloaded cracks can be nucleated and propagated around l_0 , either due to the high stress values of scattered elastic waves, or be viewed as a means to populate the initial set of in-situ cracks. Note that generation of a crack segment involves two steps; the nucleation of a crack tip and an extension from it as shown in Fig. 7.3b and Fig. 7.3c, respectively. Crack intersection, along with nucleation and extension completes the set of operations needed for

modeling the evolution of cracks in a fracture network. Both Figs. 7.3e and 7.3f demonstrate crack intersection scenarios. The fundamental difference between these cases is that the intersection in Fig. 7.3e occurs between two fracture edges in unloaded states whereas Fig. 7.3f demonstrates intersection of the loaded hydraulic fracture edge with a set of unloaded fracture edges. It is emphasized that crack intersection, in fact is a type of crack extension where the destination vertex of extension belongs to another crack segment or is a singleton nucleated crack tip.

Two different maps, disjoint set (DSET) and set to load (SET2L), are used to keep track of fracture network connectivity and their HF loading status. When an independent subset of cell(s) is generated, that subset is assigned a unique *cell set id* and *disjoint set number* with both sharing the same value initially. Both values remain unaltered unless fracture intersection occurs. The convention used in Fig. 7.3 to assign and denote cell set id and disjoint set number is DSET: *disjoint set number*{*cell set ids*}. For example, DSET: 3{1, 2} in Fig. 7.3e means that *disjoint set number* 3 includes cracks with *cell set id* 1 and 2. As it becomes apparent below, these cells were initially generated in disjoint sets with numbers 1 and 2 before their disjoint sets merged to a disjoint set with number 3.

The map SET2L is used to specify the loading states of the cells. SET2L is a map from disjoint set numbers to a set of HF loads that the disjoint set is connected to. This map is shown as the second line below each subfigure with the syntax SET2L: *disjoint set number* $\mapsto$ $\{L_j\}$, where for each disjoint set number $\{L_j\}$ is the set of the numbers of connected HF loads. The unloaded fractures in a disjoint set with number n are represented by an empty load set SET2L: $n \mapsto \{\}$; see for example SET2L: 3 $\mapsto \{\}$ in Fig. 7.3e. If a disjoint set is connected to multiple HF loads, *e.g.*, from different perforations, the applied HF load can be chosen as the maximum pressure from all these sources if constant pressure is used as in the present manuscript or a coupled hydro-mechanical formulation can use this connectivity information to derive the correct pressure in the vicinity of such intersection point.

Having defined cell connectivity information and DSET and SET2L related attributes, we can now list all data members associated with cells contained in SimpComp representation of a fracture network,

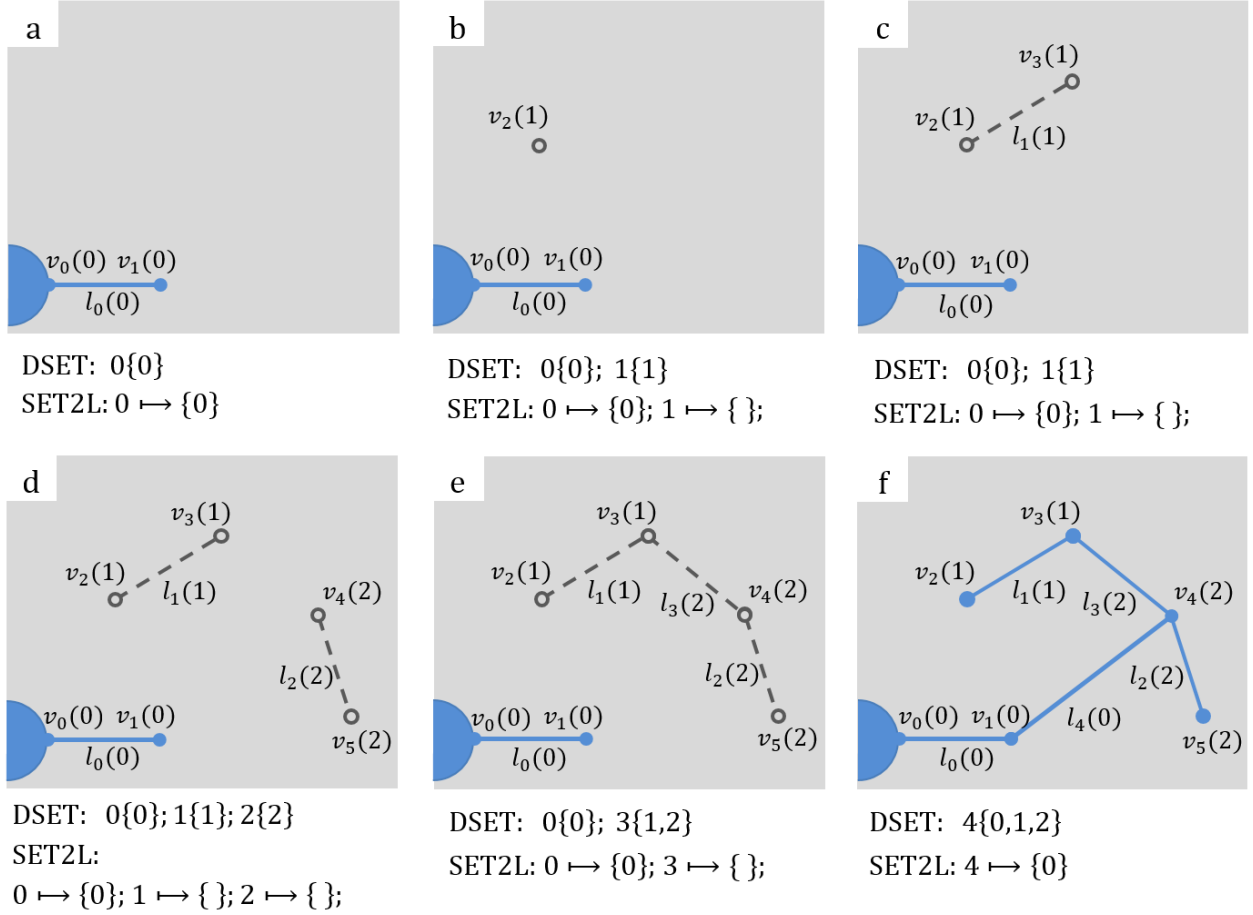


Figure 7.3: Tracking connectivity and load numbers of cracks in a fracture network. (b) and (c) show the two steps needed for nucleation and extension of a crack. These steps are repeated in (d). Crack interactions between hydraulically unloaded disjoint sets and between loaded and unloaded sets are shown in (e) and (f), respectively.

- Dimension: geometric dimension of a cell. In the crack network shown in Fig. 7.3 for a 2D problem, 0D (vertex) and 1D (edge/line) members are denoted by v and l .
- Cell id: Is an identification number unique within each dimension group of cells. They appear as subscripts for v (vertices) and l (lines) in the figure. Some examples are v_1 and l_0 in Fig. 7.3a.
- Facets: Facets of a cell are collected in a set. This set is empty for vertices.
- Cofacets: Cofacets of a cell are collected in a separate cell. The top dimensional crack segments do not have any cofacets.
- Cell set id: When a cell is initially generated, whether or not it induces the generation of a new disjoint set, it will be a part of a disjoint set. The number of this disjoint cell is assigned as the cell's *cell set id*. This number is not modified upon the intersection of its containing disjoint set with another disjoint set. The DSET map can always be used to determine what disjoint set a cell currently belongs to. For example line l_1 with cell set id 1 belongs to disjoint sets 1, 3, and 4 in Fig. 7.3c, Fig. 7.3e, and Fig. 7.3f, respectively. This is because for these three cases cell set id 1 is mapped to 1, 3, and 4 in the DSET map. In the figure the cell set id of a cell is shown in parenthesis in front of the cell name, see for example $l_0(0)$ in Fig. 7.3a.
- Physics data: Various physics related data are stored in a cell. For example, fracture aperture at edge endpoints is used in §7.2.3 to regularize the application of hydraulic load in the present manuscript.

Having defined the convention of the two global maps and cell data members, we first elaborate on crack nucleation and extension operations in Fig. 7.3. The initial network configuration is seen in Fig. 7.3a wherein a horizontal edge cell represents a hydraulically loaded fracture emanating from a circular wellbore induced by the process of hydraulic perforation. For this initial configuration, the cells representing the hydraulic fracture are assigned the unique set id 0 and corresponding disjoint set number 0. The load number zero is associated with this disjoint set; that is SET2L: $0 \mapsto \{0\}$. This load state variable

is associated with the load properties of fluid flow initiated at the wellbore origin, vertex v_0 . The process of a crack nucleation is shown in Fig. 7.3b wherein a newly generated vertex is added to the fracture network. Being disjoint from the initial hydraulic fracture, this new cell is assigned its own set id of 1 and placed in the disjoint set number 1. Since this new main set is not connected to the hydraulic fracture, and is in an unloaded state its disjoint set number is mapped to an empty set, that is in SET2L: $1 \mapsto \{\}$. Figure 7.3c demonstrates the propagation of a fracture edge from an existing vertex to a newly nucleated vertex (crack tip); this type of hydraulically unloaded fracture can indeed occur due to stress wave scattering induced by hydraulically loaded fracture(s). Since this edge extension operation was performed from an existing vertex to a newly generated vertex, the load data and disjoint set specifier are directly transferred from the existing to the new cells and no changes are made to neither the DSET nor the SET2L maps. Figure 7.3d shows a similar set of operations as Fig. 7.3c without showing the two step process of an initial vertex nucleation followed by an extension; since these new unloaded cells are generated disjointly from the other subsets of existing cells, they are assigned unique main set and set ids 2 with DSET and SET2L mappings updated accordingly.

In an event of crack intersection, the two maps DSET and SET2L are used to keep track of crack connectivity and to distinguish fracture edge extensions induced from hydraulic loading from those induced by external stress loadings, respectively. In intersections where the disjoint set number of intersecting crack and intersected vertex (crack) are distinct, three things happen; first for DSET map, a new disjoint set with the next available disjoint set number is generated. The cell set ids from the original two disjoint sets are combined and associated with the new disjoint set number. This process is used in combining DSET: $1\{1\}, 2\{2\}$ from Fig. 7.3d to DSET: $3\{1, 2\}$ in Fig. 7.3e in response to the extension of a crack from v_3 , a vertex with disjoint set number 1, to v_4 , a vertex from disjoint set number 2. The second change is related to SET2L; a new entry is added to SET2L with the new disjoint set number being mapped to a set that combines the load numbers that are associated with the two disjoint sets that are combined into the new disjoint set. For example, in Fig. 7.3d both disjoint sets 1 and 2 have empty load number sets associated with them in the SET2L map as they are unloaded. They remain unloaded after the intersection, as the union of the

two empty sets is empty. This results in $3 \mapsto \{\}$ for the SET2L map in Fig. 7.3e. In contrast, from Fig. 7.3e to Fig. 7.3f, the union of loads of loaded disjoint set 0 (with load number 0) and unloaded disjoint set 3, is the set of load numbers $\{0\}$; thus, the new merged disjoint set is mapped to $\{0\}$. That is, in SET2L we get $4 \mapsto \{0\}$. The third operation is simply deleting the entries for the two previously distinct disjoint sets from both DSET and SET2L maps. Note that for intersection scenarios where the disjoint set number of the source and destination vertices is the same, *e.g.*, when a microcrack intersects its mother crack or other microcracks emanated from it, no changes are made to DSET and SET2L maps.

Finally, to further clarify what is stored in cells in a fracture network, the data members of all cells of SimpComp at a stage shown in Fig. 7.3e are shown in table 7.1. Note that the values in the last two columns are not directly stored in a cell. Rather, they can be sequentially computed by a cell's *cell set id*. The global DSET map maps this id to disjoint set number which is subsequently mapped to a set of load numbers using the SET2L map.

Table 7.1: Data members for all cells in SimpComp data structure for the stage shown in Fig. 7.3e. The last two columns, disjoint set number and load number, are not directly stored in a cell but are obtained as described in the text.

cell	dimension	id	facets	cofacets	<u>disjoint set number</u>	<u>load number</u>
v_0	0	0	$\{\}$	$\{l_0\}$	0	$\{0\}$
v_1	0	1	$\{\}$	$\{l_0\}$	0	$\{0\}$
v_2	0	2	$\{\}$	$\{l_1\}$	3	$\{\}$
v_3	0	3	$\{\}$	$\{l_1, l_3\}$	3	$\{\}$
v_4	0	4	$\{\}$	$\{l_2, l_3\}$	3	$\{\}$
v_5	0	5	$\{\}$	$\{l_2\}$	3	$\{\}$
l_0	1	0	$\{v_0, v_1\}$	$\{\}$	0	$\{0\}$
l_1	1	1	$\{v_2, v_3\}$	$\{\}$	3	$\{\}$
l_2	1	2	$\{v_4, v_5\}$	$\{\}$	3	$\{\}$
l_3	1	3	$\{v_3, v_4\}$	$\{\}$	3	$\{\}$

7.2.3 Application of hydraulic pressure to intersected in-situ cracks

The approaches presented in [55] provide the basis for the algorithms proposed in preceding sections to track crack connectivity and to transfer hydraulic load to newly intersected in-situ cracks. However, therein the application of hydraulic load to intersected cracks was manually retarded in time to prevent some of the problems discussed below. In the following, we propose a regularization approach based on the aperture of connected hydraulically loaded cracks to a crack segment.

While the crack connectivity model is general, a spatially-constant pressure model is used for the numerical results presented in §8.5. This approximation is used in many studies and as discussed in [94], is an accurate model for the fracture analysis of shale gas reservoirs with low permeability. For such a very tight formation, the leak-off of fluid across crack faces can be neglected. Besides, low viscosity fracturing fluids such as treated water is becoming more prevalent in hydraulic fracturing. Under such conditions, the fluid pressure along fracture faces, specifically near the wellbore can be treated as a nearly constant due to the high *in-situ* stresses acting as effective confining pressures in the deep reservoirs and the low fluid viscosity. The accuracy of constant pressure approximation is also explained by the analysis in [64, 66, 42], where it is shown that for rocks with high fracture toughness and/or hydraulic fluids with low viscosity, the fluid flow approaches non-dissipative inviscid behavior. Based on these studies, [86, 66] showed that considering this behavior is reasonable.

Although the algorithms and methods from §7.2.1 to §7.2.2 allow the transferring of hydraulic load to a newly loaded segment following fracture intersection, there are adverse effects when using a phenomenological constant pressure throughout the hydraulic fracture network. The first consequence is that hydraulic load is instantaneously applied to the entire surface of the newly loaded crack; this error implies infinite fluid speed inside the newly loaded cracks which can result in unrealistic responses for relatively long fracture segments. For example, a potential problem can be immediate crack extension by hydraulic load at the two end points of the loaded crack. The second consequence is that right at the moment of intersection, the pressure on the surfaces of in-situ crack suddenly jumps from in-situ pressure

to the hydraulic pressure of the intersecting loaded crack. This induces a sharp jump in target dynamic tractions and velocities that act on these surfaces. Aside from the numerical artifacts that can arise, this sudden jump of mechanical fields requires a very fine grid around the surface of an intersected crack. Herein, we propose an aperture-based scheme that smoothen the full application of hydraulic load to an intersected crack. This regularization is motivated by [8], wherein upon a separation-to-contact mode transition again there are sudden jumps in mechanical fields at an interface, hence the need to numerically smoothen the transition.

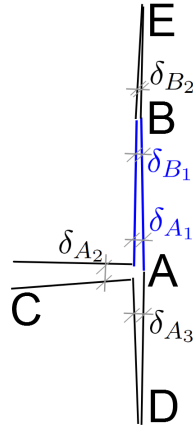


Figure 7.4: Regularization of the application of hydraulic load on crack segment AB, by using the apertures of all hydraulically loaded cracks that are connected to it.

Figure 7.4 shows the intersection of a hydraulically loaded crack, segment CA, with an in-situ or otherwise unloaded crack, *i.e.*, the extension of DE. The goal is to regularize the applied hydraulic pressure for the sample segment AB. Accordingly for an arbitrary point P, such as A or B, we define,

$$\delta_{P_{\max}} = \max_i (\delta_{P_i}) \quad (7.1)$$

where δ_{P_i} are the apertures of the hydraulically-loaded and connected cracks to point P, as shown in the figure for points A and B. Then, the *pressure factor* f_p of point P is defined as,

$$f_p(P) = \begin{cases} 0 & \delta'_P \leq 0 \\ \frac{\delta'_P}{\bar{\delta}'} & 0 < \delta'_P < \bar{\delta}' \\ 1 & \bar{\delta}' < \delta'_P \end{cases} \quad (7.2)$$

where $\delta'_P = \delta_{P_{\max}}/\tilde{\delta}$ is the maximum aperture at point P, normalized by the separation scale $\tilde{\delta}$ implied by the interfacial fracture model used for modeling crack propagation. For example, commonly used cohesive fracture models have an inherent separation scale due to the use of a *traction separation relation* (TSR) type interface constitutive equation. On the other hand, the interfacial damage model used in the present work, *cf.* §7.2.4 and [6], is characterized by a fracture strength $\tilde{\sigma}$ and a (relaxation) fracture time scale $\tilde{\tau}$. Still, by a simple dimensional analysis, an extrinsic separation scale can be derived from $\tilde{\sigma}$, $\tilde{\tau}$, and bulk material properties (*cf.* equation (39b) in [5]). Regardless of how $\tilde{\delta}$ is computed, the nondimensional parameter $\bar{\delta}'$ is chosen such that $0 < \bar{\delta}' \ll 1$. This condition ensures that the pressure regularization is only active for the very early stages of crack opening. Equation 7.2, implies that full hydraulic pressure is applied at a point, when the maximum connected aperture $\delta_{P_{\max}}$ reaches $\bar{\delta}'\tilde{\delta}$.

A few important aspects of the model are discussed. First, the locations at which apertures are measured are not right at a given point. For example, as shown in Fig. 7.4 for points A and B, there is an offset behind the point of consideration on a given crack surface. Second, the pressure factor on a crack surface is linearly interpolated based on the values at the end vertices, for example points A and B in Fig. 7.4. Third, to ensure that the regularization is not influenced by the level of mesh adaptivity, and in general element sizes, the offset is set to be a fraction of a fracture related length scale, *e.g.*, fracture process zone size (*cf.* equation (39f) in [5]). Fourth, the objective of the regularization is to activate and smoothen the sudden application of hydraulic load upon the intersection of two cracks. While in this work spatially constant hydraulic pressure is applied on crack surfaces (before regularization), the same regularization scheme can be applied to regularize the onset of the application of hydraulic pressure when other equations such as lubrication equation are used to model hydro-mechanical couplings.

7.2.4 Computational model for dynamic fracture simulation

The purpose of this section is to provide a brief overview of the computational models used for fracture simulations in §8.5. Clearly, the formulations presented in previous sections can be incorporated in a variety of other numerical methods. As explained in §8.5, crack

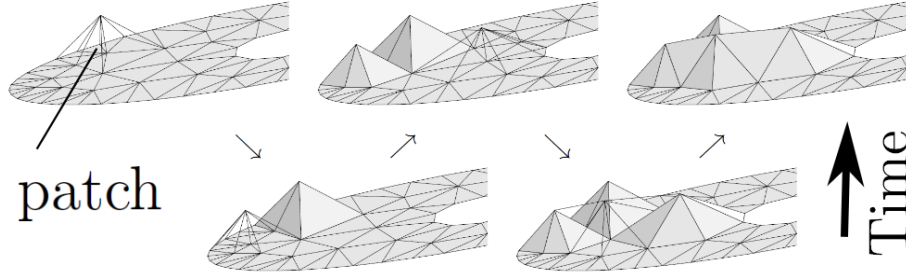


Figure 7.5: The patch-by-patch solution procedure for a $2d \times \mathbb{R}$ problem. The causality constraint limits the time duration of a patch.

propagation is modeled in transient mode as hydraulic loads are ramped up to their sustained value in milliseconds, rather than seconds and minutes. This better demonstrates the ability of the model to detect contact intersection and load transfer in complex fracture networks.

The h -adaptive asynchronous spacetime discontinuous Galerkin (aSDG) finite element method [9, 10] is used for these dynamic fracture simulations. In lieu of a conventional time marching scheme, the aSDG method advances the solution in time by directly discretizing spacetime using *causal* unstructured grids. Figure 7.5 shows the *Tent Pitcher* [3] patch-by-patch solution procedure, where each time a small collection of elements, called a *patch*, is erected around a vertex with a local time coordinate. The time advance is limited so that the outflow faces of the patch are causal, *i.e.*, the elastic waves only exit through them, thus decoupling the solution of the patch from *future* neighbor elements on these faces. Starting from an initial triangulation in 2D, the patch-by-patch solution procedure eventually fills an analysis spacetime volume.

As opposed to bulk models, *e.g.*, a continuous damage model, fracture is modeled by sharp interface cracks in the present study. The aSDG adaptive operations are used for two purposes; first, as the cracks propagate high level of resolution is needed both in the bulk regions around them (and around sharp moving wave fronts) and along the fracture surfaces. The dual adaptivity scheme from [11], ensures that all these features are accurately and efficiently resolved by refinement and coarsening operations in spacetime. In addition, fracture-specific adaptive operations are used to align inter-element boundaries with crack propagation directions that are determined by a fracture criterion [158, 6]. Thus, the limited set of inter-element edge angles around a vertex in the finite element space front does not

inhibit or affect crack propagation in arbitrary directions. This advanced feature is critical in accurate capturing of complex fracture patterns in §8.5. In practice, many of the fracture simulations by the aSDG method start from tens to a few hundreds of elements in the initial front; as cracks start to nucleate and/or propagate, the spatial front is dynamically refined and coarsened to follow high gradient solution features and crack paths. For the fracture simulations reported in this manuscript, this process results in less than a few tens of thousands of elements in the spatial front.

Finally, in lieu of a traditional cohesive model, *e.g.*, [211, 221, 43], an interfacial damage model is used to model fracture. A damage parameter D is used to interpolate between bonded and debonded states of traction and velocity at an interface. Within the debonded phase, there are two states of separation and contact, wherein contact mode itself contains two possible states of contact–stick and contact–slip. Local Riemann problems are used to derive transient target solutions for tractions and velocities within each mode [8]. The details of incorporating these solutions in a dynamic contact and fracture model can be found in [7]. Although crack propagation by hydraulic fracturing is mostly tensile-mode dominant, the numerical results in §7.3.5 demonstrate that some fractures may propagate in shear-dominant mode when crack surfaces are in contact. Thus, the use of this fracture model with contact–stick and contact–slip modes is well-justified for these simulations.

7.3 Numerical results

The problems in this section are designed to demonstrate the ability of proposed methods in tracking crack connectivity and hydraulic load transfer as cracks grow and intersect, obtaining useful information about fracture network using the representation of cracks by SimpComp data structure, and effective regularization of pressure on fracture surfaces. The first problem in §7.3.1 demonstrates the ability of the aSDG method and the interfacial damage model in predicting hydraulically-driven crack propagation directions in rock. Next, the four general classes of problems presented in §7.3.2 to §7.3.5 focus on the effect of pressure regularization (when a fluid model is not incorporated), different types of interaction between a loaded crack and in-situ cracks (crack realignment, diversion and offsetting, and

penetration), modeling and post-processing for problems with multiple hydraulic loading sources, and the simulation of 2D reservoirs with different in-situ fracture patterns. Finally, the studies in §7.3.6 demonstrate how the mode of crack interactions and the number of activated hydraulic cracks in a reservoir change as a function of the loading rate.

For all problems considered, bulk and interface material properties of rock are: elastic modulus $E = 20$ GPa, mass density $\rho = 2500$ kg/m³, Poisson’s ratio $\nu = 0.20$. In addition, rock is under confining pressure of 2.425 MPa in all directions. Hydraulic load is ramped up from this ambient pressure to sustained hydraulic pressure of 19.4 MPa in a ramp time of 1 ms or 10 ms in §7.3.2 to §7.3.5. While a single hydraulic fracturing injection often takes a duration in the order of minutes, the studies that consider the early pump-in stage in the area close to the well [227], or consider more dynamic and/or cyclic application of loading [231, 150] deal with load ramp times in the range 0.1 to 10 s [13]. These loading rates can also be associated with propellant fracturing where the pressure build-up is due to propellant burning accompanied by a gas combustion similar to pulse fracturing methods. In [101] a hybrid propellant fracturing method is proposed, where similar to hydraulic fracturing perforations are created around the wellbore. The relatively slower loading rate of propellant fracturing, compared to some other explosive methods, permits the initial crack surfaces to be effectively loaded and induce subsequent fracture formation in a reservoir. The main purpose for using fast ramp times of 1 ms or 10 ms is to induce more complex fracture patterns and intersections that better demonstrate the abilities of the proposed approaches for tracking crack connectivity and load transfer¹. In §7.3.6 ramp times up to one second are considered and it is shown that while the crack propagation patterns become simpler and approach their quasi-static limit, there is still the need to handle the interactions of hydraulically propagating cracks with in-situ cracks.

Similar to a traditional *Traction-Separation Relations* (TSRs), the contact-damage model described in §7.2.4 has a fracture strength scale $\tilde{\sigma}$, which corresponds to the material’s quasi-static strength limit. However, unlike the displacement (separation) scale $\tilde{\delta}$ used in TSRs,

¹The use of longer timescales is feasible and would be more applicable when implementing simulation parameters that mimic more realistic simulations. There is no computational restriction on the use of longer timescales in this work; however, the shorter time-scale is used to validate the capabilities of the computational framework in modeling highly dynamic problems and the subsequent complex fracture patterns.

the model has an intrinsic fracture time scale, namely the relaxation time $\tilde{\tau}$. As shown in [5], *cf.* equation (39b), an intrinsic displacement scale can be derived from $\tilde{\tau}$. Still due to different formulation approaches, even for the same $\tilde{\sigma}$ and $\tilde{\delta}$, the damage model used here and a TSR will not have identical fracture responses. The third parameter of the damage model is the mode mixity parameter β that similar to [43] combines normal and tangential tractions into a scalar effective stress, used for the evolution of damage value. Friction coefficient, k , is the only parameter of the contact model. Finally, there are two regularization parameters; a nondimensional parameter $\underline{\delta}'$ [8] controls the amount of interpenetration relative to $\tilde{\delta}$, whereas $\bar{\delta}'$ regularizes the application of hydraulic pressure, as described in §7.2.3; *cf.* (7.2). For the simulations in this section the following fracture and contact parameters are used unless otherwise mentioned for specific examples: fracture strength $\tilde{\sigma} = 2$ MPa, $\tilde{\tau} = 0.03$ ms to 0.05 ms, $\beta = 0$ to 1, and $k = 0.3$. Finally, the regularization parameters $\underline{\delta}'$ and $\bar{\delta}'$ are chosen in the range 0.1 to 0.01. For more details on the damage and contact models the reader is referred to [6] and [8], respectively.

7.3.1 Hydraulic fracture reorientation

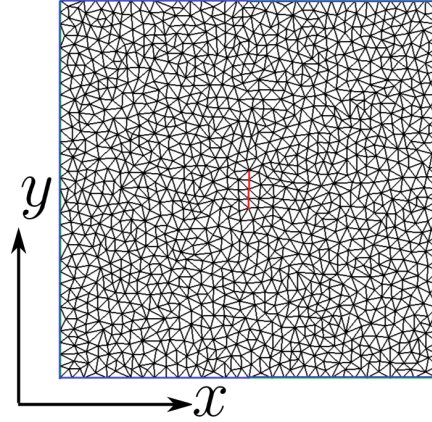


Figure 7.6: Initial computational domain and loaded crack for the hydraulic reorientation problem. The in-situ normal stresses are $\sigma_{h,xx} = 19.4$ MPa and $\sigma_{h,yy} = 9.7$ MPa.

This section provides an example of crack reorientation from an open borehole. Figure 7.6 shows the computational domain for this problem where a crack of half length $a_0 = 0.02$ m is centered in a computational square domain of edge length 0.4 m. The crack is oriented at

$\gamma = 89^\circ$ with respect to the x axis and the domain is under ambient stresses $\sigma_{h,xx} = 19.4$ MPa, and $\sigma_{h,yy} = 9.7$ MPa. The same material properties are used for the rock ($E = 20$ GPa, mass density $\rho = 2500$ kg/m³, Poisson's ratio $\nu = 0.20$), except $\tilde{\sigma} = 4$ MPa.

The interaction between the orientation of the initial crack, applied hydraulic pressure p_h , and in-situ pressure anisotropy results in different levels of crack path reorientation. Since $\sigma_{h,yy} < \sigma_{h,xx}$ the preferred crack propagation direction is along the x direction. The lower p_h the faster the crack propagating from the open borehole reorients itself with this direction. The 1° angle offset of the open borehole from the y -axis ensures that the crack propagation starts in mixed mode and the top and bottom propagations tend to extend to the right and left sides, respectively. This problem has been studied both experimentally and numerically by [217, 70, 33, 94] where for the numerical studies the *Linear Elastic Fracture Mechanics* (LEFM) theory is being used.

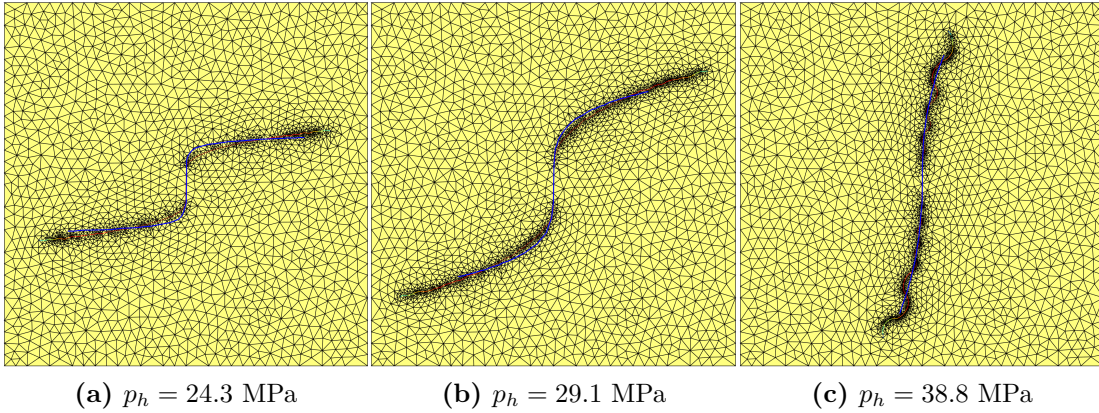


Figure 7.7: Comparison of the crack paths obtained by the aSDG method and the reference [70] (in solid blue line) for three fluid pressures p_h .

The comparison of results obtained by the aSDG method and from [70] are presented in Fig. 7.7. The crack paths from the aSDG results are shown by color-coded line segments (by their corresponding damage value) on the spatial front, while the results from by [70] are superimposed on the images. We note that the front mesh is different from the initial mesh shown in Fig. 7.6, particularly on around crack segments. The crack propagation direction is determined by the maximum circumferential effective stress criterion [6] and mesh adaptive operations in spacetime enable achieving proposed crack direction in any arbitrary direction [158, 6].

While the aSDG results are in good agreement with those from [70], two points should be clarified. First, the results in [70] are obtained by the LEFM theory, whereas herein an interfacial damage model [6] is used. It is demonstrated in [2] that even for very small load amplitudes, where the *small scale yielding* caveat of the LEFM theory holds, the results of the LEFM theory and the more realistic TSRs are different, particularly at the early stages of crack propagation. While, the interfacial damage model is different from a TSR, it still has the same intrinsic fracture scales as a TSR [5]. In fact, to compare the results with [70], we matched the fracture energy scale of the interfacial damage model, equation (39a) in [5], with the critical energy release rate value used in [70]. With the damage and TSR models providing a more realistic characterization of brittle fracture than the LEFM theory, the slight differences in crack paths in Fig. 7.7 are well expected. Second, in [70] cracks propagate in the quasi-static regime, while herein the full set of elastodynamic equations are solved. To get closer to quasi-static limit the low loading ramp time of 4 s is used for this problem. In the remainder of the manuscript, higher loading rates are used to demonstrate the capability of the method in capturing complex crack interactions (see also §7.3.6 for a detailed study of the effect of the loading rate). However, as expected only a single crack propagates from each crack tip in Fig. 7.7. The slight oscillations for $p = 38.8$ MPa are explained from the dynamic brittle fracture theory where as the loading rate or load amplitude increases cracks tend to oscillate, followed by microcracking and bifurcation to dissipate excess input energy.

In all simulations, dual adaptive error indicators control the energy error both in the bulk and on fracture surfaces [11]. Having reasonable values for the tolerances, not only prevents premature crack arrests or unsuccessful propagations, but also ensures that the crack path converges as the tolerances are tightened. Rather than reproducing similar studies for the problem in this subsection, we refer to reader to the extensive studies reported in [6] on this matter. In short, this example demonstrates the ability of the adaptive aSDG method to accurately capture crack patterns in hydraulic fracture applications.

7.3.2 Hydraulic pressure regularization

The SimpComp data structure and the algorithm described in §7.2.2 is general and does not depend on how the (hydraulic) pressure is applied on crack surfaces. The pressure acting on crack surfaces can be a spatially uniform, as in many studies in the literature, or be obtained by using lubrication equation or other coupled hydro-mechanical models. As explained in §7.2.3, pressure regularization based on the aperture of (hydraulically) loaded cracks that are connected to a crack segment provides a means to gradually apply the loads to newly loaded crack segments upon crack intersection. The two problems in this section demonstrate the need for this regularization scheme when a fluid model is not used to compute the hydraulic load. The crack nucleation is intentionally deactivated in these two problems to prevent the penetration of the hydraulic crack through the vertical crack or the nucleation of any cracks off of it. This better illustrates how the hydraulic load transmits to the vertical crack and propagates across its length.

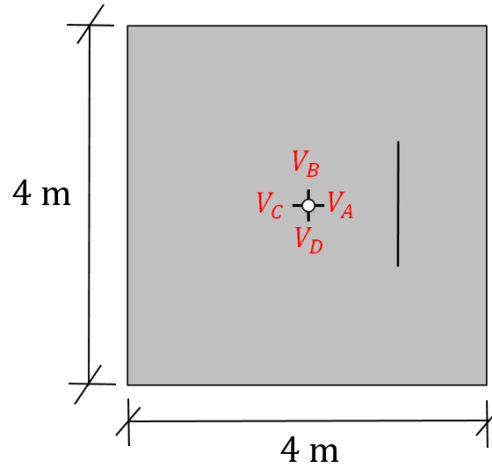


Figure 7.8: Sketch of four oriented perforations interacting with a single vertical in-situ crack.

Figure 7.8 shows the schematic of a problem where a hydraulically loaded fracture intersects a vertically oriented unloaded in-situ crack. The hydraulic load ramp time for this problem is 1 millisecond. A sequence of the solution visualization of this problem is shown in Fig. 7.9, where strain and kinetic energies are mapped to color and height fields, respectively. Figure 7.9a shows the instant at which scattered elastic waves from propagating

hydraulic fracture reach the tips of the vertical crack. Figures 7.9b to 7.9d show a time period of less than $25 \mu\text{s}$ where the leading branches of hydraulically loaded cracks intersect the vertical crack.

Herein, the application of hydraulic pressure is intentionally not regularized to illustrate the types of problems that can occur. The very short application of loads better demonstrates these problems. The first problem is the sudden jump in the pressure exerted on the vertical crack faces. At the time of intersection, $t \approx 800 \mu\text{s}$, hydraulic pressure is $p_h \approx 16 \text{ MPa}$. That is, upon intersection the pressure instantly jumps from the ambient pressure of 2.425 MPa to $p_h \approx 16 \text{ MPa}$. The spikes in these figures correspond to a sudden jump in material velocity field induced by instantaneous application of hydraulic load. The second problem is that as shown the entire crack line experiences the hydraulic load right at the time of intersection, as shown in Fig. 7.9b. Aside from these nonphysical responses, the non-regularized application of hydraulic load requires high levels of mesh refinement due to the induced numerical errors. The sharp and spread velocity spikes in Figs. 7.9b-f and particularly the high velocity spike near the point of intersection in Fig. 7.9f are some examples of numerical artifacts.

For the second problem we use a parameter $\delta'_p = 0.1$, *cf.* (7.2), to demonstrate the effect of pressure regularization. Similar to previous problem, a horizontal and hydraulically loaded crack intersects an unloaded vertical crack and the hydraulic pressure ramp time of 1 millisecond. The initial configuration is shown in Fig. 7.10. Figures 7.11 and 7.12 show the strain energy density solutions and the finite element front meshes for six different stages of solution, respectively. The solution visualization images are generated by passing a time plane through the spacetime elements and showing the solution on these constant time planes. On the other hand, front meshes are not synchronized and show the spatial view of the spacetime finite element mesh at a time when all the vertices of the front have time coordinates greater than or equal to the target time. That is why the times for the front mesh are shown as approximate values. The front mesh visualizations are used for two purposes in the entire numerical results section; first, they show the level of mesh refinement and crack patterns on the finite element front. Second, the crack segments are color-coded by the value of interfacial damage D or pressure factor f_p (the range of $[0 \ 1]$ is mapped to

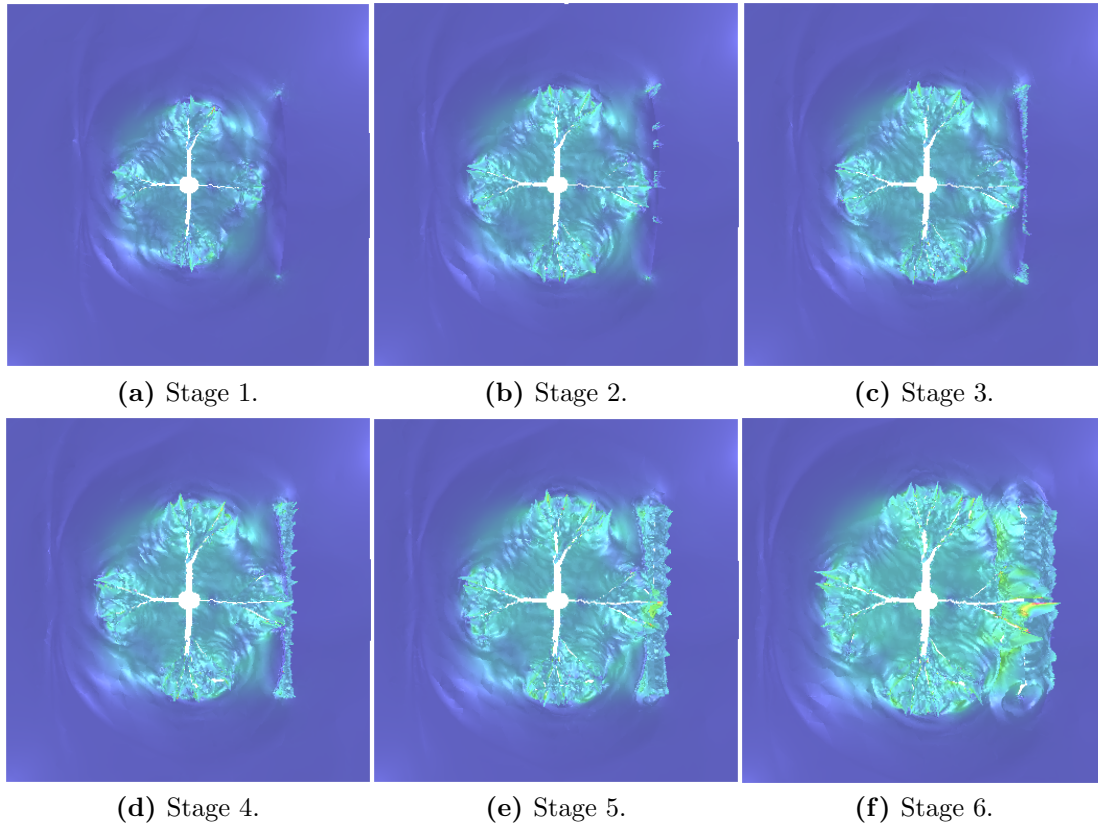


Figure 7.9: A sequence of solution visualizations of interaction of a hydraulically-loaded moving crack with an unloaded vertical crack. Lack of pressure regularization results in sharp jumps in stress and velocity. Color and height fields depict strain and kinetic energy densities, respectively.

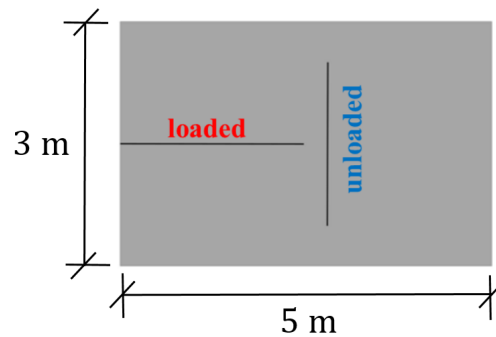


Figure 7.10: Sketch of the problem for modeling the interaction of a hydraulically-loaded horizontal crack with an unloaded in-situ vertical crack.

a blue to red color range) to demonstrate the level of damage or pressure regularization on that segment, respectively.

Figures 7.11a and Fig. 7.12a show the crack propagation slightly before the hydraulically loaded crack intersects the vertical crack. While the problem geometry and loading is symmetric with respect to the horizontal crack, the propagated crack has moved downward. This is caused by crack path oscillations that are commonly observed in dynamic fracture; at the early stages of crack propagation, cracks start to oscillate more as the crack accelerates. This mechanism enables quasi-brittle materials to dissipate more energy by increasing the overall length of propagated cracks. Figures 7.11b and 7.12b show a time slightly after the intersection of the cracks. As evident, the regularization eliminates instantaneous loading of the vertical crack and the propagation of the pressure to its entire length.

The next two figures in each sequence show the advancement of hydraulically loaded sections on the vertical crack. In Figs. 7.11c and 7.11d we observe process zone regions on the vertical crack where the interface transitions from ambient compressive stress state on the outer sides to separation mode induced by the hydraulic pressure. The high level of mesh refinement in these zones in Figs. 7.12c and 7.12d corresponds to high gradients experienced in the values of target compressive traction on the interface. As shown in solution and front mesh figures, the waves emanated from these contact transition points generate waves in the bulk with diagonal fronts. Finally, Figs. 7.11e-f and 7.12e-f correspond to times after the contact transition point reaches the tips of the vertical crack. The hydraulic load causes the propagation of new cracks off of these tips.

7.3.3 Interaction of a hydraulically loaded crack with in-situ cracks

Herein, the numerical results demonstrate the ability of the proposed scheme to handle interaction and intersections of a hydraulically loaded crack with in-situ (micro)cracks. Figure 7.13 shows the geometry of the computational domain. The length of microcracks follows a Weibull distribution and their orientation follows a uniform distribution for all possible angles. The microcracks are randomly positioned in the spatial domain, until the

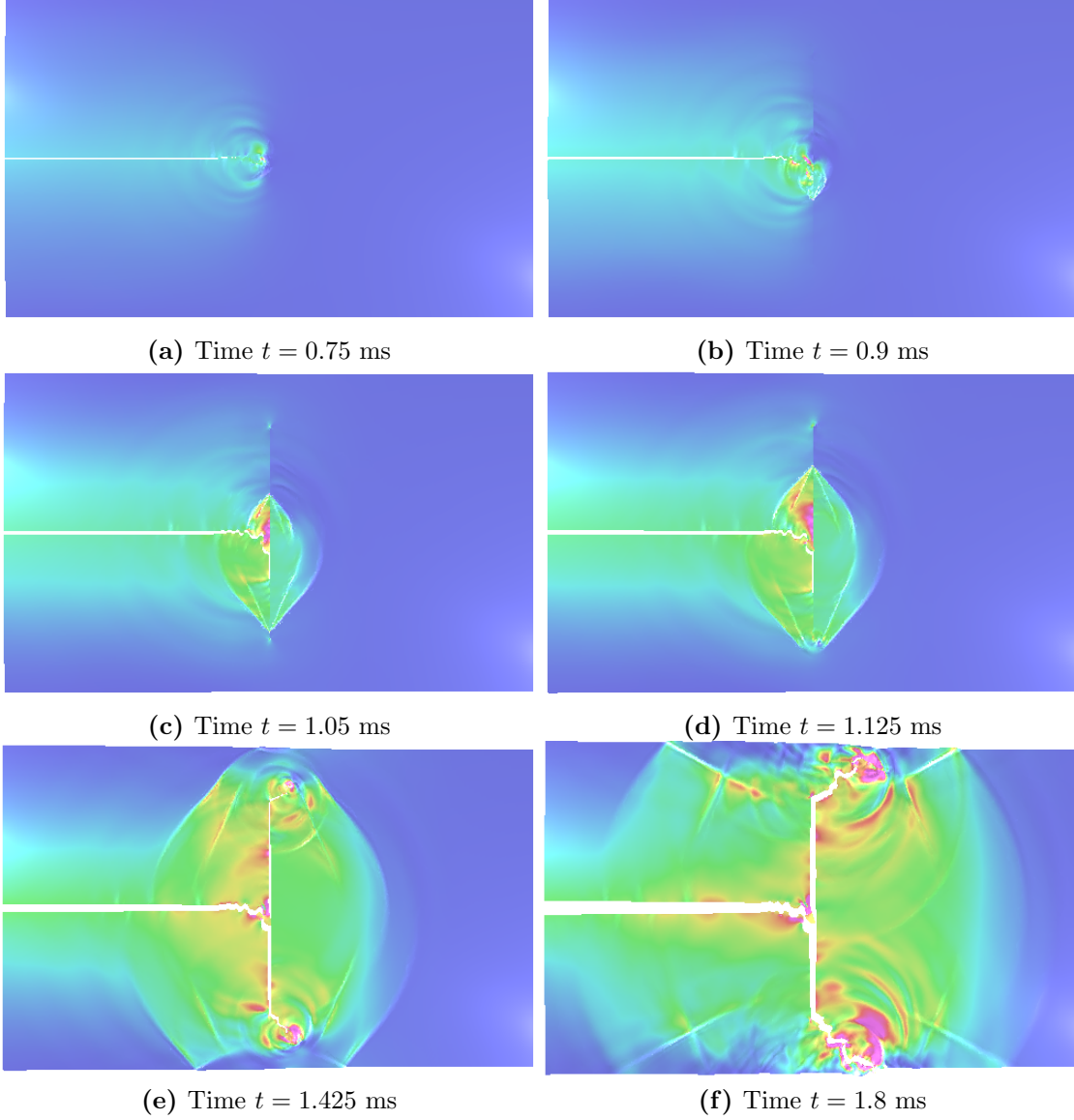


Figure 7.11: A sequence of solution visualizations for the interaction of a hydraulically-loaded moving crack with an unloaded vertical crack. Strain energy is mapped to color field.

