Literature Review and History: Damage & Fracture Mechanics

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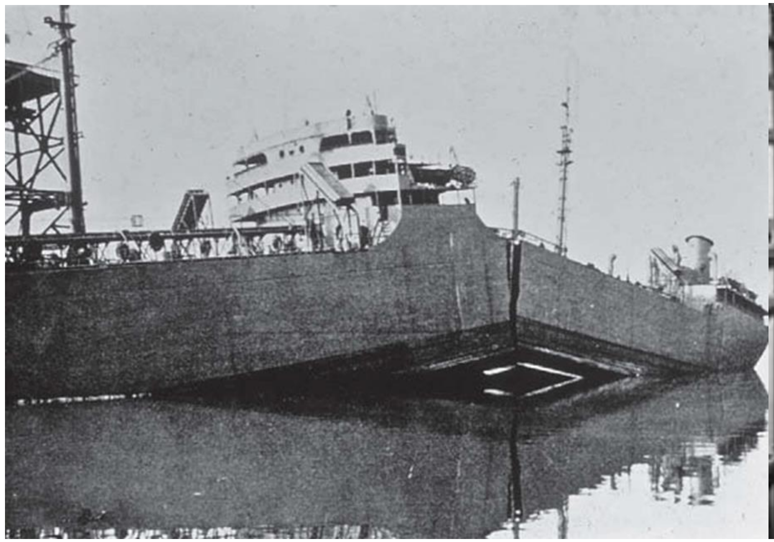
Introduction

- Damage and fracture mechanics build on existing techniques of elasticity to model the loss of load carrying capability and formation of cracks in solid bodies
- Damage is the macroscopic loss of material stiffness due to the net effect of voids and cracks on the small scale (often not observable except in the constitutive response of the material)
- Fracture is the formation of macroscopic (observable) cracks involving complete material separation
- **Goal of this report is to survey history and state-of-the-art of damage/fracture methodologies**
- **Particular attention will be paid to how each method can be used in practice, and the role of data in hypothesizing, calibrating, and testing the damage/fracture theory**

- A metal paper clip repeatedly bent back and forth will accumulate **damage** and eventually break, whereas more brittle materials like concrete tend to form sharp macroscopic **cracks**

Brief Motivation

- A structure is as an assemblage of materials intended to carry loads
- Complex engineering structures are ubiquitous: high-rise buildings, bridges and dams, airplanes, etc.
- To ensure that structures are safe, damage and fracture dominate design considerations
- **Goal of structural design is to build structures which are as cheap, light, and efficient as possible while remaining safe**
- Safe typically means having a (very) high-probability of carrying in-service loads over a specified life-time
- This requires understanding how and why structural materials become damaged, crack, and fail
- When this process is understood, the conditions which lead to unacceptable damage accumulation and crack growth can be systematically avoided with engineering design
- This has proven to be a hard problem!



- Dramatic failures of large engineering structures in mid 20th century motivated increased research in structural design and fracture mechanics
- Liberty ships during WWII cracked fully in half due to a new welding process in the hull, and Comet passenger jets had fuselage failures around square windows
- These phenomena could be explained with new theories of fracture mechanics