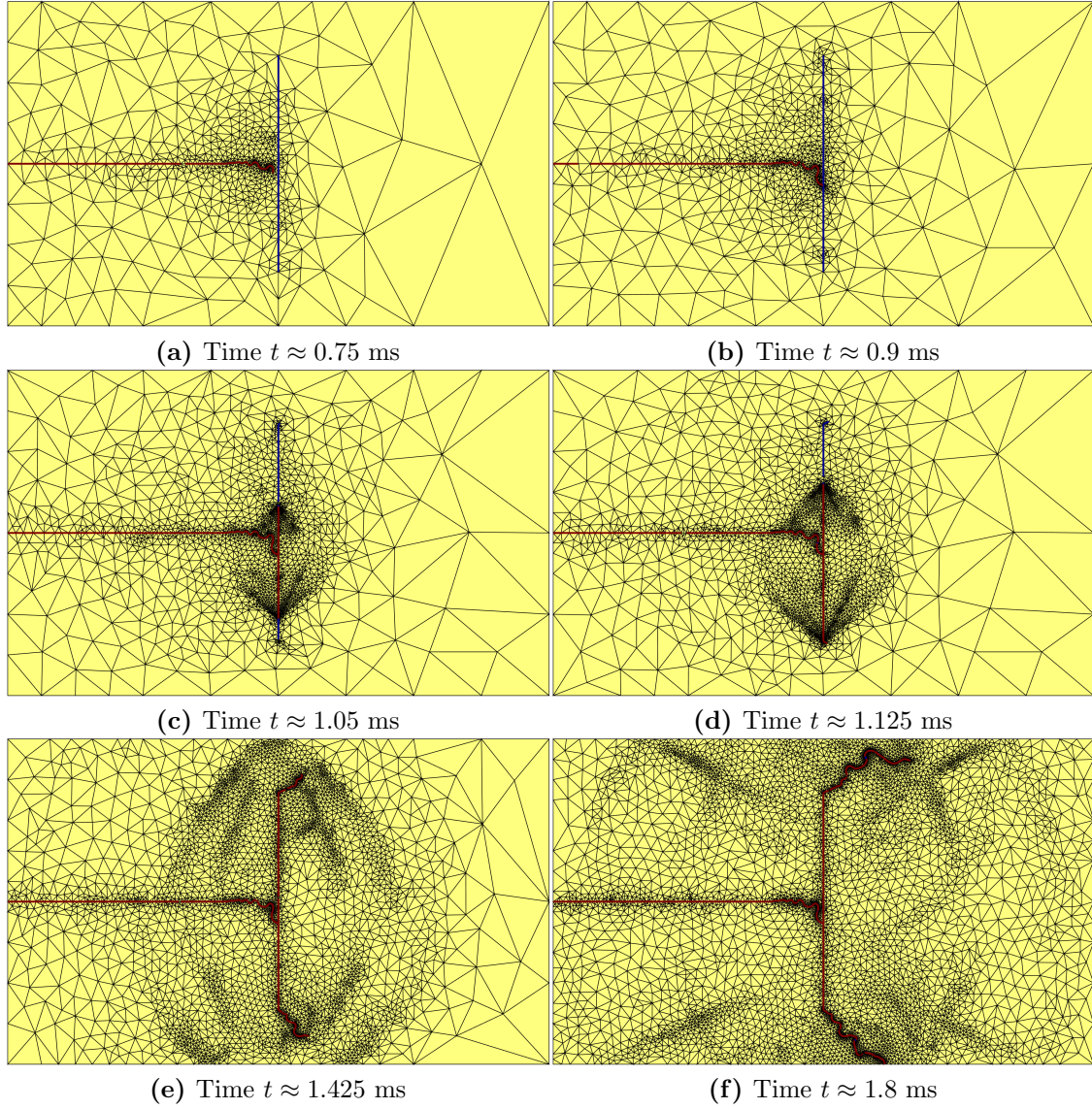


Figure 7.12: A sequence of front mesh visualizations for the interaction of a hydraulically-loaded moving crack with an unloaded vertical crack. Pressure factors on crack segments in the range, $f_p \in [0, 1]$, are mapped to a blue-to-red color range.

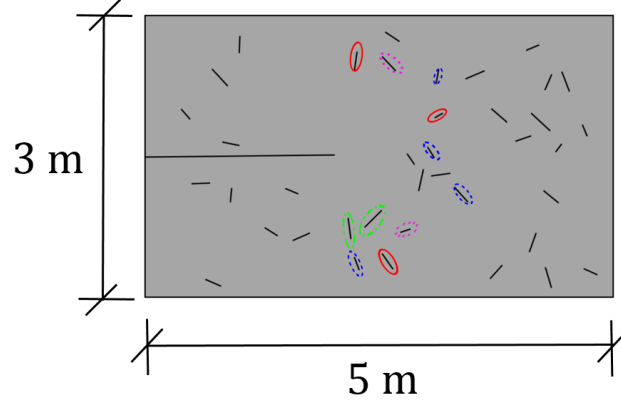


Figure 7.13: The computational domain for a problem where a horizontal hydraulically loaded crack propagates and interacts with randomly distributed in-situ cracks. The imposed ellipses are used to characterize specific crack interactions. The description of each type can be found in the caption of Fig. 7.15.

desired crack density ² of $\alpha = 0.1$ is achieved. The hydraulic load ramp time for this problem is 1 millisecond and the initial hydraulic pressure is 4.85 MPa.

Figure 7.14 shows a sequence of front mesh (left side) and solution (right side) visualizations for this problem. Figures 7.14a and 7.14b shows an early stage of hydraulic fracture propagation before its intersection with any in-situ cracks. The rather early bifurcation events (crack branchings) are due to the very dynamic nature of the hydraulic loading for this problem, wherein the maximum pressure is attained in 1 millisecond. Figures 7.14c and 7.14d illustrate a stage at which an already complex hydraulic fracture network begins to intersect in-situ cracks. The proposed algorithms from §7.2.1 can efficiently detect any intersection between the hydraulically loaded disjoint set and in-situ cracks and accordingly transfer hydraulic load to them. The intersection with in-situ cracks can happen either at one of their end points or along their length. In either case, these newly hydraulically loaded cracks can propagate from their free end point(s). A later stage of crack propagation is shown in Figs. 7.14e and 7.14f.

Several mechanisms of crack interaction can be observed in this example. The instances of these different types are encircled in Fig. 7.14e with different color and line styles. The encircled cracks can also be found in Figs. 7.13, 7.14e, and 7.15. The three instances of

²Crack density is a non dimensional quantity defined as the sum of the squares of crack lengths per unit area of the bulk for 2D problems.

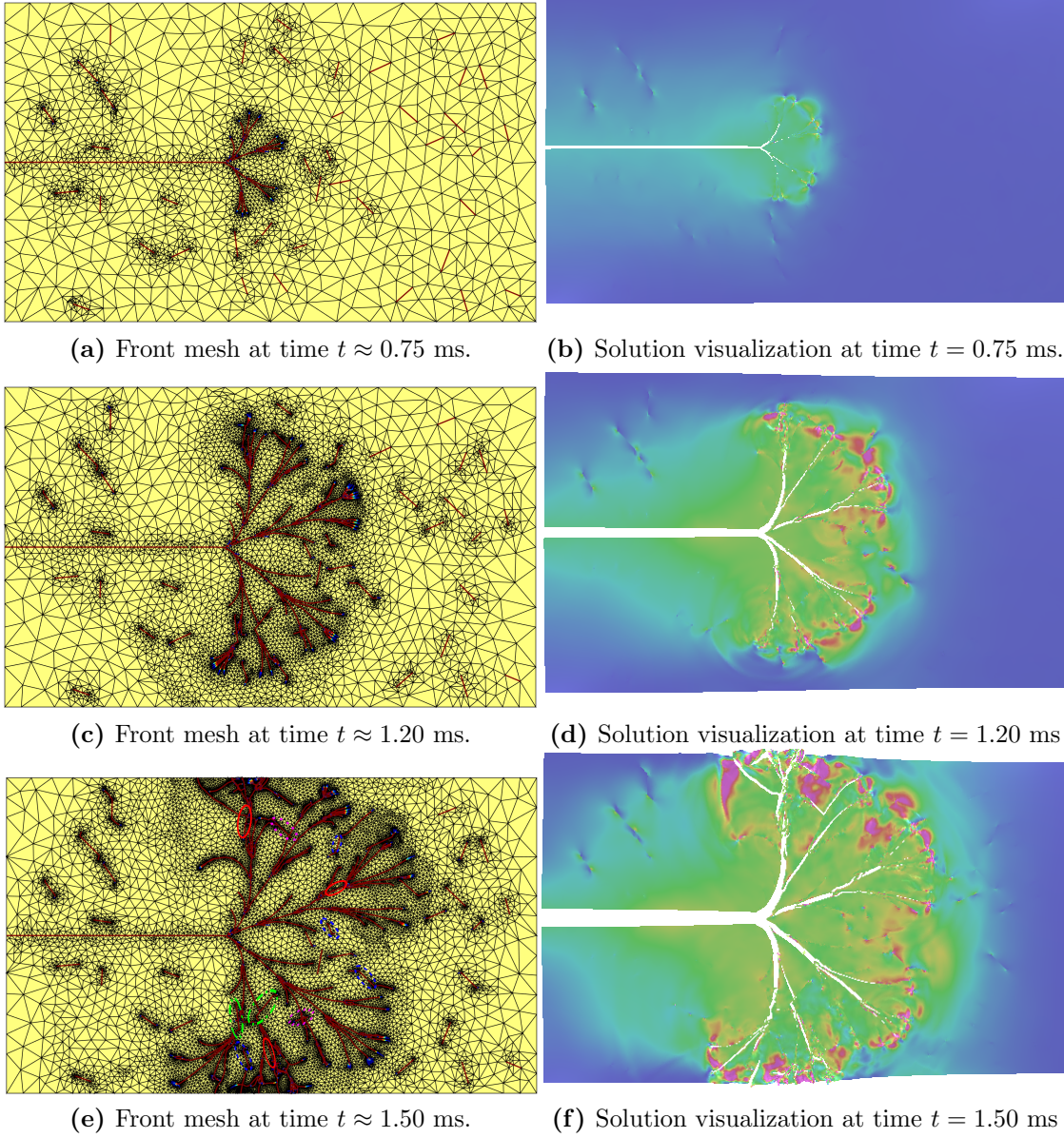


Figure 7.14: Front meshes (left side) and strain energy solution visualization (right side) for the geometry depicted in Fig. 7.13. A horizontal hydraulically loaded crack interacts with randomly distributed in-situ cracks. For the front meshes the crack segments are color-coded by the interfacial damage value D . In (f) the imposed ellipses are used to characterize specific crack interactions. The description of each type can be found in the caption of Fig. 7.15.

slight realignment, depicted by solid red ellipses, correspond to cases where the direction of hydraulically propagating crack is very close to an in-situ crack. These cracks are aligned with the in-situ cracks and exit from their far end with slight re-alignment. If the angle difference between the incoming and in-situ crack increases further, the in-situ crack diverts and offsets the hydraulically propagating crack; that is, the loaded crack's propagation direction is aligned with the in-situ crack direction before it exits from the in-situ crack's end point(s) with a continued propagation direction that may not be close to either of the in-situ or incoming crack's direction. Two instances of crack diversion and offsetting are shown by dot-dashed green ellipses in the figure. Finally, if the angle difference between incoming and in-situ cracks is so large, *e.g.*, if they are almost normal to each other, the hydraulically loaded crack may just penetrate through the in-situ crack. Two examples of crack penetration are shown by dotted purple ellipses.

It should be noted that in any of the previous cases, especially cases where the hydraulically loaded crack penetrated an in-situ crack, the incoming crack can in fact be arrested. However, capturing arrest events may require the use of a fluid model for computing fluid pressure as the pressure may not be large enough to drive the hydraulic fracture past an in-situ crack. This aspect will be studied in future works.

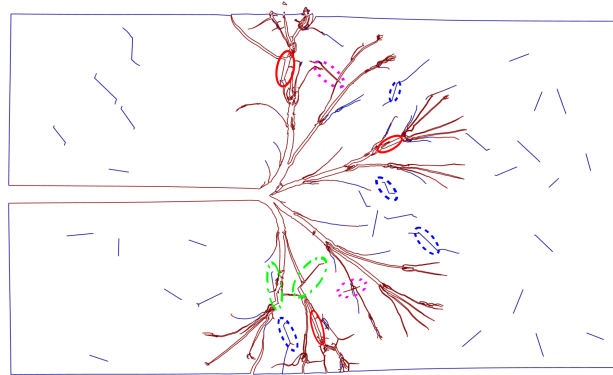


Figure 7.15: Deformed shape of the domain for the geometry shown in Fig. 7.13 at time $t = 1.50$ ms. Crack segments are color-coded by the interfacial pressure factor f_p . Solid red, dot-dashed green, and dotted purple ellipses correspond to crack path alignment, diversion and offset, and penetration events. Crack propagation by wave scattering events are shown by dashed blue ellipses.

In all previous cases there is an intersection between a hydraulically driven crack and an in-situ crack. Upon intersection the in-situ crack is connected to a loaded disjoint set and may become active and propagate if the incoming crack does not penetrate through it (or gets arrested). In dynamic setting, some of these in-situ cracks can start to propagate even before they are connected to the hydraulically loaded fracture network. Four examples are shown by dashed blue lines in Figs. 7.14e and 7.15, where each of these in-situ cracks is activated and starts to propagate when scattered waves reach one of its tips. High strain energy densities around these cracks can be observed in Figs. 7.14d and 7.14f. It is noted that in all front mesh views, only the tips of propagating cracks experience incomplete damage, which is expected as they are the active fracture process zones. The deformed shape of the domain and crack surfaces at time $t = 1.50$ ms is shown in Fig. 7.15.

7.3.4 Crack connectivity information

The facet/cofacet connectivity information in SimpComp data structure and the two maps DSET and SET2L provide very useful information about a fracture network. Some examples are total crack length for different connected sets of crack, levels of microcracks with respect to their main mother crack, and shortest distance between any two points in a connected set. Figure 7.8 shows the set-up for this problem, where the base vertices of four perforations, at angles $\{0^\circ, 90^\circ, 180^\circ, 270^\circ\}$ with respect horizon are labeled as $\{V_A, V_B, V_C, V_D\}$, respectively. Similar to the first problem in §7.3.2, these initial cracks are hydraulically loaded and will eventually intersect the in-situ vertical crack in front of V_A . The load ramp time for this problem is 10 milliseconds. Before the intersection of any of the cracks there are 5 distinct disjoint sets, four associated with vertices V_A to V_D , and one associated with the vertical crack. We demonstrate that how the crack length for each of these disjoint sets and the total crack length can be tracked for this problem.

Figures 7.16 and 7.17 show a sequence of front mesh and deformed shape for this problem, respectively. As before, the front mesh images are asynchronous and are provided to demonstrate the level of mesh adaptivity. The crack segments in Fig. 7.16 are color-coded by pressure factor, f_p , with $[0, 1]$ being mapped to a blue to color range. On the other

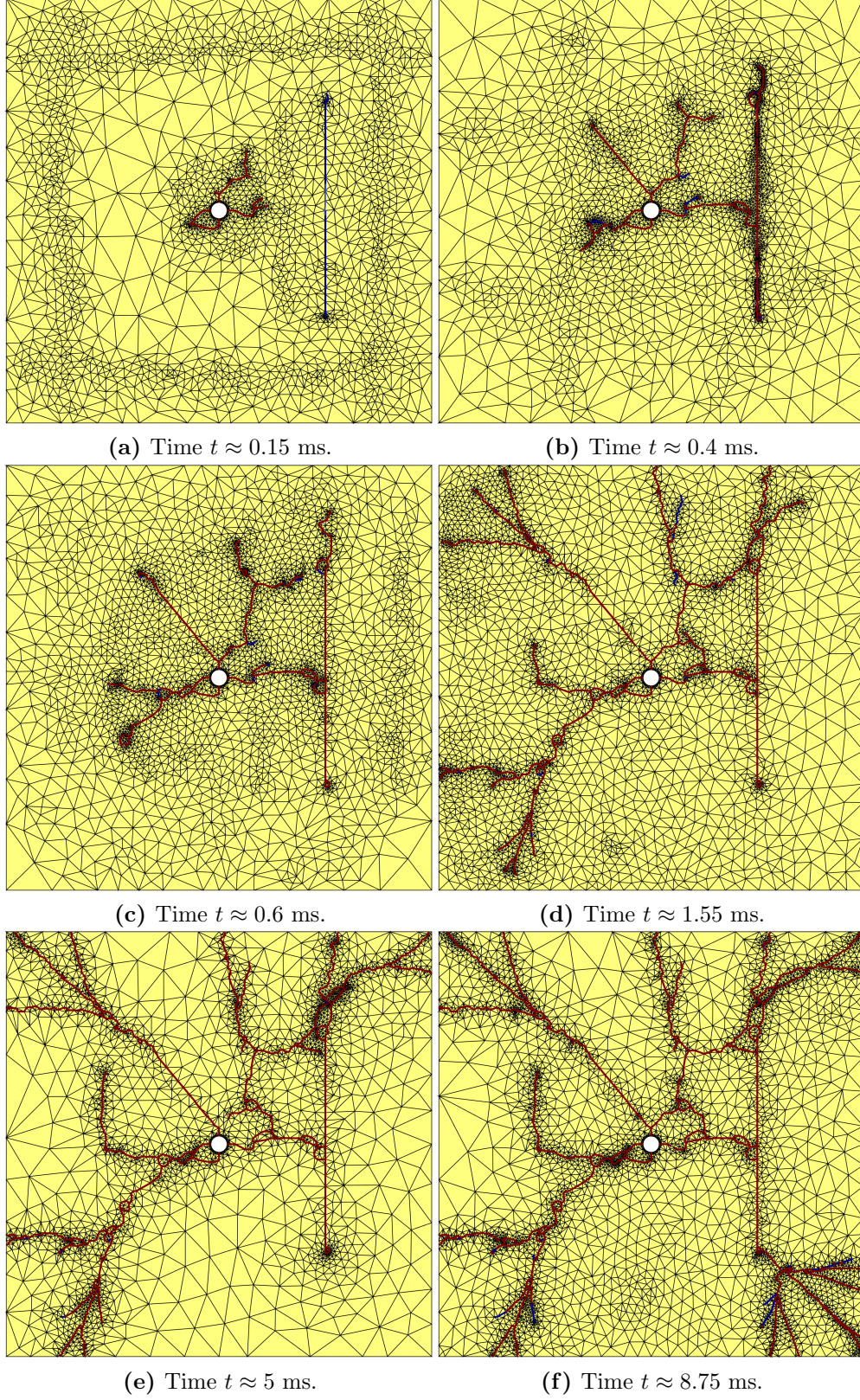


Figure 7.16: A sequence of front meshes for the problem with four oriented hydraulically loaded cracks interacting with a vertically oriented in-situ crack. Crack segments are color-coded by pressure factor $f_p \in [0, 1]$.

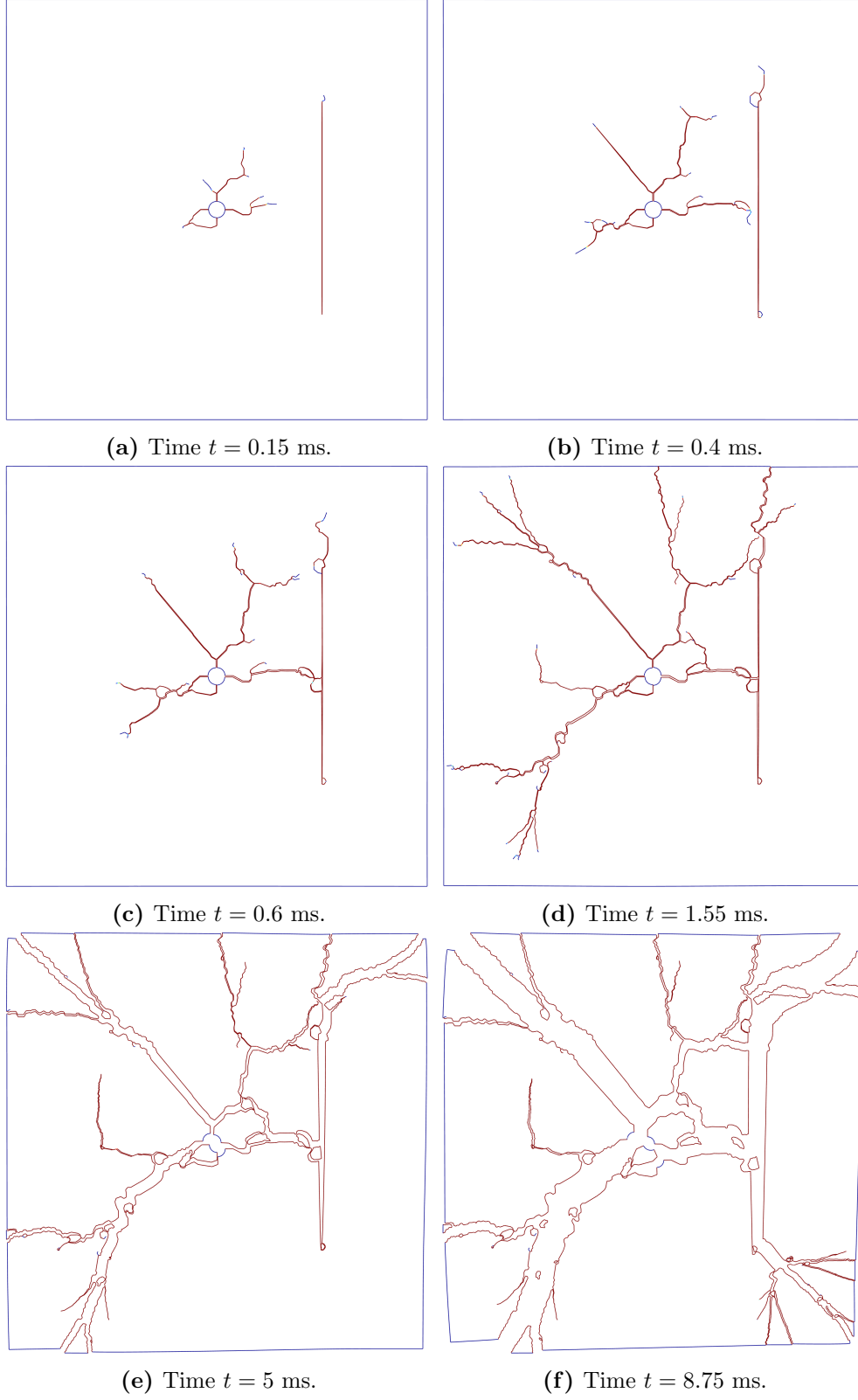


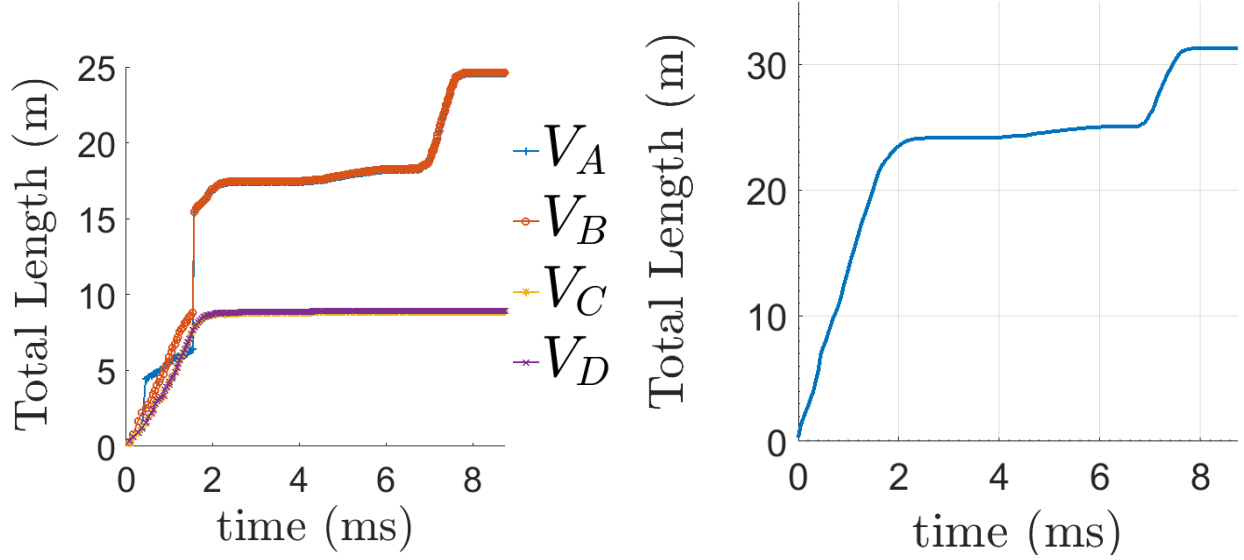
Figure 7.17: A sequence of deformed shape visualizations for the problem with four oriented hydraulically loaded cracks interacting with a vertically oriented in-situ crack. Crack segments are color-coded by the interfacial damage value $D \in [0, 1]$.

hand, the deformed shape figures are synchronous. In these figures, the damage value D is color-coded.

Figures 7.16a and 7.17a show the solution at very early stage of crack propagation. It is evident that cracks from distinct groups associated with V_C and V_D have already intersected on the lower left side of the wellbore. Figures 7.16b and 7.17b show the solution just before the crack propagated from V_A intersects the vertical crack. The blue color of the vertical crack in Figs. 7.16a is due the fact that the vertical crack is not connected to any of the loaded disjoint sets emanated from vertices V_A to V_D . The solution at time $t = 0.6$ ms is shown in Figs. 7.16c and 7.17c. As can be observed, after the intersection the crack segments in the vertical crack are in the same disjoint set that V_A belongs to. At this time, except at the tip of propagating (micro)cracks where normalized aperture is below δ'_p , all points on crack segments have a pressure factor of $f_p = 1$. The figures 7.16d and 7.17d show the solution at or slightly after time $t = 1.55$, where the disjoint sets emanating from V_A and V_B have just merged by the intersection of two microcracks in the upper right side of the wellbore. At this instant, there are only two distinct disjoint sets: one containing cracks propagated from V_A , V_B , and vertical crack, and the other containing cracks propagated from V_C and V_D . Finally in figures 7.16e, 7.17e ($t = 5$ ms) and Figs. 7.16f and 7.17f ($t = 8.75$ ms), the solutions for later times are shown. As evident, the topology of the crack pattern is not changed significantly past time $t = 1.55$; however, the crack surfaces are further separated.

It is noted that crack path oscillations, microcracking, and crack branching (bifurcation) events observed for these problems are commonly observed in quasi-brittle fracture to dissipate excessive energy input to the system under such dynamic loading scenarios. These features are much less frequent in conventional hydraulic fracturing. Also, in comparison for the results from a domain with in-situ microcracks, *cf.* Figs. 7.14 and 7.15, it is observed that such dynamic effects occur more freely in this example, as crack path oscillation, branching, and microcracking, are not inhibited or affected by in-situ cracks as for the problem in §7.3.3.

The total network crack length was tracked during solution time to demonstrate the capability of dynamically monitoring and updating the geometric and physics based information of connected fractures sets. This can be seen in Fig. 7.18. Figure 7.18a shows how the length of fractures evolves over time for the four disjoint sets associated with V_A



(a) Total length of cracks connected to each of the vertices V_A , V_B , V_C , and V_D . (b) Total length of hydraulically loaded cracks.

Figure 7.18: Progression of hydraulically loaded crack lengths versus time.

to V_D . As evident from Fig. 7.17a, the disjoint sets associated with V_C and V_D merge very early ($t \leq 0.05$ ms) due to the intersection of these two disjoint sets at the lower left side of the wellbore. Thus, their crack length curves are identical for $t \geq 0.05$ ms in Fig. 7.18a. The second major intersection occurs at $t \approx 0.4$ ms when the disjoint set associated with V_A intersects the vertical crack. Since the vertical crack is of length 2 m, there is a sudden jump in the length of this disjoint set after this intersection. Finally, the disjoint sets associated with V_A and V_B intersect at $t \approx 1.5$ ms. The merge of their corresponding crack length curves at this time, and the sudden increase to their merged disjoint set crack length (which is caused by the addition of the crack lengths of the two disjoint sets before intersection) can be observed at $t \approx 1.5$ ms in the figure. Finally, the total crack length is shown in Fig. 7.18b where as observed there is a rather slow crack length growth from time $t = 1.5$ ms to $t = 7$ ms. This is due to little change in the crack network topology and crack propagation during this period. The fast increase to total crack length past $t = 7$ ms is contributed to the propagation and bifurcation of some cracks from the lower end of the vertical crack as shown in Figs. 7.16f and 7.17f.

7.3.5 Interaction of multiple hydraulically loaded cracks with in-situ cracks in a reservoir

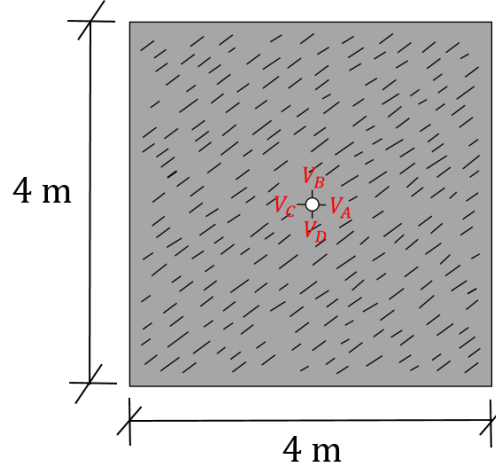


Figure 7.19: Sketch of the problem setup for a wellbore with four perforations, surrounded by in-situ cracks with density $\alpha = 0.5$ and 30° angular bias.

The objective of the examples examined in this section is to demonstrate the applicability of the proposed methods in tracking crack connectivity and load transfer in 2D reservoir simulations. Herein hydraulically loaded cracks, propagating from multiple perforations, interact with in-situ cracks. The geometry of the first problem considered is depicted in Fig. 7.19. Similar to the problem in §7.3.4, there are four perforations in the initial set-up. However, in this problem (and similar to the problem in §7.3.3), there is a population of in-situ (micro)cracks. The length of these cracks follows a Weibull distribution, while their orientation has a mean value of 30° and $\pm 3^\circ$ variation to mimic rocks with bedding planes. The ramp time for this problem is one millisecond and the initial hydraulic pressure is 4.85 MPa.

Figure 7.20 shows a sequence of solution visualizations where strain and kinetic energies are mapped to color and height fields, respectively. The 30° bias of in-situ cracks does not result in coherent and long crack propagations about 30° direction. However, they do affect the crack propagation pattern. For example, in Figs. 7.20c and 7.20d, the upward propagating vertical crack has some intermittent 30° crack propagation segments in its main branch, and in the crack branches and microcracks past the bifurcation point.

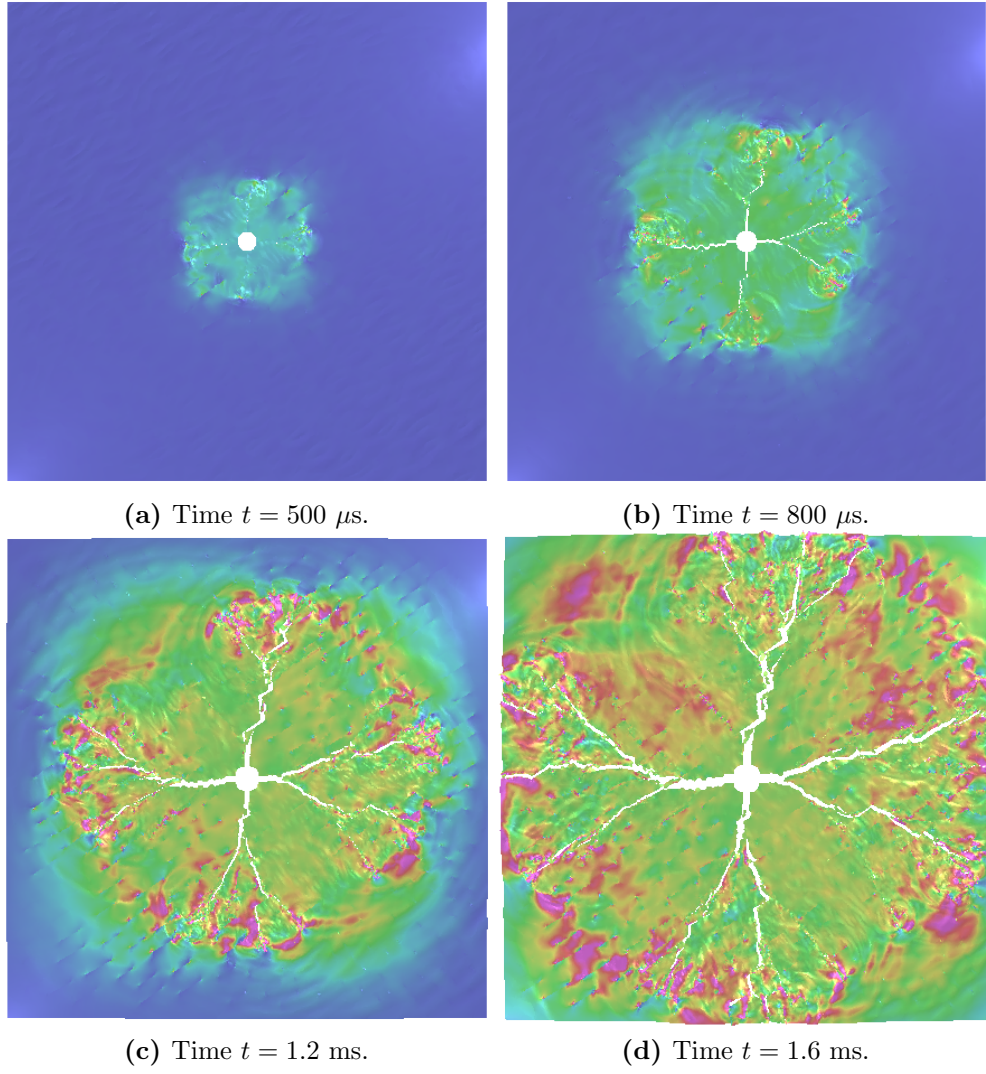


Figure 7.20: A sequence of solution visualizations for the problem set-up in Fig. 7.19. Color and height fields depict strain and kinetic energy densities, respectively.

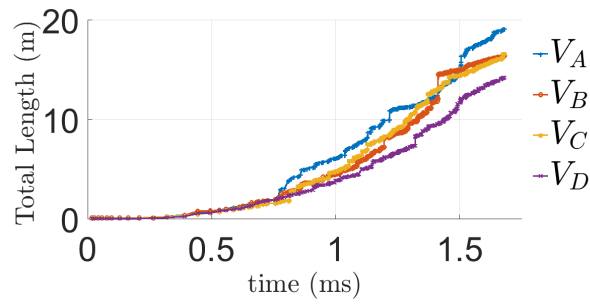


Figure 7.21: Total length of cracks connected to each of the vertices V_A , V_B , V_C , and V_D in Fig. 7.19.

Figure 7.21 compares the total crack lengths for the cracks propagation from each of the perforation bases. A few interesting observations can be made. First, at the earlier stage of crack propagation, all cracks propagate at relatively low speeds relative to Rayleigh wave speed and do not bifurcate or have microcracking events. Also in this stage, none of the main cracks interact with in-situ cracks. These two reasons contribute to all cracks experiencing the same crack growth rate at early times. Second, as the main cracks start to intersect the in-situ cracks, their propagation pattern and generated crack length are affected by the orientation of in-situ cracks. It appears that the horizontal main cracks generate a larger total length of crack in average, compared to vertical ones; the disjoint sets corresponding to V_A and V_D have the longest and shortest total lengths, respectively, while those corresponding to V_B and V_C have almost identical total crack lengths versus time. This can be attributed to easier propagation of horizontal cracks as they have a relative 30° angle with respect to in-situ cracks, as opposed to that of 60° for vertical cracks. For the same reason, it is observed that the path of vertical cracks is more affected by in-situ cracks. Third, unlike the four perforation well simulation from §7.3.4 none of the disjoint sets intersect during this simulation. We believe that in-situ cracks inhibit free propagation of the four distinct crack sets and prevent/retard their intersection. Realignment of crack orientations with 30° , occasional crack arrests and diversions, and the need for cracks to re-accelerate after their intersection with in-situ cracks can be viewed as reasons for this more inhibited crack propagation. Specifically, the need for cracks to re-accelerate automatically reduces crack branching and crack branching events as they are observed at higher crack speeds. Finally, while the computational domain is $4 \text{ m} \times 4 \text{ m}$, the total crack length for each main crack far exceeds this length ($\approx 20 \text{ m}$ propagation length). This is due to crack path oscillation, microcracking, crack branching, and merging events with in-situ cracks.

Figure 7.22 compares crack paths for different in-situ crack patterns, wherein two different crack densities ($\alpha = 0.25$ and 0.5) and orientation bias forms (no bias and 30° bias) are used. Several observations can be made. First, the 30° bias of in-situ cracks results in intermittent crack propagation segments roughly along 30° angle. These segments are more coherent for horizontal main cracks in both Figs. 7.22b and 7.22d. Conversely, main vertical cracks are more affected by in-situ cracks. Second, again for these two examples the cracks propagating

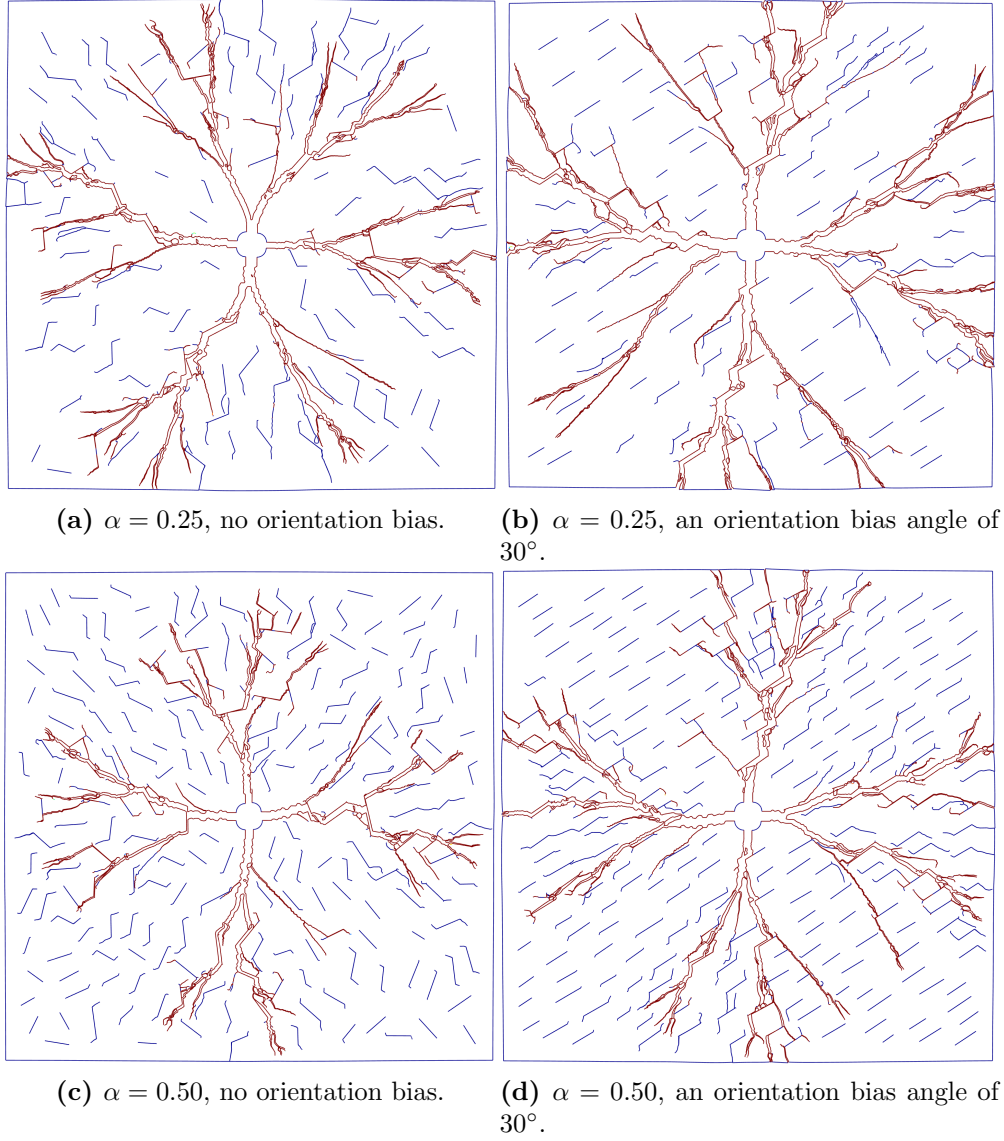


Figure 7.22: Comparison of hydraulic fracture patterns and deformed shapes for different initial in-situ crack patterns (crack density $\alpha = 0.25$ versus 0.50 , and no versus 30° orientation bias). Pressure factors on crack segments in the range, $f_p \in [0, 1]$, are mapped to a blue-to-red color range.

rather normal to in-situ cracks have smaller aperture and their propagation is mostly in shear mode. For $\alpha = 0.50$, these two cracks can be seen in both Figs. 7.22d and 7.20d on the lower side and left side of the cracks propagating from V_A and V_B , respectively. Third, there are many winged-shaped cracks in all examples considered. These cracks propagate off of the tips of in-situ cracks due to incident scattered waves and not from direct application of hydraulic load on their faces. The zero pressure factor of these cracks ($f_p = 0$), implied by their blue color, confirms that they are not connected to loaded cracks.

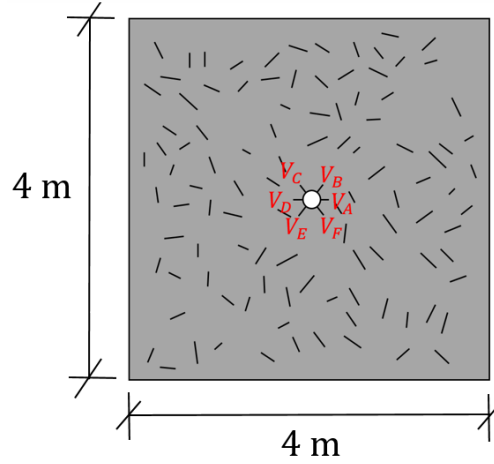


Figure 7.23: Sketch of problem setup for a wellbore with six perforations surrounded by in-situ cracks with density $\alpha = 0.5$.

The last example demonstrates the propagation of hydraulically loaded cracks in a domain with 6 perforations at angles $\{0^\circ, 60^\circ, 120^\circ, 180^\circ, 240^\circ, 300^\circ\}$ from horizontal axis with crack density $\alpha = 0.5$. A sequence of solution visualizations is shown in Fig. 7.24. As observed, all main cracks propagate in an overall angle close to their initial perforation angle, with those emanated from V_C , V_E , and V_A showing wider affected area. The total crack lengths for cracks connected to V_A to V_F and an image of the deformed geometry are shown in Figs. 7.25 and 7.26, respectively. As in previous examples in this section, none of the initial distinct loading sets intersect. One interesting observation with this problem is the activation of all six perforations. This and the activation of all perforations in the other examples herein are contributed to the short hydraulic load ramp time of one millisecond. The high height field values in Fig. 7.24 attest to dynamic nature of crack propagation. This observation is

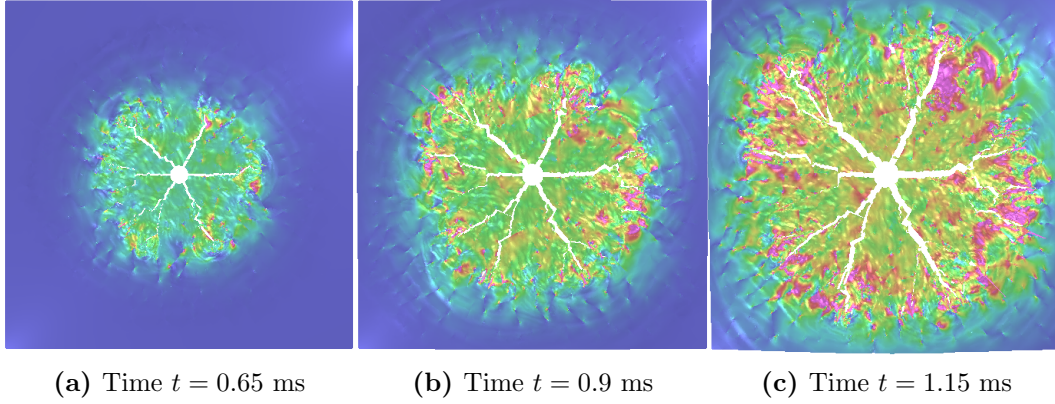


Figure 7.24: A sequence of solution visualizations for the problem set-up in Fig. 7.23. Color and height fields depict strain and kinetic energy densities, respectively.

consistent with the results in [13], wherein for load ramp times shorter than 100 milliseconds and low in-situ stress anisotropy all initial perforations become active.

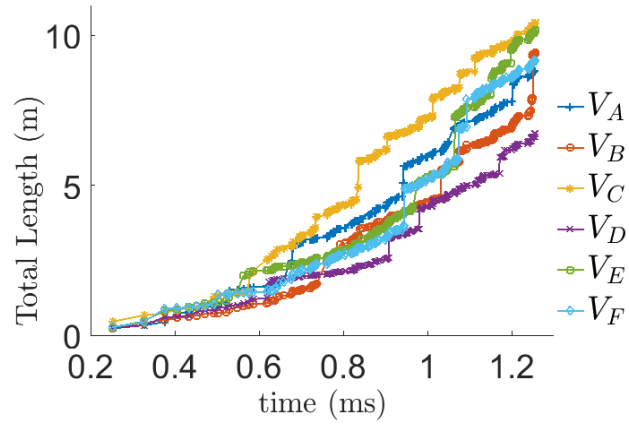


Figure 7.25: Total length of cracks connected to each of the vertices V_A to V_F in Fig. 7.23.

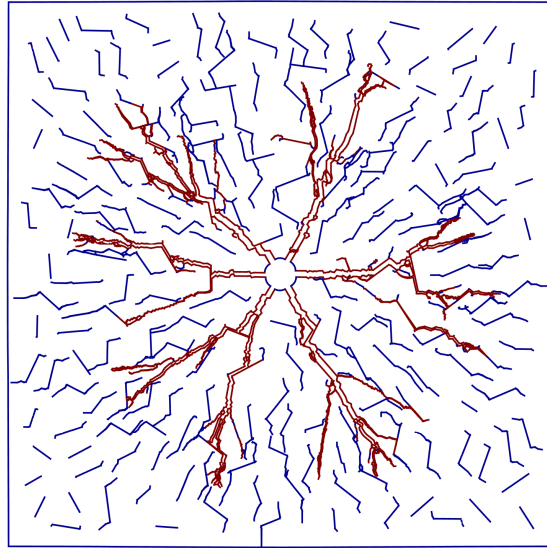
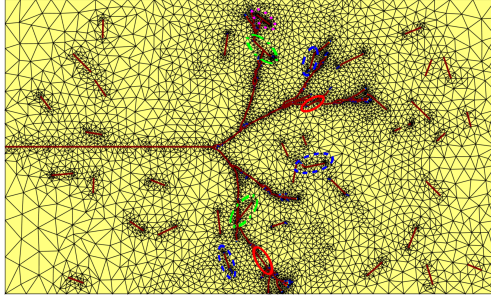
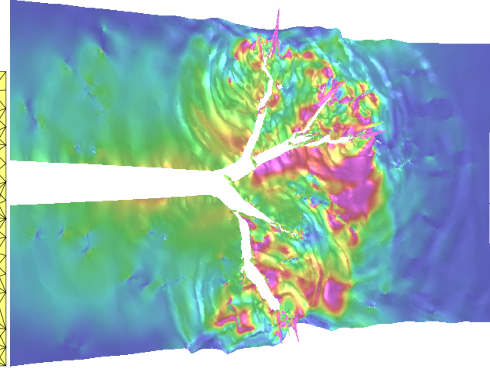


Figure 7.26: Deformed shape for the problem in Fig. 7.23 at time $t = 1.15$ ms. Pressure factor values on crack segments in the range, $f_p \in [0, 1]$, are mapped to a blue-to-red color range.

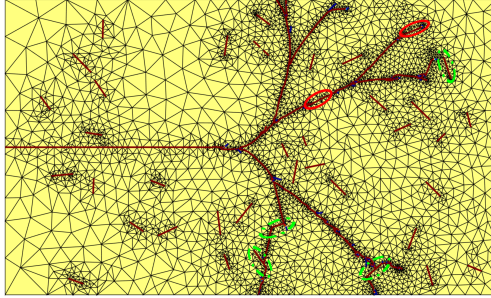
Figure 7.27: The effect of hydraulic load ramp time t_r on the interaction of a horizontal hydraulically loaded crack with in-situ cracks, with crack density $\alpha = 0.1$. The domain geometry is shown in Fig. 7.13. For the front meshes the crack segments are color-coded by the interfacial damage value D . Different types of crack interactions are decorated with the convention described in Fig. 7.15.



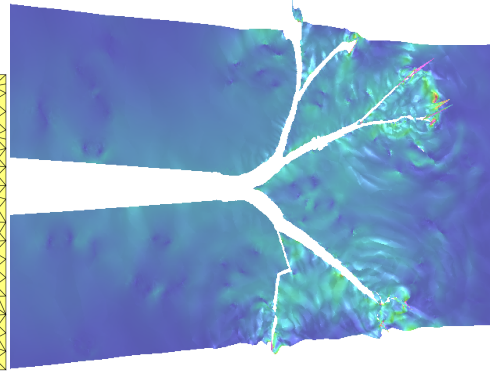
(a) $t_r = 1$ ms, front mesh.



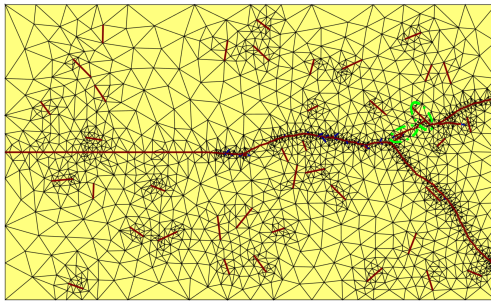
(b) $t_r = 1$ ms, solution.



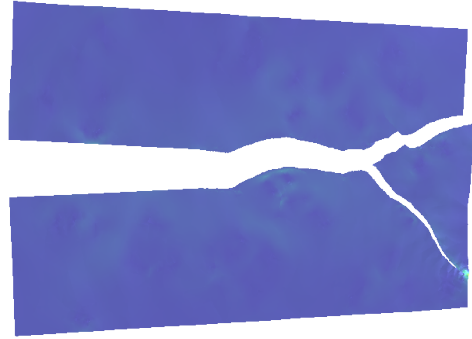
(c) $t_r = 10$ ms, front mesh.



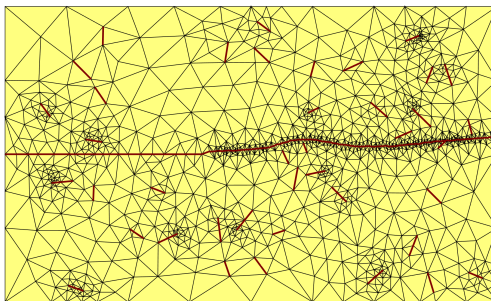
(d) $t_r = 10$ ms, solution.



(e) $t_r = 100$ ms, front mesh.



(f) $t_r = 100$ ms, solution.



(g) $t_r = 1$ s, front mesh.



(h) $t_r = 1$ s, solution.

7.3.6 The effect of hydraulic loading rate

7.3.6.1 Propagation of a hydraulically loaded crack

In this subsection we study the effect of loading rate on hydraulic fracture crack propagation pattern. In the first problem we study the interaction of a hydraulically loaded crack with in-situ cracks for the geometry shown in Fig. 7.13. Unlike the problem in §7.3.3, the hydraulic pressure ramps up from the in-situ pressure which is 2.425 MPa and the fracture strength is $\tilde{\sigma} = 20$ MPa. Similar to the other problems considered, the final value of the hydraulic load is 19.4 MPa. To study the effect of loading rate, the ramp times of $t_r = 1$ ms, 10 ms, 100 ms and 1 s are considered.

Figure 7.27 compares the crack patterns obtained from the loading rates considered. Figures 7.27a and 7.27b show the front mesh and solution for the fastest application of load, that is for $t_r = 1$ ms. Due to the high loading rate, the main crack bifurcates very quickly, following with two further levels of branching off of the bifurcated cracks. In Fig. 7.27a different types of crack interactions with the in-situ cracks can be observed, including a crack arrest by an in-situ crack at the tip of the farthest top and right propagating branch. The high strain and kinetic energies in Fig. 7.27b are due to the highly dynamic crack propagation regime for this case.

Figure 7.27c and 7.27d show the results for the ramp time $t_r = 10$ ms. In contrast to $t_r = 1$ ms, no in-situ cracks start to propagate from being impinged by elastic waves (dashed blue ellipses). This is due to the lowered amount of internal and kinetic energies as shown in Fig. 7.27d. In fact, high energy zones can be observed only around the propagating crack tips, where the high kinetic energy zones can be attributed to the quasi-singular material velocity fields around dynamically propagating cracks [11]. It is also noted that the crack bifurcates later than that for $t_r = 1$ ms.

The results for $t_r = 100$ ms are shown in Figs. 7.27e and 7.27f. First it is observed that the main crack bifurcates much later compared to the previous two cases. In fact, the bifurcation even is facilitated by the interaction of the main crack with an in-situ crack with a close orientation (first encircled crack in green). The upward diversion of the crack path before the bifurcation event is caused by the presence of two in-situ cracks below the crack

path diversion. The authors believe that the rather unfavorable direction of these two in-situ cracks relative to the propagating crack has a repulsive effect. In Fig. 7.27f, we observe that the crack path is significantly less dynamic as even the high energy zones around the moving crack tips have significantly shrunk.

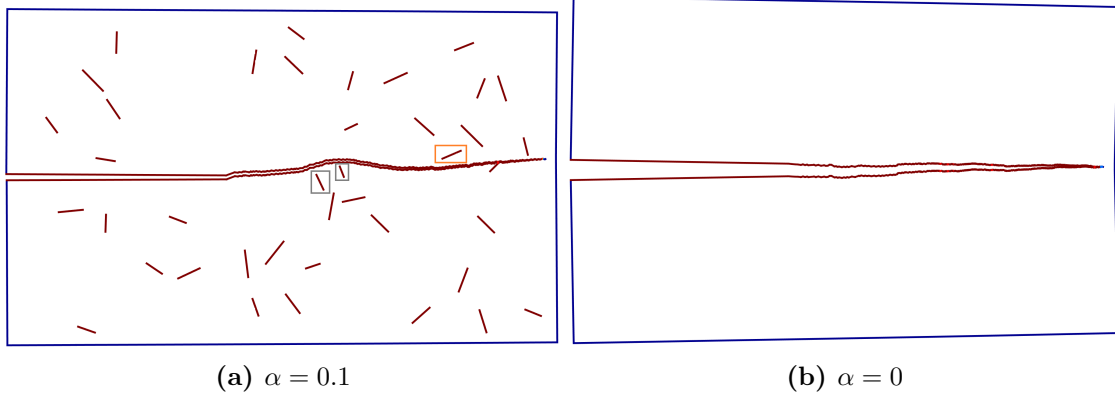


Figure 7.28: Deformed shape of the domain for a horizontally loaded main crack and the ramp time $t_r = 1$ s. The results are compared for the domain with crack density $\alpha = 0$ and a domain with no in-situ cracks. The enclosed in-situ cracks in Fig. 7.28a are described in the body.

Finally, the results for the lowest loading rate are shown in Figs. 7.27g and 7.27h. The deformed shape of the domain is shown in Fig. 7.28a. Similar to the results for $t_r = 100$ ms, the two near vertical in-situ cracks on the path of main crack propagation crack, enclosed in gray rectangles in Fig. 7.28a, cause an upward diversion of the crack path. However, in this case the driving energy of the propagation crack is not high enough to make it join with the in-situ crack enclosed in the orange rectangle in Fig. 7.28a and unlike the results for $t_r = 100$ ms no bifurcation occurs close to this location. Moreover, in Fig. 7.27h we observe much subdued internal and kinetic energy fields which are due to the quasi-static mode of crack propagation. Finally, it is noted that for this slow rate of loading, where the results approach their quasi-static limit, the crack will propagate on a straight line in the absence of any microcracks. This is demonstrated in Fig. 7.28b where the crack propagates on a smooth and almost horizontal line. The slight deviations from the straight line are due to the discretization errors and the propagation of the crack in an intermittent manner by one element edge propagation at a time. However, unlike many existing algorithms no crack

path smoothing algorithms are employed in the adaptive aSDG method; the results shown in Fig. 7.28 demonstrate the high fidelity of the method.

7.3.6.2 The effect of loading rate on the activation of wellbore initial perforations

We study the effect of loading rate for the problem in §7.3.5, where in addition to the stimulation of the reservoir shown in Fig. 7.19 with a load with ramp time $t_r = 1$ ms, the slower ramp times of $t_r = 10$ ms, 100 ms, and 1 s are used. The terminal hydraulic load is 19.4 MPa. As the loading rate decreases, the mode of crack propagation and interaction with in-situ cracks, with density $\alpha = 0.5$ and 30° angular bias, changes. The solutions and deformed crack geometries are shown in Figs. 7.29 and 7.30.

Similar to the problem in §7.3.6.1 for the fastest application of the hydraulic load in Fig. 7.29a, high internal and kinetic energy densities are observed. As the ramp time increases tenfold, the top perforation does not activate in Fig. 7.29b and both energy fields decrease correspondingly. In fact, only mild elastic wave scatterings can be observed close to the propagating cracks due to their propagation and interaction with in-situ cracks. As the ramp time further increases, only the two horizontal cracks are activated and the number of crack branching / microcracking events decreases in Fig. 7.29c. This trend continues for $t_r = 1$ s in Fig. 7.29d, where again only two main cracks are activated and they propagate much farther before any bifurcation occurs. In the last two cases the kinetic energy density is practically zero, signifying the quasi-static crack propagation regime.

The deformed crack geometries are shown in Fig. 7.30. As mentioned for this problem in §7.3.5, the dominant mode of crack interaction of the horizontally propagating cracks with in-situ cracks is crack path alignment while the vertically propagating cracks experience a higher resistance propagating through in-situ cracks; due to the higher angle difference relative to in-situ cracks the latter group of cracks tend to be diverted or offset by the in-situ cracks. This trend can be seen for the upward-propagating and downward-propagating cracks in Figs. 7.30a and 7.30b, respectively. As the loading rate decreases the number of activated perforation decreases. For this problem, there are preferred directions due to the orientation of in-situ cracks. So, in Figs. 7.30b and 7.30c one and two of the vertical cracks

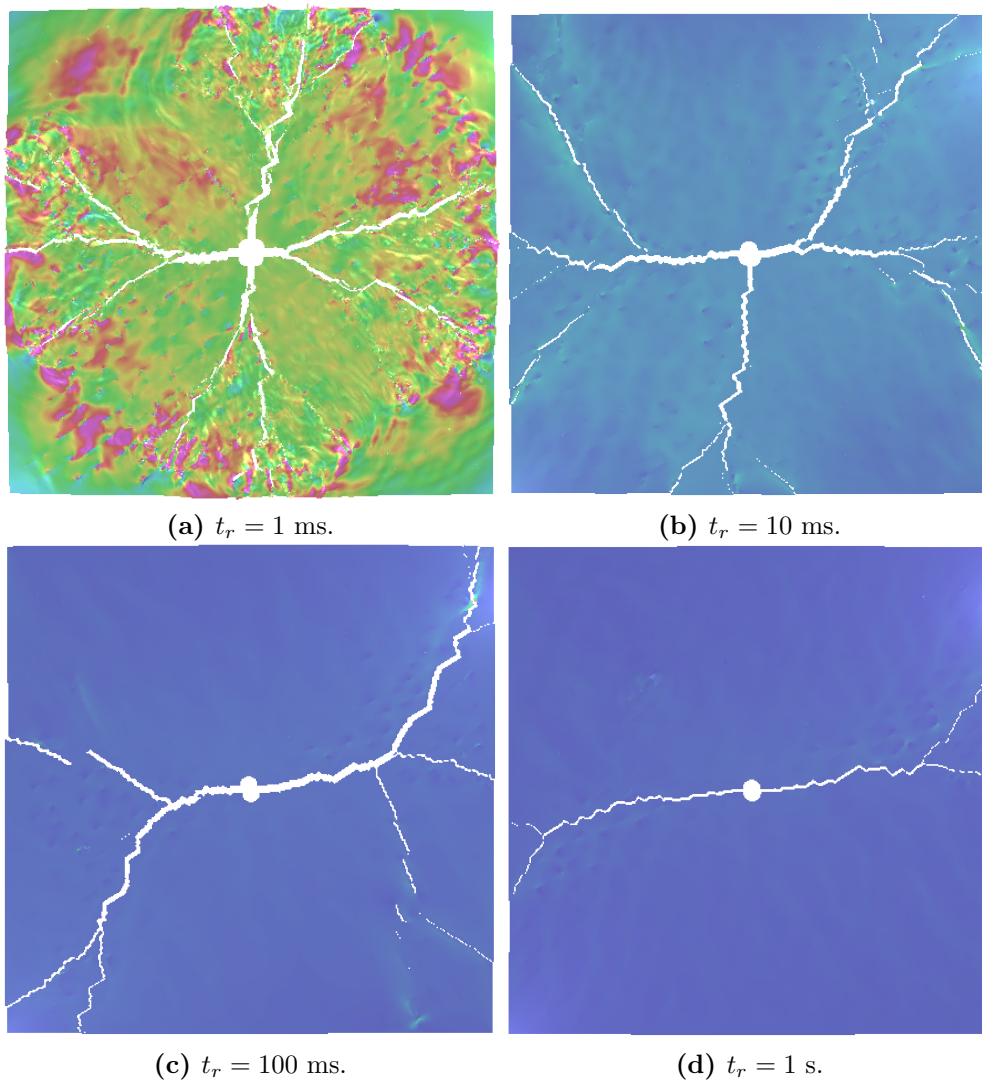


Figure 7.29: The effect of loading ramp time on energy fields for the problem set-up in Fig. 7.19. Color and height fields depict strain and kinetic energy densities, respectively.

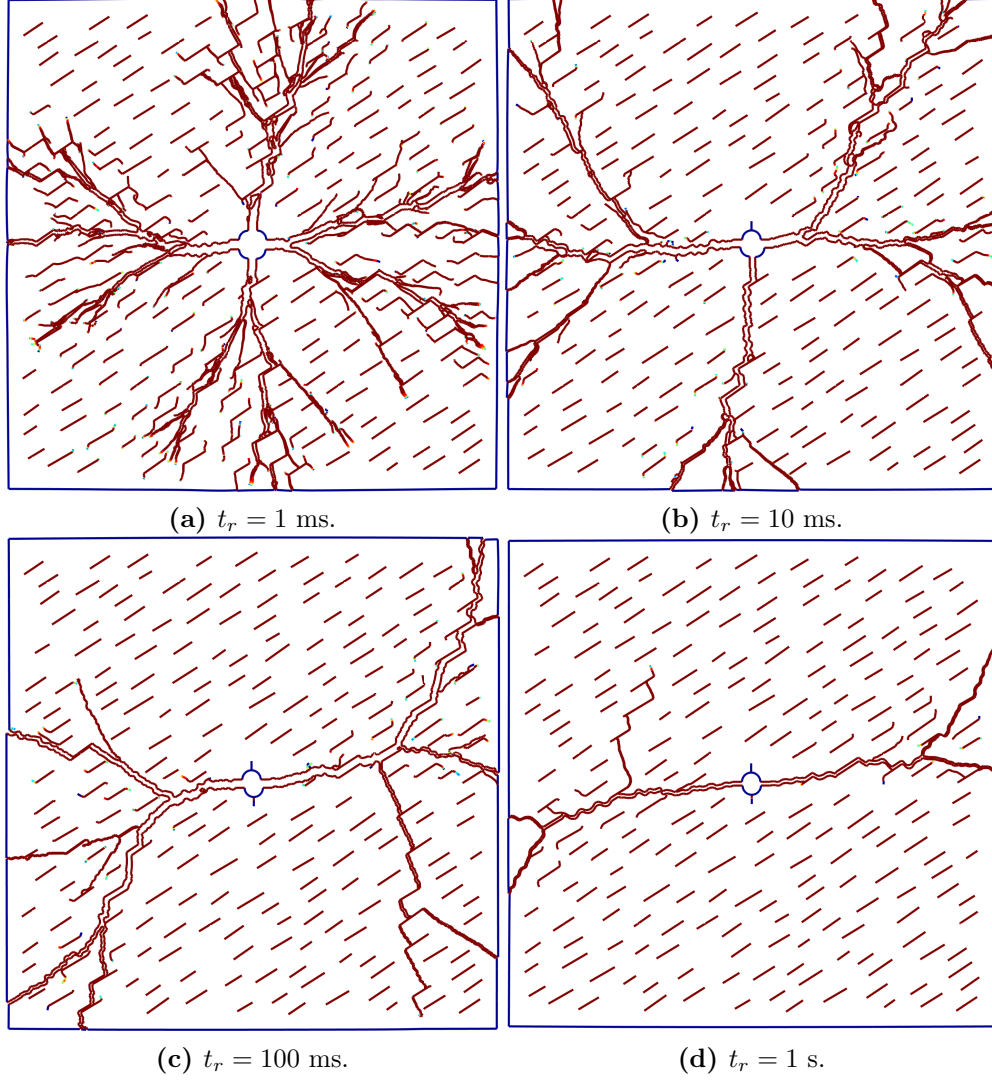


Figure 7.30: The effect of loading rate on fracture pattern for the problem set-up in Fig. 7.19. The damage D in the range of $[0 \ 1]$ is mapped to a blue to red color range on crack surfaces.

do not propagate, respectively. In addition, in Fig. 7.30c we observe that for the downward-propagating macro crack bifurcated from the right propagating main crack, again multiple diversion and offsetting events are observed due to its unfavorable propagation direction relative to in-situ cracks. Finally, the crack path for Fig. 7.30 is smoother and as observed in Fig. 7.29d bifurcations occur farther out. The few crack arrests observed on the upper side of the left propagating crack are due to the lowered driving force of the propagating cracks. In summary, the trends of crack propagation and reduction of the number of activated perforations agrees with other similar studies, for example hydraulic fracturing in reservoirs with no in-situ cracks in [13].

7.4 Conclusion

The interaction of an advancing hydraulic fracture and an in-situ fracture network in rock can yield highly complex patterns throughout the hydraulic fracturing process. It is therefore crucial to have an accurate representation of the network, specifically the connectivity of crack segments, to track proppant transport and fluid motion in the hydraulically generated and expanded network. We presented a representation of crack connectivity in a fracture network by means of a simplicial complex data structure approach, wherein the geometry of a dynamic network configuration is analyzed based on an extension of graph theory. The one dimension down facet and one dimension up cofacet neighborhood information enables concise, yet comprehensive neighborhood information between geometric cells in a fracture network. In the present work, simplices, *i.e.*, vertices, lines, triangles, and tetrahedron, are used to represent the finite element computational domain and the geometry of fracture network. Once the simplicial complex design is combined with a disjoint set data structure, explicit algorithms can be used to efficiently track network connectivity and load transfer between independent fracture sets. This also permits to impose independent loading conditions on arbitrary set of connected fractures in a hydraulic fracture simulation.

The simplicial complex and disjoint set data structures were used to study the interaction of hydraulically loaded perforations with in-situ cracks for several problems. In general it was observed that as the angle difference between an incoming hydraulically loaded fracture and

an in-situ crack increases, the effect of in-situ crack shifts from slight realignment, to diversion / offsetting of the loaded crack. As the angle difference approaches the normal angle, the loaded crack tends to directly penetrate through the in-situ crack. These data structures were used to compute the length of cracks generated by hydraulic fracturing, from each individual perforation around a wellbore. It was also demonstrated that as the hydraulic loading rate increases, more initial perforations in a wellbore result in active crack propagation. This ranged from about two perforations with favorable directions relative in-situ cracks to all perforations becoming active at lowest and highest loading rates considered, respectively. It is noted that the use of highly efficient h -adaptive aSDG method and its exact crack tracking adaptive operations where necessary to capture complex fracture patterns observed for dynamic problems considered herein.

We proposed a scheme based on the apertures of all hydraulically loaded cracks that are adjacent to a crack segment to regularize the application of hydraulic load. Two problems can occur when a hydraulically loaded crack intersects an in-situ crack; first the sudden jump of pressure from ambient to hydraulic pressure induces numerical artifacts and/or requires very fine finite element grids to resolve these transitions. Second, the entire length of in-situ crack is suddenly loaded at the very moment the two cracks intersect. The proposed regularization scheme addresses both problems when hydraulic pressure is initially applied uniformly for the entire spatial domain. Although a heuristic approach, the relationship between the crack aperture and effects of applied fluid pressure on fracture surfaces serves as the basis from which more physical relationships, *i.e.*, fully coupled hydro-mechanical models as in [95], can be derived in future works.

There are several other extensions to this work. The data structures designed to model crack connectivity and neighborhood information can be used in a post-processing stage to estimate the increased yield of a hydraulically stimulated reservoir by modeling fluid flow through the fracture network and its coupling with the solid rock body. They can also shed light on the formation of fractal-like fracture patterns in quasi-brittle materials such as rock in dynamic setting. For example, they provide better understanding on how microcracks are formed and connected or emanated from mother cracks, and on their contribution to total generated crack length and dissipated energy at different fractal levels.

Chapter 8

Effects of material inhomogeneity on
fracture induced by tensile loading:

An implicit microstructure
representation of Weibull-based
fracture strength

An original version of the following article was published in the International Journal of Fracture: Special Issue for Integrated Computational Structure-Material Modeling of Deformation & Failure Under Extreme Conditions An IUTAM Symposium [6]. The article was originally published under the title “Effect of random defects on dynamic fracture in quasi-brittle materials” but for more comprehensive inclusion into this dissertation, the title was revised to emphasis the concept of interest. The paper presents a formulation of an interfacial damage model that combines separation (fracture), contact–stick, and contact–slip modes by using dynamically consistent Riemann solutions. In the *implicit realization* approach, the Weibull statistical model is used to assign stochastic fracture strength values at the vertices of the finite element discrete mesh to model material inhomogeneity and randomness. In the *explicit realization* approach, randomly sampled microcracks are distributed in the computational domain. The paper demonstrates the effect of inhomogeneity and anisotropy in fracture response on brittle materials for tensile-dominant dynamic loading scenarios.

Abstract: We propose an asynchronous Spacetime Discontinuous Galerkin (aSDG) method combined with a novel rate-dependent interfacial damage model as a means to simulate crack nucleation and propagation in quasi-brittle materials. Damage acts in the new model to smoothly transition the aSDG jump conditions on fracture surfaces between Riemann solutions for bonded and debonded conditions. We use the aSDG method’s powerful adaptive meshing capabilities to ensure solution accuracy without resorting to crack-tip enrichment functions and extend those capabilities to support fracture nucleation, extension and intersection. Precise alignment of inter-element boundaries with flaw orientations and crack-propagation directions ensures mesh-independent crack-path predictions. We demonstrate these capabilities in a study of crack-path convergence as adaptive error tolerances tend to zero.

The fracture response of quasi-brittle materials is highly sensitive to the presence and properties of microstructural defects. We propose two approaches to modeling these inhomogeneities. In the first, we represent defects explicitly as crack-like features in the analysis domain’s geometry with random distributions of size, location, and orientation.

In the second, we model microscopic flaws implicitly, with probabilistic distributions of strength and orientation, to drive nucleation of macroscopic fractures. Crack-path oscillation, microcracking, and crack branching make numerical simulation of dynamic fracture particularly challenging. We present numerical examples that explore the influence of model parameters and inhomogeneities on fracture patterns and the aSDG model’s ability to capture complex fracture patterns and interactions.

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8.1 Introduction

8.1.1 Literature review

Stochastic distributions of material defects play a critical role in fracture processes. Stress concentrations induced by existing crack tips and by local material inhomogeneities can initiate and accelerate failure at these weaker sites. These local failures absorb energy and relax stress to shield surrounding material and can result in highly non-uniform failure patterns. Size-effects, in which fracture strength decreases as a specimen’s size increases, and stochastic fracture response with respect to fracture pattern, ultimate load, and absorbed energy exemplify the influence of micro-defects on macroscopic response. These effects are more pronounced in quasi-brittle materials than in ductile materials where plastic yielding can redistribute stress.

Material models and computational methods can represent material heterogeneities and defects either *explicitly* or *implicitly*. In *explicit* approaches, individual defects, microcracks, and other inhomogeneities are incorporated directly in the model. For example, in *lattice models* [189, 131], the *Discrete Element Method* (DEM) [111], and *peridynamics* [77], heterogeneities can be modeled by varying the constitutive parameters that govern interacting particles. In the context of continuum-based models, such as finite element methods, microcracks and other defects can be explicitly embedded in the initial domain

description and the corresponding numerical mesh. This requires a highly refined mesh to ensure that the initial microcrack distribution is precisely represented.

While explicit approaches can provide a detailed representation of material heterogeneities, the requirement to directly resolve the material microstructure generally limits their application to small space and time scales. *Implicit* approaches, on the other hand, incorporate the collective effect of microstructure into phenomenological models or continuum constitutive relations. For example, [215, 216] introduced a well-known probabilistic model that provides a good representation of the size effect in quasi-brittle materials. Material microstructure can also be used to calibrate continuum fracture models such as the damage models in [194]. Homogenization approaches, on the other hand, derive macroscopic effective constitutive parameters by solving the underlying problem in a *Volume Element* (VE). If the VE is large enough to effectively homogenize material properties (*i.e.*, if the material is macroscopically homogeneous), it is called a *Representative Volume Element* (RVE). In contrast, *Stochastic Volume Elements* (SVEs), such as those in [160, 122, 183], are formulated for smaller VE sizes to preserve material heterogeneities and statistical variability. SVEs preserve microstructure variability while averaging it to a larger and more manageable length scale and can be very effective in fracture analysis of quasi-brittle materials.

Dynamic fracture of quasi-brittle materials poses additional modeling and computational challenges. Dynamic fracture patterns can be quite complicated. As a crack accelerates, it may oscillate, emit microcracks, interact with or intersect other cracks, or bifurcate to form two or more crack tips. Strong interactions of advancing macrocracks with in-situ microcracks makes their dynamic behavior sensitive to random variations of microscale defects. In addition, the large and growing number of moving crack tips, whose fracture process zone sizes shrink dramatically as the tips accelerate, pose serious computational challenges.

Stationary and dynamically propagating cracks can be represented individually as sharp interfaces, or their collective effect can be modeled by a nonlinear continuum model, such as a bulk damage model. We also note recent applications of variational [40], phase-field [24], and thick level-set [46] methods to brittle fracture. However, we focus in this work on sharp-interface finite element fracture models. These can be classified by three features: a

discontinuous response model that supports jumps in displacement and velocity across crack surfaces, a *fracture process model*, and a *crack representation method* that models global crack paths and patterns. Various permutations of the available choices for these features distinguish alternative schemes for modeling dynamic fracture.

Discontinuous-response models suitable for brittle fracture include interface elements, discontinuous and singular intra-element enrichment functions, and inter-element discontinuous basis functions. Interface elements coincide with facets of adjacent bulk elements and have paired nodes that accommodate displacement jumps across the interface and couple with adjacent bulk-element nodes. Discontinuous and singular enrichment functions within elements are hallmarks of extended and generalized finite element methods, while inter-element discontinuous basis functions are characteristic of discontinuous Galerkin (DG) methods (see discussions below).

Cohesive Zone Models (CZMs), introduced by [221] and based on work by [25] and [74], are a popular class of fracture-process constitutive models in which a *traction–separation law* (TSL) defines the cohesive tractions acting on a fracture surface as a function of the separation (or displacement jump) across the interface. They are commonly implemented with interface elements, as in [221, 43, 164]. [147], use a stabilized DG discretization in space to model quasi-static bulk response, but still use interface elements to implement a cohesive zone model. They call this hybrid approach a discontinuous Galerkin – cohesive zone model (DG–CZM). CZMs can also be implemented as inter-element jump conditions in DG methods without resorting to interface elements. For example, [11] propose an asynchronous spacetime discontinuous Galerkin (aSDG) model for dynamic fracture in which a spacetime formulation of linear elastodynamics [9] models the bulk response, and DG inter-element jump conditions weakly enforce a cohesive TSL along fracture surfaces. Powerful h -adaptive spacetime meshing and high-order basis functions enable very high-resolution renderings of crack-tip fields in this approach, as seen in comparisons with Xu and Needleman’s solutions in [11].

Interfacial damage models (*cf.*, *e.g.*, [21, 165]) offer an alternative to CZM fracture process models. [1] propose an enhanced aSDG dynamic fracture model using a rate-dependent interfacial damage model; [213] propose a damage-based variant of the DG-CZM

method. Although the damage models in [1] and [213] share some similarities, there are also fundamental differences. The former rate-dependent model represents the fracture process as a damage-controlled transition between Riemann solutions for bonded and debonded conditions in DG jump conditions, where the debonded Riemann solutions account for dynamic contact–stick and contact–slip response during crack closure. In contrast, the latter model derives from a free-energy potential that depends on the current value of a damage parameter and the numerical fluxes acting on a fracture interface.

Extended Finite Element Methods (XFEMs) [35, 149, 68, 181] and Generalized Finite Element Methods (GFEMs) [73, 203, 204] typically draw on Linear Elastic Fracture Mechanics (LEFM) theory to determine crack-tip enrichment functions. In lieu of an explicit fracture process model, they use LEFM crack propagation criteria to control crack extension, orientation, and branching. These methods may face difficulties when cracks intersect, branch, or approach domain boundaries since LEFM solutions are not generally available in these situations.

There are two broad categories of crack representation methods for problems where the crack paths are not prescribed a priori: *crack capturing* and *crack tracking*. Crack capturing involves approximating crack paths within a finite-dimensional space of candidate crack paths. For example, crack paths may be constrained to follow inter-element boundaries in a fixed mesh. This implies that only a small number of possible crack orientations are available in the neighborhood of any point within the domain and that crack-segment length scales are similarly limited by the mesh. [221] pioneered this approach by introducing cohesive interface elements on every inter-element boundary in fixed, but highly refined, meshes. Two problems commonly arise in this approach. *Artificial compliance* [173, 39], occurs when potential fracture interfaces exhibit finite compliance before the onset of an active fracture process. This disturbs the properties and wave speeds of the bulk medium, especially as the mesh is refined, and can lead to erroneous fracture results. Artificial compliance is typical of intrinsic cohesive models, such as the one proposed by Xu and Needleman, as well as certain interfacial damage models, *e.g.*, [21, 165]. [43] and [164] introduced interface elements with extrinsic CZMs to avoid artificial compliance in a crack capturing method. Similarly, certain interfacial damage models, such as [1, 213], do not suffer finite initial

compliance and are not subject to the artificial compliance problem when used in crack capturing schemes.¹ The second problem involves mesh-dependent results due to geometric constraints imposed on the fracture pattern by the restriction to a finite set of fracture orientations and length scales. This can distort the fracture pattern and artificially impede crack nucleation, propagation, and branching, even on highly refined meshes, by precluding energetically favored paths. [201] combine polygonal finite elements with limited element refinement and splitting operations in a crack capturing method to possibly mitigate, but not eliminate this problem.

Crack-tracking methods mitigate or eliminate mesh-dependent solutions by approximating crack paths within infinite-dimensional spaces in which local crack orientations and, in some cases, crack-segment lengths are continuously variable. Tracking methods generally do not insert fracture surfaces on all inter-element boundaries, so artificial bulk compliance is never a problem. Crack-tracking methods may produce mesh-independent results in the sense that discrete crack path representations converge to a continuum solution in the limit of mesh refinement. XFEM and GFEM methods implement a form of crack tracking in which discontinuous enrichments allow cracks to traverse element interiors. Thus, the orientation of a new crack segment from the point of entry on an element's boundary is continuously variable and not constrained by the mesh. However, since typical XFEM and GFEM implementations use singular enrichments from LEFM theory to avoid adaptive mesh refinement and because the discontinuous enrichments usually support only a single crack segment within each element, the lengths of crack segments generally remain mesh-dependent. Thus, XFEM and GFEM methods mitigate, but do not eliminate, mesh dependence. [176] propose a new crack-tracking scheme based on *universal meshes* [177] and LEFM theory. So far, applications are limited to quasi-static crack propagation where microcracking and crack branching are uncommon. The aSDG fracture model in [1] implements a form of crack tracking in which a sharp-interface fracture model is restricted to space-time inter-element boundaries. However, in contrast to crack-capturing methods, the orientations and length scales of incremental crack extensions are treated as continuously

¹[1] uses a crack-tracking scheme, so his method would not suffer artificial compliance even if he chose an interfacial damage model with finite initial compliance.

variable. Dynamic adaptive space-time meshing creates inter-element boundaries that conform exactly to physically determined incremental orientations and length scales. This version of crack tracking is, in principle, capable of converging to continuum crack paths as adaptive tolerances are tightened.

There is growing recognition that probabilistic modeling is essential to realistic fracture simulations. Assumptions of uniform material properties are inconsistent with most real materials and can lead to unrealistic fracture patterns and overestimation of fracture resistance. For example, [129] introduce a stochastic variation of macroscopic fracture strength to enhance a fixed-mesh model based on an extrinsic cohesive model. [1] introduced a stochastic representation of various properties of microscopic defects, including orientation and nucleation strength, that determine the initiation of new fracture surfaces in the macroscopic model.

8.1.2 Scope and original content

In this work, we propose an h -adaptive (aSDG) finite element method [9] and an interfacial damage model to simulate dynamic fracture in quasi-brittle materials. Advantages of the aSDG method include arbitrarily high-order accuracy in space and time, per-element satisfaction of balance laws, an asynchronous local solution scheme, and powerful spacetime adaptive meshing operations. In lieu of a traditional cohesive model, we propose a rate-dependent interfacial damage model. Our model also incorporates dynamically consistent contact–stick and contact–slip response modes to simulate crack closure. We emphasize that the exceptional flexibility, fidelity and efficiency of the adaptive aSDG method are critical to the accurate resolution of crack paths and of fracture process zones that undergo dramatic shrinkage and growth as crack tips accelerate and arrest.

The new modeling techniques proposed in this work build on previous applications of aSDG methods to dynamic fracture mechanics: [3, 9, 10, 5, 8]. The novel content includes specializations of spacetime meshing techniques for crack nucleation, extension, and intersection, an interfacial damage model that represents fracture as a continuous transition of Riemann fluxes from bonded to debonded conditions, and techniques for explicit and implicit realizations of stochastic distributions of microstructural defects with randomized

strength and orientation. Much of this content is based on previously unpublished material from [1]. We also present a set of original numerical examples that demonstrate the modeling capabilities and crack-path convergence of the proposed methods.

The organization of the remainder of this paper is as follows. We briefly review the aSDG method in §8.2. We introduce the interfacial damage and contact models in §9.2. In §9.3, we propose explicit and implicit realizations of random material defects, novel spacetime adaptive meshing operations for precise tracking of dynamic crack propagation paths, and techniques for introducing angular bias in fracture strength. We present numerical studies that demonstrate the capabilities of the explicit and implicit defect models and a qualitative investigation of various model parameters on fracture patterns in §8.5. Discussion and conclusions appear in §8.6.

8.2 Adaptive Spacetime Discontinuous Galerkin Finite Element Method

This section reviews key concepts and features of the adaptive aSDG method that provides the underlying computational framework for our dynamic fracture model. Please see [9, 10, 1] for further details.

8.2.1 Causality-based spacetime meshing and solution scheme

As with any *Discontinuous Galerkin* (DG) finite element method, the aSDG method employs basis functions that are discontinuous across element boundaries. In lieu of a conventional time-marching scheme, we directly discretize the spacetime analysis domain using unstructured grids that satisfy a special causality constraint as discussed below. Applying this approach to the solution of hyperbolic partial differential equations yields a unique combination of properties, including arbitrarily high orders of spatial and temporal accuracy, exact (to within machine precision) per-element balance, a localized, asynchronous solution scheme that lends itself to fine-grain adaptive meshing and parallel algorithms, and excellent performance in resolving shocks and high gradient features in wave propagation

problems. Each of these properties is critical to the success of our proposed numerical model for dynamic fracture.

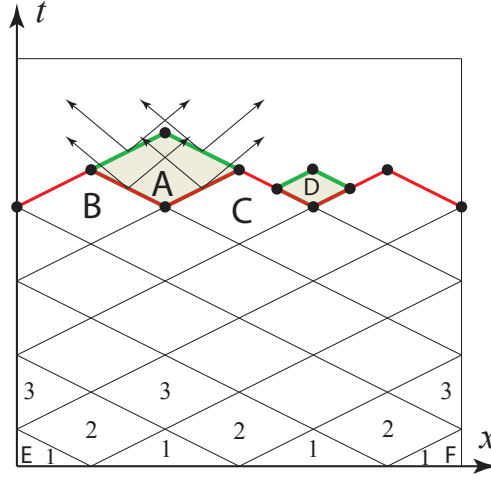


Figure 8.1: aSDG Solution scheme on causal spacetime mesh in $1d \times \text{time}$.

Figure 8.1 depicts a simple unstructured *causal* spacetime mesh in $1d \times \text{time}$ (*i.e.*, one spatial dimension and time) that suffices to explain the basic concepts of the aSDG solution procedure. The inclined arrows indicate the fastest characteristic directions under the simplifying assumptions of uniform wave speeds and equal maximum wave speeds to the left and right. We enforce a *causality constraint* on all facets in the spacetime mesh to enable a scalable, local solution scheme. Specifically, each facet must be faster (*i.e.*, closer to horizontal in Fig. 8.1) than the fastest characteristic direction traversing the facet. A mesh in which all facets conform to the causality constraint is a causal mesh, and a causal mesh implies an asymmetric dependency graph between the solutions on adjacent elements. For example, the solution on element A depends only on the solutions on the earlier neighbor elements, B and C, while the solutions on B and C do not depend on A. In other words, the earlier facets of element A, shown in red, are pure inflow edges. The remaining facets, shown in green, are pure outflow edges.

In general, the solution on any element in a causal mesh depends only on prescribed initial and boundary data and the solutions on its earlier immediate neighbors. The asymmetric dependency graph implies a partial element ordering by which the global solution can be computed locally, one element at a time. For example, the solutions on level-1 elements

in the figure depend only on initial conditions (and boundary conditions in the cases of elements E and F). Thus, the solutions on the level-1 elements can be computed locally, in any order or simultaneously in parallel. A level-2 element can be solved as soon as its earlier neighbors are solved; there is no need to wait for all level-1 elements to be solved. Assuming the computational complexity of solving a single element is bounded, causal aSDG meshes enable asynchronous, element-by-element solutions with linear computational complexity in the number of spacetime elements.

Rather than generate an entire causal spacetime mesh in a single operation, we add one causal element at a time. We immediately solve the local problem on each new element and locally advance the front mesh to the element’s outflow facets. This interleaving of spacetime element generation and solution operations provides a framework for exceptionally fine-grained adaptive mesh refinement. For example, we can check an element-level error indicator immediately after each element’s solution. If an element-level error tolerance is exceeded, we locally refine the old front mesh by bisecting edges along the element’s inflow faces before discarding the element and resuming the spacetime meshing procedure. This procedure generates new elements that are locally refined in both space and time, such as element D in Fig. 8.1.

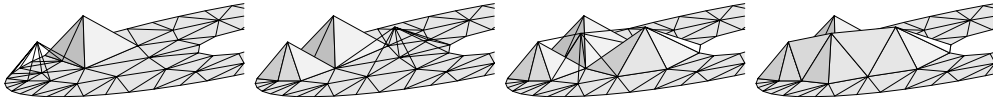


Figure 8.2: Tent-Pitcher in $2d \times \text{time}$; the time-axis is vertical. Wireframe renderings depict new patches of tetrahedra to be solved. Patches with opaque surfaces are already solved (reproduced from [9]).

In practice, we replace the individual elements with small clusters of simplex elements called *patches*, where only the exterior patch facets must be causal. For example, clusters of tetrahedral elements in $2d \times \text{time}$ comprise causal patches in Fig. 8.2. The *Tent Pitcher* algorithm and solution procedure, described in [3], is an advancing-front scheme in which causal patch construction and patch solution operations are interleaved. It generates a sequence of causal spacetime patches that conform to the causal partial ordering such that each patch can be solved as soon as it is generated. In each step, the *Tent Pitcher* algorithm defines a local update of the space-like front mesh, as depicted in Fig. 8.2, by advancing a

local-minimum vertex in the *front mesh* in time. We form the new patch by constructing a small cluster of spacetime simplices to cover the region between the old and new fronts. The causality constraint determines the maximum allowable increment of time advancement for the front-mesh vertex and, thereby, the maximum duration of the new patch. We form and solve new patches as local problems and update the front mesh until the entire spacetime analysis domain is solved. Figure 8.2 illustrates this procedure for the first four patches in a Tent Pitcher solution sequence.

8.2.2 Adaptive schemes for tracking cracks

We use a flexible and efficient h -adaptive aSDG analysis scheme to model the fine details of complex fracture patterns. In addition to conventional adaptive refinement operations on the front mesh, we use special patch configurations to perform other familiar remeshing operations (*e.g.*, vertex deletion, edge flips, and vertex repositioning for mesh smoothing and object tracking) in spacetime *within* the patches [3, 10]. The inflow and outflow facets of these adaptive patches conform with the old and new configurations of the front mesh, so there is no need for error-prone projections of the solution from the old front mesh onto the new one. For this reason, and in contrast to conventional adaptive methods, our spacetime adaptive meshing procedure maintains the full convergence rates of high-order aSDG models.

We present an adaptive crack tracking scheme based on this technology in §8.4.4 that can align element boundaries with any desired direction of crack extension. In addition to the bulk energy dissipation error indicator that drives the adaptive analysis of elastodynamics in [10], we check an indicator specific to interfacial energy error in discrete fracture models [11]. Taken together, the localized asynchronous aSDG solution scheme and the adaptive crack tracking technology, provide an accurate and efficient simulation tool for dynamic fracture that is capable of rendering complex fracture patterns in considerable detail.

8.2.3 Formulation of linear elastodynamics

Details of the aSDG formulation for linear elastodynamics using spacetime differential forms, including the relevant spacetime jump conditions, can be found in [9, 1]. For our present

purposes, it suffices to review the governing equations for elastodynamics in direct tensor notation:

$$\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{b} = \dot{\mathbf{p}} \quad (8.1a)$$

$$\boldsymbol{\sigma} = \mathbf{C} \boldsymbol{\epsilon}, \quad \mathbf{p} = \rho \mathbf{v} \quad (8.1b)$$

$$\dot{\boldsymbol{\epsilon}} = \frac{1}{2}(\nabla \mathbf{v} + \nabla^T \mathbf{v}), \quad \mathbf{v} = \dot{\mathbf{u}} \quad (8.1c)$$

where $\mathbf{u}$, $\mathbf{v}$, $\boldsymbol{\epsilon}$, $\mathbf{p}$, $\boldsymbol{\sigma}$, and $\mathbf{b}$ are displacement, velocity, strain, linear momentum density, stress, and body force fields, respectively. Equation (8.1a) is the familiar equation of motion. The constitutive equations (8.1b) express the force-like fields as functions of the kinematic fields, the elasticity tensor $\mathbf{C}$, and the mass density ρ . Equations (8.1c) are the kinematic compatibility equations. In the case of an isotropic material, the components of the elasticity tensor are given by

$$C^{ijkl} = \lambda \delta^{ij} \delta^{kl} + \mu (\delta^{ik} \delta^{jl} + \delta^{il} \delta^{jk}), \quad (8.2)$$

where λ and μ are the Lamé parameters.

In addition to the governing equations listed above, jump conditions derived from the governing equations must be weakly enforced in aSDG formulations. Rather than write these as jumps between interior traces on adjacent elements, it is useful to work instead with jumps between specified *target values* and interior traces from just one element at a time. Initial and boundary conditions determine the target values on the corresponding segments of the boundary of the spacetime analysis domain. Riemann solutions define unique target values for the characteristic variables along inter-element boundaries on the interior of the spacetime analysis domain. Once the target values are determined on all element faces, jump conditions that enforce initial and boundary conditions as well as inter-element balance and compatibility conditions can be written in a common format and weakly enforced in the same way. The interfacial damage model presented in §9.2 addresses both fracture and contact by using a damage parameter to interpolate between the target values for bonded, intact material and debonded material.

8.3 A rate-dependent interfacial damage model for fracture and contact

Cohesive models are a popular means for representing debonding processes in computational fracture mechanics. In this approach, a *traction–separation relation* (TSR) models the tractions acting across an interface as nonlinear functions of the displacement jump across the interface. However, the enforcement of impenetrability conditions and modeling frictional contact during crack closure are more difficult in this approach. A penalty method, in which the slope of the normal component of the compressive branch of the TSR serves as the penalty parameter, is often used to approximate the impenetrability condition. A large penalty value effectively limits the amount of nonphysical penetration. However, choosing the penalty value can be challenging: small values imply loose approximation of impenetrability, while large values result in overly stiff systems that are difficult to solve numerically. Contact–slip modes with friction cannot be directly modeled with a TSR, and their seamless integration with a cohesive model can be quite challenging. We note that, while the impenetrability condition alone is sufficient in quasi-static problems, it does not encompass the full set of contact conditions in dynamic problems. When applied to all inter-element boundaries, cohesive models introduce the artificial compliance problem noted in [173]. However, restricting the cohesive model to a mesh-independent set of fracture surfaces circumvents this problem.

Damage mechanics provides an alternative means to represent material failure, including applications to fracture; see [133] for a recent example. Typically, a scalar damage parameter, $D \in [0, 1]$, is used to degrade the material stiffness. For example, in bulk damage models, an effective material stiffness tensor can be expressed as, $\mathbf{C}_{\text{eff}} = (1 - D)\mathbf{C}$. A damage evolution law, possibly describing rate-dependent response, completes the model. [22] used an interfacial damage model that similarly degrades an interfacial stiffness parameter in a model for interlaminar fracture. However, the treatment of contact–separation and contact–slip modes remains problematic in traditional damage mechanics methods.

In this section, we present an interfacial damage model, first introduced in [1], that represents dynamic processes of debonding and contact on *fracture interfaces*, *i.e.*, surfaces

where a fracture already exists or may develop in the future. Rather than degrade an interfacial stiffness, as in [22], we use a scalar damage field, D , to interpolate between dynamically consistent Riemann solutions for fully bonded (intact) and fully debonded material on fracture surfaces. The Riemann solutions for the debonded case cover a complete set of subcases for separation, contact–stick, and contact–slip modes, including friction effects, as described in [8]. We note that enforcing the appropriate Riemann solutions ensures satisfaction of the impenetrability condition for crack closure without resorting to penalty or other constraint methods.

In the following subsections we present dynamically consistent Riemann solutions for intact material as well as the various separation and contact modes for debonded material, a constitutive model that governs the evolution of the interfacial damage field on fracture surfaces, and the construction of target values for traction and velocity using the interfacial damage field to interpolate between the Riemann solutions for intact and debonded material.

8.3.1 Riemann solutions for intact material and the contact–separation modes of debonded material

The solutions for individual contact modes are obtained by solving local Riemann problems at a contact interface. A local coordinate frame at an arbitrary spacetime location P on contact interface Γ is illustrated in Fig. 9.1. The local coordinates are (ξ_1, ξ_2, t) , and the frame is oriented such that the ξ_1 -direction aligns with the spatial normal vector on Γ .

We label quantities on opposing sides of the interface with superscripts $+$ and $-$ and define the initial data for the Riemann problem as the distinct velocity traces, $\mathbf{v}^\pm$, and tractions, $\mathbf{s}^\pm$, defined by $\mathbf{s} = \boldsymbol{\sigma} \cdot \mathbf{n}$ in which the same spatial normal vector, $\mathbf{n}$, is used to compute $\mathbf{s}^+$ and $\mathbf{s}^-$ from the distinct traces of the stress field on the interface, $\boldsymbol{\sigma}^\pm$. The Riemann values at any point on the interface include components of the traction vector acting on the interface and traces of the velocity components from each side of the interface. We denote these by $(\check{\mathbf{s}}, \check{\mathbf{v}}^\pm)$, as shown in the figure. Balance of linear momentum requires equality between the traction vectors obtained from the stress fields on opposite sides of the interface. That is, $\check{\mathbf{s}}^+ = \check{\mathbf{s}}^- := \check{\mathbf{s}}$.

The kinematic compatibility conditions on the interface depend on whether the material interface is intact (perfectly bonded), or in the debonded case, on the specific contact mode. For intact interfaces and for contact–stick mode in the debonded case, the kinematic jump condition for velocity enforces continuity of all velocity components. In separation mode, no jump condition on velocity is enforced, since $\mathbf{v}^+$ and $\mathbf{v}^-$ are independent. In contact–slip mode, the velocity jump condition only enforces continuity of the normal velocity component. In general, we must allow for distinct Riemann velocity values, $\check{\mathbf{v}}^\pm$, to accommodate the separation and contact–slip modes.

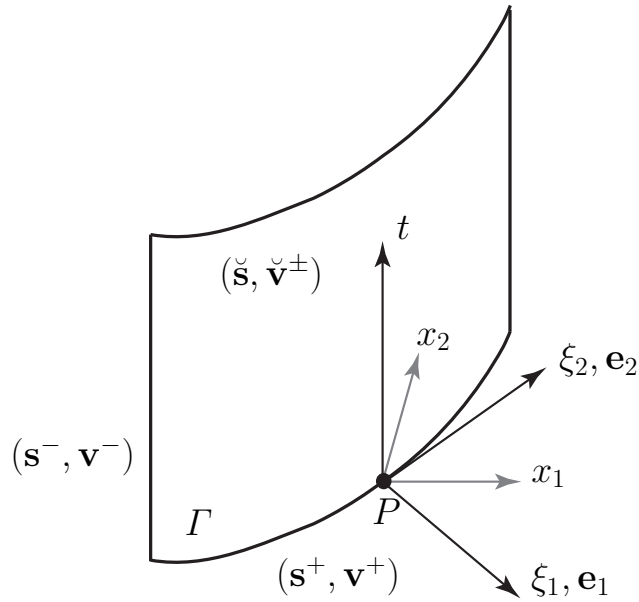


Figure 8.3: Local coordinate frame at arbitrary spacetime location P on a spacetime fracture surface Γ for a problem in two spatial dimensions.

Characteristic values in linear hyperbolic problems are preserved along the characteristic directions in spacetime. For an isotropic material in linear elastodynamics, the spacetime characteristic trajectories in all directions are determined by the dilatational and shear wave speeds, $c_d^\pm$ and $c_s^\pm$, in which

$$c_d = \sqrt{\frac{\lambda + 2\mu}{\rho}}, \quad c_s = \sqrt{\frac{\mu}{\rho}}. \quad (8.3)$$

We determine the Riemann solutions by enforcing the preservation of characteristic values across the interface. To this end, we first define material impedances,

$$Z^{i\pm} := \begin{cases} (c_d\rho)^\pm & i = 1 \\ (c_s\rho)^\pm & i = 2, 3 \end{cases} \quad (8.4)$$

in which the index i indicates spatial directions in the local coordinate frame.

The components of the Riemann values for the contact–stick and bonded modes are,

$$\check{s}^i = \frac{s^{i+}Z^{i-} + s^{i-}Z^{i+}}{Z^{i-} + Z^{i+}} + \frac{Z^{i-}Z^{i+}}{Z^{i-} + Z^{i+}}(v_i^+ - v_i^-) \quad (8.5a)$$

$$\check{v}_i = \frac{s^{i-} - s^{i+}}{Z^{i-} + Z^{i+}} + \frac{v_i^+Z^{i+} + v_i^-Z^{i-}}{Z^{i-} + Z^{i+}} \quad (8.5b)$$

in which, here and in all subsequent equations, the summation convention does not apply for repeated indices i . Recall, also, that $\check{\mathbf{v}}^+ = \check{\mathbf{v}}^- := \check{\mathbf{v}}$ for bonded and contact–stick solutions.

In separation mode, $\check{\mathbf{v}}^+$ and $\check{\mathbf{v}}^-$ are independent. The Riemann tractions are, however, set equal to $\mathbf{S}$, the tractions specified by a particular fracture model or crack-surface loading. Preservation of characteristic values across the interface leads to the Riemann solutions for separation mode:

$$\check{s}^i = S^i \quad (8.6a)$$

$$\check{v}_i^\pm = v_i^\pm + \frac{s^{i\pm} - S^i}{Z^{i\pm}} \quad (8.6b)$$

The prescribed tractions can take different forms. For example, similar to TSRs, $\mathbf{S}$ can be expressed as a function of the displacement jump across the interface. Another option is to set $\mathbf{S} = \mathbf{0}$, as discussed in [1]. When nonzero tractions act as loads on the crack surfaces, $\mathbf{S}$ is determined by the specified loads, *cf.* §8.5.2.

The Riemann solutions for contact–slip mode are more complex and depend on the type of friction model employed at the interface. We refer the reader to [8] for detailed derivations and expressions for all the Riemann solutions.

8.3.2 Evolution of the interfacial damage field

This section describes the constitutive model that governs the evolution of the damage field D on fracture surfaces. In general, damage fields can be computed using a static equation or by integrating an evolution equation. However, static damage models cannot properly describe fracture processes unless they introduce a microscopic length scale [23]. This is similar to the requirement for a microscopic length scale in bulk damage models, where numerical simulations based on models without a microscopic length scale predict undesirable mesh-dependent response in the strain-softening regime [31]. Alternatively, a time scale associated with the microscopic fracture process can be combined with a velocity scale, such as an elastic wave speed, to introduce an implicit microscopic length scale. These time scales have reduced or eliminated mesh sensitivity in numerical simulations of dynamic fracture using bulk damage models [154]. This is the approach we follow in this work, in which we consider a damage-delay evolution model that is similar in structure, but not identical, to those proposed in [57, 23]. We assume that the damage rate is bounded. This precludes instantaneous finite changes in D due to load variations.

Motivated by the evolution law in [22], we adopt the damage evolution rule,

$$\dot{D} = \begin{cases} \frac{1}{\tilde{\tau}}[1 - H(\langle D_t - D \rangle)] & D < 1 \\ 0 & D = 1 \end{cases}, \quad (8.7)$$

where $\tilde{\tau}$ is a *relaxation time*, and the *target damage value*, D_t , is the long-term damage value for the current applied load under quasi-static conditions. The function H has the value of unity at zero and monotonically decreases to 0 at infinity. Following [22], the particular form of H used in this work is given as $H(x) = \exp(-ax)$. The relaxation time $\tilde{\tau}$ is the time scale associated with local fracture processes. When the time scales over which the applied loads vary are much larger than $\tilde{\tau}$, we have $\langle D_t - D \rangle \rightarrow 0$. In the limit of this quasi-static behavior, the damage evolution takes the form,

$$D(t) = \sup_{s \leq t} D_t(s). \quad (8.8)$$

That is, D takes the maximum value of the stationary damage over time.

The property, $H(0) = 1$, ensures that $\dot{D} = 0$ when the stationary damage value is less than or equal to the current damage value. Furthermore, the maximum damage rate is bounded by $1/\tilde{\tau}$, as $D_t - D < \infty$. Note that the delay effect decreases as H tends less strongly to 0.

In general, the target damage value D_t can be a function of the traction, velocity, and displacement traces on opposing sides of the interface. However, here we focus on tractions, specifically the Riemann tractions for the bonded condition given in (9.3a), as the driving force that generates new damage beyond the current level. We explain this choice as follows. At some microscopic level, a partially damaged interface can be idealized as having some area fraction that is already debonded, and a complementary area fraction that remains bonded. Additional damage involves microscopic debonding events within the remaining bonded area fraction, where the bonded Riemann solutions in (9.3a) best reflect the local tractions generated by impinging elastic waves. Accordingly, we combine normal and tangential components of the bonded Riemann traction vector to define an *effective Riemann stress*,

$$\check{s} := \sqrt{\langle \check{s}_B^1 \rangle^2 + \beta^2 \sum_{j=2}^d (\check{s}_B^j)^2}, \quad (8.9)$$

where β is the *shear stress factor* that controls mode mixity, and subscripts B indicate bonded-mode Riemann tractions obtained from (9.3a). The positive-part operator $\langle \cdot \rangle$ ensures that only tensile normal components of the traction vector drive the damage evolution. Finally, we write D_t as a function of $\check{s}$,

$$D_t = \begin{cases} 0 & \check{s} < \underline{s} \\ \frac{\check{s} - \underline{s}}{\bar{s} - \underline{s}} & \underline{s} \leq \check{s} < \bar{s} \\ 1 & \bar{s} \leq \check{s} \end{cases}, \quad (8.10)$$

where $\underline{s}$ and $\bar{s}$ denote, respectively, effective traction thresholds for the onset of additional damage evolution and for attainment of the maximum damage rate, $1/\tilde{\tau}$. From here on, we refer to $\bar{s}$ as the *fracture strength*. If $\check{s} < \underline{s}$, we get $D_t = 0$, and (9.10) delivers $\dot{D} = 0$. We

call the ratio, $c_0 := \underline{s}/\bar{s}$ ($\Rightarrow 0 < c_0 < 1$), the *brittleness factor* because higher values of c_0 imply a more brittle fracture process. Although we assume here a linear relation between $\check{s}$ and D_t (*cf.* second branch in (9.14)), more general relations can be considered and calibrated by experimental measurements. The third branch of (9.14) ensures that D_t is bounded by unity.

8.3.3 Target values for traction and velocity

The target tractions and velocities used to construct aSDG jump conditions on a fracture surface are a weighted average of the *bonded* and *debonded* Riemann solutions:

$$\mathbf{s}^* := (1 - D)\check{\mathbf{s}}_B + D\check{\mathbf{s}}_D \quad (8.11a)$$

$$\mathbf{v}^{*\pm} := (1 - D)\check{\mathbf{v}}_B + D\check{\mathbf{v}}_D^\pm \quad (8.11b)$$

where subscripts B and D indicate Riemann values for bonded (*cf.* (9.3)) and debonded conditions. Recall that the debonded Riemann values may arise from separation (*cf.* (9.4)), contact–stick (*cf.* (9.3)), or contact–slip (*cf.* [8]) conditions.

Discontinuous changes in the Riemann solutions across contact-mode transitions are known to cause problems in numerical simulations. For example, [172] reports mode chatter and non-convergence associated with discontinuous response at stick–slip transitions for Coulomb friction models. Various numerical remedies are proposed for this problem in the literature [118, 152, 172, 146]. However, there is no physical basis for these discontinuities, and for the case of isotropic Coulomb friction models, [8] proposed an equivalent reformulation of the Coulomb model that eliminates the discontinuity as well as the need for special numerical treatments. We use the same revised friction model in this work. On the other hand, tractions and velocities exhibit genuine discontinuous response across separation-to-contact transitions where dynamic impact generates weak shocks. Suitably robust numerical methods are required to model these events accurately without Gibbs effects or other numerical artifacts. We use the regularization in [8] to suppress numerical problems at these transitions.

8.4 Stochastic nucleation and extension of fracture surfaces

Interfacial damage in real materials can accumulate on mesoscopic structures, such as grain boundaries and material interfaces. Alternatively, randomly distributed microscopic flaws, such as voids, inclusions, and microcracks, can trigger spontaneous nucleation and extension of fracture surfaces in seemingly homogeneous regions, even when no macroscopic feature, such as a notch or crack, is present. In the latter case, models that assume macroscopically homogeneous material can predict very nonphysical fracture patterns. Therefore, some means to account for random distributions of microscopic flaws and inhomogeneities is required in numerical simulations of fracture in quasi-brittle materials.

In this study, we assume the microscopic defects take the form of micro-cracks and use two strategies to model their influence on macroscopic response. In an *explicit realization*, the description of the analysis domain includes an explicit representation of a set of initial microcracks that fits a specified statistical distribution. In an *implicit realization*, a probabilistic crack nucleation model incorporates the influence of microcracks on the macroscopic response without explicitly representing the microscopic flaws in their original state. In this study, neither model is calibrated with experimental results for an actual material microstructure. Our purpose is only to demonstrate the qualitative influence of microscopic flaws, modeled by the two aforementioned realizations, on macroscopic fracture patterns.

Both realizations make use of the notion of *Active Crack Tips* (ACTs). An ACT is a vertex in the spacetime mesh from which a new fracture surface segment may be extended. ACTs appear at the endpoints of existing fractures in both realizations. In addition, isolated ACTs arise in implicit realizations during nucleations of new fracture surfaces.

Four special capabilities enable aSDG simulations of dynamic crack propagation: 1) a direction-dependent effective stress measure, 2) criteria for the identification of ACTs, 3) criteria for extension of fracture surfaces, and 4) adaptive procedures that allow the aSDG mesh to conform to any desired crack-propagation direction. In §8.4.5, we discuss methods for

incorporating an angular bias in the fracture algorithm to model anisotropies, such as those produced by bedding planes in rock formations. To simplify the presentation, we restrict our attention to fracture models in two spatial dimensions and assume that microscopic flaws are modeled as microcracks from here on.

8.4.1 A direction-dependent effective stress measure

We introduce here a direction-dependent measure of effective stress that controls nucleation of new cracks in implicit realizations as well as extensions of existing fracture surfaces in both types of realizations. Figure 8.4 shows the spatial projection of the top facets of a previously solved aSDG patch in which vertex V is the top vertex shared by all of the tetrahedral elements in the patch (*cf.* Fig. 8.2). The new effective stress measure at V is similar to the effective Riemann stress in (8.9), except it is used at stages in our algorithm where a fracture surface segment is not yet available to determine the orientation of a local coordinate frame, as in Fig. 9.1. Instead, we construct local coordinate frames relative to rays emanating from V in spatial directions determined by a variable angle θ , such that s^1 and s^2 are the normal and tangential components of the traction vectors acting on the rays.

Following [43], we now define a *directional effective stress*, $s_{\text{eff}}(\theta)$,

$$s_{\text{eff}}(\theta) := \sqrt{\langle s^1(\theta) \rangle_+^2 + \beta^2 (s^2(\theta))^2} \quad (8.12)$$

in which β is a shear stress factor similar to the one in (8.9), and we use stress fields within elements surrounding V to evaluate the tractions $s^1(\theta)$ and $s^2(\theta)$. Since the stress and velocity fields are continuous on the element interiors but not across element boundaries, we conclude that the tractions in (9.11) are identical to the tractions for the bonded condition in (8.9) for almost every angle θ . Thus, the effective stresses in (8.9) and (9.11) are equivalent, aside from the angular dependence of (9.11). This observation justifies the use of the same notation, $\mathfrak{s}$, for both versions of effective stress.

8.4.2 Identification of active crack tips

Active crack tips play important roles in our models of dynamic fracture for both explicit and implicit realizations of microscopic flaws. In this subsection, we describe how ACTs are identified in each model.

8.4.2.1 Identification of ACTs in explicit realizations

In an explicit realization, the initial distribution of microcracks is explicitly represented in the initial description of the analysis domain as well as the initial finite element mesh. We mark the tips of every initial microcrack as ACTs.

We first generate an initial distribution of microcracks to satisfy specified statistical properties. The microcrack lengths, l_i , must fit a specified probability distribution from a Weibull model. We quantify the density of initial microcracks with a nondimensional crack density ratio,

$$\alpha = \frac{\sum_{i=1}^{\text{nc}} l_i^2}{A_c} \quad (8.13)$$

in which A_c is a reference spatial area, and nc is the number of microcracks in A_c . We assume that the positions of initial microcracks are uniformly distributed in space and either assume that the microcrack orientations are uniformly distributed or that there is a preferred orientation, as discussed in §8.4.5.

We use a “take and place” method to construct a distribution of initial microcracks that satisfies the given statistical properties. We create a candidate microcrack by sampling the distributions for each probabilistic variable, and tentatively add the candidate to the analysis domain according to its size, orientation and location. We discard the candidate crack if it intersects an existing crack. Otherwise, the candidate is accepted as a permanent part of the model. We repeat this procedure until we attain the target crack density. Then we generate an initial finite element mesh that resolves all of the microcracks.

8.4.2.2 Identification of ACTs in implicit realizations

Multi-scale simulation of fracture with explicit treatment of all relevant length scales, from the macroscopic domain geometry down to the smallest microscopic flaw, remains a daunting computational challenge. In implicit realizations, we replace explicit representations of microscopic flaws with a probabilistic model that determines the nucleation of macroscopic cracks. This provides a more tractable simulation problem that can still incorporate the influence of microscopic features on macroscopic fracture.

We base our probabilistic crack nucleation criteria on the Weibull model [215, 216], a reasonable choice for modeling failure in quasi-brittle materials. The *probability distribution function* (PDF) for fracture strength $\bar{s}$, cf. (9.14), is given by,

$$p(\bar{s}) = \begin{cases} 0 & \bar{s} < s_{\min} \\ \frac{A}{A_0} \frac{m}{s_0} \left(\frac{\bar{s} - s_{\min}}{s_0} \right)^{m-1} e^{-\frac{A}{A_0} \left(\frac{\bar{s} - s_{\min}}{s_0} \right)^m} & \bar{s} \geq s_{\min} \end{cases} \quad (8.14)$$

in which A_0 is a reference area, such as the area of an experimental specimen used to calibrate the Weibull model, s_0 is a strength scale, m is the Weibull modulus (or shape parameter), and $s_{\min}$ is a lower bound for the fracture strength. Lower values for s_0 imply lower fracture strengths, $\bar{s}$. Similarly, for a given area A , smaller values for A_0 reduce the fracture strength, $\bar{s}$, and imply a higher microcrack density in the context of an implicit realization. We use the *inverse CDF method* to sample fracture strengths $\bar{s}$ consistent with the Weibull PDF (9.17) at the vertices of aSDG mesh.

Consider again the patch and vertex V in Fig. 8.4. We set A in (9.17) equal to the patch's projected area to determine a PDF for fracture strength in the patch. Next, we sample an angle-independent strength, $\bar{s}$, from the patch PDF (plotted as a circle around vertex V) and a direction-dependent effective stress, $s_{\text{eff}}(\theta)$, using (9.11). If $s_{\text{eff}}(\theta) > \bar{s}$ for any angle θ , such as the one corresponding to P in the figure, we mark vertex V as an ACT and store its sampled fracture strength, $\bar{s}$. Vertex V will be checked for potential crack extension using its stored strength every time a patch is erected over it, so long as it remains an ACT. Any

crack extension from the isolated ACT at V constitutes the nucleation of a new fracture surface.

8.4.3 Criteria for extension of fracture surfaces

We model crack propagation by extending a new fracture surface segment from an ACT. The damage field on the new segment is initialized to zero (fully-bonded condition), so initially there is no change in mechanical response across the new segment. Actual crack propagation is delayed until sufficient damage accumulates to start debonding the new segment. We describe below the criteria and procedures for deciding when to extend a fracture surface, for determining the direction of extension, and for adapting the mesh to generate a new segment in the correct direction.

The criteria and procedures for extending new fracture segments in explicit and implicit realizations are essentially the same, except for one difference. In explicit realizations, the fracture strength, $\bar{s}$, associated with an ACT is a deterministic parameter because all probabilistic variations are encoded in the initial layout of microcracks. On the other hand, fracture strength is a probabilistic parameter in implicit realizations, so it is important to always use the sampled value of $\bar{s}$ that was stored when the ACT was first created.

Before generating a new patch over an ACT, we first check the extension criterion. The setup is mostly the same as in Fig. 8.4, except now V is a local minimum and its adjacent elements are in previously solved patches constructed over the neighbor vertices of V . Let $\check{s}_{\max} := \max_{\theta} \check{s}(\theta)$. If $\check{s}_{\max} < \bar{s}$ there is no propagation, and we proceed with the construction of a new patch over vertex V , which retains its status as an ACT. Otherwise, we choose extension directions for which $\check{s}(\theta)$ is a local maximum and its value exceeds $\bar{s}$. For example, for the stress state shown in Fig. 8.4, we extend the fracture surface in the V - P direction.

8.4.4 Adaptive alignment of element boundaries with extension directions

When the crack propagation criterion, $\check{s}_{\max} \geq \bar{s}$, is satisfied, the computed crack-growth direction(s) can be accommodated by the aSDG method's powerful adaptive meshing

capabilities. Figure 8.5 depicts a front-mesh fragment in which vertex A is an ACT that has been assigned a crack-propagation direction along line l . As is typical, l is not aligned with any of the element boundaries in the front mesh.

There are two adaptive meshing options for aligning an element boundary with the propagation direction. The first is illustrated in Fig. 8.5(a), where vertex E is inserted on edge BC to create a new edge AE that is aligned with the crack direction. This operation subdivides front-mesh element e into elements e_1 and e_2 in a manner very similar to the edge-bisection operation in the newest-vertex refinement procedure that is heavily used in aSDG adaptive meshing. Accordingly, this method works best when E lands near the center of edge BC. Note that vertex E must be marked as an ACT, while A loses its ACT status to complete the operation.

The second option, depicted in Fig. 8.5(b), is favored when line l is closer to one of the existing element boundaries (AB in this example), than it is to the bisector of element e . In this case, the best option might be to use a tilted-tent-pole patch to move the top vertex, B', over line l . In this scenario, the tilted patch must be generated and solved before the fracture surface can be extended over edge AB'. A more detailed discussion of these adaptive strategies can be found in [1].

8.4.5 Adding angular bias to the fracture strength

In some materials, such as sedimentary rocks with bedding planes, the fracture strength has an angular bias. We can introduce a similar angular bias in either style of realization. In an explicit realization, we would generate a nonuniform distribution of initial microcrack orientations, with the highest probability densities centered on the given (bias) orientation. In an implicit realization, an angular profile for $\bar{s}$ is chosen. The maximum strength about a vertex V is obtained from the Weibull probabilistic failure model in §8.4.2.2. Thus, the profile of $\bar{s}$ versus angle θ and its maximum value fully characterize $\bar{s}(\theta)$ for a given vertex V. We note that the angular profile of $\bar{s}$ can be made spatially inhomogeneous and statistically random by using random variables to characterize, for example, the angle and value of minimum strength. An example of a model of this type is presented in §8.5.2.2. The crack

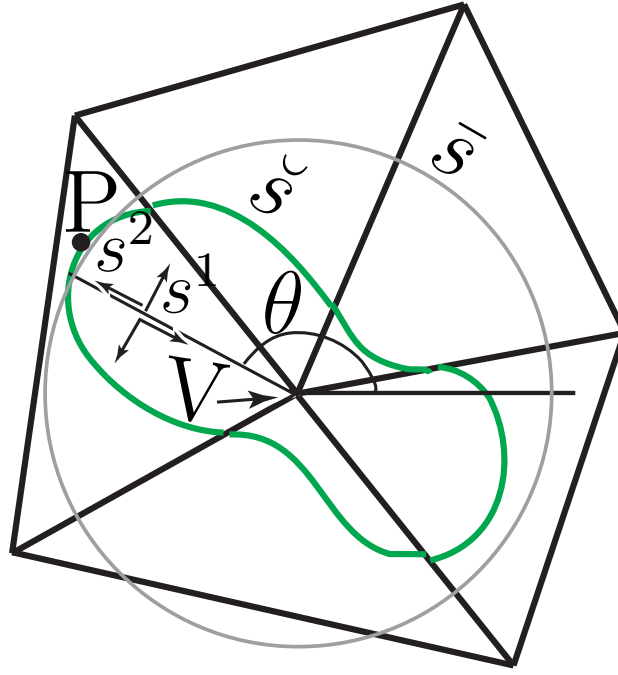


Figure 8.4: The angular distribution of effective stress s_{eff} and fracture strength $\bar{s}$ around vertex V at the top of a patch. The magnitude of these parameters for a given angle θ is mapped to radial distance from V . The maximum value of s_{eff} at V occurs in the direction of P , where it slightly exceeds the fracture strength, $\bar{s}$.

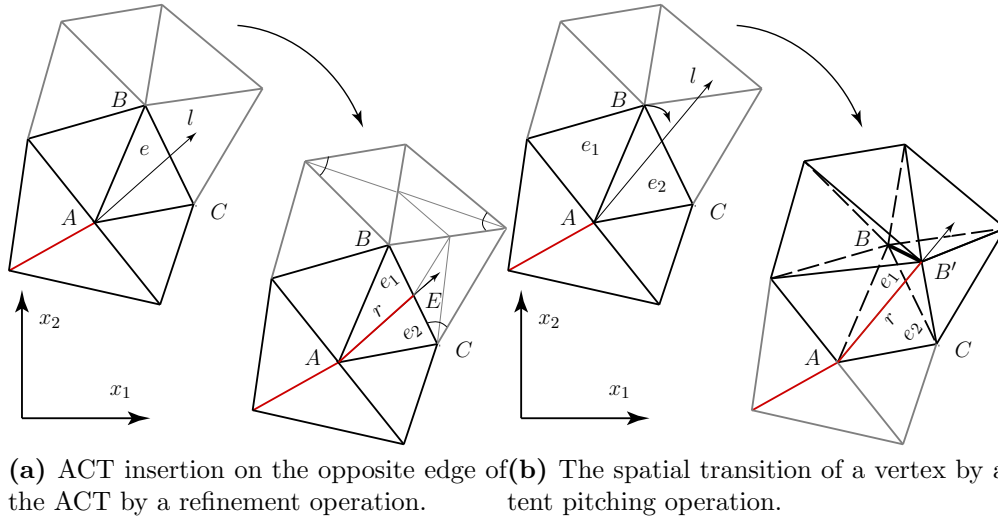


Figure 8.5: The extension of a crack in the space mesh through refinement and tent pitching operations.

propagation direction is no longer the same as in §8.4.3, since now both the fracture strength, $\bar{s}(\theta)$, and the effective stress, $s_{\text{eff}}(\theta)$, are non-uniform functions.

8.5 Numerical Examples

In this section, we first demonstrate crack-path convergence using the proposed damage model and the adaptive aSDG method. Then we examine the influence of various material parameters on fracture patterns in quasi-brittle materials, using both explicit and implicit realizations of flaws. We use the following parameters in the damage model in all examples in this section: $\beta = 1$, $c_0 = 0.8$, and $a = 10$ (*cf.* (9.10), (8.9), and (9.14)).

8.5.1 Crack-path convergence study

In this subsection, we investigate crack-path convergence as tighter adaptive tolerances increase the resolution of our discrete models. In view of the stochastic nature of the nucleation model proposed in §8.4.2.2, we do not expect to obtain precisely the same fracture pattern on distinct meshes, even when the solution is well resolved. Therefore, in order to study the convergence properties of the underlying aSDG crack growth model, we disable the stochastic nucleation model. We retain, however, the adaptive meshing operations described in §8.4.4 to ensure that incremental fracture-surface extensions match precisely the directions given by the maximum effective stress criterion in §8.4.1.

Figure 8.6 shows the geometry, supports, and loading conditions for a problem defined on an L-shaped domain in which a quarter-circle fillet with a 10 mm radius spans the re-entrant corner. A spatially uniform, prescribed-velocity boundary condition, $\bar{\mathbf{v}}(t)$, is applied over a 30 mm boundary segment as shown. The magnitude of the prescribed velocity ramps smoothly from an initial zero value to a sustained value of 1 m/s in 100 μs . In lieu of the stochastic nucleation model, we prescribe a single nucleation site in the center of the fillet. The bulk material and interface fracture properties are; Young’s modulus $E = 20$ GPa, mass density $\rho = 2400$ kg/m³, Poisson’s ratio $\nu = 0.18$, fracture strength $\bar{s} = 30$ MPa, shear stress factor $\beta = 0$, and relaxation time $\tilde{\tau} = 1$ μs .

We introduce two error indicators, one that measures the numerical energy dissipation over each spacetime element and one that measures the energy induced on each spacetime fracture-surface facet by the mismatch between the tractions generated by the trace of the

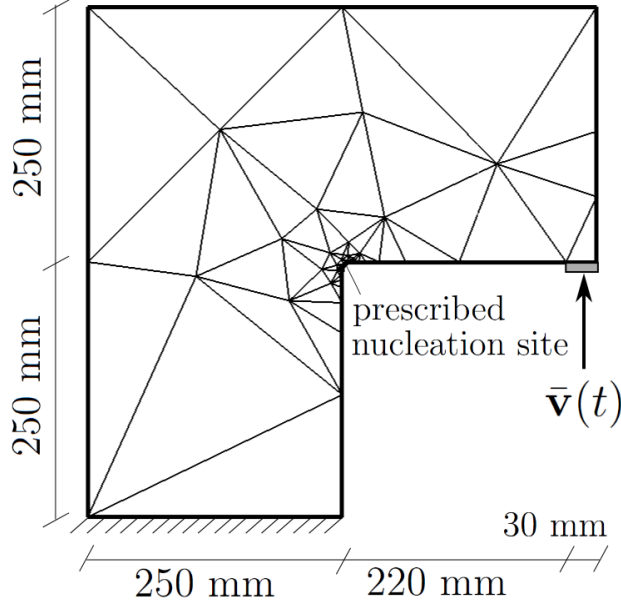
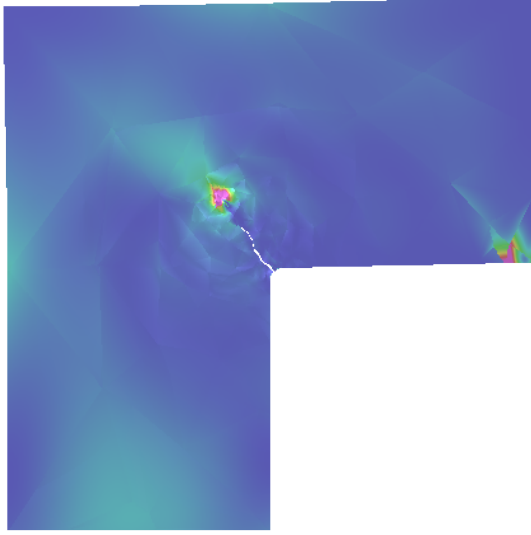


Figure 8.6: Schematic of the domain, loading condition, and initial space mesh for the L-shaped problem in §8.5.1.

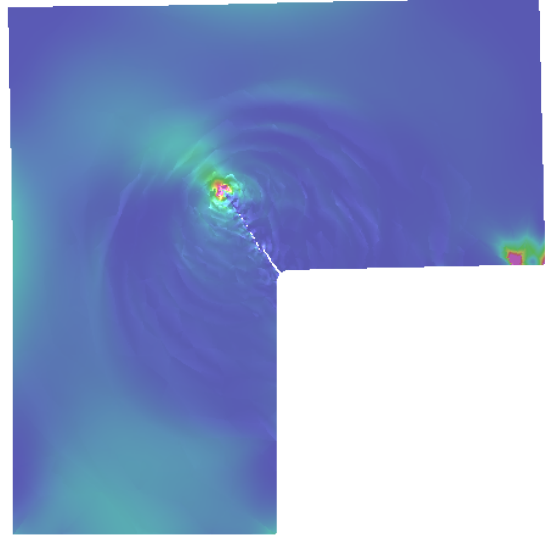
aSDG stress solution and the target Riemann tractions determined by our interfacial damage model; *cf.* §8.2.2, (9.7), and [3, 10, 11]. User-specified tolerances, $\tilde{\epsilon}_D$ and $\tilde{\epsilon}_C$ respectively, independently control the magnitudes of these energy errors. In the present study, we assume $\tilde{\epsilon}_D = \tilde{\epsilon}_C =: \tilde{\epsilon}$, and compute solutions for $\tilde{\epsilon} = 10^{-5}$, 10^{-6} , 10^{-7} , 10^{-8} , and 10^{-9} J. As described in [11], simultaneously reducing $\tilde{\epsilon}_D$ and $\tilde{\epsilon}_C$ ensures that the aSDG solution resolves crack-tip fields and propagating wave fronts while rendering the fracture process zone accurately.

Figure 8.7 shows solutions for the L-shaped domain problem at an intermediate time, $t = 430 \mu\text{s}$. Figure 8.8 shows the corresponding front meshes at $t = 880 \mu\text{s}$, slightly after the time when the crack tip should exit the domain. The simulation with the coarsest adaptive tolerances falsely predicts crack arrest before the fracture exits the domain, as seen in Fig. 8.8a. The smeared crack-tip fields, under-resolved wave fronts, and mesh-related artifacts evident in Fig. 8.7a contribute to this erroneous prediction. Things improve as we tighten the adaptive tolerances until all solution features and the crack path are well resolved for $\tilde{\epsilon} = 10^{-9}$ J; *cf.* Figs. 8.7d and 8.8d.

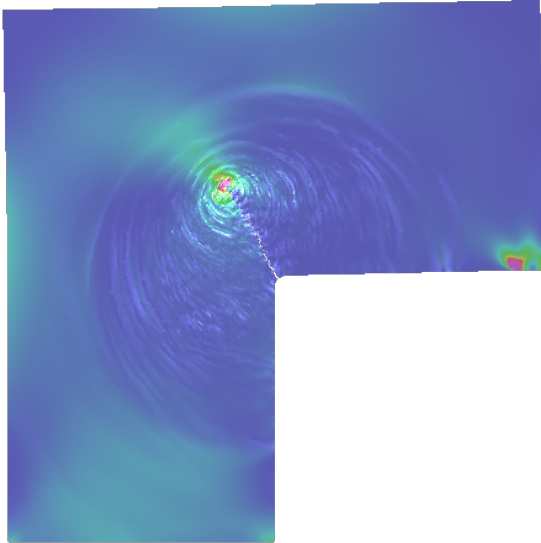
The front mesh for $\tilde{\epsilon} = 10^{-9}$ J at $t = 430 \mu\text{s}$ in Fig. 8.9 demonstrates the adaptive aSDG method’s ability to capture the fine details of dynamic solutions. Regions of intense mesh refinement correspond to the local crack-tip field, sharp wave fronts emitted by the



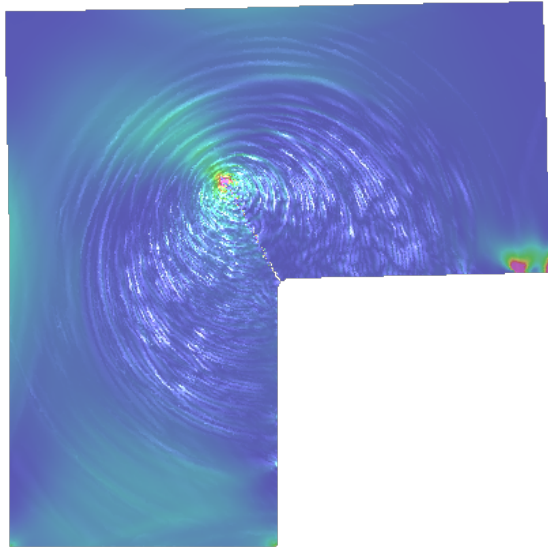
(a) $\tilde{\epsilon} = 10^{-5} \text{ J}$.



(b) $\tilde{\epsilon} = 10^{-7} \text{ J}$.



(c) $\tilde{\epsilon} = 10^{-8} \text{ J}$.



(d) $\tilde{\epsilon} = 10^{-9} \text{ J}$.

Figure 8.7: Front meshes for the L-shaped domain problem at time $t = 430 \mu s$ for various values of $\tilde{\epsilon}$. Color and height fields depict internal and kinetic energy densities, respectively.

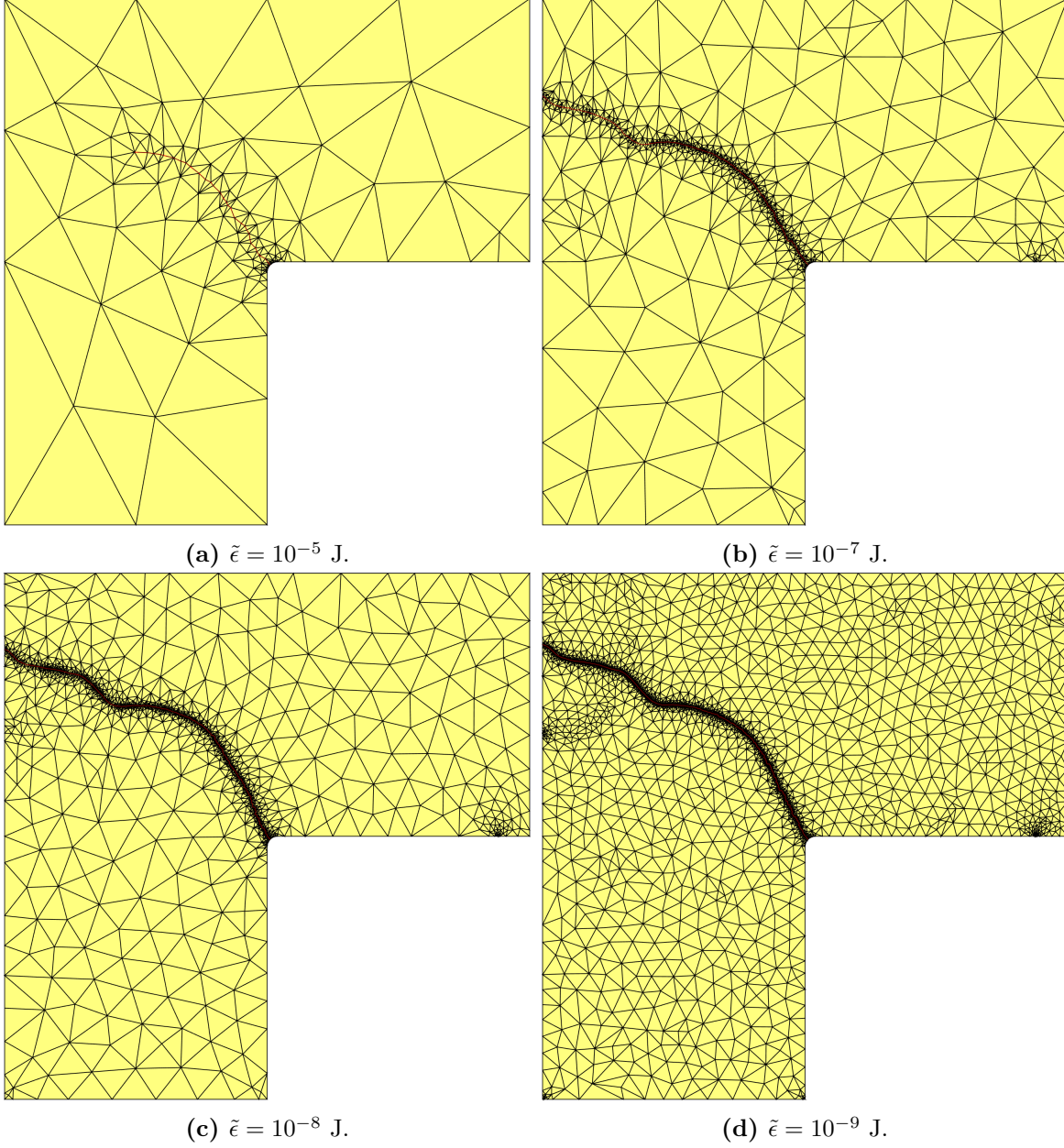


Figure 8.8: Front meshes for the L-shaped domain problem at $t = 880 \mu\text{s}$ for various values of $\tilde{\epsilon}$. The crack path is rendered with red line segments.

propagating crack, and the stress concentration at the edge of the prescribed-velocity loading, as depicted in Fig. 8.7d. It is noteworthy that the complex front mesh in Fig. 8.9 with 22948 triangles evolved from the same coarse mesh in Fig. 8.6, with only 115 triangles, that we used to initiate all the simulations in this study.

Figure 8.10 compiles crack paths at $t = 800 \mu\text{s}$ for adaptive tolerances ranging from $\tilde{\epsilon} = 10^{-5}$ to 10^{-9} J. The false crack arrest for $\tilde{\epsilon} = 10^{-5}$ attests to the unreliability of predictions based on under-resolved numerical simulations in dynamic fracture mechanics. On the other hand, evidence of crack-path convergence is observed in the results for $\tilde{\epsilon} = 10^{-8}$ and 10^{-9} J. The convergence is most convincing in the earlier stages of crack propagation, while a small difference between the two crack-path predictions develops in the later stages. Close inspection suggests that this discrepancy might be due to modest mesh coarsening along the crack path for $\tilde{\epsilon} = 10^{-8}$ J when the crack tip traverses a less energetic region in the later stages of the simulation. In contrast, the mesh is well refined along the entire crack path for $\tilde{\epsilon} = 10^{-9}$ J.

Based on this study, we summarize requirements for convergent crack-path predictions in sharp-interface fracture models as follows. The model must be able to accurately resolve transmitted and reflected wavefronts produced by dynamic loading as well as crack initiation and arrest events. The model must resolve all relevant time and length scales, such as process zone diameter. Crack-tip fields must be rendered with sufficient continuity and smoothness to support reliable computation of directions for incremental crack extensions, and the numerical model must be sufficiently flexible to support fracture extension precisely in the computed directions. Finally, there must be competent control of the length of incremental crack extensions to support convergent integration of crack path geometry. Although our aSDG method addresses all of these requirements, lengths of incremental crack extensions are only controlled indirectly via adaptive mesh refinement in the vicinity of crack tips. Since our use of high-order basis functions tends to reduce the amount of mesh refinement, a more direct means to address this issue is worth investigating.

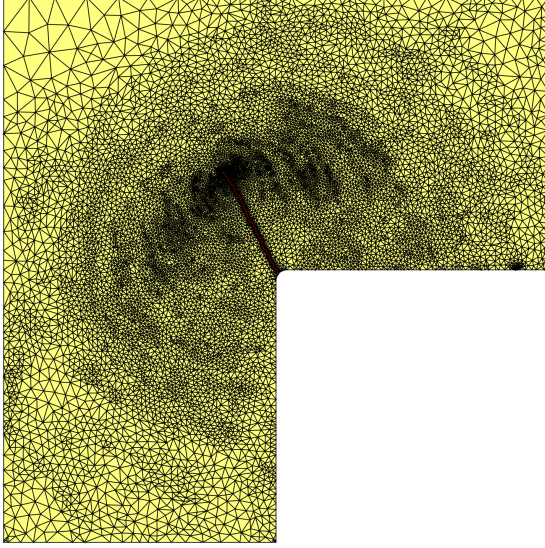


Figure 8.9: Front mesh at $t = 430 \mu\text{s}$ for $\tilde{\epsilon} = 10^{-9} \text{ J}$.

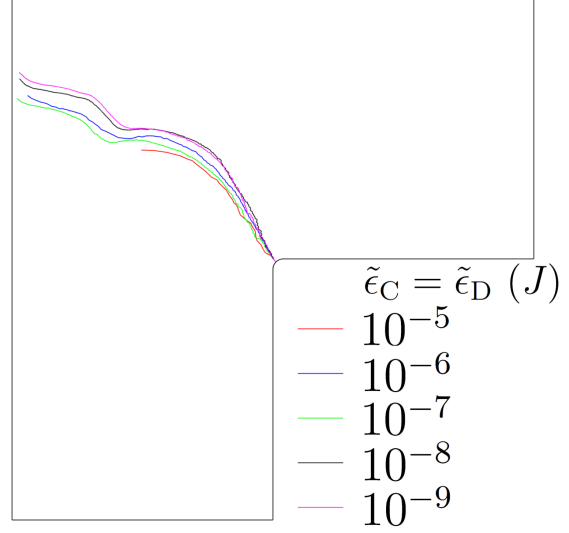


Figure 8.10: Comparison of crack paths at $t = 430 \mu\text{s}$ for various values of $\tilde{\epsilon}$.

8.5.2 Crack propagation under an ambient hydrostatic pressure field

This example demonstrates the aSDG method's ability to model crack propagation in a medium with initial microcracks under ambient hydrostatic pressure in which the surfaces of an initial crack are rapidly loaded with a uniform pressure to simulate dynamic hydraulic loading. This provides a favorable setting for studying the interaction of a main crack with microcracks because, in contrast to a problem loaded by far-field tensile loads, in this problem the microcracks propagate only when triggered by interactions with the main crack tip.

Figure 8.11 shows the problem geometry and loading. A rock sample is loaded by an ambient hydrostatic pressure, $\sigma_H = 4.85 \text{ MPa}$. The four sides of the computational domain are treated with transmitting boundary conditions consistent with the hydrostatic pressure. The domain dimensions are $L_x = 5\text{m}$, $L_y = 3\text{m}$, and the initial crack length, from the boundary to tip V, is $L_c = 2\text{m}$. The material properties are: Young's modulus $E = 20 \text{ GPa}$, mass density $\rho = 2500 \text{ kg/m}^3$, and Poisson's ratio $\nu = 0.2$, and relaxation time $\tilde{\tau} = 0.03 \text{ s}$ (cf. (9.10)). The faces of the initial crack are dynamically loaded with a uniform pressure that ramps over one second from σ_H to a sustained value of 19.4 MPa . This loading rate is similar to dynamic hydraulic loading [231] and slower than explosive loading [87, 171]

which has a load-ramp duration of about 10 to 100 microseconds. The relatively rapid loading in the example tests the proposed model's ability to capture various features of dynamic fracture in quasi-brittle materials, including crack-path oscillation, microcracking, and crack bifurcation. During the course of the simulation, we extend the pressure loading to all fracture surfaces that become connected to the initial macroscopic crack by the growing complex of crack propagation. We present numerical results at times shortly after the loading reaches its sustained value.

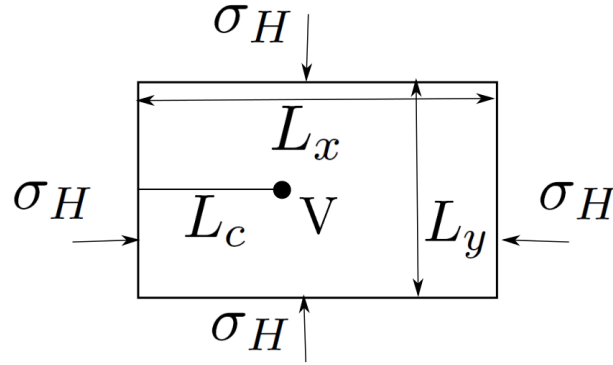


Figure 8.11: Schematic of the domain and hydrostatic loading for the numerical studies in §8.5.2.

8.5.2.1 Explicit realization under ambient hydrostatic pressure

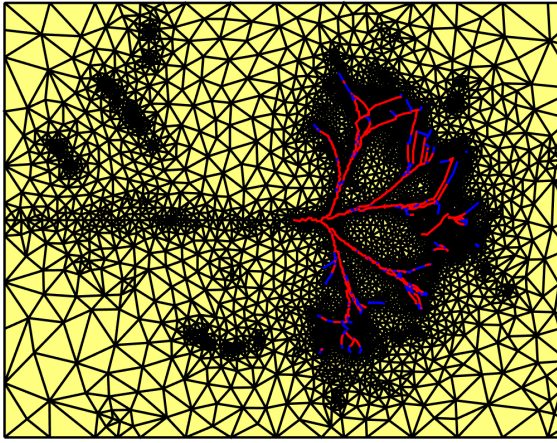
We present results in Fig. 8.12 for explicit realizations with microcrack densities, $\alpha = 0.1, 0.25, 0.50$, and a uniform (isotropic) distribution of microcrack orientations. The fracture strength threshold is $\bar{s} = 0.01E = 200$ MPa. The solution visualizations on the right, in Figs. 8.12(b,d,f), map strain energy density to color and kinetic energy density to a synthetic height field. The visualizations on the left, in Figs. 8.12(a,c,e), show spatial projections of the asynchronous aSDG front mesh at a stage where the vertex time coordinates are very close to, but not precisely equal to, the uniform sample time used in the solution visualizations. The front mesh plots reveal the crack pattern as well as the level of mesh refinement around the initial microcracks, macroscopic crack paths, and propagating crack tips. We use color to highlight new fracture surfaces generated during the simulation by crack propagation. Red indicates complete debonding (*i.e.*, $D = 1$) while blue — mostly observed near the crack

tips — highlights fracture process zones and other fracture surface segments with incomplete debonding ($D < 1$).

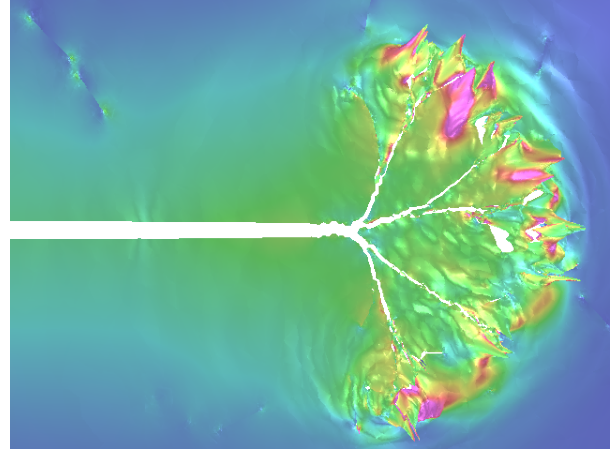
Figs. 8.12(a,b) show results for the lowest microcrack density, $\alpha = 0.10$. In Fig. 8.12(a), the regions with strong mesh refinement to the left of the fractured region reveal initial microcracks generated in the explicit realization. Elastic waves emitted by the initial macroscopic crack tip at V and by new macroscopic crack tips generated by the crack propagation model interact with the system of initial microcracks. Our analysis shows that this interaction induces contact-mode transitions on crack surfaces (between stick, slip, and separation modes) that are captured by the contact model described in §9.2. We use very tight regularization parameters in the contact model to ensure high accuracy; this accounts for the strong mesh refinement seen along crack path segments that are remote from crack tips, but within the range of elastic waves generated by the active fracture region.

Initial microcracks start to propagate when triggered by interactions with the system of loaded, actively propagating cracks. Our analysis shows that microcracks start to propagate either when they are intersected by a loaded propagating crack or when triggered by sufficiently strong elastic waves generated by the system of propagating cracks. In either case, they eventually join the network of propagating cracks that connects back to the original crack-tip position V. However, the initial microcrack density is not high enough to significantly influence the pattern of propagating macrocracks.

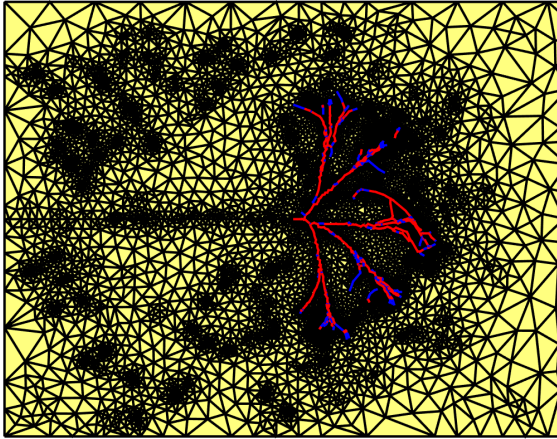
Figures 8.12(c,d) show results for $\alpha = 0.25$. The fracture pattern does not change significantly compared to $\alpha = 0.10$, however we observe more wave scattering by microcracks behind the propagating cracks. Results for the highest microcrack density, $\alpha = 0.50$, are shown in Figs. 8.12(e,f). In this case, we observe strong interactions between the initial and propagating macrocracks that substantially alter the fracture pattern. The active fracture zone becomes flatter than the more circular patterns observed in the previous cases, and stronger waves are emitted behind the active fracture zones. For purposes of comparisons of computational complexity, the front meshes corresponding to $\alpha = 0.10$, 0.25, 0.50 include, respectively, 15697, 15838, and 23402 elements and 3270, 2417, and 2961 newly generated crack segments.



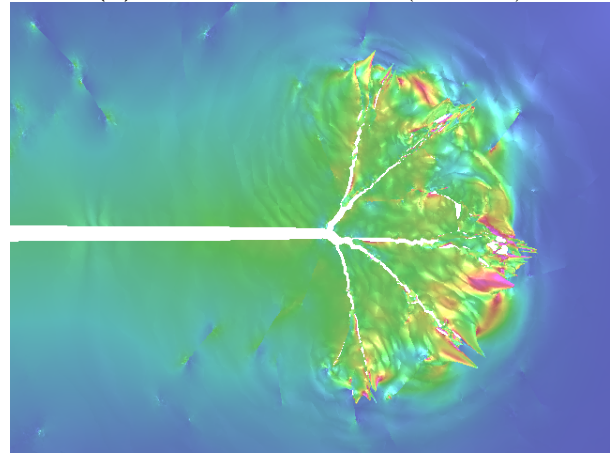
(a) Front mesh ($\alpha = 0.10$)



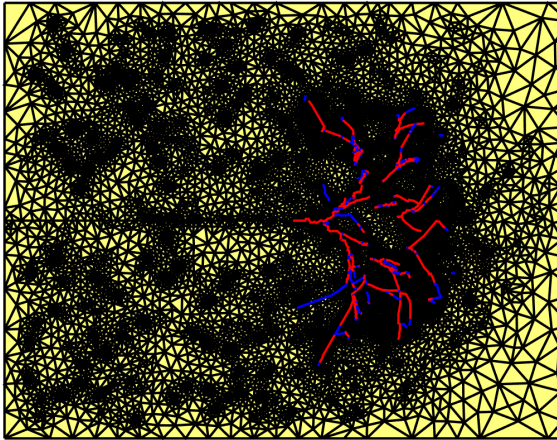
(b) Solution visualization ($\alpha = 0.10$)



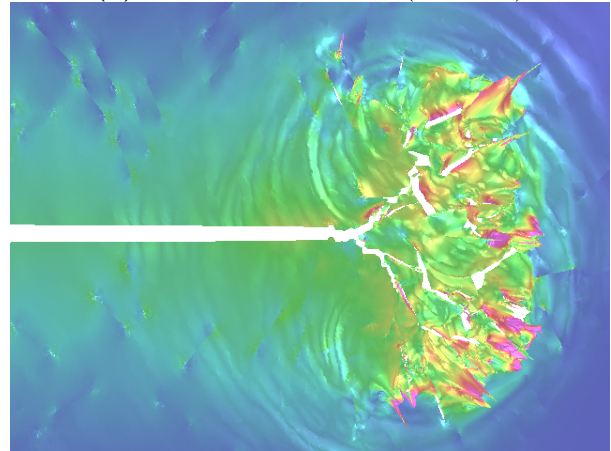
(c) Front mesh ($\alpha = 0.25$)



(d) Solution visualization ($\alpha = 0.25$)

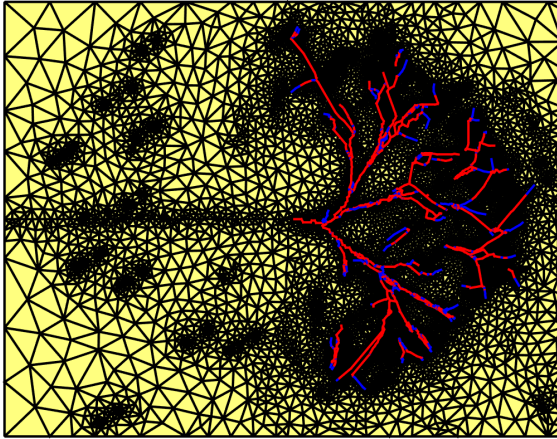


(e) Front mesh ($\alpha = 0.50$)

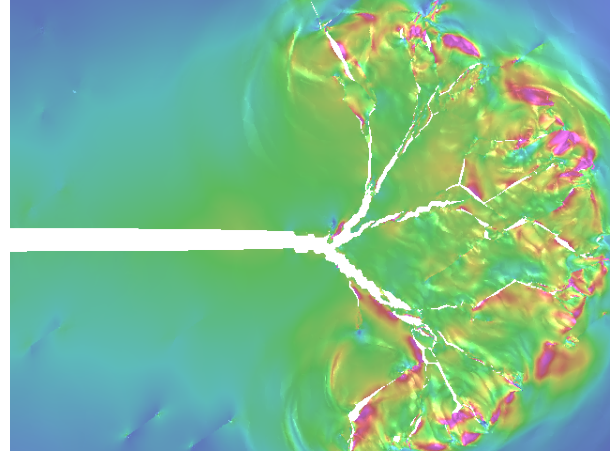


(f) Solution visualization ($\alpha = 0.50$)

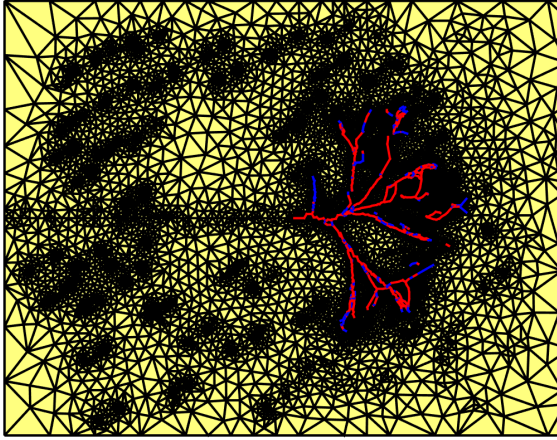
Figure 8.12: Interaction of a loaded macrocrack with explicit realizations of random distributions of initial microcracks at densities, $\alpha = 0.10, 0.25, 0.50$.



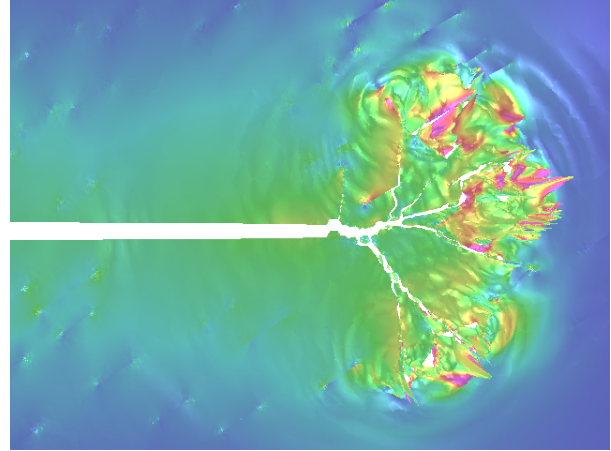
(a) Front mesh ($\alpha = 0.10$)



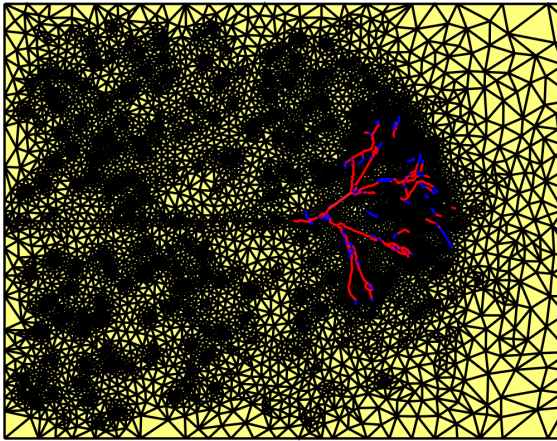
(b) Solution visualization ($\alpha = 0.10$)



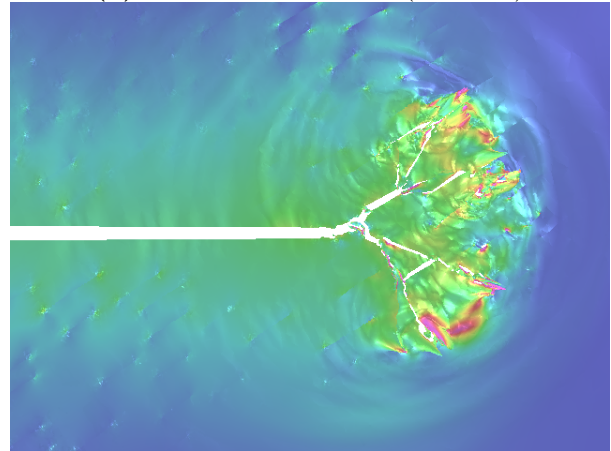
(c) Front mesh ($\alpha = 0.25$)



(d) Solution visualization ($\alpha = 0.25$)



(e) Front mesh ($\alpha = 0.50$)



(f) Solution visualization ($\alpha = 0.50$)

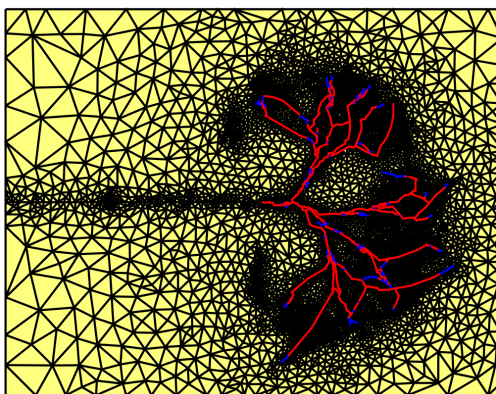
Figure 8.13: Interaction of a loaded macrocrack with explicit realizations of random distributions of initial microcracks with 30° orientation bias and densities, $\alpha = 0.10, 0.25, 0.50$.

Figure 8.13 shows results obtained with explicit realizations of the same three microcrack densities when the initial-crack orientations cluster about a 30° angle. Specifically, we use a uniform distribution of microcrack orientations between 25° and 35° . The purpose of this test is to investigate the influence of the angular bias of the initial fissures on the macroscopic crack pattern. Results for $\alpha = 0.10$ are shown in Figs. 8.13(a,b). There are no significant differences relative to the results without angular bias in Figs. 8.12(a,b). The same assertion can be made for results obtained with the intermediate microcrack density, $\alpha = 0.25$, depicted in Figs. 8.13(c,d). However, we do observe asymmetric changes in the macroscopic crack pattern in the results for the highest microcrack density, $\alpha = 0.5$, shown in Figs. 8.13(e,f). The upper major branch of the fracture zone is larger and has advanced further than the lower branch, and there is a noticeable tendency for the orientations of local fracture segments to align close to 30° . Apparently, higher initial microcrack densities are required to significantly influence macroscopic crack patterns.

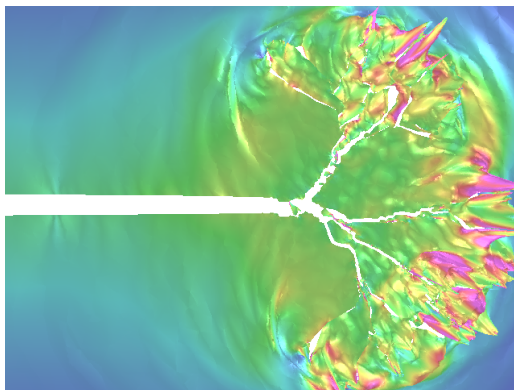
8.5.2.2 Implicit realization under ambient hydrostatic pressure

Next, we study the influence of microcracks on macroscopic fracture patterns obtained with implicit realizations based on the probabilistic nucleation model described in §8.4.2.2. We fix three of the Weibull model parameters, $m = 4$, $s_0 = 380$ MPa and $s_{\min} = 50$ MPa, but vary the reference area, $A_0 = 1, 10, 100$, and 1000 m^2 to adjust the likelihood of crack nucleation. We note that smaller reference areas give higher likelihoods of nucleation, and implicitly, higher microcrack densities. While some of these values for A_0 might be unrealistic, our goal is to understand how the value of A_0 influences fracture patterns. The values of other Weibull parameters might also be influential, but their investigation is beyond the scope of this study.

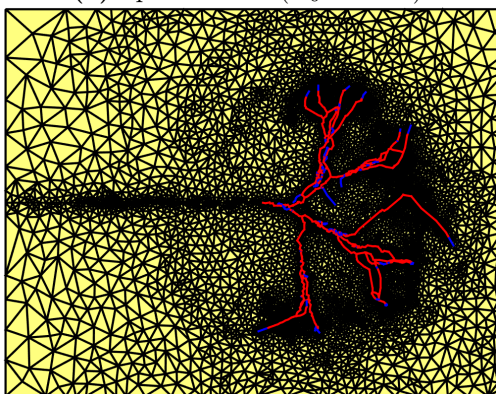
Figure 8.14: Propagation of a loaded macrocrack in random media modeled with implicit realizations of microcracks for reference areas, $A_0 = 1, 10, 100, 1000 \text{ m}^2$.



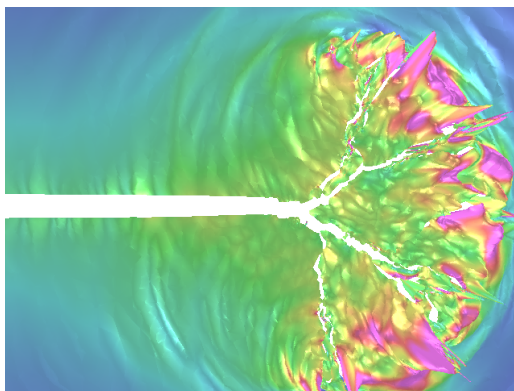
(a) Spatial mesh ($A_0 = 1 \text{ m}^2$)



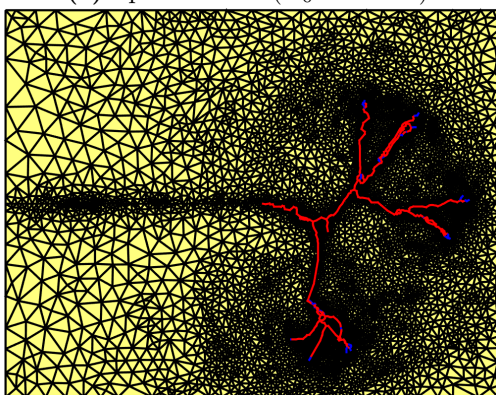
(b) Solution visualization ($A_0 = 1 \text{ m}^2$)



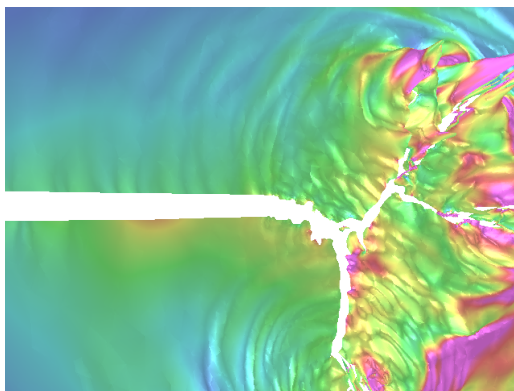
(c) Spatial mesh ($A_0 = 10 \text{ m}^2$)



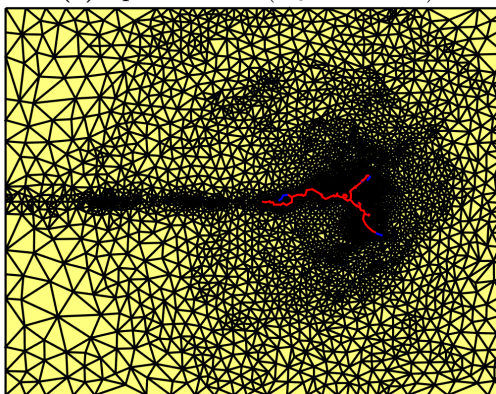
(d) Solution visualization ($A_0 = 10 \text{ m}^2$)



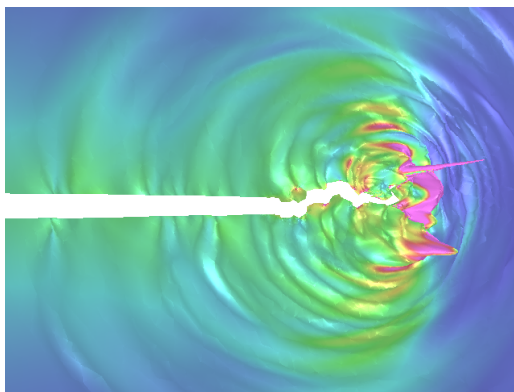
(e) Spatial mesh ($A_0 = 100 \text{ m}^2$)



(f) Solution visualization ($A_0 = 100 \text{ m}^2$)



(g) Spatial mesh ($A_0 = 1000 \text{ m}^2$)



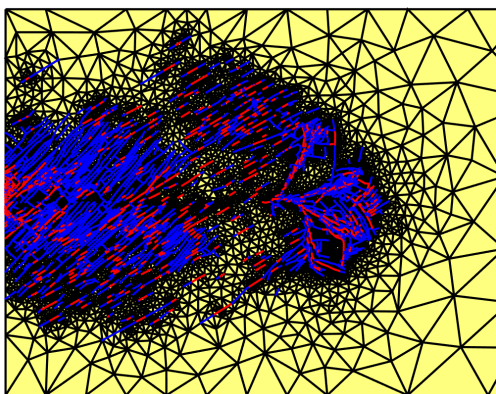
(h) Solution visualization ($A_0 = 1000 \text{ m}^2$)

We first consider the case where the probabilistic fracture strength, $\bar{s}$, does not depend on orientation. That is, the fracture strength at a given location is the same for all potential crack-propagation directions. As discussed in §8.4.2.2, the probability distribution of fracture strength $\bar{s}$ for the tent pole top vertex V of a patch with area A is fully characterized by the Weibull model (9.17), from which we sample a random strength at V.

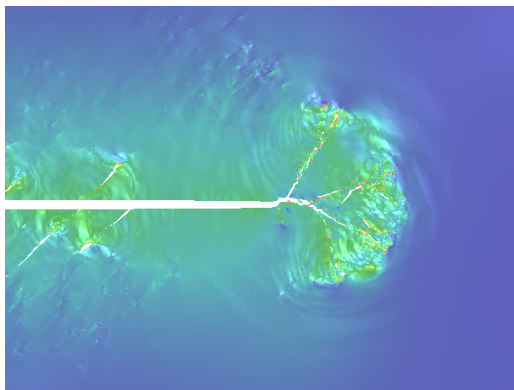
Results for varying values of A_0 are shown in Fig. 8.14. The crack patterns for $A_0 = 1 \text{ m}^2$ in Figs. 8.14(a,b) and $A_0 = 10 \text{ m}^2$ in Figs. 8.14(c,d) show realistic dynamic fracture patterns. As expected, the results from $A_0 = 1 \text{ m}^2$ exhibit a denser fracture pattern, since a smaller A_0 implies lower values for fracture strength from (9.17). However, as A_0 increases to 100 m^2 in Figs. 8.14(e,f) and 1000 m^2 in Figs. 8.14(g,h) it becomes extremely difficult to nucleate a crack, and the fracture patterns start to deviate from what is expected for quasi-brittle materials under dynamic loading. Specifically, for $A_0 = 1000 \text{ m}^2$ there is only one main crack that eventually bifurcates. The regions around the crack tips experience very high stress values, but given the low probability of fracture, it is difficult for any cracks to nucleate from these regions. For purposes of comparison, the space meshes corresponding to $A_0 = 1, 10, 100$, and 1000 m^2 include 17872, 16358, 15582, and 7835 elements and 4339, 3278, 2220, and 634 newly generated crack segments.

Figure 8.15 also shows results obtained with implicit realizations, but this time with angle-dependent fracture strengths, $\bar{s}(\theta)$, in which the angle θ describes the potential crack-extension direction. We assume that $\bar{s}(\theta)$ attains its lowest value, $\bar{s}_{\min}$, at $\theta_{\min}$ and $\theta_{\min} + \pi$ and its highest value, $\bar{s}_{\max}$, at $\theta_{\min} \pm \frac{\pi}{2}$. We sample values of $\bar{s}_{\max}$ similarly to the uniform angle values for $\bar{s}$ in Fig. 8.14. That is, they are based on the same Weibull parameters and local patch areas, A . However, we treat the fracture-strength ratio, $\bar{s}_{\min}/\bar{s}_{\max}$, as a random variable with small variations around 0.1 and the minimum-strength angle, $\theta_{\min}$, as a random variable with a mean value of 30° and $\pm 5^\circ$ of variation. As in Fig. 8.14, results are presented for $A_0 = 1, 10, 100$, and 1000 m^2 . Although all other model parameters are the same as in the model with angle-independent strength depicted in Fig. 8.14, we emphasize that the angle-dependent strength, $\bar{s}(\theta)$, and the specified fracture-strength ratio imply a roughly ten-fold weaker medium in the present example.

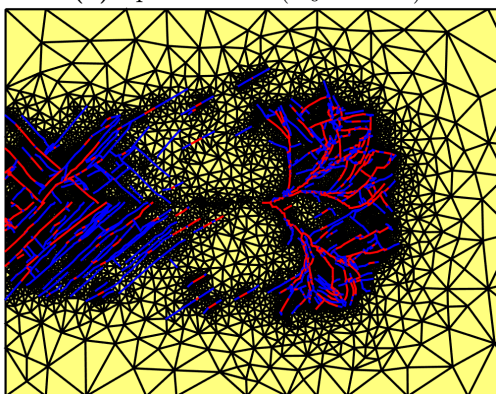
Figure 8.15: Propagation of a loaded macrocrack in random media modeled with implicit realizations of microcracks for reference areas ($A_0 = 1, 10, 100, 1000\text{m}^2$) and bias angles near 30° .



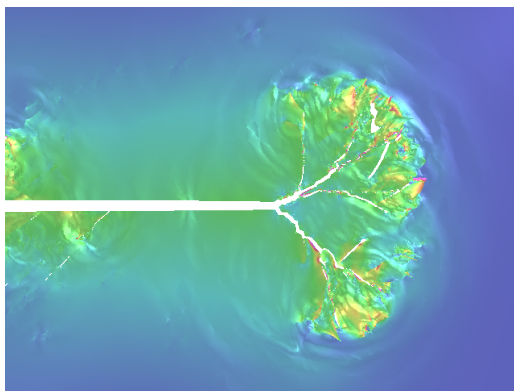
(a) Spatial mesh ($A_0 = 1 \text{ m}^2$)



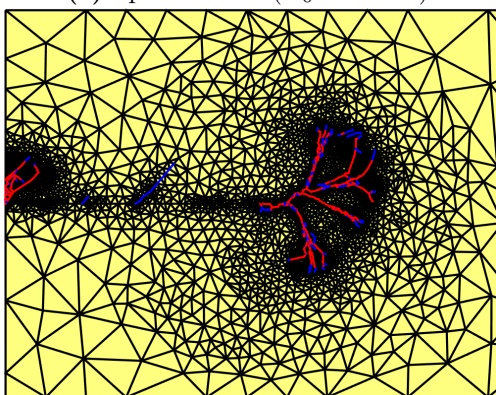
(b) Solution visualization ($A_0 = 1 \text{ m}^2$)



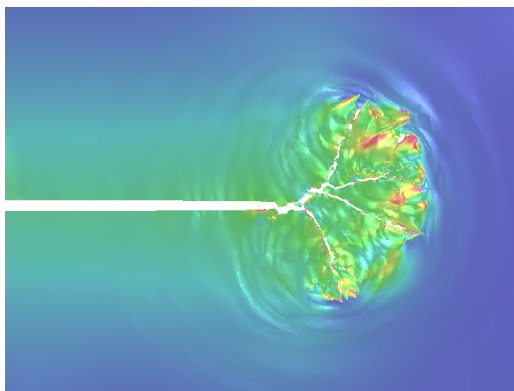
(c) Spatial mesh ($A_0 = 10 \text{ m}^2$)



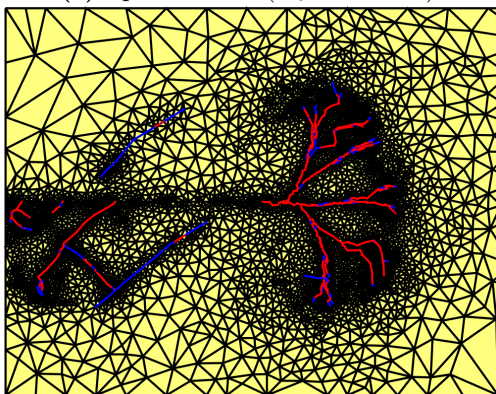
(d) Solution visualization ($A_0 = 10 \text{ m}^2$)



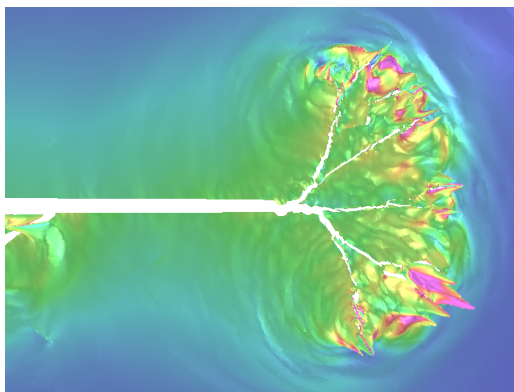
(e) Spatial mesh ($A_0 = 100 \text{ m}^2$)



(f) Solution visualization ($A_0 = 100 \text{ m}^2$)



(g) Spatial mesh ($A_0 = 1000 \text{ m}^2$)



(h) Solution visualization ($A_0 = 1000 \text{ m}^2$)

Figures 8.15(a,b) show results for $A_0 = 1 \text{ m}^2$, a low value that implies a very weak material according to (9.17) where for patch areas, $A \ll A_0$, the probability of crack nucleation is very high at relatively low stress values. The dynamic hydraulic loading generates compressive waves that perturb the background hydrostatic pressure field adjacent to the initial crack, generating shear stresses with maximum values at $\pm 45^\circ$ that, for this very weak material, are sufficient to nucleate and propagate a dense field of microcracks. A large subset of these roughly aligns with the $+45^\circ$ maximum shear stress direction which is not too far removed from the minimum strength direction at $+30^\circ$. Notably, there is insufficient energy in the perturbed stress state to drive the majority of these cracks beyond low levels of damage (rendered in blue). A much smaller subset aligns with the -45° maximum shear stress direction which is far from the minimum-strength direction. Finally, there is a subset of microcracks that align with the minimum strength direction at $+30^\circ$. These are distinguished by full damage (rendered in red), at least over short distances. The under-developed fracture network in front of the main crack tip is another important feature. Here, too, there are many nucleated cracks but only a small fraction of them sustain major damage. We emphasize that this choice of A_0 yields a model that is physically unrealistic for common materials. We observe similar behavior for $A_0 = 10 \text{ m}^2$ in Figs. 8.15(c,d). However, fewer cracks nucleate due to the higher sampled fracture strengths, $\bar{s}(\theta)$, and the probabilistic aspect of the model is more apparent than in the results for $A_0 = 1 \text{ m}^2$.

Figures 8.15(e – h) show results for $A_0 = 100$ and 1000 m^2 . As expected, fewer cracks nucleate and propagate, and most of these attain full damage. There are still a few cracks adjacent to the main crack; their random locations are a consequence of the stochastic nucleation model. We observe more fracture formation in these results than in the results for angle-independent strength displayed in Fig. 8.14(e) – (h). This is due to the reduction of fracture strength in most directions, especially the ten-fold decrease for $\theta \approx 30^\circ$. To quantify this, we observe that for nonuniform $\bar{s}(\theta)$, the space meshes corresponding to $A_0 = 1, 10, 100$, and 1000 m^2 include 31717, 27453, 12608, and 14558 elements and 17137, 10530, 3839, and 3513 newly generated crack-path segments. That is from two to six times more crack segments compared to the uniform-strength study.

8.5.3 Fragmentation under uniform applied tensile stress

Cracks nucleating at random sites under dynamic loading can propagate and intersect to form complex fracture patterns that include isolated fragments. The simulation example presented here demonstrates the aSDG method's ability to model fragmentation through crack nucleation, propagation, and intersection. To facilitate normalization, we set all dimensions and material properties to unity without reference to a specific system of units. The computational domain is a square with unit edge length, centered at $(0, 0)$. We specify plane strain conditions and the following material properties: Young's modulus $E = 1$, mass density $\rho = 1$, and Poisson's ratio $\nu = 0.3$. The relaxation time, *cf.* (9.10), is $\tilde{\tau} = 0.0116$. This implies a reference fracture displacement scale $\tilde{u} = \bar{s}\tilde{\tau}/c_d\rho = 0.001$; *cf.* [5] .

We apply initial and boundary conditions consistent with a uniform, isotropic tension field that ramps linearly in time. The components of the displacement field are

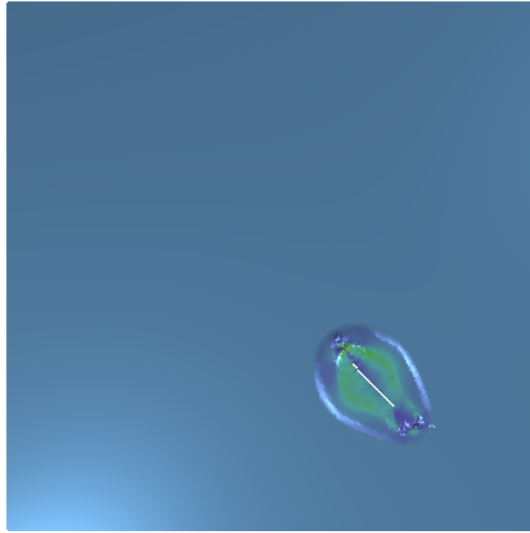
$$u_1(x_1, x_2, t) = ax_1t, \quad u_2(x_1, x_2, t) = ax_2t \quad (8.15)$$

in which $a > 0$ is the loading coefficient. For simplicity, we apply Dirichlet boundary conditions, *i.e.*, a prescribed velocity field derived from (8.15), on the entire boundary of the unit square at all times, even though the uniform, isotropic tension field is broken once cracks start to form.

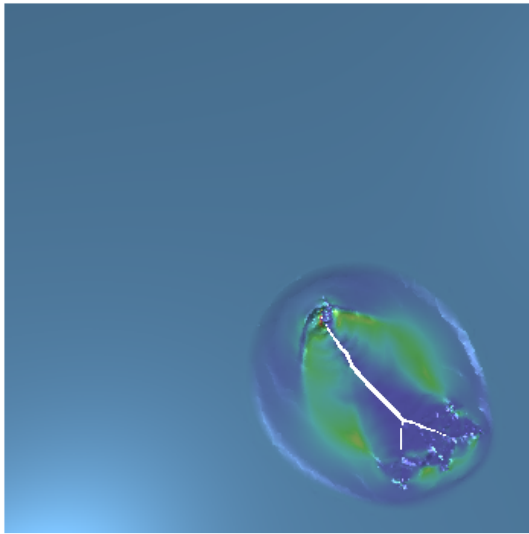
Figure 8.16: Fragmentation simulation for a domain subjected to uniform isotropic tension; $\tilde{\tau} = 0.0116$. Color and height fields depict internal and kinetic energy densities, respectively.



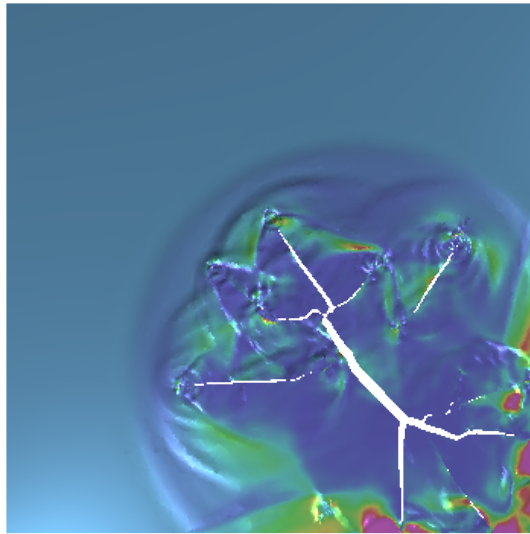
(a) $t = 7.13$



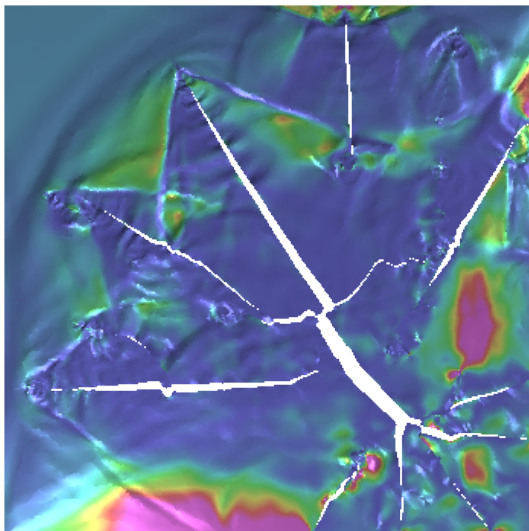
(b) $t = 7.20$



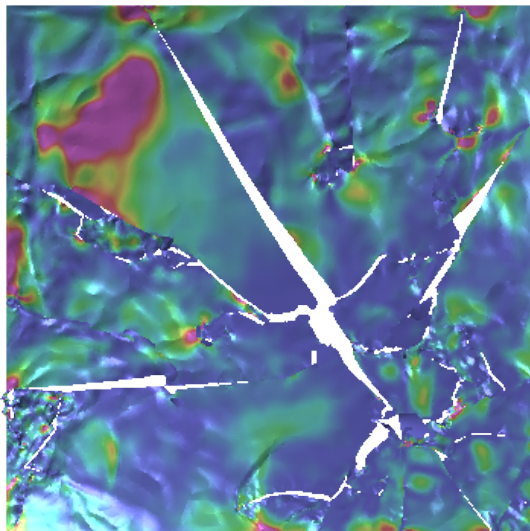
(c) $t = 7.30$



(d) $t = 7.50$



(e) $t = 7.80$



(f) $t = 8.40$

Figure 8.16 present results for $a = 0.013$. As before, the color and height fields depict strain and kinetic energy densities. The Weibull parameters are $m = 4$, $s_0 = 0.2E = 0.2$, $s_{\min} = 0.03$, and $A_0 = 1$. This corresponds to a mean strength value, $\langle \bar{s} \rangle = 0.211$, with a standard deviation of 0.0508 for random strength, $\bar{s}$, defined by (9.17). For the given material properties, the applied uniform tension field reaches the mean strength $\langle \bar{s} \rangle$ at $t_{\langle \bar{s} \rangle} = 8.44$. In view of the random strength model used in this example, we expect the first crack to nucleate at a somewhat earlier time. Indeed, we observe the first nucleation at about $t = 7.13$, as seen in Fig. 8.16(a). Since the location and time of first crack nucleation depends on the particular sampling of the random strength model in a given simulation, the location and time of first nucleation can vary from one run to the next for the same Weibull parameters.

Figures 8.16(b-f) show a sequence of crack propagation and fragmentation. The initial crack propagates (Fig. 8.16b) before branching (Fig. 8.16c). The fracture pattern continues to develop in Figs. 8.16(d-f) with additional nucleations, propagation, branching and crack intersections. The fracture process accelerates as the applied load increases. This sequence is notable, relative to other fragmentation studies, for the detailed resolution of waves emitted by individual crack tips and their influence on neighboring fractures, *cf.* Figs. 8.16(d,e). Eventually, crack intersections generate a few fragments near the initial nucleation site, as seen in Fig. 8.16f.

Figure 8.17 shows the influence of the relaxation time, $\tilde{\tau}$, on the fracture pattern, with a ten times larger value in Fig. 8.17a and a ten times smaller value in Fig. 8.17b relative to the reference value, $\tilde{\tau} = 0.0116$, used in Fig. 8.16e. Figure 8.17a ($\tilde{\tau} = 0.116$, displacement scale $\tilde{u} = 0.01$) shows only a single main crack, a much simpler fracture pattern, and more ductile response than the reference case, Fig. 8.16e. In contrast, Fig. 8.17b ($\tilde{\tau} = 0.00116$, $\tilde{u} = 0.0001$) shows more nucleation sites, faster moving crack tips, more propagating cracks, and overall a more brittle response than the reference case. In short, the response becomes more brittle as the relaxation time decreases. This is expected as the fracture toughness scale, $\bar{s}\tilde{\tau}$ [5], decreases as $\tilde{\tau}$ decreases.

This example highlights the importance of stochastic strength variations in numerical modeling of brittle fracture. If material properties, including fracture strength, are modeled as perfectly homogeneous, every point in the analysis domain should, in theory,

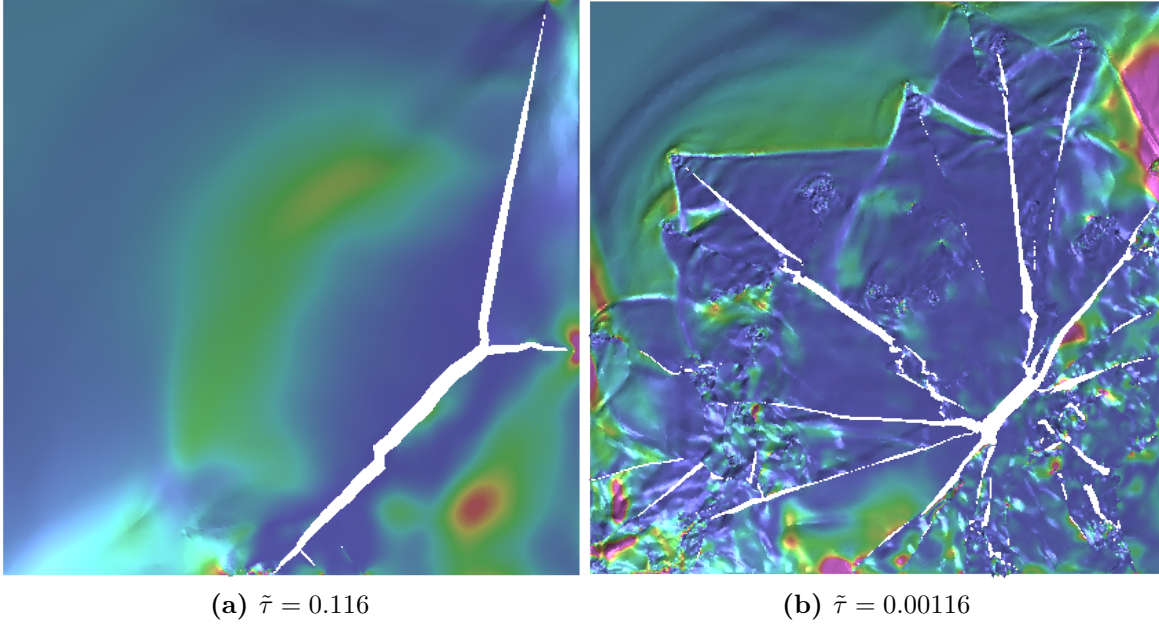


Figure 8.17: Effect of relaxation time on fracture patterns at time $t = 7.80$.

simultaneously nucleate a crack at the instant when the rising uniform tension field reaches the fracture strength. Real materials contain defects and various other heterogeneities that generate stochastic variations in fracture strength that preclude this unnatural response. Numerical error or problem domains with notches, pre-cracks, or other stress-concentrating features may break stress uniformity to mask this issue in numerical models that lack stochastic variations in fracture strength. Nonetheless, models with perfectly homogeneous material properties tend to overestimate system strength and otherwise predict nonphysical response in many practical problems. In fact, we believe this example provides a stringent and suitable test case for computational models of fracture in brittle and quasi-brittle materials.

8.6 Discussion and conclusions

We combined the adaptive spacetime discontinuous Galerkin finite element method with a dynamically consistent interfacial damage model to create a powerful simulation tool for dynamic fracture in quasi-brittle materials. We proposed two alternative realizations of microscopic distributions of flaws. In explicit realizations, we generate distributions of

initial microcracks to match a given statistical description. In implicit realizations, we use a phenomenological nucleation criterion based on a Weibull model to incorporate the influence of the initial microcrack distribution on macroscopic response.

In §8.5.2 we studied the influence of fracture strength and its angular distribution on the macroscopic fracture pattern. We adjusted crack density, α , in an explicit realization and modified the Weibull model parameters, specifically the reference area, A_0 , in an implicit realization as a means to vary the material's fracture strength. We found that extreme values of A_0 produced unrealistic fracture patterns for quasi-brittle materials. Very high values suppressed crack nucleation, resulting in fracture patterns with a single main crack, while very low values combined with strong, orientation-dependent reductions in fracture strength resulted in extensive fractures with incomplete damage adjacent to the main crack. Another, not unexpected, finding was that higher microcrack densities in explicit realizations of models involving angular bias in fracture strength produce stronger anisotropic effects in the fracture patterns. Similarly, implicit realizations of strength models with angular bias having smaller reference areas (implying higher microcrack densities), produced more anisotropic fracture patterns. We obtained much stronger anisotropic results with the implicit realizations, presumably because much higher microcrack densities than we used are required to get similar results with explicit realizations.

We used the L-shaped domain example in §8.5.1 to demonstrate mesh-independent crack-path convergence as we tighten the adaptive tolerances in our aSDG model. In general, we found the robust aSDG adaptive meshing capabilities to be critical for ensuring adequate resolution of solution fields, accurate tracking of solution-dependent crack paths, as well as supporting crack intersections and nucleations of new fracture surfaces. With these adaptive capabilities, there is no need to introduce special enrichment functions that are generally unavailable in geometrically complex situations, such as crack intersections, and in problems where the assumptions of LEFM are unsuitable. Robust adaptive meshing capabilities also support the highly nonlinear contact and interfacial damage model at the heart of our formulation.

In this work we demonstrated the potential of an interfacial damage model, in combination with the adaptive capabilities of the aSDG method, to model complex processes

in brittle fracture mechanics. Additional research and various extensions are needed to transform this approach into a practical tool for modeling real materials. These include extending our model to address a broader set of microscopic defects and calibrating it to predict the response of specific materials. Another avenue for development involves the use of *stochastic volume elements* (SVEs) to represent a material’s spatial inhomogeneities and statistical variability. For example, we could apply the moving window method advanced by [26] to develop covariance functions of our random fields. Alternatively, since the size-effect responses of actual quasi-brittle materials do not necessarily follow a Weibull distribution [80], we could replace our current Weibull size-effect model with a new model calibrated by careful analysis of SVEs with different sizes.

Chapter 9

Effects of material inhomogeneity on fracture induced by compressive loading: An implicit microstructure representation of Weibull-based fracture strength

An original version of the following article was submitted for publications in the conference proceedings of the 52th US Rock Mechanics/Geomechanics Symposium (ARMA 2018) [4]. The article was originally submitted under the title “Modeling of rock inhomogeneity and anisotropy by explicit and implicit representation of microcracks” but for more comprehensive inclusion into this dissertation, the title was revised to emphasis the concept of interest. This paper presents a formulation similar to [6], with the main difference that fracture is under compressive stress state (relevant in rock fracture). This requires the definition of a new effective stress model, based on the Mohr-Coulomb failure criterion. The interaction of material weakest planes (a result of fracture strength anisotropy) and natural angles that rock tend to fracture under uniaxial compressive load, results in interesting fracture patterns. Moreover, the response of explicit and implicit models for this problem is different from those observed for tensile-dominant problems in [6].

Abstract: Fracture patterns experienced under a dynamic uniaxial compressive load are highly sensitive to rock microstructural defects due to its brittleness and the absence of macroscopic stress concentration points. We propose two different approaches for modeling rock microstructural defects and inhomogeneity. In the *explicit realization* approach, microcracks with certain statistics are incorporated in the computational domain. In the *implicit realization* approach, fracture strength values are sampled using a Weibull probability distribution. We use the Mohr-Coulomb failure criterion to define an effective stress in the context of an interfacial damage model. This model predicts crack propagation at angles $\pm\phi_{ch} = \pm(45 - \phi/2)$ relative to the direction of compressive load, where ϕ is the friction angle. By using appropriate models for fracture strength anisotropy, we demonstrate the interaction of rock weakest plane and ϕ_{ch} . Numerical results demonstrate the greater effect of strength anisotropy on fracture pattern when an explicit approach is employed. In addition, the density of fractures increases as the angle of the weakest planes approaches $\pm\phi_{ch}$. The fracture simulations are performed by an h -adaptive asynchronous spacetime discontinuous Galerkin (aSDG) method that can accommodate crack propagation in any directions.

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9.1 Introduction

Heterogeneities in elastic properties and fracture strength can be either *explicitly* or *implicitly* incorporated in rock mechanics. In *explicit* approaches defects, microcracks, and other inhomogeneities are directly incorporated in the model. For example, in lattice models, the bulk is represented as a network of particles connected by springs. The inhomogeneity can be readily incorporated in lattice models by sampling the strength of springs from an assumed probability distribution [188, 130]. For *Finite Element Methods* (FEMs), the explicit modeling of defects such as microcracks often requires a considerably finer discrete grid to capture the geometries of the defects. This in turn can substantially increase the computational cost. *Discrete Element Method* (DEM) and *peridynamics* methods model the media as a collection of interacting particles. Similar to lattice models, the material inhomogeneity can be *explicitly* modeled by assigning different bond stiffness between the particles. Some hybrid methods such as combined finite-discrete element method (FDEM) [153], have been proposed to combine the computational advantages of the FEMs and flexibility of discrete methods in modeling inhomogeneity. For example, [141, 142] represents cracked regions by discrete elements while the intact parts are discretized by finite elements.

While accurate, explicit approaches can become quite expensive if defects of all sizes are directly incorporated in the computational model. The *implicit* approaches only include the collective effect of microstructures in macroscopic material models. Homogenization approaches derive macroscopic properties such as elastic moduli by solving the underlying problem in a *Volume Element* (VE). Similar approaches can also be used to calibrate continuum damage models, see for example [208, 107, 194, 138]. For a macroscopically homogeneous material, the derived values converge to a unique value as the VE size approaches the size of the *Representative Volume Element* (RVE)—referred to

as *Representative Elementary Volume* (REV) in rock mechanics. However, by using RVEs the statistical variations of properties from sample to sample, and spatial inhomogeneities of the material are lost. As an alternative, *Statistical Volume Elements* (SVEs), such as those in [122], use small enough VEs that such variations are preserved. Finally, phenomenological models attempt to represent material inhomogeneity and statistical variation without formally homogenizing its properties. The Weibull model [215, 216], is one of such models that can provide an accurate representation of statistical nature of fracture strength of brittle materials such as rock.

In [54, 13], it is shown that incorporating material inhomogeneity plays an important role in predicting realistic fracture patterns. For rock, material anisotropy also plays a crucial role; the existence of bedding planes not only affects the elastic properties, but also makes the rock weaker normal to these planes. There are two main approaches to model the anisotropy of rock fracture properties. In [168, 167], a failure criterion is expressed in terms of invariants of stress tensor and a second order so-called microstructure tensor. While based on sound continuum mechanics theories, it is not straightforward to extract the fracture strength of rock for a given direction. In the second approach, typical failure criteria such as Mohr-Coulomb or Hoek-Brown are generalized such that for each direction, the parameters of these models are angle dependent; see for example [198].

We propose two approaches to model rock heterogeneities. In the *explicit realization* approach, we use certain statistics for microcrack density, location, and length to generate random realizations that contain a large number of microcracks. In the *implicit realization* approach, rather than using SVEs to homogenize effective properties, we use the phenomenological Weibull model to sample fracture strength values at the vertices of a discrete finite element mesh. As for modeling rock anisotropy, we adopt the second general approach described above for implicit realizations, in that the parameters of a failure criterion (Mohr-Coulomb) are angle dependent. For explicit realizations, the realized cracks are heavily oriented around a given angle. The problem specifically studied is the fracture of rock under dynamic uniaxial compressive load. For an isotropic model, the friction angle of rock dictates a preferable angle for the formation of cracks. However, when anisotropy is included, the competition of the natural angle of fracture under compressive load and the

angle corresponding to weakest plane results in interesting fracture patterns for both explicit and implicit methods. The underlying elastodynamic problem is solved by an h -adaptive *asynchronous Spacetime Discontinuous Galerkin* (aSDG) method [9, 10, 2]. The fracture is modeled using an interfacial damage model [6]. A brief overview of the contact/fracture models and certain extensions for modeling anisotropic fracture based on Mohr Coulomb failure criterion are presented in the next two sections. Finally, §9.4 the effect of fracture strength anisotropy is studied for a problem where rock is under compressive dynamic load.

9.2 A rate-dependent interfacial damage model

This section provides an overview of the damage model presented in [6]. One difference will be the use of an effective stress model that is appropriate for the compressive mode fracture analysis presented in §9.4.

Instead of a traditional cohesive model, we present an interfacial damage model to represent fracture and contact modes on a crack surface. A scalar damage parameter, D , is used to interpolate between fully bonded ($D = 0$) and debonded ($D = 1$) states of an interface. It should be noted that in the majority of damage formulations, the stiffness of the bulk is degraded by the damage value. However, in our formulation, the damage model degrades the state on an interface. The contact modes include contact–stick and contact–slip modes as described in [8] as well as a separation mode which corresponds to fracture or crack opening. The use of Riemann solutions ensures that correct interface kinematic compatibility conditions are satisfied without resorting to penalty methods that are often combined with traditional cohesive models.

The formulation of traction and velocity values on a fracture section is comprised for two stages: First, the solutions within each of the three contact modes are presented in §9.2.1. Second, by using interpolation values such as D interface traction and velocity are obtained by forming a weighted average of individual contact mode solutions. This is described in §9.2.2. Finally, an effective stress model for fracture under compressive stress is presented in §9.2.3.

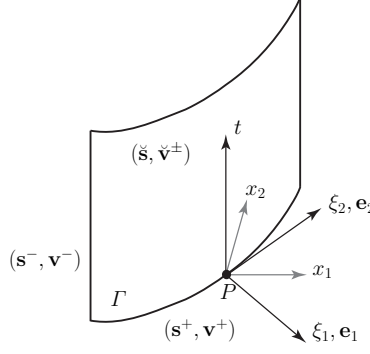


Figure 9.1: Local coordinate frame at an arbitrary location P on a spacetime fracture surface Γ .

9.2.1 Riemann solutions for contact modes

Figure 9.1 shows a local coordinate system at an arbitrary location P on contact interface Γ in spacetime. The local coordinate (ξ_1, ξ_2, t) is chosen such that ξ_1 -direction is normal to Γ . The quantities from opposite sides of Γ , decorated with superscripts $+$ and $-$, define the initial data for the Riemann problem. Distinct velocity traces, $\mathbf{v}^\pm$, and tractions, $\mathbf{s}^\pm$, defined by $\mathbf{s} = \boldsymbol{\sigma} \cdot \mathbf{n}$ in which the same spatial normal vector, $\mathbf{n}$, is used to compute $\mathbf{s}^+$ and $\mathbf{s}^-$ from the traces of the stress tensor field on the interface, $\boldsymbol{\sigma}^\pm$. The Riemann solutions include the traction vector $\check{\mathbf{s}}$ and velocity vectors $\check{\mathbf{v}}^\pm$ that act on the interface. The Riemann solutions are obtained by preserving the characteristic values of the elastodynamic problem on each sides of the fracture interface and enforcing the appropriate type of kinematic compatibility (relation between $\check{\mathbf{v}}^+ = \check{\mathbf{v}}^-$) for each type of contact solution. The Riemann solutions depend on material impedance values from the two sides $\pm$,

$$Z^{i\pm} := \begin{cases} (c_d \rho)^\pm & i = 1 \\ (c_s \rho)^\pm & i = 2, 3 \end{cases} \quad (9.1)$$

in which the index i corresponds to spatial directions in the local frame shown in Fig. 9.1 and the longitudinal and shear wave speeds are given by,

$$c_d = \sqrt{\frac{\lambda + 2\mu}{\rho}}, \quad c_s = \sqrt{\frac{\mu}{\rho}}. \quad (9.2)$$

where ρ is mass density and λ, μ are Lamé parameters.

The Riemann solutions for contact–stick and bonded modes, decorated with subscripts ST and B respectively, are

$$\check{s}_B^i = \check{s}_{ST}^i = \check{s}^i = \frac{s^{i+}Z^{i-} + s^{i-}Z^{i+}}{Z^{i-} + Z^{i+}} + \frac{Z^{i-}Z^{i+}}{Z^{i-} + Z^{i+}}(v_i^+ - v_i^-) \quad (9.3a)$$

$$\check{v}_i^B = \check{v}_i^{ST} = \check{v}_i = \frac{s^{i-} - s^{i+}}{Z^{i-} + Z^{i+}} + \frac{v_i^+Z^{i+} + v_i^-Z^{i-}}{Z^{i-} + Z^{i+}} \quad (9.3b)$$

In separation mode, $\check{\mathbf{v}}^+$ and $\check{\mathbf{v}}^-$ are independent. The target tractions are, however, set to $\mathbf{S}$, which in particular is obtained by the particular fracture model used at the interface. Similar to [54] we set $\mathbf{S} = \mathbf{0}$. The Riemann solutions for the separation case, decorated by S, are,

$$\check{s}_S^i = \check{s}^i = S^i \quad (9.4a)$$

$$\check{v}_i^{S^\pm} = \check{v}_i^\pm = v_i^\pm \pm \frac{S^i - s^{i\pm}}{Z^{i\pm}} \quad (9.4b)$$

In contact mode, a friction model determines which of the two contact–stick or contact–slip modes holds. This requires the definition of the *magnitude of tangential traction for bonded Riemann solutions* as,

$$\check{\tau}_B := \begin{cases} \sqrt{(\check{s}_B^2)^2 + (\check{s}_B^3)^2} & d = 3 \\ |\check{s}_B^2| & d = 2 \end{cases} \quad (9.5)$$

where d is the spatial dimension. For the transition between contact–stick and contact–slip modes we use the Mohr–Coulomb friction law, which states that contact–slip mode holds if,

$$|\check{\tau}_B| > k \langle -\check{s}_B^1 \rangle_+ \quad (9.6)$$

in which k is the friction coefficient and $\langle \cdot \rangle_+$ is the positive operator. Under these conditions, the magnitude of target shear traction is given by $k \langle -\check{s}_B^1 \rangle_+$. The normal component of the traction and velocity vectors are enforced using the bonded Riemann solutions (9.3) (for $i = 1$) and the tangential velocities are obtained by preserving the characteristic values in

directions $i \neq 1$ and using Mohr-Coulomb model for the tangential traction. For brevity, these solutions are not presented here and can be found in [8].

9.2.2 Macroscopic target values

The macroscopic, *i.e.*, averaged, solutions on Γ are obtained by interpolating between *bonded* and *debonded* solutions, using the damage parameter D ,

$$\mathbf{s}^* := (1 - D)\check{\mathbf{s}}_B + D\check{\mathbf{s}}_D \quad (9.7a)$$

$$\mathbf{v}^{*\pm} := (1 - D)\check{\mathbf{v}}_B + D\check{\mathbf{v}}_D^\pm \quad (9.7b)$$

in which subscripts B and D denote Riemann values for bonded and debonded conditions.

The bonded solutions $(\check{\mathbf{s}}_B, \check{\mathbf{v}}_B)$ are obtained from (9.3), while any of the separation, contact-stick, or contact-slip solutions can hold for the debonded values $\check{\mathbf{s}}_D, \check{\mathbf{v}}_D^\pm$. First, it should be determined whether the debonded part is in contact or separation model. Separation mode holds if the normal bonded traction $\check{s}_B^1$ is positive or the normal displacement jump is positive at P on Γ . Physically, the separation to contact mode transition is nonsmooth. Hence, a regularization scheme is proposed in [8] where the *relative contact fraction* transitions debonded solutions from complete separated values at $\eta = 0$ to full contact values at $\eta = 1$. On the other hand, [8] shows that stick to slip transitions are in fact smooth. Thus, the binary state *relative stick fraction*, $\gamma \in \{0, 1\}$ is used to transition between contact-stick ($\gamma = 1$) and contact-slip ($\gamma = 0$) modes. The Mohr-Coulomb condition (9.6) is used to determine whether stick or slip conditions hold.

In summary, $\check{\mathbf{s}}_D$ and $\check{\mathbf{v}}_D^\pm$ are interpolations of separation solutions (9.4), bonded/contact-stick solutions (9.3), and contact-slip [8] solutions. Considering the three relative fractions, D , η , and γ , it is easy to show that $\mathbf{s}^*$ and $\mathbf{v}^{*\pm}$ in (9.7) can be expressed as linear sums of the Riemann solutions from three distinct response modes, bonded/contact-stick (B),

contact–slip (SL), and separation (S):

$$\mathbf{s}^* := a_B \check{\mathbf{s}}_B + a_{SL} \check{\mathbf{s}}_{SL} + a_S \check{\mathbf{s}}_S \quad (9.8a)$$

$$\mathbf{v}^{*\pm} := a_B \check{\mathbf{v}}_B + a_{SL} \check{\mathbf{v}}_{SL}^\pm + a_S \check{\mathbf{v}}_S^\pm \quad (9.8b)$$

with the coefficients

$$a_B = 1 - D + D\eta\gamma \quad (9.9a)$$

$$a_{SL} = D\eta(1 - \gamma) \quad (9.9b)$$

$$a_S = D(1 - \eta) \quad (9.9c)$$

9.2.3 Damage evolution law

Bulk damage models that lack an intrinsic length scale, may result in non-convergent numerical solutions where damage localizes to layers whose width continues to shrink without limit as the mesh is refined[31, 23]. Similar problems exist for the interfacial damage models that lack a length scale. Instead of directly incorporating a length scale in the model, a length scale can be introduced through a time scale in the damage evolution law, as in [154] for a bulk model and [57, 23] for an interfacial model. We follow a similar approach and adopt the model in [22],

$$\dot{D} = \begin{cases} \frac{1}{\tilde{\tau}}[1 - H(\langle D_t - D \rangle)] & D < 1 \\ 0 & D = 1 \end{cases}, \quad (9.10)$$

in which $\tilde{\tau}$ is a *relaxation time*, and D_t is a *target damage value* that corresponds to the damage value under quasi-static loading conditions. The function H has unit value at zero and decreases to zero at infinity. Following [22], we use $H(x) = \exp(-ax)$. From the form of H , a maximum damage rate of $1/\tilde{\tau}$ is implied by (9.10).

In general, D_t depends on the states on both sides of the interface. We focus on a model where damage is mostly stress driven. In [6] we introduced a scalar *effective stress*, as $\check{s} := \sqrt{\langle \check{s}_B^1 \rangle^2 + (\beta \check{\tau}_B)^2}$, where as in [43] β is the *shear stress factor*, and the positive operator,

$\langle \cdot \rangle$, ensures that no damage evolve incurs under compressive normal stress. There are two problems with this effective stress model. First, the shear strength of rock does not increase as the confinement pressure increases. Second, it predicts failure along $\pm 45^\circ$ for a uniaxial compressive test. As a result, in [7] we proposed an effective stress model that is based on Mohr-Coulomb failure criterion,

$$\check{s} := \check{\tau}_B + k\check{\sigma}_B^1 \quad (9.11)$$

where k is the friction coefficient introduced in (9.6). The *angle of friction* ϕ is defined as,

$$\phi = \tan^{-1}(k) \quad (9.12)$$

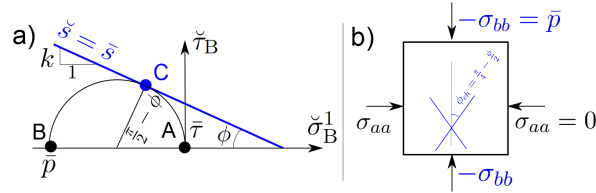


Figure 9.2: The compressive strength, $\bar{p}_{MC}$, and the critical angle, θ_{MC} , for the Mohr–Coulomb model.

The condition $\check{s} = \bar{s}$ corresponds to the Mohr-Coulomb *failure criterion* as shown in Fig. 9.2a) and fracture strength based on (9.11) corresponds to cohesion, often denoted by c . This model also captures the correct compressive strength; as shown in Fig. 9.2b), for a compressive loading scenario where σ_{bb} is set to the uniaxial compressive strength of rock $\bar{p}_{MC}$, based on its corresponding stress state in 9.2a), for isotropic rock the value of $\bar{p}_{MC}$ and the orientation of fracture plane with this load are determined as,

$$\bar{p}_{MC} = 2\bar{\sigma} \frac{\cos(\phi)}{1 - \sin(\phi)} = 2\bar{\sigma} \frac{1}{\sqrt{1 + k^2} - k} \quad (9.13a)$$

$$\theta_{MC} = \pm \left(\frac{\pi}{4} - \frac{\phi}{2} \right) \quad (9.13b)$$

Once the effective stress is formulated based on the Mohr-Coulomb failure criterion, D_t is determined by,

$$D_t = \begin{cases} 0 & \check{s} < \underline{s}, \\ \frac{\check{s}-\underline{s}}{\bar{s}-\underline{s}} & \underline{s} \leq \check{s} < \bar{s}, \\ 1 & \bar{s} \leq \check{s} \end{cases} \quad (9.14)$$

where $0 < \underline{s} < \bar{s}$ are quasi-static strength thresholds for the initiation of damage evolution and complete failure, respectively. $\bar{s}$ is referred to as the *fracture strength*.

9.3 Statistical aspects

9.3.1 Spatial inhomogeneity

In the explicit realization approach, microcracks are explicitly incorporated in the computational domain. The end points of these cracks are called *fracture surface tips* (FSTs). In the implicit realization approach, the effect of the in-situ defects can be homogenized to form an implicit representation of rock strength. In this approach, cracks can nucleation from points with lower strength and/or high stress values. In short, the tips of all active cracks in a computational domain, where pre-existed or nucleated afterward, is called a FST. In the aSDG method, used for the analyses in §9.4, cracks can only propagate from FSTs.

Figure 9.3 shows the distribution of $\check{s}$ and $\bar{s}$ around the FSF V. The definition of effective for any arbitrary angle θ follows the definition (9.11) on fracture surfaces,

$$\check{s}(\theta) := \check{\tau}_B(\theta) + k(\theta)\check{\sigma}_B^1(\theta) \quad (9.15)$$

A crack is extended for which the ratio $\check{s}/\bar{s}$ is a local maximum with a value greater than or equal to unity. Once a crack propagation direction is assigned to an FST, the underlying numerical method should accommodate an extension along the proposed direction. Unlike *eXtended finite element methods* (XFEMs) [35, 149] and *generalized finite element methods* (GFEMs) [204] where the underlying finite element mesh is not modified, mesh adaptive schemes, *e.g.*, [177, 176], move finite element vertices such that a finite element boundary is

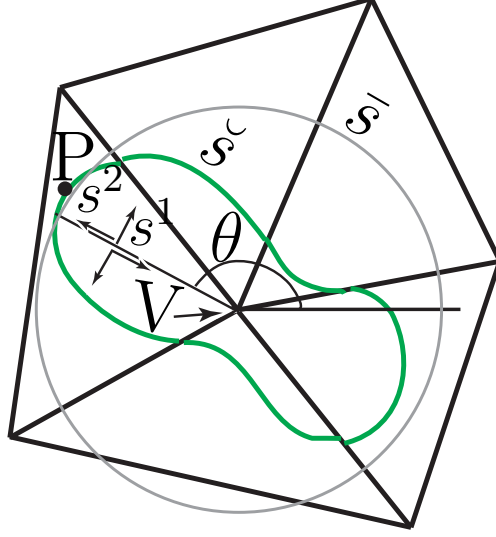


Figure 9.3: The angular distributions of effective stress $\check{s}$ and fracture strength $\bar{s}$ around the FST V. The terms in (9.15) are $s^1 = \check{\sigma}_B^1$ and $s^2 = \check{\tau}_B$.

aligned with the proposed direction. Herein, we take the latter approach in that adaptive operations in spacetime can align element boundaries with any proposed crack propagation direction; *cf.* [158, 6] for more details. Once the crack is extended in the proposed direction, the vertex V becomes inactive and the new crack tip becomes an active FST.

9.3.1.1 Explicit Realization

In this method, the cracks are already included in the initial discretization. To generate the in-situ cracks, a certain statistics of cracks is assumed. Perhaps the most important statistics, the density of initial cracks is defined as,

$$\alpha = \frac{\sum_{i=1}^{nc} l_i^2}{A_c} \quad (9.16)$$

where l_i is the length of crack number i in a 2D domain with area A_c and nc is the number of cracks inside A_c . We assume the crack length to follow a Weibull distribution, and that their position in space to follow a uniform distribution. We use the “take and place” approach to sample and insert one crack in the computational domain at a time, until the target crack density is reached.

9.3.1.2 Implicit Realization

Incorporating in-situ microcracks and defects of rock in a computational domain can result in very expensive simulations. Instead, one can implicitly consider the effect of cracks that are short enough to enable the application of homogenization theories. Instead of using SVEs to homogenize the properties of rock and derive their statistical distribution, we employ a phenomenological model for the fracture strength of rock. The Weibull model [215, 216] has proved to be an accurate statistical model for fracture strength of brittle and quasi-brittle materials. The *cumulative distribution function* (CDF) for $\bar{s}$ for a region with area A is,

$$P(\bar{s}) = 1 - e^{-\frac{A}{A_0} \left(\frac{\bar{s} - s_{\min}}{s_0} \right)^m} \quad (9.17)$$

The model parameters are a strength scale s_0 , minimum fracture strength $s_{\min}$, and the Weibull modulus m . A_0 is the area for which the Weibull parameters are calibrated.

The way in which (9.17) is used in a computational setting is as follows. For any vertex V in the computational domain, this CDF is used to sample a fracture strength $\bar{s}$. The value A is chosen as an area that is associated with the vertex. For example, in Fig. 9.3, A is set to the total area of the 5 surrounding triangles.

9.3.2 Anisotropy

Material properties of rock, including fracture strength, can be highly anisotropic, for example due to the existence of bedding planes. Two different approaches are used to incorporate rock anisotropy for the explicit realization and implicit realization methods. In the explicit method, crack orientation is biased around certain angles instead of following a uniform distribution in the range $[0, \pi]$. For example, to model bedding planes around the angle $\theta_0 = 30^\circ$ a uniform distribution $[\theta_0 - \Delta\theta/2, \theta_0 + \Delta\theta/2]$ may be considered for crack orientation, where $\Delta\theta$ is the span of the angles of cracks.

For the implicit approach, fracture strength is not only assumed to be a function of location, through material inhomogeneity, but also anisotropic. The first aspect, inhomogeneity, is addressed by sampling a location-dependent (and angle-independent)

strength $\bar{s}(V)$, as described in §9.3.1.2. To model anisotropy, the strength is made angle-dependent with the relation,

$$\bar{s}(V, \theta) = \bar{s}(V)f(\theta) \quad (9.18)$$

where $f(\theta)$ is a modulation function. Modulation of the parameters of a fracture strength model is one of the approaches to incorporate rock anisotropy in the literature. For example, [169] and [127] modify the parameters of the Mohr-Coulomb and Hoek-Brown [106] models, respectively.

In the discrete setting, the function $f(\theta)$ is sampled separately for each vertex V of the discrete domain. The function $f(\theta)$ is characterized by θ_0 and f_0 the angle and minimum modulation of the function $f(\theta)$; that is $f(\theta)$ takes the minimum value of f_0 at $\theta_0 \pm \pi$. As discussed in §9.4, some randomness is incorporated in the sampling of f_0 and θ_0 for each vertex. Finally, once fracture strength is fully characterized by (9.18) for V at all angles θ , the direction of extension is determined as the angle that maximizes $\check{s}(\theta)/\bar{s}(V, \theta)$. A propagation from V is not realized until this maximum ratio exceeds unity.

In conclusion, in the explicit realization approach, fracture strength is not inhomogeneous nor anisotropic. That is, a unique angle independent value is used for $\bar{s}$ in contrast to the model (9.18) for the implicit realization method. In addition, no cracks are permitted to nucleated inside the domain. These are consequences of the assumption that the random and explicit distribution of cracks is the only source of randomness for the explicit realization approach.

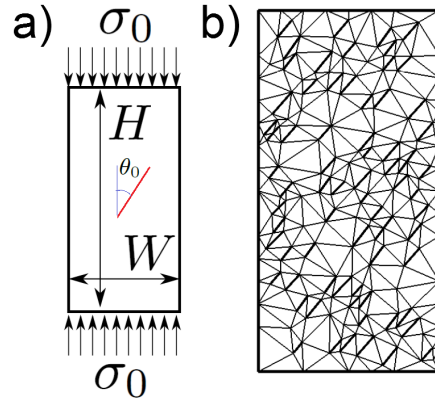


Figure 9.4: Compressive fracture of a rectangular domain: a) Domain geometry and loading; b) The discrete initial mesh for an explicit realization with $\alpha = 0.5$ and angular bias $\theta_0 = 40^\circ$.

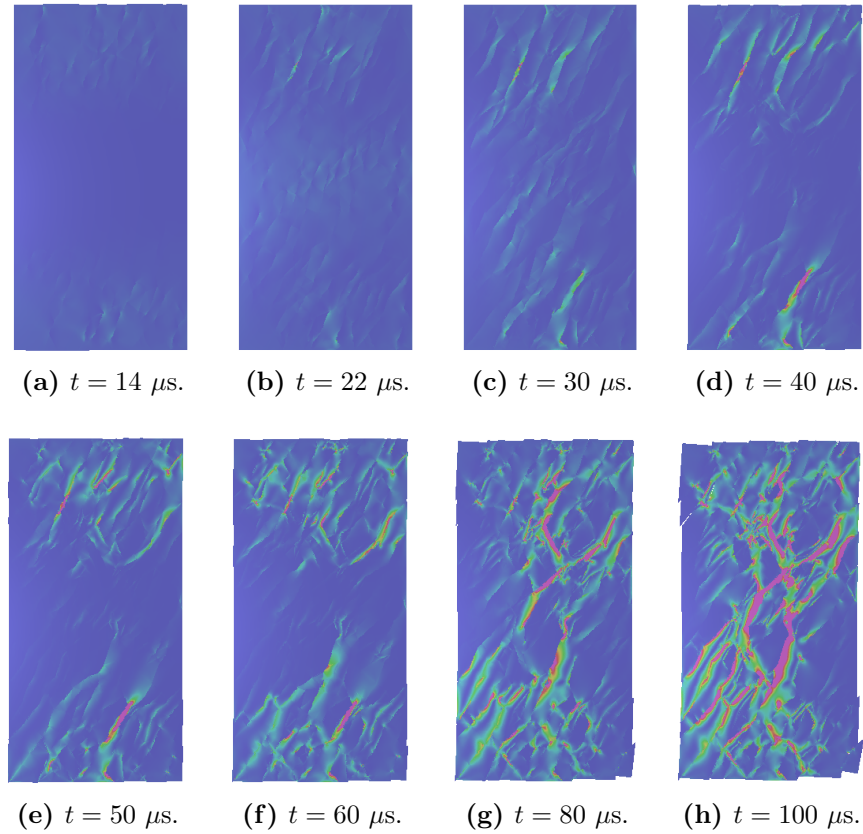


Figure 9.5: A sequence of solutions for an explicit realization with $\alpha = 0.5$ and angular bias $\theta_0 = 20^\circ$. Strain energy density is mapped to color with blue-to-red range indicating low to high values.

9.4 Numerical results

Figure 9.4a) diagrams a problem involving compressive uniaxial loading applied to a rectangular domain in which the load ramps from zero to a sustained value of $\sigma_0 = 2.5\text{MPa}$ over 10 microseconds. The domain dimensions are $W = 0.08\text{ m}$ and $H = 0.16\text{ m}$. The angle of weak planes for both implicit and explicit realizations with respect to the load direction (vertical direction) is denoted by θ_0 in the clock-wise direction as shown. Similar to θ_0 , all the angles are measured relative to the vertical direction in the clock-wise direction. The material properties are: Young's modulus $E = 65\text{ GPa}$, mass density $\rho = 2600\text{ kg/m}^3$, and Poisson's ratio $\nu = 0.27$. The friction coefficient is $k = 0.3$, corresponding to $\phi = 16.9^\circ$. In the absence of fracture strength anisotropy we would expect cracks along $\pm\phi_{ch}$, where $\phi_{ch} = (45^\circ - \phi/2) = 36.65^\circ$; *cf.* (9.13b) and Fig. 9.2b).

The two different explicit and implicit realization models are used for this study. Figure 9.4b) shows an explicit realization spatial mesh for crack density $\alpha = 0.5$. The realized microcrack orientations are sampled from a uniform distribution with the average angle $\theta_0 = 40^\circ$ and a span of $\Delta\theta = 10^\circ$. The fracture strength is set to $\bar{s} = 1.344\text{ MPa}$, which from (9.13a) yields a uniaxial fracture strength of $\bar{p}_{MC} = 3.612\text{ MPa}$. Thus, in the absence of microcracks the compressive load of $\sigma_0 = 2.5\text{MPa}$ is not large enough to cause any crack nucleation before the magnitude of the load doubles when the waves propagating from the top and bottom intersect in the middle of the domain. However, the presence of microcracks implies that cracks can propagate from their tips even under this applied load.

Figure 9.5 shows the solution visualization for an explicit realization with $\alpha = 0.5$ and mean microcrack angle $\theta_0 = 20^\circ$; *cf.* Fig. 9.4a). In the presence of microcracks, two things happen; first, between the two angles $\pm\phi_{ch} = \pm 36.65^\circ$ the $+\phi_{ch}$ has a much closer direction to in-situ cracks. So, if there are long distances between cracks more cracks with the angle ϕ_{ch} , rather than $-\phi_{ch}$, are expected. Second, the microcrack directions to a large extent direct crack propagation directions as they create weak planes along the θ_0 direction. From the energy density visualizations in Fig. 9.5 both expectations are verified. First, not many cracks are observed with negative angles with respect to the load direction. Second, the majority of cracks propagate along $\theta_0 = 20$ and its only between the cracks that angles

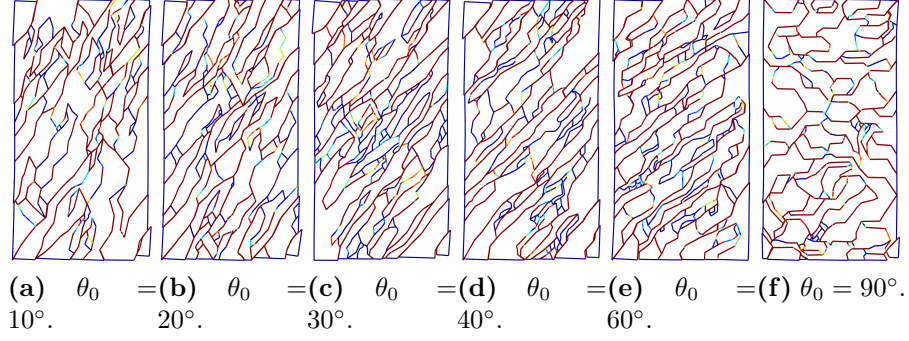


Figure 9.6: Comparison of fracture patterns and deformed shapes for the explicit realization model for crack density $\alpha = 0.5$ and different values for angular bias θ_0 at time $t = 90 \mu\text{s}$. The crack segments are color coded with the damage value $D \in [0, 1]$ mapped to the blue to red color range.

closer to anticipated $\phi_{ch} = 36.65^\circ$ connects the cracks. The competition between θ_0 and ϕ_{ch} and high stress concentrations in the fracture process zones around the crack tips and on the sides of the crack surfaces, due to frictional sliding, can clearly be seen in Figs. 9.5(f-h).

Figure 9.6 compares the results for explicit realization simulations for different mean values of microcrack orientation θ_0 . As mentioned, the natural angles of crack extension are along $\pm\phi_{ch} = \pm 36.65^\circ$. In Fig. 9.6a, the cracks are too close to vertical direction and their direction is not close to $\pm\phi_{ch}$, however, still ϕ_{ch} is closer to crack directions and more of this angle of crack propagation is expected between microcracks. The reorientation of propagating cracks in this direction can clearly be seen in the figure. This trend continues in Fig. 9.6b but with slightly more straight path for cracks. Finally, in Fig. 9.6c and especially Fig. 9.6d, the angle of in-situ cracks gets so close to ϕ_{ch} that first much more straight crack path is observed and second due to the energetically favorable propagation of cracks, a denser fracture network is observed. As the crack angles get farther away from ϕ_{ch} in Fig. 9.6e, crack paths start to become more complex. Finally, for $\theta_0 = 90^\circ$ in Fig. 9.6f there is no preferred direction between $\pm\phi_{ch}$ and cracks with both directions are observed. In addition, the very unfavorable direction of microcracks greatly inhibits crack propagation under the compressive stress loading.

Next, the results for the implicit approach are presented. Two aspects need to be addressed; first, the inhomogeneity of fracture strength is realized by sampling $\bar{s}$ from (9.17).

The values $m = 4$, $s_{\min} = 0.74$ MPa, $s_0 = 2.69$ MPa, and $A_0 = 0.01$ m² imply a mean strength $\mathbb{E}(\bar{s}) = 3.03$ MPa for $A = W \times H = 0.0128$ m² in (9.17). This corresponds to a mean compressive strength of $\mathbb{E}(\bar{p}_{\text{MC}}) = 8.14$ MPa which is significantly larger than the applied load $\sigma_0 = 2.5$ MPa. However, the statistical variation of sampled $\bar{s}$ implies that for the points whose sampled compressive strength is smaller than $\sigma_0 = 2.5$ MPa, a crack can be nucleated.

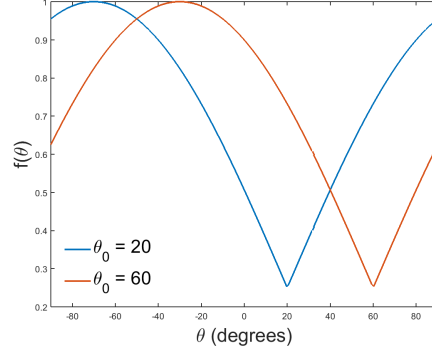


Figure 9.7: Sample $f(\theta)$ functions, *cf.* (9.18), for $f_0 = 0.25$ and $\theta_0 = 20^\circ$ and $\theta_0 = 60^\circ$.

The anisotropy of the fracture strength is modeled by the function $f(\theta)$, *cf.* (9.18). For all the implicit realizations $f(\theta)$ ranges from one to its minimum value $f_0 = 0.25$ at an angle with $\pm 5^\circ$ variation around a specified angle θ_0 . Figure 9.7 shows two samples for $f(\theta)$ for $\theta_0 = 20^\circ$ and $\theta_0 = 60^\circ$, where as shown in Fig. 9.4 and evident in this figure, θ_0 and $\theta_0 \pm 90^\circ$ correspond to the weakest and strongest planes.

A sequence of solutions for an implicit realization with angle bias $\theta_0 = 20^\circ$ is shown in Fig. 9.8. Comparing corresponding times in Figs. 9.8(a-d) with those from explicit realization in Figs. 9.5(a-d), we observe that fewer cracks are observed for the implicit approach. This is expected for the two particular set-ups considered, as in the explicit approach the large microcracks can greatly increase stress fields around the crack tips and cause further crack propagation. Also apparent in Figs. 9.8(a-d) is that most cracks propagation along positive angles, which is expected by having weakest plane at $\theta_0 = 20^\circ$. The results in Figs. 9.8(e-h) show high level of compaction near the top and bottom boundaries. Also, while more cracks are observed close to θ_0 to ϕ_{ch} , see for example Figs. 9.8(g-h), there are also cracks close to $-\phi_{ch}$. In comparison to Fig. 9.5, we observe that the explicit representation of microcracks results in much more focused propagation of cracks in the range θ_0 to ϕ_{ch} .

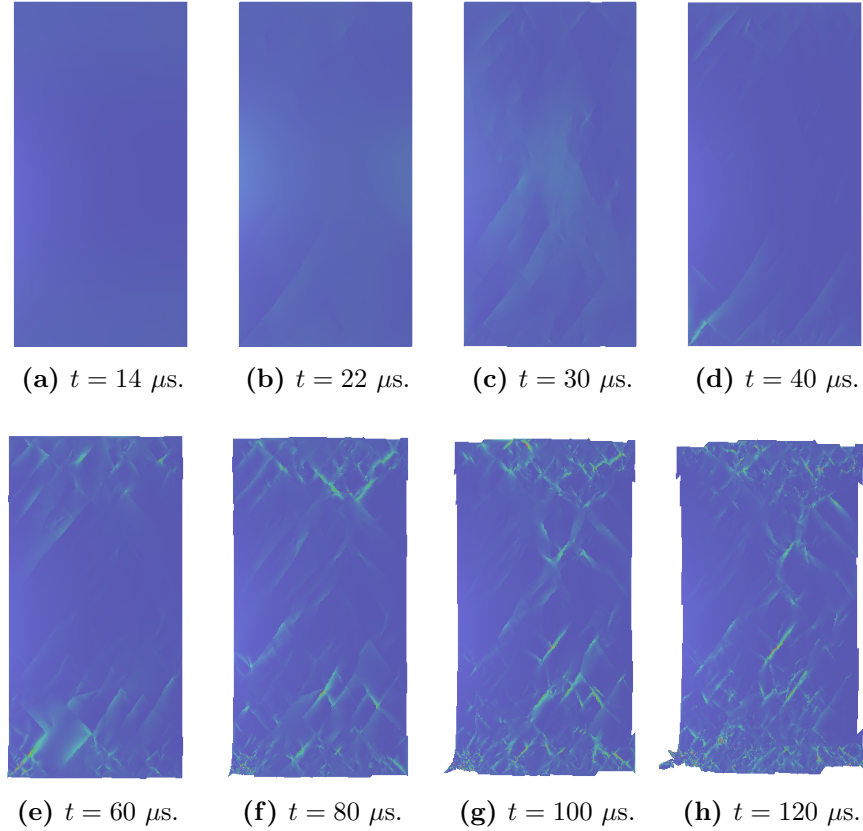


Figure 9.8: A sequence of solutions for an implicit realization with min stress ratio $f_0 = 0.25$ and angular bias $\theta_0 = 20^\circ$. Strain energy density is mapped to color with blue-to-red range indicating low to high values.

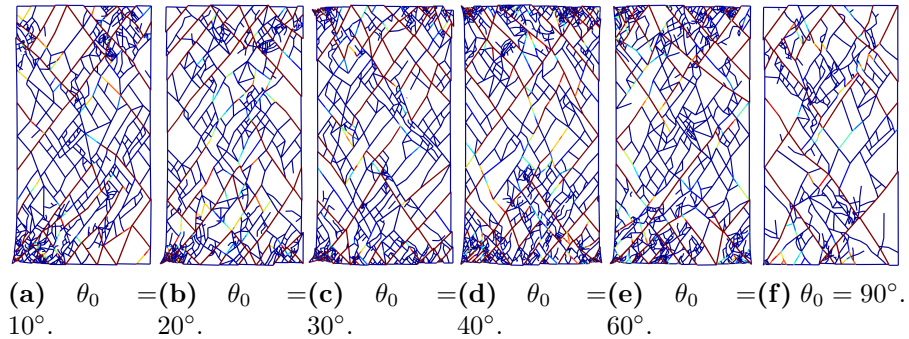


Figure 9.9: Comparison of fracture patterns and deformed shapes for the implicit realization model for minimum strength factor $f_0 = 0.25$ and different values for angular bias θ_0 at time $t = 90 \mu\text{s}$. The crack segments are color coded with the damage value $D \in [0, 1]$ mapped to the blue to red color range.

Figure 9.9 compares fracture patterns for different angles of the weakest plane θ_0 for the implicit realization model. Similar to the explicit realization model, the highest density of cracks are observed when weakest planes are close to natural angle of fracture $\phi_{ch} = 36.65^\circ$, that is for $\theta_0 = 30^\circ$ and $\theta_0 = 40^\circ$, in Figs. 9.9(c-d). Moreover, unlike the explicit model, where the orientation of microcracks at positive angles heavily prevented crack propagation at negative angles, for the implicit model a considerable density of cracks can be observed at negative angles. However, by closer examination, the majority of cracks with substantial damage, red color, are in positive directions.

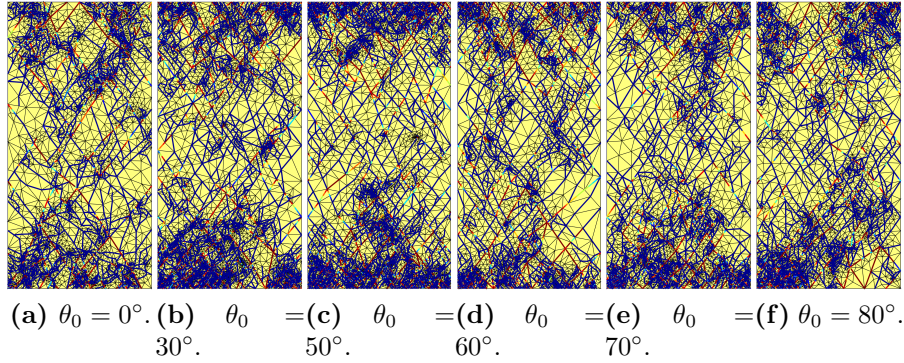


Figure 9.10: Comparison of the front meshes and a_{SL} for the implicit realization model for minimum strength factor $f_0 = 0.25$ and different values for angular bias θ_0 at time $t = 150 \mu s$. The crack segments are color coded with $a_{SL} \in [0, 1]$ mapped to the blue to red color range.

Finally, Fig. 9.10 shows the finite element front meshes for the implicit realization approach for different angles θ_0 at a later time $t = 150 \mu s$. These figures demonstrate the level of mesh refinement and adaptivity close to the top and bottom boundaries that are caused by the compaction of rock. This is a testament to the aSDG methods powerful meshing operations that accommodate crack propagation in arbitrary directions. The map of a_{SL} to color also demonstrate which crack segments are in slip mode. As evident, at this time the majority of crack segments are in contact-stick mode. The local sliding of certain crack segments at different times is responsible for the deformed shapes observed in Fig. 9.9.

9.5 Conclusions

We presented the explicit and implicit realization approaches to model rock inhomogeneity. Modeling of rock inhomogeneity is essential in problems that lack initial stress concentration points, such as rock fracture under axial compressive load studied in this manuscript. In addition, for this problem in an isotropic rock medium, cracks tend to nucleation and propagate along $\pm\phi_{ch} = \pm(45^\circ - \phi/2)$ directions with respect to the compressive load direction. We studied the effect of rock anisotropy on the angles at which cracks propagate. It was demonstrated that in the explicit approach where the microcracks were directly incorporated in the computational domain, the angle of weakest plane of rock had a more major role on fracture patterns. Moreover, for both approaches, more cracks propagated when the weakest plane direction tended to the natural fracture angle ϕ_{ch} .

There are several extensions to this work. First, the homogenization of SVEs, rather than using the phenomenological Weibull model, can greatly improve the accuracy of rock inhomogeneity with the implicit realization approach. Similarly, for explicit realization of crack actual microcrack statistics such as those reported in [156] and more robust approaches for their generation [108] can be employed. Moreover, for a more quantitative analysis quantities of interest such as maximum attainable compressive stress and dissipated fracture energy can be derived as a function loading rate and material inhomogeneity and anisotropy; as shown in [159, 13], modeling rock inhomogeneity becomes more important at higher loading rates and models that treat rock as a homogeneous medium greatly overestimate the induced density of cracks.

Chapter 10

Effects of material inhomogeneity on fracture patterns: An implicit microstructure representation of spatially correlated fracture strength

An original version of the following article was published in the conference proceedings of International Mechanical Engineering Congress & Exposition 2017 (AMSE IMECE 2017) [54]. The article was originally published under the title “Effect of the spatial inhomogeneity of fracture strength on fracture pattern for quasi-brittle materials” but for more comprehensive inclusion into this dissertation, the title was revised to emphasis the concept of interest. This article expands upon the topics introduced in chapter 4 section 5; However, rather than employing hydraulic loading, uniaxial tensile loading is imposed on material domain modeled with continuum fracture strength random field to investigate fracture initiation and growth in an otherwise “pristine” material. The uniaxial loading is imposed in such a way that produces uniform stresses throughout the domain, which is a very difficult computational problem to model for material of homogeneous fracture strength. This modeling setup shows a greater sensitivity to the implicit representation of heterogeneity and produces fracture responses that are better correlated to the spatial variation of the fracture strength field.

Abstract: The response of quasi-brittle materials is greatly influenced by their microstructural architecture and variations. To model such statistical variability, Statistical Volume Elements (SVEs) are used to derive a scalar fracture strength for domains populated with microcracks. By employing the moving window approach the probability density function and covariance function of the scalar fracture strength field are obtained. The Karhunen-Loève method is used to generate realizations of fracture strength that are consistent with the SVE-derived statistics. The effect of homogenization scheme, through the size of SVE, on fracture pattern is studied by using an asynchronous spacetime discontinuous Galerkin (aSDG) finite element method, where cracks are exactly tracked by the method’s adaptive operations.

Acknowledgments: The authors gratefully acknowledge partial support for this work via the U.S. National Science Foundation (NSF), CMMI - Mechanics of Materials and Structures (MoMS) program grant numbers 1538332 and 1654198.

10.1 Introduction

Due to the lack significant bulk energy dissipative mechanisms for quasi-brittle materials, their mechanical response is greatly influenced by microscale distribution of defects [80]. Size effect, the decrease of fracture strength as the size of a specimen increases, and variations in crack patterns, ultimate loads, *e.g.*, *cf.* [20, 200] are some consequences of the high sensitivity of quasi-brittle materials to their microstructural defects. Randomness and inhomogeneity of material is considered in geometry [20, 219, 200], initial damage state [102, 45], elasticity [59, 67], strength [45, 128], or fracture toughness and cohesive strength [60, 193].

The variability in a material property can be either *explicitly* modeled, by direct modeling of microstructural constituents, *e.g.*, [189, 131, 12], or *implicitly*. In implicit approaches phenomenological models, *e.g.*, Weibull model [215], is used as in [13] or macroscopic effective constitutive quantities are derived with a homogenization approach wherein the elemental problem is solved in a thermodynamically consistent *Volume Element* (VE). There are two commonly used classes of VEs known as *Representative Volume Element* (RVE) and *Statistical Volume Elements* (SVEs) [210, 190]. Employing SVEs in random media can be a more accurate averaging approach than utilizing RVEs for two reasons; first, they maintain spatial inhomogeneity of material property which is important in generation of stress concentration and nucleation of cracks from weak sites. Second, due to their statistical nature they can model macroscopic probabilistic variations in ultimate load and fracture energy.

The authors have previously employed implicit approaches based on Weibull model in [13], and SVE homogenization in [53]. We choose an approach similar to the latter work by using SVEs to generate random fields for fracture strength. But, we study the impact of SVE size on generated random fields and investigate how they will influence the induced fracture pattern. In addition, unlike the prior work, there is no approximation involved in the Karhunen-Loève (KL) approach by forcing the Probability Density Function (PDF) of the random field to be lognormal. Specifically, we use the CDF-inverse approach to map back and forth between the original statistics of the random fracture field and a standard normal field used for the generation of the KL grid. Finally, the asynchronous Spacetime

Discontinuous Galerkin (aSDG) method is used to simulate crack propagation on random fields realized based on different SVE window sizes. As demonstrated, more realistic fracture patterns are obtained for realizations that are based on smaller SVE window sizes.

10.2 Formulation

In this section we review the derivation of fracture strength, by using SVEs with microcracks, and the generation of statistically consistent grids for fracture strength based on SVE results.

10.2.1 Computation of Fracture Strength for an SVE

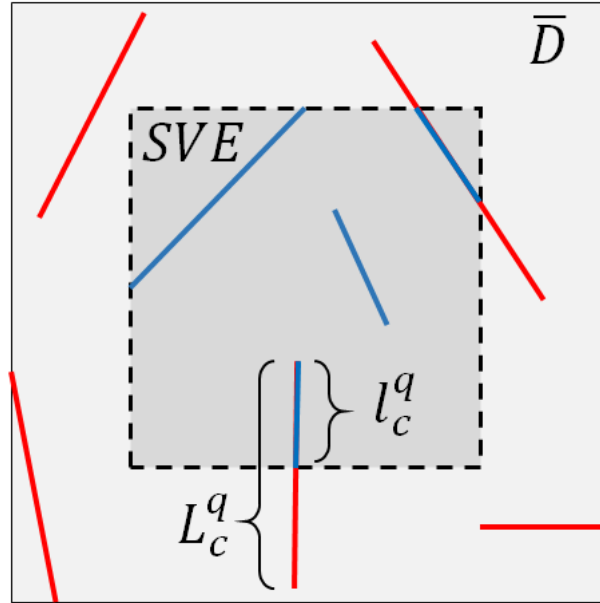


Figure 10.1: Cracks considered for computation of effective strength for an SVE; blue and red colors correspond to crack segments inside and outside the SVE, respectively.

Figure 10.1 shows a sample SVE in domain $\bar{D}$. The cracks that are fully or partially in the SVE are considered in the computation of its fracture strength $\bar{\sigma}$. The fracture strength is computed by finding the minimum tensile stress, along all directions, such that at least for one of the crack tips in the SVE, $K = K_c$ where K is the stress intensity factor at the crack tip and K_c is the fracture toughness of the given material.

Clearly, the microcrack propagation criterion at the SVE level is assumed to follow the linear elastic fracture mechanics (LEFM) theory. The association of the stress that result in propagation of one SVE with the SVE's fracture strength is motivated by the behavior of quasi-brittle materials where there is a very small difference between the stresses that initiate fracture and the ultimate stress (fracture stress); *cf.* the results in [155]. For our model the point of departure from linear elasticity and initiation of failure corresponds to the stress at which the first microcrack propagates. Finally, instead of doing a full FE analysis, we assume that the stress intensity factor of each crack can be approximated by that of a crack in an infinite domain. While this is still expected to model spatial variation of fracture strength relatively well, in forthcoming works we aim to use FEM analyses for this purpose.

Let L_c and l_c be the original length and length of the i th microcrack within the SVE, respectively. The critical stress for this specific i th microcrack within the SVE is given by the equation

$$\bar{s}^i = \left(\frac{L_c^i}{l_c^i} \right)^\alpha \frac{K_c}{\sqrt{\pi L_c^i/2}}, \quad (10.1)$$

where as mentioned K_c is the fracture toughness and α is a constant value coefficient. The values of $\alpha = 0$ and $\alpha = \frac{1}{2}$ consider the full length of the crack, L_c^i , and the length of the crack inside the SVE, l_c^i , respectively; accordingly, similar to [53] we choose $\alpha = \frac{1}{4}$ to consider an intermediate length of the crack between L_c^i and l_c^i when it intersects the SVE boundaries. After computing critical stresses $\bar{s}^i$ for all cracks $i \in \mathcal{I}$, the strength of the SVE $\bar{s}$ is defined as,

$$\bar{s} = \min_{i \in \mathcal{I}} \{\bar{s}^i\}. \quad (10.2)$$

By this definition, a fracture strength value $\bar{s}$ is assigned to SVEs constructed at all spatial positions and for all random realizations that are generated based on the statistics of microcracks. The point values of $\bar{s}$ are used to compute its probability density function (PDF). The covariance function needed for the Karhunen-Loève method is obtained by the moving technique [26], where the sampling SVE is gradually moved in the domain to determine the trend on which fracture strength changes spatially.

10.2.2 Karhunen-Loeve (KL) Expansion

For a given domain $\bar{D}$ the Karhunen-Loève (KL) method enables generating random fields for a variable ξ , consistent with its underlying statistics, in this case its point-wise PDF and two-point covariance function. The value of the random field ξ is derived based on a random variable ω , that is $\xi = \xi(\mathbf{x}, \omega)$. Having these functions (at all points), it is possible to derive a simple formula which approximates the mean and covariance of the known random variable distribution; the truncated KL expansion of the random field $\xi = \xi(\mathbf{x}, \omega)$ yields the following representation of the field,

$$\xi(\mathbf{x}, \omega) = \mu_\xi(\mathbf{x}) + \sum_{i=1}^{n_{KL}} \sqrt{\lambda_i} b_i(\mathbf{x}) Y_i(\omega) \quad (10.3)$$

where $\{\lambda_i, b_i(\mathbf{x})\}_{i=1}^{n_{KL}}$ are eigen-pairs determined from the covariance of the random field and $Y_i(\omega)$ are centered, uncorrelated random variables¹ which derive the probability distribution of the random field. For an arbitrary PDF function for $\xi(\mathbf{x}, \omega)$, Y_i are only uncorrelated. To make this formula practical and be able to generate random variables Y_i *independent* of each other, they should be independent random variables. The latter condition holds if $\xi(\mathbf{x}, \omega)$ is point-wise Gaussian. Thus, Eqn. (10.3) is to be used for a normal field. In our prior work [53], we approximated the fracture strength field by a lognormal field to be able to directly use Eqn. (10.3) on $\log(\bar{s})$. However, in general we need to transfer a random field ξ to η , a random field with point-wise Gaussian distribution before using the KL method. Then a random field for the mapped normal field η is generated, and finally the random field is transferred back to its original form. The KL expansion for the Gaussian random field $\eta(\mathbf{x}, \omega) \sim N(\mu_\eta, \sigma_\eta)$ is,

$$\eta(\mathbf{x}, \omega) = \mu_\eta(\mathbf{x}) + \sum_{i=1}^{n_{KL}} \sqrt{\lambda_i} b_i(\mathbf{x}) y_i, \quad (10.4)$$

where μ_η and σ_η are the mean value and standard deviation of η . The aforementioned eigen-pairs of the spatial eigenfunctions $b_i(\mathbf{x})$ and eigenvalues λ_i are obtained by solving a generalized eigenvalue problem (EVP) that can be solved by finite element method (FEM) discretization; *cf.* [82].

¹ $\mathbb{E}(Y_i(\omega)) = 0$, and $\mathbb{E}(Y_i(\omega)Y_j(\omega)) = 0$

As mentioned, a general non-Gaussian random field $\xi(\mathbf{x}, \omega)$ is first mapped to a Gaussian random field $\eta(\mathbf{x}, \omega)$. This map is expressed through the *Inverse Transformation Method*,

$$\eta(\mathbf{x}, \omega) = F_\eta^{-1}(F_\xi(\xi(\mathbf{x}, \omega))), \quad (10.5)$$

where F_ξ and F_η are the Cumulative Density Functions (CDF) of the non-Gaussian and Gaussian random fields, respectively. We use a standard normal, *i.e.*, $\mu_\eta = 0$ and $\sigma_\eta = 1$, for the Gaussian field. Finally, for any of the random field realizations of η , obtained by Eqn. (10.4), we use the inverse of the map in Eqn. (10.5) to transfer it back to ξ . This transformation for ξ (equal to fracture strength $\bar{s}$) is expressed as,

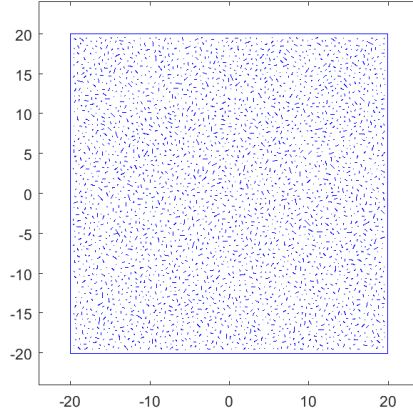
$$\bar{s}(\mathbf{x}) = \xi(\mathbf{x}) = F_\xi^{-1}\left(\frac{1}{2}\left[1 + \text{Erf}\left(\frac{\eta(\mathbf{x})}{\sqrt{2}}\right)\right]\right). \quad (10.6)$$

This is a more accurate extension of [53] wherein the original field $\xi(\mathbf{x}, \omega)$ and CDF F_ξ assumed a Log-normal probability distribution. We note that the covariance function for $\eta(\mathbf{x}, \omega)$, which is required in solving the KL eigen-problem, is characterized by a moving window approach; *cf.* [53] for more details.

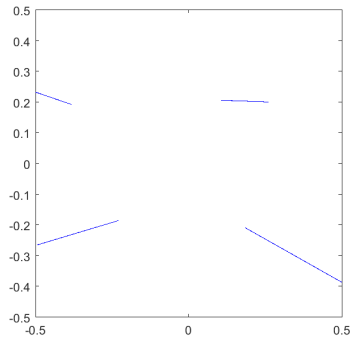
10.3 Numerical Results

The spatial domain $\bar{D}$ used for generating the following statistical data is a simple rectangular domain centered at the Cartesian position $\mathbf{x}_{center} = (0, 0)$ and spanning 40 length units ($L_{\bar{D}} = 40$ mm) in both $\mathbf{e}_1$ and $\mathbf{e}_2$ directions.

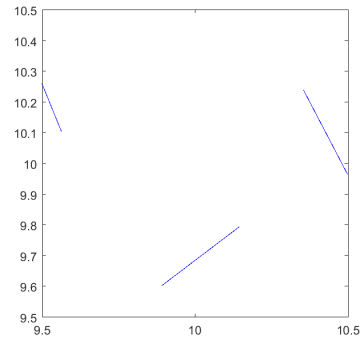
To generate domain microstructural realizations with microcracks, we assume that the microcrack length follows a Weibull distribution [215, 216] and its angle a uniform distributed between $[0, 2\pi]$. Furthermore, the average and standard deviation of microcrack length are 330 μm and 170 μm , respectively. Finally, we use a take-and-place algorithm to distribute generated cracks within domain $\bar{D}$. A sample realization is shown in Fig. 10.2a. Two sample SVEs generated from the domain in Fig. 10.2a are shown in Fig. 10.2b and Fig. 10.2c. The center points of sampled SVEs form a nonuniform grid, with a denser spacing near zero distance, to have a more accurate derivation of covariance function.



(a) Example of realization $\bar{D}$ with random microstructure architecture.



(b) SVE ($L_{VE} = 1$) sample from Fig. 10.2a centered at $\mathbf{x} = (0, 0)$.



(c) SVE ($L_{VE} = 1$) sample from Fig. 10.2a centered at $\mathbf{x} = (10, 10)$.

Figure 10.2: A 40 mm $\times$ 40 mm domain and two sampled SVEs.

10.3.1 The effect of the SVE size on random field statistics

The size of the SVE directly influences the statistics of the random field characterized. To study the relation between the SVE size and the fracture strength random field statistics, square SVEs with edge sizes of 1, 2, 4, 8 and 16 mm were considered. The PDFs of the fracture strength field in Fig. 10.3 are accordingly labeled by $\text{SVE}1 \times 1$, $\text{SVE}2 \times 2$, $\text{SVE}4 \times 4$, $\text{SVE}8 \times 8$, and $\text{SVE}16 \times 16$.

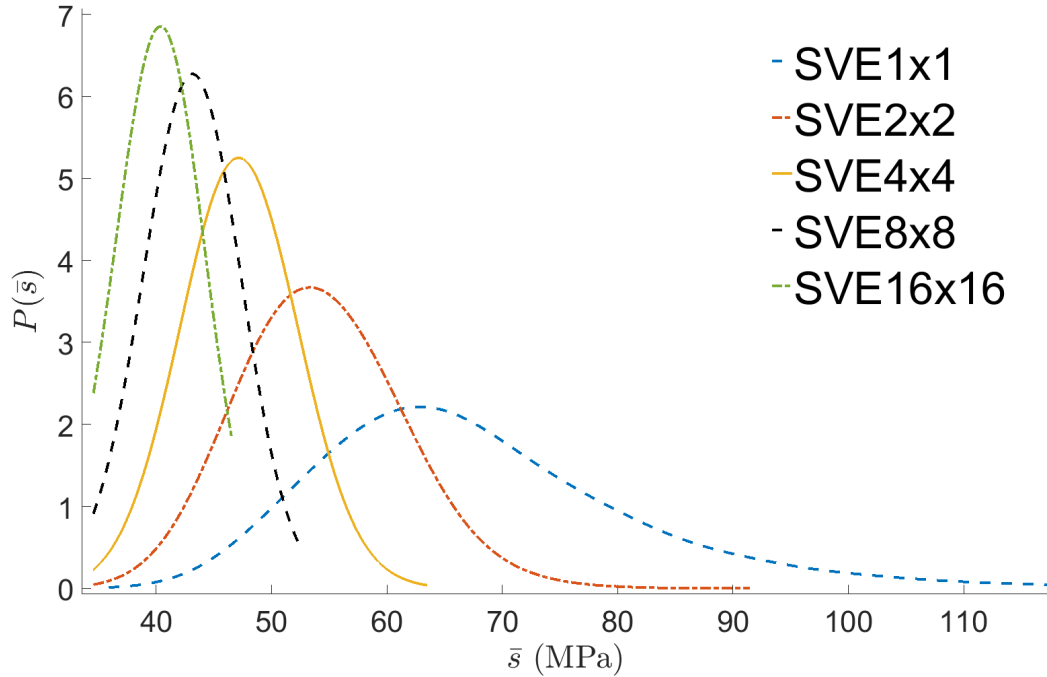


Figure 10.3: The effect of the SVE size on the pdf of random field $\bar{s}$.

As the SVE size becomes larger, the peak of the PDF curve shifts to the left, that is a weaker material is represented. This is the well-known size effect for quasi-brittle materials; as the size of the domain increases there is a larger likelihood that a more critical crack or defect exists in it. That is why larger samples tend to have lower fracture strengths. In fact, domain size calibrated Weibull model and many other stochastic models in the literature attempt to represent this phenomenon.

Another observation is that as the window size decreases, the sampled fracture strength values are more likely to have wider variations. The reason is that at small sizes, the SVE may land in a region with long crack(s) or a short one, thus yielding a low or a high fracture

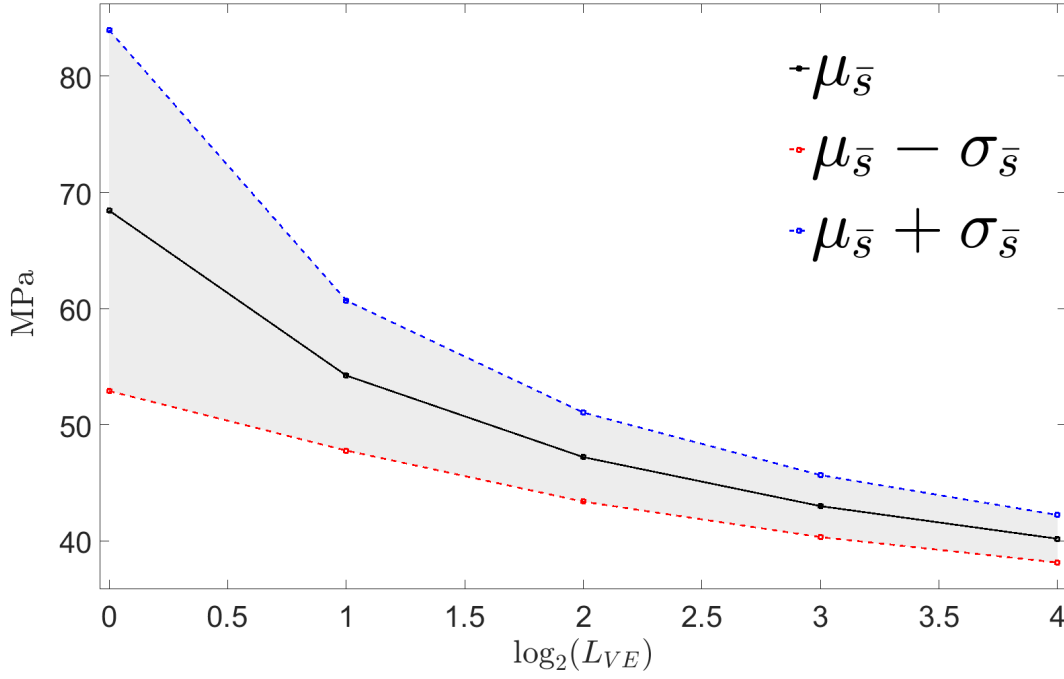


Figure 10.4: The effect of the SVE size on random field $\bar{s}$ statistics.

strength, respectively. This is demonstrated by higher standard deviations for smaller SVE window sizes in Fig. 10.4. On the contrary, as the SVE window size increases, the standard deviation decreases, *i.e.*, PDF function becomes narrower. This is expected, because as the window size increases many defects (microcracks) are included in the SVE and all SVEs tend to have roughly the same critical crack length.

10.3.2 KL random fields

The KL random field meshes were generated based on the assumption that the material modeled was isotropic with a rotationally invariant scalar fracture strength, and the covariance function depending only on distance between two arbitrary points. Moreover, the covariance function for fracture strength—casted to a standard normal Gaussian distribution, *cf.* η in Eqn. (10.5)—is interpolated by the exponentially decaying function,

$$COV(\eta(\mathbf{x}^1), \eta(\mathbf{x}^2)) = e^{-\left(\frac{|\mathbf{x}^1 - \mathbf{x}^2|}{d_c}\right)^2}, \quad (10.7)$$

where d_c is a characteristic correlation length scale implied by the form of the function. It is noted that, the exponential function from Eqn. (10.7) is a very good fit for the numerically obtained covariance functions. The correlation lengths for different SVE sizes are $d_c^{1 \times 1} = 0.52$ mm, $d_c^{2 \times 2} = 0.96$ mm, $d_c^{4 \times 4} = 1.84$ mm, $d_c^{8 \times 8} = 3.98$ mm, and $d_c^{16 \times 16} = 8.19$ mm respectively, and their covariance functions are shown in Fig. 10.5. To ensure that accurate KL grids are constructed, enough number of terms should be considered in Eqn. (10.3) so that last eigenvalues are very close to zero; for the SVE1 $\times$ 1 sampling, at $n_{KL} \approx 1500$ eigenvalues are extremely close to zero, and even fewer terms are needed for larger sampling window sizes. For all the KL grids generated subsequently, $n_{KL} = 2000$ eigenvalues / eigenvectors are considered.

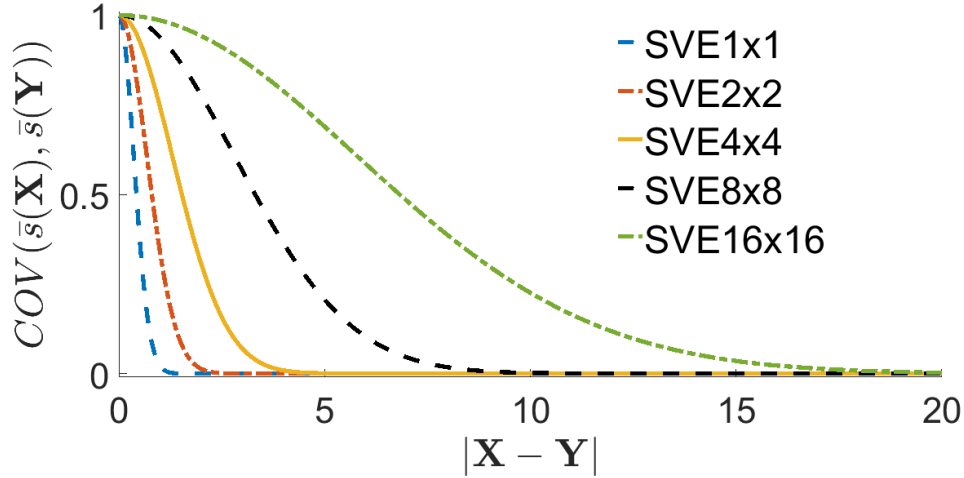


Figure 10.5: One-dimensional covariance functions based on variable SVE sizes.

10.3.3 Discrete grids for fracture strength and FEM solution

We use two different discrete grids for our fracture simulations. The *material grid* is used for the generation and storage of fracture strength and the *aSDG spatial grid* is the finite element discrete mesh used for fracture simulation. The former is a uniform grid on which the KL eigenvalue problem is solved; *cf.* the formulation section and [82]. The latter is used for the solution of dynamic fracture problem, which is nonuniform. Adaptive operations are used to control solution discretization error and accommodate arbitrary oriented crack paths. For fracture simulations in this manuscript a 16mm $\times$ 16mm domain is considered.

Note that this domain is different from the $40\text{mm} \times 40\text{mm}$ domains used in Fig. 10.2a. In the latter case, domains with micro-structure (microcracks herein) are generated to derive the first and second moments needed for the KL method, while in the former case the KL grids are generated based on such derived statistics. It should be noted that the sizes of these domains do not need to be the same. Finally, the KL domains generated subsequently do not include any microcracks, as the effect of microcracks is already incorporated in the inhomogeneous and randomly sampled fracture strength field.

Accordingly, a structured 2D mesh of dimensions $[-8, 8] \text{ mm} \times [-8, 8] \text{ mm}$ is used for the KL expansion method. For this grid, 2D quadrilateral elements (60×60 elements) of equal element size are used for solving the eigenvalue problem and generating random field realizations. The KL discretization mesh is shown in Fig. 10.6.

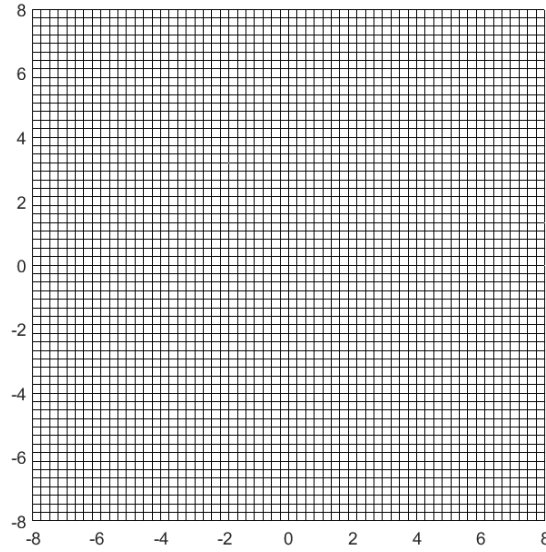
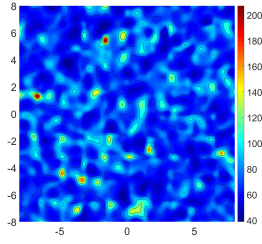
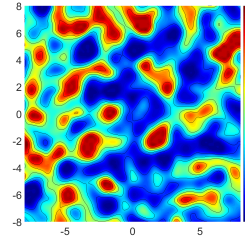


Figure 10.6: structured mesh for KL eigenvalue problem and random field realizations.

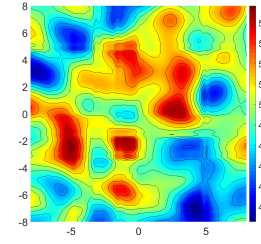
One KL random field realization for fracture strength $\bar{s}$ for each of the available SVE sizes is depicted in Fig. 10.7. The decrease of each SVE size yielded a greater variability in fracture strength randomness within a given length-scale; this behavior agrees with theoretical expectations of how SVE sizes affect random field value scatter.



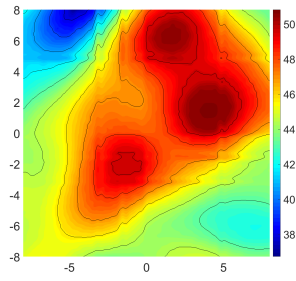
(a) random $\bar{s}$ field for SVE1 $\times$ 1



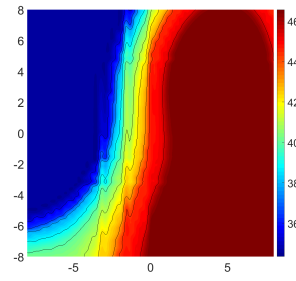
(b) random $\bar{s}$ field for SVE2 $\times$ 2



(c) random $\bar{s}$ field for SVE4 $\times$ 4

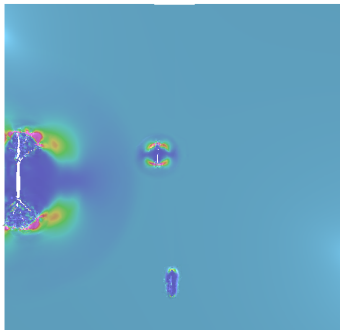


(d) random $\bar{s}$ field for SVE8 $\times$ 8

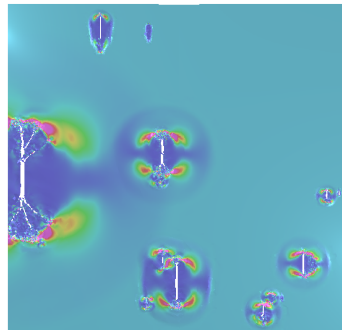


(e) random $\bar{s}$ field for VE16 $\times$ 16

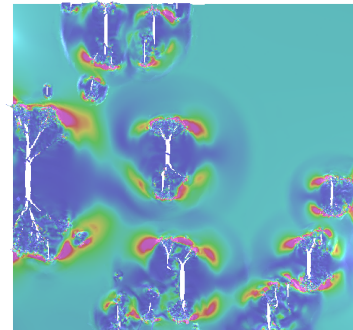
Figure 10.7: The first realization of KL-generated random field meshes for fracture strength $\bar{s}$ (in MPa) with respect to different SVE sizes.



(a) Time $t = 7.250 \mu s$.

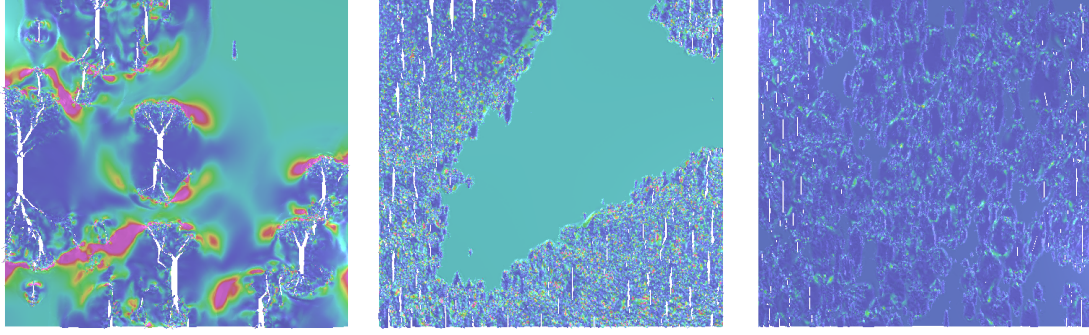


(b) Time $t = 7.875 \mu s$.



(c) Time $t = 8.625 \mu s$.

Figure 10.8: A sequence of fracture solution visualizations for SVE1 $\times$ 1 mm.



(a) SVE1 $\times$ 1, time $t = 9.25 \mu\text{s}$. (b) SVE8 $\times$ 8, time, $t = 8.65 \mu\text{s}$. (c) Homogeneous $\bar{s}$, time $t = 3.9 \mu\text{s}$.

Figure 10.9: Fracture solution visualization with varying fracture strength randomness.

10.3.4 Dynamic fracture under uniform uniaxial applied tensile stress

We use an h -adaptive asynchronous spacetime discontinuous Galerkin (aSDG) finite element method [9, 10] for our dynamic fracture simulations. The aSDG method directly discretizes spacetime using nonuniform grids that satisfy a special causality constraint [3] yielding unique properties such as local and asynchronous solution scheme, arbitrarily high and local temporal order of accuracy, and linear solution scaling with number of elements. This numerical scheme, implemented in C++, utilizes the aforementioned features as well as advanced adaptive operations in spacetime to very accurately and efficiently capture complex fracture patterns by a *crack tracking* adaptive scheme [1, 158]. The solution is mesh independent and accommodates crack propagation in any desired direction, a feature similar to the popular XFEM and GFEM methods, but removes the need to enrich element basis functions. All these features make the aSDG method ideal for dynamic quasi-brittle fracture simulations reported herein.

This section aims to validate the method's ability to capture fracture nucleation at domain locations of weaker fracture strength as well as track the development of a possibly complex crack network. The FEM domain is a 2D quadrilateral of side length 8 centered at $\mathbf{x} = (0, 0)$. The bulk material properties are: Young's Modulus $E = 3.24 \text{ GPa}$, mass density $\rho = 1190 \text{ kg/m}^3$, and Poisson's ratio $\nu = 0.35$. The values of fracture strength $\bar{s}(\mathbf{x})$

are extracted from the independent KL random field solution discretization. The fracture strength equation parameters used in the SVE sampling algorithm are fracture toughness $K_c = 1.5\text{MPa}\sqrt{m}$ and coefficient $\alpha = \frac{1}{4}$. The initial and boundary conditions are specified consistent with displacement field $\mathbf{u}(\vec{x}, t) = (u_1(\vec{x}, t), u_2(\vec{x}, t)) = (ax_1t, 0.0)$ where $a > 0$ and $(\mathbf{x}, t)$ is the spacetime coordinate of a point. This corresponds to a spatially uniform stress field in x_1 direction, a condition that will no longer hold after the nucleation/propagation of the first crack. As will be discussed below, this uniform stress field very well demonstrates the shortcoming of models that use a spatially constant fracture strength. For the following results, the value of $a = 1.062/\text{ms}$ is chosen.

10.3.4.1 Comparative study: random vs homogeneous fracture strength fields

To understand the effect of incorporating randomness into a fracture model of quasi-brittle material, fracture solutions generated from the use of a spatially *homogeneous* fracture strength field is compared to solutions which facilitate KL-generated random fracture strengths. Specifically, the first KL mesh realizations for 1×1 and 8×8 SVEs are used for nonuniform fields for $\bar{s}$; *cf.* Figures 10.7a and 10.7d.

We first study the development of the SVE 1×1 fracture network to demonstrate how the variability of the fracture strength influences random nucleation locations as well as fracture patterns characteristics. Figure 10.8 shows the visualization of intermediate fracture solutions on deformed geometry. The color and height fields correspond to strain and kinetic energy densities, respectively. As the solution time progresses a clear correlation between the fracture strength distribution and the site of fracture nucleation is demonstrated; *cf.* Figure 10.7a. As the boundary loading increases cracks accelerate and characteristics of brittle fracture such as microcracks / crack bifurcations are observed.

In Figure 10.9 the effect of SVE sampling window size, and consequently correlation length scale, on developed fracture patterns is studied. As the sve size increases, there is a decrease in the degree of spatial variation of the strength values and potentially larger areas of weaker strength. Fractures based on 1×1 mm SVE homogenization in Fig. 10.9a are closer to what is expected from brittle fracture by forming distinct cracks with microcracking and crack branching events. The solution for 8×8 mm SVE homogenization are shown in Fig.

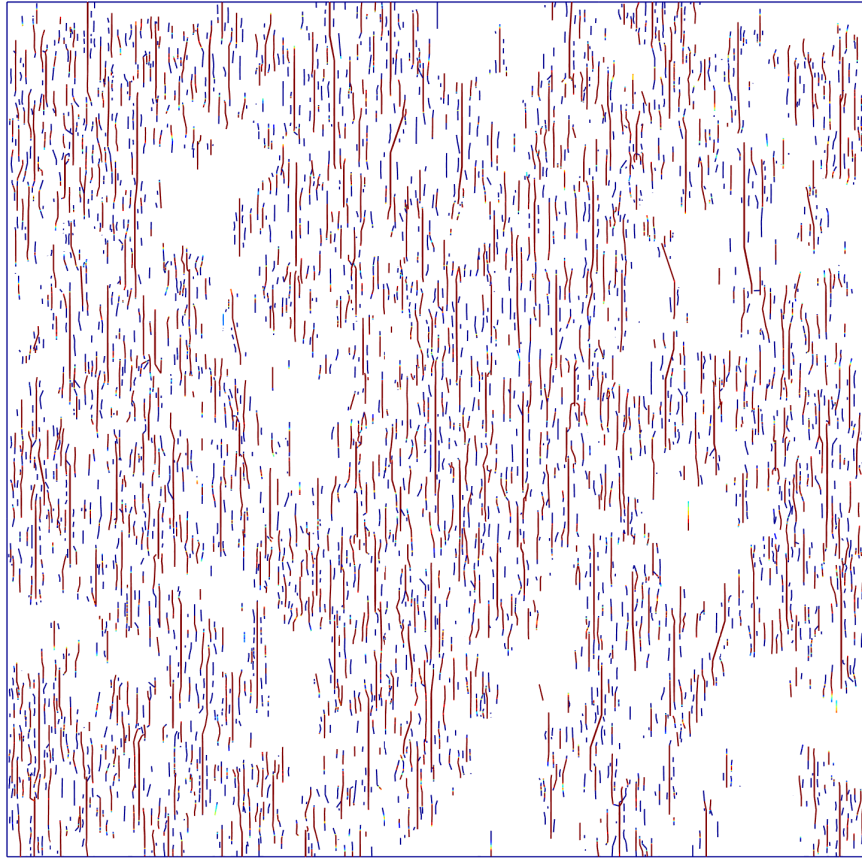


Figure 10.10: Homogeneous solution deformed shape at time, $t \approx 3.9 \mu s$.

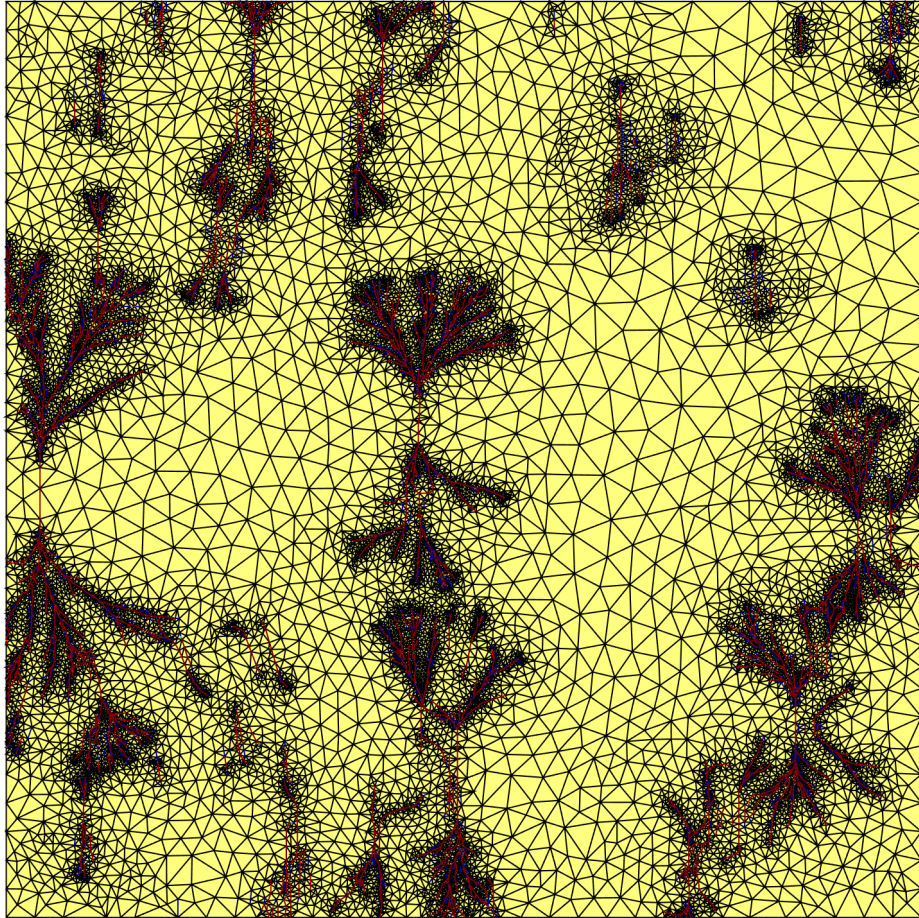


Figure 10.11: $\text{SVE1} \times 1$ solution discretization at time, $t \approx 9.648 \mu\text{s}$.

10.9b; as can be seen there is an excellent agreement between regions with fracture and those with lower fracture strength $\bar{s}$ from the first realization used in Fig. 10.7d. Within these large weaker areas with almost the same fracture strength, greater number of nucleation sites occur resulting in clusters of relatively smaller cracks. Finally, Fig. 10.9c demonstrates fracture pattern predicted when a homogeneous fracture strength is used for the entire domain; the fracture network can be better seen in Fig. 10.10, where the deformed solution geometry represented by linear segments is color-coded based on a scalar damage value (blue segments are undamaged and red segments are beyond a critical damage value). The fracture network is densely populated compared to the $\text{SVE1} \times 1$ case; also, since the domain contains no variation in fracture strength value, the location of these fracture sites is merely based on numerical errors in the FEM solution rather than microstructure variations.

The importance of mesh adaptivity is demonstrated in Fig. 10.11 for $\text{SVE1} \times 1$ results, where crack segments are represented by red 2D line segments in the space front; adaptive operations enable exact tracking of crack direction and accurate resolution of fracture process zone size.

10.4 Conclusion

SVEs and the moving window approach were used to derive the statistics of a scalar fracture strength field for domains with random distribution of microcracks. The Inverse Transform Method was used to transform the derived non-Gaussian random field to a standard normal field to enable the generation of statistically consistent random fields with the Karhunen-Loève method, and to transfer the generated random field back to its non-Gaussian form. The fracture simulations, obtained by the aSDG method, demonstrated the effect of the size of SVE on fracture formation where microcracking, crack branching and other features of brittle fracture were more evident with smaller SVE sizes.

Chapter 11

Conclusion

Through the efforts presented in this document, relationships between brittle material heterogeneity and the material's inelastic responses induced by dynamic loading were investigated. The meat of the matter is shown in the macroscale simulations of Chapter 6, but some intrinsic relationships are seen in the preceding chapters.

By utilizing in-house or collaborative methods, various material microstructures were generated and studied. This included material architectures range from the distribution of simplistic non-overlapping rectilinear microcracks, which can represent such systems as natural fractures within a rock matrix, to circular inclusions representing a fiber reinforced composite material. It is a bit intuitive that these discrete descriptions introduce levels of material biases in that they assume material constitutions that either overestimate or underestimate the true responses of the material; the intent of the overall framework is the capacity to sufficiently represent a (quasi-)brittle material independent of the makeup of the initial microstructure. Therefore, to have a more consistent relation between the material micro- to macroscale it was necessary to describe the microstructure on a continuum mechanics basis; this rendered statistically averaged material properties obtained using SVE based homogenization at select spatial locations. As theoretically expected, there was a clear demonstration of how micromechanics-based homogenization within these SVEs allowed material uncertainty to propagate from the microscale to the macroscale, and how this multiscale relation is influenced by the SVE geometry and size. The first instance of this concept was seen when the statistics of the effective properties were analyzed for the various SVE sizes.

Using the probability density function (PDF) as well as the first and second statistical moments (*i.e.*, mean value about zero, and variance about the mean value respectively) of the averaged values, statistical characteristics numerically captured the phenomenon known as the size-effect of brittle materials. This is essentially the representation of a material having lower and more statistically uniform effective fracture strength values when it is homogenized by larger SVEs. The trend is evident by the shifting of the peak value of PDF (*i.e.*, average value) for fracture strength to lower values and a transition of the smooth PDF curve to a dirac delta function. This delta function is indicative of an RVE homogenized material of uniform strength. Another means of quantifying the size-effects from the above

computed statistics was an evident decrease in both the mean and variance of the averaged effective properties as the SVE size tended to the RVE limit. Exploiting the statistical information influenced by the microstructure, the Karhunen-Loève method was then used to construct a continuous approximation of the average properties. This discretized quantity provided independently meshed inputs to the solid mechanics finite element solver as the material micro(meso-)structure representation. When the discretized approximation was derived from an SVE tending to the RVE limit there was a decrease in the spatial variability of the continuum-based property representing the material. This was expected as we are aware that RVEs are incapable of preserving a materials inherent spatial randomness.

With both random explicit structure realizations and the continuum based material property approximation, we were able to study how various material domain representations responded to highly dynamic loading conditions; specifically from the standpoints of hydro-elastics and purely elasto-dynamics. Each case study contributed to the overall comparison of dynamic responses for material micro(meso-)structures modeled i) homogeneously or heterogeneously, or ii) discretely versus continuously in a random sense. For the former modeling cases, modeling a uniform stress distribution for a material subject to uniaxial tensile far field loading demonstrated how homogeneous fracture strengths can give unrealistic instantaneous initiation of large amounts of macrocracks. Contrary to the previous homogeneous model, implicit heterogeneous spatially correlated fracture strengths were found to give a more brittle-like fracture response. In the later comparisons for the specific studies of compressive and tensile loading conditions, both sets of findings gave interesting insight on how explicit crack density and level of microstructure anisotropy affected the fracture patterns. For tensile loading study cases, it was seen that an increase in the explicit or implied crack density of a material greatly increases the amount of crack growth and pattern complexity; this is especially true for materials that were modeled with anisotropic explicit crack distribution or implicit strength. The tensile studies also revealed a ductile to brittle material behavior transition when the interfacial damage model relaxation time τ decreased. This is a direct result of a reduction in fracture toughness that is directly proportional to the relaxation time. Utilizing a damage model effective stress based on Mohr-Coulomb failure criterion, compressive test studies demonstrated how anisotropy affected crack propagation when an

imposed angular bias favors failure in the critical directions $\pm\phi_{ch} = (45^\circ - \phi/2)$ for angle of friction ϕ . Whether the material microstructure explicitly resolves weak bedding planes by discrete cracks oriented at specific angles or implicitly describes fracture strength values having angular bias, these compressive studies demonstrated how there is a greater level of crack initiation and growth when the microstructure characterizing angles tend to this critical angle ϕ_{ch} . Similar to the far field tensile and compressive loading cases, the hydraulic fracture problems illustrated the effects of material matrix crack density. An increase in the crack density resulted in much more significant fracture patterns and well as reduction in penetration depth of the hydraulically loaded fracture. It was also seen that there is a greater sensitivity to material heterogeneity when the hydraulic fracture is subject to a higher loading rate; slower rates result in a smoother and straighter path that would not otherwise deviate and interact with distributed natural fractures due to low energy zones about the propagating crack tip.

The work in this dissertation will be expanded in future to address certain concepts worth visiting. One of which is regarding the generation of the statistical data used in the Karhunen-Loève expansion. Although the spatially-correlated random fields share the statistical structure of the underlying microstructure, it may be argued that the effective property statistics generated thus far mimic the *ad hoc* probability structure used to generate the material microstructure rather than any real material. To remedy this concern, works are currently being conducted to obtain microstructure realizations from image processing of a real microstructure sample; this will ensure that the ensemble statistics mimic that of real material samples. A significant portion of the numerical results are generated utilizing random inhomogeneous fracture strength properties, while the elastic properties such as material elastic modulus and mass density are modeled homogeneously. In the future, the incorporation of cross-correlated elastic properties and fracture related properties will be introduced to the model to account for randomness in the material fracture mechanics as well as material constitutive relations. Finally, efforts are presently underway to study anisotropy in terms of elastic properties such as with stiffness tensors of brittle materials which are inherently directional dependent. The aSDG numerical solver utilizes Reimann solutions in the interfacial damage model which are determined for isotropic bulk wave

speeds. The primary goal in this regard will be to use anisotropic dilatational and shear bulk wavespeeds determined using the previously mentioned Christoffel equation solver to compute higher tensor order Reimann solutions to adopt into the damage model. The secondary goal will then be to develop a means of generating a continuum representation of these stiffness tensors in the same manner that the KL random fracture strength fields are computed. This introduces the main hurdles of determining consistent cross-correlation (covariance) functions between each of the possibly 21 independent elastic constants defining the Voigt stiffness; we must then adapt the KL method to generate anisotropic random tensor fields rather than an isotropic scalar field.

Bibliography

- [1] Abedi, R. (2010). *Spacetime damage-based cohesive model for elastodynamic fracture with dynamic contact*. PhD thesis, Department of Theoretical and Applied Mechanics, University of Illinois at Urbana–Champaign. [60](#), [72](#), [150](#), [151](#), [152](#), [153](#), [154](#), [157](#), [159](#), [162](#), [171](#), [232](#)
- [2] Abedi, R. (2016). A comparative and parametric study of dynamic cohesive and linear elastic fracture mechanics models. *International Journal of Solids and Structures*, 102-103:163–75. [115](#), [202](#)
- [3] Abedi, R., Chung, S.-H., Erickson, J., Fan, Y., Garland, M., Guoy, D., Haber, R., Sullivan, J. M., Thite, S., and Zhou, Y. (2004). Spacetime meshing with adaptive refinement and coarsening. In *Proceedings of the Twentieth Annual Symposium on Computational Geometry*, SCG '04, pages 300–309. ACM. [60](#), [110](#), [153](#), [156](#), [157](#), [175](#), [232](#)
- [4] Abedi, R. and Clarke, P. (2018). Modeling of rock inhomogeneity and anisotropy by explicit and implicit representation of microcracks. *Proceeding: 52th US Rock Mechanics/Geomechanics Symposium, June 17-June 20, Seattle, Washington USA*, pages ARMA 18–1094 (10 pages). [199](#)
- [5] Abedi, R. and Haber, R. (2011). Spacetime dimensional analysis and self-similar solutions of linear elastodynamics and cohesive dynamic fracture. *International Journal of Solids and Structures*, 48(13):2076–87. [109](#), [113](#), [115](#), [153](#), [191](#), [194](#)
- [6] Abedi, R., Haber, R., and Clarke, P. (2017a). Effect of material randomness on dynamic fracture of quasi-brittle materials. *International Journal of Fracture: Special Issue for Integrated Computational Structure-Material Modeling of Deformation & Failure Under Extreme Conditions An IUTAM Symposium*. Accepted. [97](#), [109](#), [110](#), [113](#), [114](#), [115](#), [147](#), [199](#), [202](#), [206](#), [209](#)
- [7] Abedi, R., Haber, R., and Elbanna, A. (2017b). Mixed-mode dynamic crack propagation in rocks with contact-separation mode transitions. *Proceeding: 51th US Rock Mechanics/Geomechanics Symposium, June 25-June 28, San Francisco, California USA*, pages ARMA 17–0679 (12 pages). [111](#), [207](#)

- [8] Abedi, R. and Haber, R. B. (2014). Riemann solutions and spacetime discontinuous Galerkin method for linear elastodynamic contact. *Computer Methods in Applied Mechanics and Engineering*, 270:150 – 177. [97](#), [108](#), [111](#), [113](#), [153](#), [160](#), [162](#), [165](#), [202](#), [205](#)
- [9] Abedi, R., Haber, R. B., and Petracovici, B. (2006a). A spacetime discontinuous Galerkin method for elastodynamics with element-level balance of linear momentum. *Computer Methods in Applied Mechanics and Engineering*, 195:3247–3273. [xvii](#), [25](#), [59](#), [97](#), [110](#), [150](#), [153](#), [154](#), [156](#), [157](#), [202](#), [232](#)
- [10] Abedi, R., Haber, R. B., Thite, S., and Erickson, J. (2006b). An h -adaptive spacetime-discontinuous Galerkin method for linearized elastodynamics. *Revue Européenne de Mécanique Numérique (European Journal of Computational Mechanics)*, 15(6):619–42. [25](#), [59](#), [67](#), [97](#), [110](#), [153](#), [154](#), [157](#), [175](#), [202](#), [232](#)
- [11] Abedi, R., Hawker, M. A., Haber, R. B., and Matouš, K. (2009). An adaptive spacetime discontinuous Galerkin method for cohesive models of elastodynamic fracture. *International Journal for Numerical Methods in Engineering*, 1:1–42. [83](#), [85](#), [87](#), [110](#), [115](#), [139](#), [150](#), [157](#), [175](#)
- [12] Abedi, R., Omid, O., and Clarke, P. (2016). Numerical simulation of rock dynamic fracturing and failure including microscale material randomness. *Proceeding: 50th US Rock Mechanics/Geomechanics Symposium, June 26-June 29, Houston, Texas - USA*, pages ARMA 16–0531 (13 pages). [51](#), [221](#)
- [13] Abedi, R., Omid, O., and Clarke, P. (2017c). A numerical study on the effect of loading and randomness on fracture patterns in a tight formation. *Proceeding: 51th US Rock Mechanics/Geomechanics Symposium, June 25-June 28, San Francisco, California USA*, pages ARMA 17–0641 (12 pages). [112](#), [135](#), [144](#), [201](#), [218](#), [221](#)
- [14] Acton, K., Baxter, S., Bahmani, B., Clarke, P., and Abedi, R. (November 3-9, 2017). Mesoscale models characterizing material property fields used as a basis for predicting fracture patterns in quasi-brittle materials. In *Proceedings of ASME 2017 International Mechanical Engineering Congress & Exposition IMECE 2017*, pages IMECE2017–71500,

5 pages, Tampa, Florida, USA. ASME International Mechanical Engineering Congress & Exposition. [24](#)

- [15] Acton, K. and Graham-Brady, L. (2009a). Fitting an anisotropic yield surface using the generalized method of cells. In *Advances in mathematical modeling and experimental methods for materials and structures*, pages 27–41. Springer. [26](#)
- [16] Acton, K. and Graham-Brady, L. (2009b). Meso-scale modeling of plasticity in composites. *Computer Methods in Applied Mechanics and Engineering*, 198(9):920–932. [26](#)
- [17] Acton, K. and Graham-Brady, L. (2010). Elastoplastic mesoscale homogenization of composite materials. *Journal of engineering mechanics*, 136(5):613–624. [xi](#), [13](#), [26](#)
- [18] Ahn, B. and Curtin, W. (1997). Strain and hysteresis by stochastic matrix cracking in ceramic matrix composites. *Journal of the Mechanics and Physics of Solids*, 45(2):177–209. [77](#)
- [19] Akulich, A. V. and Zvyagin, A. V. (2008). Interaction between hydraulic and natural fractures. *Fluid Dynamics*, 43(3):428–435. [95](#)
- [20] Al-Ostaz, A. and Jasiuk, I. (1997). Crack initiation and propagation in materials with randomly distributed holes. *Engineering Fracture Mechanics*, 58(5-6):395–420. [xi](#), [8](#), [9](#), [25](#), [50](#), [77](#), [80](#), [221](#)
- [21] Alfano, G. and Sacco, E. (2006). Combining interface damage and friction in a cohesive-zone model. *International Journal for Numerical Methods in Engineering*, 68(5):542–582. [150](#), [151](#)
- [22] Allix, O. and Corigliano, A. (1999). Modeling and simulation of crack propagation in mixed-modes interlaminar fracture specimens. *International Journal of Fracture*, 38:111–140. [159](#), [160](#), [163](#), [206](#)
- [23] Allix, O., Feissel, P., and Thevenet, P. (2003). A delay damage mesomodel of laminates under dynamic loading: basic aspects and identification issues. *Computers and Structures*, 81(12):1177–1191. [163](#), [206](#)

- [24] Ambati, M., Gerasimov, T., and De Lorenzis, L. (2015). A review on phase-field models of brittle fracture and a new fast hybrid formulation. *Computational Mechanics*, 55:383–405. [149](#)
- [25] Barenblatt, G. I. (1962). The mathematical theory of equilibrium of cracks in brittle fracture. *Advanced Applied Mechanics*, 7:55–129. [150](#)
- [26] Baxter, S. and Graham, L. (2000). Characterization of random composites using moving-window technique. *Journal of Engineering Mechanics*, 126(4):389–397. [8](#), [13](#), [26](#), [31](#), [50](#), [197](#), [223](#)
- [27] Baxter, S., Hossain, M., and Graham, L. (2001). Micromechanics based random material property fields for particulate reinforced composites. *International Journal of Solids and Structures*, 38(50-51):9209–20. [11](#)
- [28] Bazant, Z. and Liu, K. (1985). Random creep and shrinkage in structures: sampling. *Journal of Structural Engineering*, 111(5):1113–1134. [38](#)
- [29] Bazant, Z. and Novak, D. (2000). Probabilistic nonlocal theory for quasibrittle fracture initiation and size effect- II: Application. *Journal of Engineering Mechanics*, 126(2):175–185. [25](#)
- [30] Bažant, Z. P. (1999). Size effect on structural strength: a review. *Archive of Applied Mechanics*, 69(9):703–725. [10](#)
- [31] Bazant, Z. P., Belytschko, T. B., and Chang, T.-P. (1984). Continuum theory for strain-softening. *Journal of Engineering Mechanics*, 110(12):1666–1692. [163](#), [206](#)
- [32] Bažant, Z. P., Tabbara, M. R., Kazemi, M. T., and Pijaudier-Cabot, G. (1990). Random particle model for fracture of aggregate or fiber composites. *Journal of engineering mechanics*. [11](#)
- [33] Behnia, M., Goshtasbi, K., Fatehi Marji, M., and Golshani, A. (2012). On the crack propagation modeling of hydraulic fracturing by a hybridized displacement

- discontinuity/boundary collocation method. *Journal of Mining and Environment*, 2(1):1–16. [114](#)
- [34] Behnia, M., Goshtasbi, K., Marji, M. F., and Golshani, A. (2015). Numerical simulation of interaction between hydraulic and natural fractures in discontinuous media. *Acta Geotechnica*, 10(4):533–546. [95](#)
- [35] Belytschko, T. and Black, T. (1999). Elastic crack growth in finite elements with minimal remeshing. *International Journal for Numerical Methods in Engineering*, 45(5):601–620. [96](#), [151](#), [208](#)
- [36] Besterfield, G., Liu, W., Lawrence, M., and Belytschko, T. (1990). Brittle-fracture reliability by probabilistic finite-elements. *Journal of Engineering Mechanics-ASCE*, 116(3):642–659. [38](#)
- [37] Biner, S. (1995). Fem analysis of crack growth in microcracking brittle solids. *Engineering Fracture Mechanics*, 51(4):555–573. [79](#)
- [38] Biner, S. and Morris, J. (2002). A two-dimensional discrete dislocation simulation of the effect of grain size on strengthening behaviour. *Modelling and Simulation in Materials Science and Engineering*, 10(6):617–635. [11](#), [77](#)
- [39] Blal, N., Daridon, L., Monerie, Y., and Pagano, S. (2012). Artificial compliance inherent to the intrinsic cohesive zone models: criteria and application to planar meshes. *International Journal of Fracture*, 178(1):71–83. [151](#)
- [40] Bourdin, B., Larsen, C. J., and Richardson, C. L. (2011). A time-discrete model for dynamic fracture based on crack regularization. *International Journal of Fracture*, 168(2):133 – 143. [149](#)
- [41] Brencich, A. and Carpinteri, A. (2000). Heuristic approach to microcracking and fracture for ceramics with statistical consideration. *Theoretical and Applied Fracture Mechanics*, 33(2):135–143. [79](#)

- [42] Bungler, A. P. and Detournay, E. (2005). Asymptotic solution for a penny-shaped near-surface hydraulic fracture. *Engineering Fracture Mechanics*, 72(16):2468–2486. [107](#)
- [43] Camacho, G. T. and Ortiz, M. (1996). Computational modelling of impact damage in brittle materials. *International Journal of Solids and Structures*, 33:2899–2938. [111](#), [113](#), [150](#), [151](#), [167](#), [206](#)
- [44] Cannillo, V. and Carter, W. (2005). A stochastic model of damage accumulation in complex microstructures. *Journal of Materials Science*, 40(15):3993–4004. [77](#)
- [45] Carmeliet, J. and Hens, H. (1994). Probabilistic nonlocal damage model for continua with random field properties. *Journal of Engineering Mechanics*, 120(10):2013–2027. [25](#), [50](#), [79](#), [221](#)
- [46] Cazes, F. and Moës, N. (2015). Comparison of a phase-field model and of a thick level set model for brittle and quasi-brittle fracture. *International Journal for Numerical Methods in Engineering*, 103(2):114–143. nme.4886. [149](#)
- [47] Charalambides, P. and McMeeking, R. (1987). Finite element method simulation of crack propagation in a brittle microcracking solid. *Mechanics of Materials*, 6(1):71–87. [79](#)
- [48] Chen, C., Cui, J., Duan, H., Feng, X., He, L., Hu, G., Huang, M., Huo, Y., Ji, B., Liu, B., Peng, X., Shi, H., Sun, Q., Wang, J., Wang, Y., Zhao, H., Zhao, Y., Zheng, Q., and Zou, W. (2011). Perspectives in mechanics of heterogeneous solids. *Acta Mechanica Sinica*, 24(1):1 – 26. [14](#)
- [49] Chen, Y., Hu, S., Zhou, C., and Jing, L. (2014). Micromechanical modeling of anisotropic damage-induced permeability variation in crystalline rocks. *Rock Mechanics and Rock Engineering*, 47(5):1775–1791. [95](#)
- [50] Chernov, L. and Silverman, R. (1960). *Wave Propagation in a Random Medium*. Dover Books on Physics. Dover Publications. [7](#), [76](#)
- [51] Chudnovsky, A. and Wu, S. (1991). Elastic interaction of a crack with a random array of microcracks. *International Journal of Fracture*, 49(2):123–140. [79](#)

- [52] Clarke, P. and Abedi, R. (2018). Modeling the connectivity of propagating cracks with in-situ cracks in rock. *International Journal for Numerical and Analytical Methods in Geomechanics*. Under review. [93](#)
- [53] Clarke, P. and Abedi, R. (June 25-28, 2017). Fracture modeling of rocks based on random field generation and simulation of inhomogeneous domains. In *Proceeding: 51th US Rock Mechanics/Geomechanics Symposium*, pages ARMA 17-0643 (11 pages), San Francisco, California, USA. [34](#), [48](#), [221](#), [223](#), [224](#), [225](#)
- [54] Clarke, P., Abedi, R., Bahmani, B., Acton, K., and Baxter, S. (November 3-9, 2017). Effect of the spatial inhomogeneity of fracture strength on fracture pattern for quasi-brittle materials. In *Proceedings of ASME 2017 International Mechanical Engineering Congress & Exposition IMECE 2017*, pages IMECE2017-71515, 11 pages, Tampa, Florida, USA. accepted. [201](#), [204](#), [220](#)
- [55] Clarke, P., Omid, O., and Abedi, R. (2016). Modeling crack connectivity of induced fractures in a naturally fractured formation. *Proceeding: 50th US Rock Mechanics/Geomechanics Symposium, June 26-June 29, Houston, Texas - USA*, pages ARMA 16-0532 (13 pages). [107](#)
- [56] Clayton, J. (2005). Dynamic plasticity and fracture in high density polycrystals: Constitutive modeling and numerical simulation. *Journal of the Mechanics and Physics of Solids*, 53(2):261–301. [77](#)
- [57] Corigliano, A. and Ricci, M. (2001). Rate-dependent interface models: formulation and numerical applications. *International Journal of Solids and Structures*, 38:547–576. [163](#), [206](#)
- [58] Cosmi, F. (2004). Two-dimension estimate of effective properties of solid with random voids. *Theoretical and Applied Fracture Mechanics*, 42(2):183–189. [77](#)
- [59] Cox, S. and Paterson, L. (1989). Tensile fracture of heterogeneous solids with distributed breaking strengths. *Physical Review B (Condensed Matter)*, 40(7A):4690–4695. [79](#), [221](#)

- [60] Curtin, W. (1997). Toughening in disordered brittle materials. *Physical Review B-Condensed Matter*, 55(17):11270–11276. [79](#), [221](#)
- [61] Daphalapurkar, N., Ramesh, K., Graham-Brady, L., and Molinari, J. (2011). Predicting variability in the dynamic failure strength of brittle materials considering pre-existing flaws. *Journal of the Mechanics and Physics of Solids*, 59(2):297–319. [11](#), [50](#), [77](#), [79](#), [80](#)
- [62] de Borst, R., Gutierrez, M., Wells, G., Remmers, J., and Askes, H. (2004). Cohesive-zone models, higher-order continuum theories and reliability methods for computational failure analysis. *International Journal for Numerical Methods in Engineering*, 60(1):289–315. [38](#)
- [63] Dershowitz, W. S. and Fidelibus, C. (1999). Derivation of equivalent pipe network analogues for three-dimensional discrete fracture networks by the boundary element method. *Water Resources Research*, 35(9):2685–91. [96](#), [97](#)
- [64] Desroches, J., Detournay, E., Lenoach, B., Papanastasiou, P., Pearson, J., Thiercelin, M., and Cheng, A. (1994). The crack tip region in hydraulic fracturing. *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 447(1929):39–48. [107](#)
- [65] Destrade, M. and Saccomandi, G. (2012). *Continuum Mechanics*, volume II. EOLSS Publishers, Oxford, UK. [xiv](#), [87](#), [90](#), [91](#)
- [66] Detournay, E. (2004). Propagation regimes of fluid-driven fractures in impermeable rocks. *International Journal of Geomechanics*, 4(1):35–45. [107](#)
- [67] Dimas, L., Giesa, T., and Buehler, M. (2014). Coupled continuum and discrete analysis of random heterogeneous materials: Elasticity and fracture. *Journal of the Mechanics and Physics of Solids*, 63(1):481–490. [xii](#), [41](#), [42](#), [79](#), [81](#), [221](#)
- [68] Dolbow, J., Moës, N., and Belytschko, T. (2000). Discontinuous enrichment in finite elements with a partition of unity method. *Finite Elements in Analysis and Design*, 36(3-4):235–260. [96](#), [151](#)

- [69] Doltsinis, I. and Dattke, R. (2005). Numerical experiments on the rupture of brittle solids - variation of microstructure, loading and dimensions. *International Journal of Solids and Structures*, 42(2):565–579. [77](#)
- [70] Dong, C. and de Pater, C. (2001). Numerical implementation of displacement discontinuity method and its application in hydraulic fracturing. *Computer Methods in Applied Mechanics and Engineering*, 191(8):745–760. [xv](#), [83](#), [95](#), [114](#), [115](#)
- [71] Doostan, A., Ghanem, R., and Red-Horse, J. (2007). Stochastic model reduction for chaos representations. *Computer Methods in Applied Mechanics and Engineering*, 196(37-40):3951–3966. [39](#)
- [72] Du, X. and Ostoja-Starzewski, M. (2006). On the scaling from statistical to representative volume element in thermoelasticity of random materials. *Networks and Heterogenous Media*, 1(2):259 – 274. [50](#), [52](#)
- [73] Duarte, C. A., Babuška, I., and Oden, J. T. (2000). Generalized finite element methods for three-dimensional structural mechanics problems. *Computers & Structures*, 77(2):215–232. [97](#), [151](#)
- [74] Dugdale, D. S. (1960). Yielding of steel sheets containing slits. *Journal of the Mechanics and Physics of Solids*, 8:100–104. [150](#)
- [75] Espinosa, H. and Zavattieri, P. (2000). In *Modeling of ceramic microstructures: dynamic damage initiation and evolution*, number 505, pages 333–338, AIP Conference Proceedings. [77](#)
- [76] Espinosa, H. and Zavattieri, P. (2003). A grain level model for the study of failure initiation and evolution in polycrystalline brittle materials. Part II: Numerical examples. *Mechanics of Materials*, 35(3-6):365–394. [11](#), [12](#), [77](#), [78](#)
- [77] Evangelatos, G. I. and Spanos, P. D. (2012). A collocation approach for spatial discretization of stochastic peridynamic modeling of fracture. *Journal of Mechanics of Materials and Structures*, 6(7-8):1171 – 1195. [148](#)

- [78] Evans, A. and Faber, K. (1984). Crack-growth resistance of microcracking brittle materials. *Journal of the American Ceramic Society*, 67(4):255–260. [79](#)
- [79] Fedorov, F. (1968). *Theory of elastic waves in crystals*. Springer Science+Business Media, New York. [87](#)
- [80] Genet, M., Couegnat, G., Tomsia, A., and Ritchie, R. (2014). Scaling strength distributions in quasi-brittle materials from micro- to macro-scales: A computational approach to modeling nature-inspired structural ceramics. *Journal of the Mechanics and Physics of Solids*, 68(1):93–106. [xi](#), [10](#), [11](#), [25](#), [30](#), [197](#), [221](#)
- [81] Ghaffari, H., Nasser, M., and Young, R. (2012). Fluid flow complexity in fracture networks: analysis with graph theory and LBM. Cornell University Library. [96](#), [97](#)
- [82] Ghanem, R. and Spanos, P. (1991). *Stochastic finite elements: a spectral approach*. Springer-Verlag. [xii](#), [31](#), [39](#), [40](#), [41](#), [43](#), [54](#), [224](#), [229](#)
- [83] Ghoniem, N. M., Busso, E. P., Kioussis, N., and Huang, H. (2003). Multiscale modelling of nanomechanics and micromechanics: an overview. *Philosophical Magazine*, 83(31-34):3475–3528. [14](#)
- [84] Gogotsi, G., Lugovoi, N., and Slyunyaev, V. (2002). Statistical evaluation of microcracking of inelastic ceramics. *Strength of Materials*, 34(4):349–358. [77](#)
- [85] Gogotsi, G. and Lugovy, M. (2001). Local stochastic analysis of microcracking and non-elastic behavior of ceramics. *Theoretical and Applied Fracture Mechanics*, 36(2):115–123. [77](#)
- [86] Gordeliy, E. and Peirce, A. (2013). Coupling schemes for modeling hydraulic fracture propagation using the {XFEM}. *Computer Methods in Applied Mechanics and Engineering*, 253(0):305–322. [107](#)
- [87] Grady, D. and Kipp, M. (1980). Continuum modeling of explosive fracture in oil shale. *International Journal of Rock Mechanics and Mining Sciences & Geomechanics Abstracts*, 17(3):147–157. [179](#)

- [88] Graham, L. and Baxter, S. (2001). Simulation of local material properties based on moving-window GMC. *Probabilistic Engineering Mechanics*, 16(4):295–305. [14](#), [26](#)
- [89] Graham, L., Gurley, K., and Masters, F. (2003). Non-gaussian simulation of local material properties based on a moving-window technique. *Probabilistic Engineering Mechanics*, 18(3):223–234. Random fields;. [12](#)
- [90] Graham-Brady, L. (2010). Statistical characterization of meso-scale uniaxial compressive strength in brittle materials with randomly occurring flaws. *International Journal of Solids and Structures*, 47(18-19):2398–2413. [74](#)
- [91] Graham-Brady, L., Siragy, E., and Baxter, S. (2003). Analysis of heterogeneous composites based on moving-window techniques. *Journal of engineering mechanics*, 129(9):1054–1064. [26](#)
- [92] Grasselli, G., Lisjak, A., Mahabadi, O. K., and Tatone, B. S. (2015). Influence of pre-existing discontinuities and bedding planes on hydraulic fracturing initiation. *European Journal of Environmental and Civil Engineering*, 19(5):580–597. [95](#), [96](#)
- [93] Grogan, D., Brdaigh, C., and Leen, S. (2015). A combined XFEM and cohesive zone model for composite laminate microcracking and permeability. *Composite Structures*, 120:246–261. [79](#)
- [94] Gupta, P. and Duarte, C. (2014). Simulation of non-planar three-dimensional hydraulic fracture propagation. *International Journal for Numerical and Analytical Methods in Geomechanics*, 38(13):1397–1430. [97](#), [107](#), [114](#)
- [95] Gupta, P. and Duarte, C. A. (2016). Coupled formulation and algorithms for the simulation of non-planar three-dimensional hydraulic fractures using the generalized finite element method. *International Journal for Numerical and Analytical Methods in Geomechanics*, 40(10):1402–1437. [145](#)
- [96] Gutierrez, M. (2006a). The random dimension in computational failure mechanics. *Probabilistic Engineering Mechanics*, 21(3):257–266. [38](#)

- [97] Gutierrez, M. (2006b). Size sensitivity for the reliability index in stochastic finite element analysis of damage. *International Journal of Fracture*, 137(1-4):109–120. [25](#)
- [98] Gutierrez, M. and de Borst, R. (1999). Deterministic and stochastic analysis of size effects and damage evolution in quasi-brittle materials. *Archive of Applied Mechanics*, 69(9-10):655–676. [79](#)
- [99] Gutierrez, M. and de Borst, R. (2000). Stochastic aspects of localised failure: material and boundary imperfections. *International Journal of Solids and Structures*, 37(48-50):7145–7159. [38](#)
- [100] Hamidi, F. and Mortazavi, A. (2014). A new three dimensional approach to numerically model hydraulic fracturing process. *Journal of Petroleum Science and Engineering*, 124:451–467. [96](#)
- [101] Hanson, J., Schmidt, R., Cooley, C., Schatz, J., et al. (1984). Multiple fracture stimulation using controlled pulse pressurization. In *SPE Unconventional Gas Recovery Symposium*. Society of Petroleum Engineers. [70](#), [112](#)
- [102] Hassold, G. and Srolovitz, D. (1989). Brittle fracture in materials with random defects. *Physical Review B (Condensed Matter)*, 39(13):9273–9281. [221](#)
- [103] Heap, M., Xu, T., and Chen, C. (2014). The influence of porosity and vesicle size on the brittle strength of volcanic rocks and magma. *Bulletin of Volcanology*, 76(9):1–15. [77](#)
- [104] Hfner, S., Eckardt, S., Luther, T., and Knke, C. (2006). Mesoscale modeling of concrete: Geometry and numerics. *Computers & Structures*, 84(7):450 – 461. [11](#)
- [105] Hill, R. (1963). Elastic properties of reinforced solids – some theoretical principles. *Journal of Mechanics and Physics of Solids*, 11(5):357–372. [13](#)
- [106] Hoek, E. and Brown, T. (1980). *Underground Excavations in Rock*. Geotechnics and foundations. Taylor & Francis. [211](#)
- [107] Homand-Etienne, F., Hoxha, D., and Shao, J. (1998). A continuum damage constitutive law for brittle rocks. *Computers and Geotechnics*, 22(2):135–151. [50](#), [200](#)

- [108] Huq, F., Brannon, R., and Graham-Brady, L. (2016). An efficient binning scheme with application to statistical crack mechanics. *International Journal for Numerical Methods in Engineering*, 105(1):33–62. [74](#), [218](#)
- [109] Hutchinson, J. (1987). Crack tip shielding by micro-cracking in brittle solids. *Acta Metallurgica*, 35(7):1605–1619. [79](#)
- [110] Huyse, L. and Maes, M. (2001). Random field modeling of elastic properties using homogenization. *Journal of Engineering Mechanics*, 127(1):27–36. [13](#)
- [111] Ibrahimbegovic, A. and Delaplace, A. (2003). Microscale and mesoscale discrete models for dynamic fracture of structures built of brittle material. *Computers & Structures*, 81(12):1255–65. [148](#)
- [112] Iman, R. and Conover, W. (1980). Small sample sensitivity analysis techniques for computer models, with an application to risk assessment. *Communications in Statistics - Theory and Methods*, A9(17):1749–1842. [38](#)
- [113] Izadi, G. and Elsworth, D. (2014). Reservoir stimulation and induced seismicity: Roles of fluid pressure and thermal transients on reactivated fractured networks. *Geothermics*, 51:368–379. [95](#)
- [114] Jaeken, J. and Cottenier, S. (2016). Solving the christoffel equation: Phase and group velocities. *Computer Physics Communications*, 207:445 – 451. [87](#), [88](#)
- [115] Kachanov, M., Montagut, E., and Laures, J. (1990). Mechanics of crack-microcrack interactions. *Mechanics of Materials*, 10(1-2):59–71. [79](#)
- [116] Kaminski, M. and Kleiber, M. (2000a). Numerical homogenization of n-component composites including stochastic interface defects. *International Journal for Numerical Methods in Engineering*, 47(5):1001–1027. [77](#)
- [117] Kaminski, M. and Kleiber, M. (2000b). Perturbation based stochastic finite element method for homogenization of two-phase elastic composites. *Computers & Structures*, 78(6):811 – 826. [38](#)

- [118] Karnopp, D. (1985). Computer simulation of stick-slip friction in mechanical dynamic systems. *Journal of Dynamic Systems, Measurement and Control, Transactions of the ASME*, 107(1):100 – 103. [165](#)
- [119] Khoei, A. R., Hirmand, M., Vahab, M., and Bazargan, M. (2015). An enriched FEM technique for modeling hydraulically driven cohesive fracture propagation in impermeable media with frictional natural faults: Numerical and experimental investigations. *International Journal for Numerical Methods in Engineering*, 104(6):439–468. [95](#)
- [120] Khoei, A. R., Vahab, M., and Hirmand, M. (2016). Modeling the interaction between fluid-driven fracture and natural fault using an enriched-FEM technique. *International Journal of Fracture*, 197(1):1–24. [95](#)
- [121] Khoroshun, L. and Shikula, E. (1997). Effect of the strength scatter of the components on the deformation of a particulate composite with microcracks. *International Applied Mechanics*, 33(8):626–631. [79](#)
- [122] Koyama, T. and Jing, L. (2007). Effects of model scale and particle size on micro-mechanical properties and failure processes of rocks—a particle mechanics approach. *Engineering Analysis with Boundary Elements*, 31(5):458 – 472. [50](#), [149](#), [201](#)
- [123] Kozicki, J. and Tejchman, J. (2007). Effect of aggregate structure on fracture process in concrete using 2D lattice model. *Archives of Mechanics*, 59(4-5):365–84. [xi](#), [8](#), [10](#)
- [124] Kraft, R. and Molinari, J. (2008). A statistical investigation of the effects of grain boundary properties on transgranular fracture. *Acta Materialia*, 56(17):4739–4749. [77](#)
- [125] Laalai, I. and Sab, K. (1996). A stochastic nonlocal damage model. *International Journal of Fracture*, 76(2):121–140. [79](#)
- [126] Lane, C. (2014). *The development of a 2D ultrasonic array inspection for single crystal turbine blades*. Cham: Springer. [87](#)
- [127] Lee, Y.-K. and Pietruszczak, S. (2008). Application of critical plane approach to the prediction of strength anisotropy in transversely isotropic rock masses. *International Journal of Rock Mechanics and Mining Sciences*, 45(4):513–23. [211](#)

- [128] Levy, S. and Molinari, J. (2010). Dynamic fragmentation of ceramics, signature of defects and scaling of fragment sizes. *Journal of the Mechanics and Physics of Solids*, 58(1):12–26. [79](#), [221](#)
- [129] Levy, S., Molinari, J., and Radovitzky, R. (2012). Dynamic fragmentation of a brittle plate under biaxial loading: strength or toughness controlled? *International Journal of Fracture*, 174(2):203–15. [153](#)
- [130] Li, H., Bai, Y., Xia, M., Ke, F., and Yin, X. (2000). Damage localization as a possible precursor of earthquake rupture. *pure and applied geophysics*, 157(11):1929–1943. [200](#)
- [131] Li, J. (2000). Debonding of the interface as ‘crack arrestor’. *International Journal of Fracture*, 105(1):57–79. [50](#), [95](#), [148](#), [221](#)
- [132] Li, J. and Yu, J. (2005). Computational simulations of intergranular fracture of polycrystalline materials and size effect. *Engineering Fracture Mechanics*, 72(12):2009–2017. [77](#)
- [133] Li, T., Marigo, J.-J., Guilbaud, D., and Potapov, S. (2016). Gradient damage modeling of brittle fracture in an explicit dynamics context. *International Journal for Numerical Methods in Engineering*, 108(11):1381–1405. nme.5262. [159](#)
- [134] Lin, T., Evans, A., and Ritchie, R. (1987). Stochastic modeling of the independent roles of particle size and grain size in transgranular cleavage fracture. *Metallurgical Transactions A (Physical Metallurgy and Materials Science)*, 18A(4):641–651. [77](#)
- [135] Lisjak, A., Kaifosh, P., He, L., Tatone, B., Mahabadi, O., and Grasselli, G. (2017). A 2D, fully-coupled, hydro-mechanical, FDEM formulation for modelling fracturing processes in discontinuous, porous rock masses. *Computers and Geotechnics*, 81:1–18. [95](#)
- [136] Liu, X., Wang, S., Wang, S., and Wang, E. (2015). Fluid-driven fractures in granular materials. *Bulletin of Engineering Geology and the Environment*, 74(2):621–36. [94](#)

- [137] Loehnert, S. and Belytschko, T. (2007). A multiscale projection method for macro/microcrack simulations. *International Journal for Numerical Methods in Engineering*, 71(12):1–17. [79](#)
- [138] Lu, Y., Elsworth, D., and Wang, L. (2013). Microcrack-based coupled damage and flow modeling of fracturing evolution in permeable brittle rocks. *Computers and Geotechnics*, 49:226–44. [50](#), [200](#)
- [139] Lua, Y., Liu, W., and Belytschko, T. (1992a). A stochastic damage model for the rupture prediction of a multi-phase solid. i. parametric studies. *International Journal of Fracture*, 55(4):321–340. [79](#)
- [140] Lua, Y., Liu, W., and Belytschko, T. (1992b). A stochastic damage model for the rupture prediction of a multi-phase solid. ii. statistical approach. *International Journal of Fracture*, 55(4):341–361. [79](#)
- [141] Mahabadi, O., Lisjak, A., Munjiza, A., and Grasselli, G. (2012). Y-geo: New combined finite-discrete element numerical code for geomechanical applications. *International Journal of Geomechanics*, 12(6):676–688. [96](#), [200](#)
- [142] Mahabadi, O., Tatone, B., and Grasselli, G. (2014). Influence of microscale heterogeneity and microstructure on the tensile behavior of crystalline rocks. *Journal of Geophysical Research: Solid Earth*, 119(7):5324–5341. [11](#), [77](#), [78](#), [79](#), [200](#)
- [143] Massart, T. and Selvadurai, A. (2014). Computational modelling of crack-induced permeability evolution in granite with dilatant cracks. *International Journal of Rock Mechanics and Mining Sciences*, 70:593–604. [95](#)
- [144] Matthies, H., Brenner, C., Bucher, B., and Soares, C. (1997). Uncertainties in probabilistic numerical analysis of structures and solids-stochastic finite elements. *Structural Safety*, 19(3):283–336. [38](#)
- [145] McWilliams, B., Ramesh, K., and Yen, C. (2013). Probabilistic response of heterogeneous particle reinforced metal matrix composites with particle size dependent strengthening. *Computational Materials Science*, 79:15–24. [77](#)

- [146] Meguid, S. and Czekanski, A. (2008). Advances in computational contact mechanics. *International Journal of Mechanics and Materials in Design*, 4(4):419 – 443. [165](#)
- [147] Mergheim, J., Kuhl, E., and Steinmann, P. (2005). A finite element method for the computational modelling of cohesive cracks. *International Journal for Numerical Methods in Engineering*, 63:276–289. [150](#)
- [148] Miehe, C. and Mauthe, S. (2016). Phase field modeling of fracture in multi-physics problems. Part III. Crack driving forces in hydro-poro-elasticity and hydraulic fracturing of fluid-saturated porous media. *Computer Methods in Applied Mechanics and Engineering*, 304:619–655. [95](#), [96](#)
- [149] Moës, N., Dolbow, J., and Belytschko, T. (1999). A finite element method for crack growth without remeshing. *International Journal for Numerical Methods in Engineering*, 46(1):131–150. [96](#), [151](#), [208](#)
- [150] Mohammadnejad, T. and Andrade, J. (2016). Numerical modeling of hydraulic fracture propagation, closure and reopening using XFEM with application to in-situ stress estimation. *International Journal for Numerical and Analytical Methods in Geomechanics*, 40(15):2033–2060. [112](#)
- [151] Montagut, E. and Kachanov, M. (1988). On modelling a microcracked zone by ‘weakened’ elastic material and on statistical aspects of crack-microcrack interactions. *International Journal of Fracture*, 37(4):55–62. [79](#)
- [152] Mostaghel, N. and Davis, T. (1997). Representations of Coulomb friction for dynamic analysis. *Earthquake Engineering and Structural Dynamics*, 26(5):541 – 548. [165](#)
- [153] Munjiza, A. (2004). *The combined finite-discrete element method*. Wiley. [97](#), [200](#)
- [154] Needleman, A. (1988). Material rate dependence and mesh sensitivity in localization problems. *Computer Methods in Applied Mechanics and Engineering*, 67(1):69 – 85. [163](#), [206](#)

- [155] Nguyen, V. P., Lloberas-Valls, O., Stroeven, M., and Sluys, L. J. (2011). Homogenization-based multiscale crack modelling: From micro-diffusive damage to macro-cracks. *Computer Methods in Applied Mechanics and Engineering*, 200(9):1220–36. [30](#), [58](#), [223](#)
- [156] Olarewaju, J., Ghorri, S., Fuseni, A., Wajid, M., et al. (1997). Stochastic simulation of fracture density for permeability field estimation. In *Middle East Oil Show and Conference*. Society of Petroleum Engineers. [74](#), [218](#)
- [157] Olson, J. E. and Taleghani, A. D. (January 19-21, 2009). Modeling simultaneous growth of multiple hydraulic fractures and their interaction with natural fractures. In *Society of Petroleum Engineers Hydraulic Fracturing Technology*, The Woodlands, Texas, USA. [95](#)
- [158] Omid, O., Abedi, R., and Enayatpour, S. (2015). An adaptive meshing approach to capture hydraulic fracturing. *The 49th US Rock Mechanics/Geomechanics Symposium, June 28-July 1, San Francisco, CA, USA*, (ARMA 15-572). [25](#), [34](#), [60](#), [67](#), [97](#), [110](#), [114](#), [209](#), [232](#)
- [159] Omid, O., Abedi, R., and Enayatpour, S. (June 26-29, 2016). Well stimulation in tight formations: a dynamic approach. In *Proceeding: 50th US Rock Mechanics/Geomechanics Symposium*, pages ARMA 16–0150 (12 pages), Houston, Texas, USA. [70](#), [218](#)
- [160] Ostoj-Starzewski, M. (2002). Microstructural randomness versus representative volume element in thermomechanics. *Journal of Applied Mechanics-Transactions of the ASME*, 69(1):25–35. [12](#), [13](#), [149](#)
- [161] Outters, N. and Shuttle, D. (2000). Sensitivity analysis of a discrete fracture network model for performance assessment of aberg. *Swedish Nuclear Fuel and Waste Management Co.*, 32(17):11–12. [96](#), [97](#)
- [162] Paley, M. and Aboudi, J. (1992). Micromechanical analysis of composites by the generalized method of cells. *Mechanics of Materials*, 14:127 – 139. [14](#)

- [163] Paliwal, B. and Ramesh, K. (2008). An interacting micro-crack damage model for failure of brittle materials under compression. *Journal of the Mechanics and Physics of Solids*, 56(3):896–923. [11](#), [12](#)
- [164] Pandolfi, A. and Ortiz, M. (2002). An efficient adaptive procedure for three-dimensional fragmentation simulations. *Engineering with Computers*, 18:148–159. [150](#), [151](#)
- [165] Parrinello, F., Failla, B., and Borino, G. (2009). Cohesive-frictional interface constitutive model. *International Journal of Solids and Structures*, 46(13):2680–2692. [150](#), [151](#)
- [166] Pelissou, C., Baccou, J., Monerie, Y., and Perales, F. (2009). Determination of the size of the representative volume element for random quasi-brittle composites. *International Journal of Solids and Structures*, 46(1415):2842 – 2855. [50](#)
- [167] Pietruszczak, S., Lydzba, D., and Shao, J. (2002). Modelling of inherent anisotropy in sedimentary rocks. *International Journal of Solids and Structures*, 39(3):637–648. [201](#)
- [168] Pietruszczak, S. and Mroz, Z. (2000). Formulation of anisotropic failure criteria incorporating a microstructure tensor. *Computers and Geotechnics*, 26(2):105–112. [201](#)
- [169] Pietruszczak, S. and Mroz, Z. (2001). On failure criteria for anisotropic cohesive-frictional materials. *International Journal for Numerical and Analytical Methods in Geomechanics*, 25(5):509–524. [211](#)
- [170] Pindera, M.-J., Khatam, H., Drago, A. S., and Bansal, Y. (2009). Micromechanics of spatially uniform heterogeneous media: A critical review and emerging approaches. *Composites Part B: Engineering*, 40(5):349 – 378. [14](#)
- [171] Pramanik, R. and Deb, D. (2014). Implementation of smoothed particle hydrodynamics for detonation of explosive with application to rock fragmentation. *Rock Mechanics and Rock Engineering*, 48(4):1683–1698. [179](#)

- [172] Quinn, D. D. (2004). A new regularization of Coulomb friction. *Journal of Vibration and Acoustics, Transactions of the ASME*, 126(3):391 – 397. [165](#)
- [173] Radovitzky, R., Seagraves, A., Tupek, M., and Noels, L. (2011). A scalable 3D fracture and fragmentation algorithm based on a hybrid, discontinuous Galerkin, cohesive element method. *Computer Methods in Applied Mechanics and Engineering*, 200(1-4):326–344. [151](#), [159](#)
- [174] Rahman, M. M. and Rahman, S. S. (2013). Studies of hydraulic fracture-propagation behavior in presence of natural fractures: Fully coupled fractured-reservoir modeling in poroelastic environments. *International Journal of Geomechanics*, 13(6):809–826. [95](#)
- [175] Rahman, S. and Chakraborty, A. (2011). Stochastic multiscale fracture analysis of three-dimensional functionally graded composites. *Engineering Fracture Mechanics*, 78(1):27–46. [77](#), [80](#)
- [176] Rangarajan, R., Chiaramonte, M. M., Hunsweck, M. J., Shen, Y., and Lew, A. J. (2015). Simulating curvilinear crack propagation in two dimensions with universal meshes. *International Journal for Numerical Methods in Engineering*, 102(3-4):632–70. [82](#), [97](#), [152](#), [208](#)
- [177] Rangarajan, R. and Lew, A. J. (2014). Universal meshes: A method for triangulating planar curved domains immersed in nonconforming meshes. *International Journal for Numerical Methods in Engineering*, 98(4):236–64. [82](#), [97](#), [152](#), [208](#)
- [178] Rao, B. and Rahman, S. (2002). Stochastic meshless analysis of elastic-plastic cracked structures. In *ASME Pressure Vessels and Piping Conference*, volume 438, pages 133–146, Vancouver, BC, Canada. [38](#)
- [179] Rasmussen, C. and Williams, K. (2006). *Gaussian Processes for Machine Learning*. the MIT Press. [39](#)
- [180] Reddy, R. and Rao, B. (2008). Stochastic fracture mechanics by fractal finite element method. *Computer Methods in Applied Mechanics and Engineering*, 198(3-4):459–474. [38](#)

- [181] Remmers, J. J. C., de Borst, R., and Needleman, A. (2003). A cohesive segments method for the simulation of crack growth. *Computational Mechanics*, 31:69–77. [151](#)
- [182] Rinaldi, A. and Mastilovic, S. (2014). The krajcinovic approach to model size dependent fracture in quasi-brittle solids. *Mechanics of Materials*, 71:21–33. [8](#)
- [183] Sakata, S., Ashida, F., and Enya, K. (2012). A microscopic failure probability analysis of a unidirectional fiber reinforced composite material via a multiscale stochastic stress analysis for a microscopic random variation of an elastic property. *Computational Materials Science*, 62:35–46. [38](#), [149](#)
- [184] Sakata, S., Ashida, F., and Ohsumimoto, K. (2013). Stochastic homogenization analysis of a porous material with the perturbation method considering a microscopic geometrical random variation. *International Journal of Mechanical Sciences*, 77:145–154. [38](#)
- [185] Sakata, S., Ashida, F., and Zako, M. (2008). Kriging-based approximate stochastic homogenization analysis for composite materials. *Computer Methods in Applied Mechanics and Engineering*, 197(21-24):1953–1964. [38](#)
- [186] Salmi, M., Auslender, F., Bornert, M., and Fogli, M. (2012). Apparent and effective mechanical properties of linear matrix-inclusion random composites: Improved bounds for the effective behavior. *International Journal of Solids and Structures*, 49(10):1195–1211. [26](#)
- [187] Schicker, J. and Pfuff, M. (2006). Statistical modelling of fracture in quasi-brittle materials. *Advanced Engineering Materials*, 8(5):406–410. [79](#)
- [188] Schlangen, E. and Garboczi, E. (1997a). Fracture simulations of concrete using lattice models: Computational aspects. *Engineering Fracture Mechanics*, 57(23):319–332. [50](#), [200](#)
- [189] Schlangen, E. and Garboczi, E. (1997b). Fracture simulations of concrete using lattice models: computational aspects. *Engineering Fracture Mechanics*, 57(2-3):319–332. [148](#), [221](#)

- [190] Segurado, J. and LLorca, J. (2006). Computational micromechanics of composites: The effect of particle spatial distribution. *Mechanics of Materials*, 38(8-10):873–883. [11](#), [13](#), [50](#), [221](#)
- [191] Sfantos, G. and Aliabadi, M. (2007). A boundary cohesive grain element formulation for modelling intergranular microfracture in polycrystalline brittle materials. *International Journal for Numerical Methods in Engineering*, 69(8):1590–1626. [11](#), [77](#), [80](#)
- [192] Shang, S. and Yun, G. J. (2013). Stochastic finite element with material uncertainties: Implementation in a general purpose simulation program. *Finite Elements in Analysis and Design*, 64:65 – 78. [51](#)
- [193] Shanmugam, V., Penmetsa, R., Tuegel, E., and Clay, S. (2013). Stochastic modeling of delamination growth in unidirectional composite DCB specimens using cohesive zone models. *Composite Structures*, 102:38–60. [79](#), [221](#)
- [194] Shao, J. and Rudnicki, J. (2000). A microcrack-based continuous damage model for brittle geomaterials. *Mechanics of Materials*, 32(10):607 – 619. [50](#), [149](#), [200](#)
- [195] Sharon, E. and Fineberg, J. (1996). Microbranching instability and the dynamic fracture of brittle materials. *Physical Review B*, 54(10):7128–7139. [79](#)
- [196] Sharon, E. and Fineberg, J. (1999). Confirming the continuum theory of dynamic brittle fracture for fast cracks. *Nature*, 397(6717):333–335. [79](#)
- [197] Shi, F., Wang, X., Liu, C., Liu, H., and Wu, H. (2017). An XFEM-based method with reduction technique for modeling hydraulic fracture propagation in formations containing frictional natural fractures. *Engineering Fracture Mechanics*, 173:64–90. [95](#), [96](#)
- [198] Shi, X., Yang, X., Meng, Y., and Li, G. (2016). An anisotropic strength model for layered rocks considering planes of weakness. *Rock Mechanics and Rock Engineering*, 49(9):3783–92. [201](#)
- [199] Simpson, G., Guèguen, Y., and Schneider, F. (2001). Permeability enhancement due to microcrack dilatancy in the damage regime. *Journal of Geophysical Research: Solid Earth*, 106(B3):3999–4016. [95](#)

- [200] Sobczyk, K. (2008). Morphological complexity of material microstructures: From stochastic models to fracture estimation. *Probabilistic Engineering Mechanics*, 23(4):444–455. [25](#), [50](#), [77](#), [221](#)
- [201] Spring, D. W., Leon, S. E., and Paulino, G. H. (2014). Unstructured polygonal meshes with adaptive refinement for the numerical simulation of dynamic cohesive fracture. *International Journal of Fracture*, 189(1):33 – 57. Adaptive refinement;Cohesive model;Cohesive zone element;Dynamic fractures;Polygonal meshes;. [152](#)
- [202] Srivastava, A., Ponson, L., Osovski, S., Bouchaud, E., Tvergaard, V., and Needleman, A. (2014). Effect of inclusion density on ductile fracture toughness and roughness. *Journal of the Mechanics and Physics of Solids*, 63:62–79. [77](#)
- [203] Strouboulis, T., Babuška, I., and Copps, K. (2000). The design and analysis of the generalized finite element method. *Computer Methods in Applied Mechanics and Engineering*, 181:43–69. [97](#), [151](#)
- [204] Strouboulis, T., Copps, K., and Babuka, I. (2001). The generalized finite element method. *Computer Methods in Applied Mechanics and Engineering*, 190(3233):4081–4193. [97](#), [151](#), [208](#)
- [205] Taleghani, A. D. and Olson, J. E. (2011). Numerical modeling of multistranded-hydraulic-fracture propagation: Accounting for the interaction between induced and natural fractures. *Society of Petroleum Engineers*, 16(3):575–581. [95](#)
- [206] Tamuzs, V. and Petrova, V. (1999). Modified model of macro-microcrack interaction. *Theoretical and Applied Fracture Mechanics*, 32(2):111–117. [79](#)
- [207] Tandon, S. and Faber, K. T. (1993). *Cements Research Progress*, chapter Fracture of Brittle and Quasi-Brittle Engineering Materials, pages 209–239. American Ceramic Society, Columbus, OH. [7](#)
- [208] Taylor, L. M., Chen, E.-P., and Kuszmaul, J. S. (1986). Microcrack-induced damage accumulation in brittle rock under dynamic loading. *Computer Methods in Applied Mechanics and Engineering*, 55(3):301 – 320. [50](#), [200](#)

- [209] Tomar, V. and Zhou, M. (2005). Stochastic analyses of dynamic fracture in composite ceramic microstructures. volume 6, pages 4556–61, Turin, Italy. [77](#)
- [210] Tregger, N., Corr, D., Graham-Brady, L., and Shah, S. (2006). Modeling the effect of mesoscale randomness on concrete fracture. *Probabilistic Engineering Mechanics*, 21(3):217–225. [13](#), [50](#), [221](#)
- [211] Tvergaard, V. and Hutchinson, J. W. (1992). The relation between crack growth resistance and fracture process parameters in elastic-plastic solids. *Journal of the Mechanics and Physics of Solids*, 40:1377–1397. [111](#)
- [212] Valentini, L., Perugini, D., and Poli, G. (2007). The 'small-world' topology of rock fracture networks. *Physica A: Statistical Mechanics and its Applications*, 377(1):323–28. [96](#)
- [213] Versino, D., Mourad, H. M., Davila, C. G., and Addessio, F. L. (2015). A thermodynamically consistent discontinuous galerkin formulation for interface separation. *Composite Structures*, 133:595–606. [150](#), [151](#)
- [214] Wang, Z., Kwan, A., and Chan, H. (1999). Mesoscopic study of concrete i: generation of random aggregate structure and finite element mesh. *Computers & Structures*, 70(5):533 – 544. [11](#)
- [215] Weibull, W. (1939). A statistical theory of the strength of materials. *R. Swed. Inst. Eng. Res.*, page Res. 151. [10](#), [50](#), [62](#), [149](#), [169](#), [201](#), [210](#), [221](#), [225](#)
- [216] Weibull, W. (1951). A statistical distribution function of wide applicability. *Journal of Applied Mechanics*, 18:293–297. [10](#), [50](#), [62](#), [149](#), [169](#), [201](#), [210](#), [225](#)
- [217] Weijers, L. (1995). *The near-wellbore geometry of hydraulic fractures initiated from horizontal and deviated wells*. PhD thesis, TU Delft, Delft University of Technology. [114](#)
- [218] Wittmann, F., Roelfstra, P., and Sadouki, H. (1985). Simulation and analysis of composite structures. *Materials Science and Engineering*, 68(2):239 – 248. [11](#)

- [219] Wriggers, P. and Moftah, S. (2006). Mesoscale models for concrete: Homogenisation and damage behaviour. *Finite Elements in Analysis and Design*, 42(7):623–636. [11](#), [77](#), [221](#)
- [220] Xu, X. and Graham-Brady, L. (2005). A stochastic computational method for evaluation of global and local behavior of random elastic media. *Computer Methods in Applied Mechanics and Engineering*, 194(4244):4362 – 4385. [xii](#), [39](#), [40](#), [42](#), [43](#), [51](#)
- [221] Xu, X. P. and Needleman, A. (1994). Numerical simulations of fast crack growth in brittle solids. *Journal of the Mechanics and Physics of Solids*, 42:1397–1434. [111](#), [150](#), [151](#)
- [222] Xu, Z., Ma, G., and Li, S. (2014). A graph-theoretic pipe network method for water flow simulation in a porous medium: GPNM. *International Journal of Heat and Fluid Flow*, 45:81–97. [95](#), [96](#)
- [223] Yan, C., Zheng, H., Sun, G., and Ge, X. (2016). Combined finite-discrete element method for simulation of hydraulic fracturing. *Rock Mechanics and Rock Engineering*, 49(4):1389–1410. [95](#), [96](#)
- [224] Yin, X., Chen, W., To, A., McVeigh, C., and Liu, W. (2008). Statistical volume element method for predicting microstructure-constitutive property relations. *Computer Methods in Applied Mechanics and Engineering*, 197(43-44):3516–3529. [49](#)
- [225] Zavattieri, P. and Espinosa, H. (2001). Grain level analysis of crack initiation and propagation in brittle materials. *Acta Materialia*, 49(20):4291–4311. [11](#), [77](#)
- [226] Zavattieri, P. and Espinosa, H. (2003). An examination of the competition between bulk behavior and interfacial behavior of ceramics subjected to dynamic pressure-shear loading. *Journal of the Mechanics and Physics of Solids*, 51(4):607–35. [77](#)
- [227] Zazovsky, A. et al. (2004). Propellant fracturing revisited. In *Gulf Rocks 2004, the 6th North America Rock Mechanics Symposium (NARMS)*. American Rock Mechanics Association. [112](#)

- [228] Zhang, Q.-H. and Yin, J.-M. (2014). Solution of two key issues in arbitrary three-dimensional discrete fracture network flow models. *Journal of Hydrology*, 514:281–96. [95](#)
- [229] Zhang, X. and Jeffrey, R. G. (2008). Reinitiation or termination of fluid-driven fractures at frictional bedding interfaces. *Journal of Geophysical Research: Solid Earth*, 113(B8). [95](#)
- [230] Zhang, X., Jeffrey, R. G., and Thiercelin, M. (2007). Deflection and propagation of fluid-driven fractures at frictional bedding interfaces: A numerical investigation. *Journal of Structural Geology*, 29(3):396–410. [95](#)
- [231] Zhang, Z., Peng, S., Ghassemi, A., and Ge, X. (2015). Lattice bond cell modeling of dynamic hydraulic fracture. In *The 49th US Rock Mechanics/Geomechanics Symposium, June 28-July 1, San Francisco, CA, USA*, number ARMA 15-258. [112](#), [179](#)
- [232] Zhou, C., Li, K., and Pang, X. (2011). Effect of crack density and connectivity on the permeability of microcracked solids. *Mechanics of Materials*, 43(12):969–978. [12](#), [95](#), [96](#)
- [233] Zhou, F. and Molinari, J. (2004a). Dynamic crack propagation with cohesive elements: A methodology to address mesh dependency. *International Journal for Numerical Methods in Engineering*, 59(1):1–24. [79](#)
- [234] Zhou, F. and Molinari, J. (2004b). Stochastic fracture of ceramics under dynamic tensile loading. *International Journal of Solids and Structures*, 41(22-23):6573–6596. [77](#), [79](#)
- [235] Zhou, F., Molinari, J., and Ramesh, K. (2005). A cohesive model based fragmentation analysis: Effects of strain rate and initial defects distribution. *International Journal of Solids and Structures*, 42(18-19):5181–5207. [77](#), [79](#)

Vita

A native of the commonwealth of the Bahamas, Philip Clarke came to the United States in 2006 to begin his collegiate career. Philip briefly attended Fisk University (Nashville, Tennessee) where he begun pursuing a B.S. in Physics; however, he ultimately graduated from Florida International University in 2011 with a B.S. in Mechanical Engineering. Since 2012, Philip has attended graduate school at the University of Tennessee Knoxville/Space Institute, pursuing a Ph.D. in Mechanical Engineering under the pupillage of Dr. Reza Abedi. While at the University of Tennessee, Philip has conducted research with a concentration on Applied Mechanics and Computational Mechanics, even achieving such accolades as the Mechanical, Aerospace and Biomedical Engineering (MABE) department's Outstanding Graduate Student Award in 2017.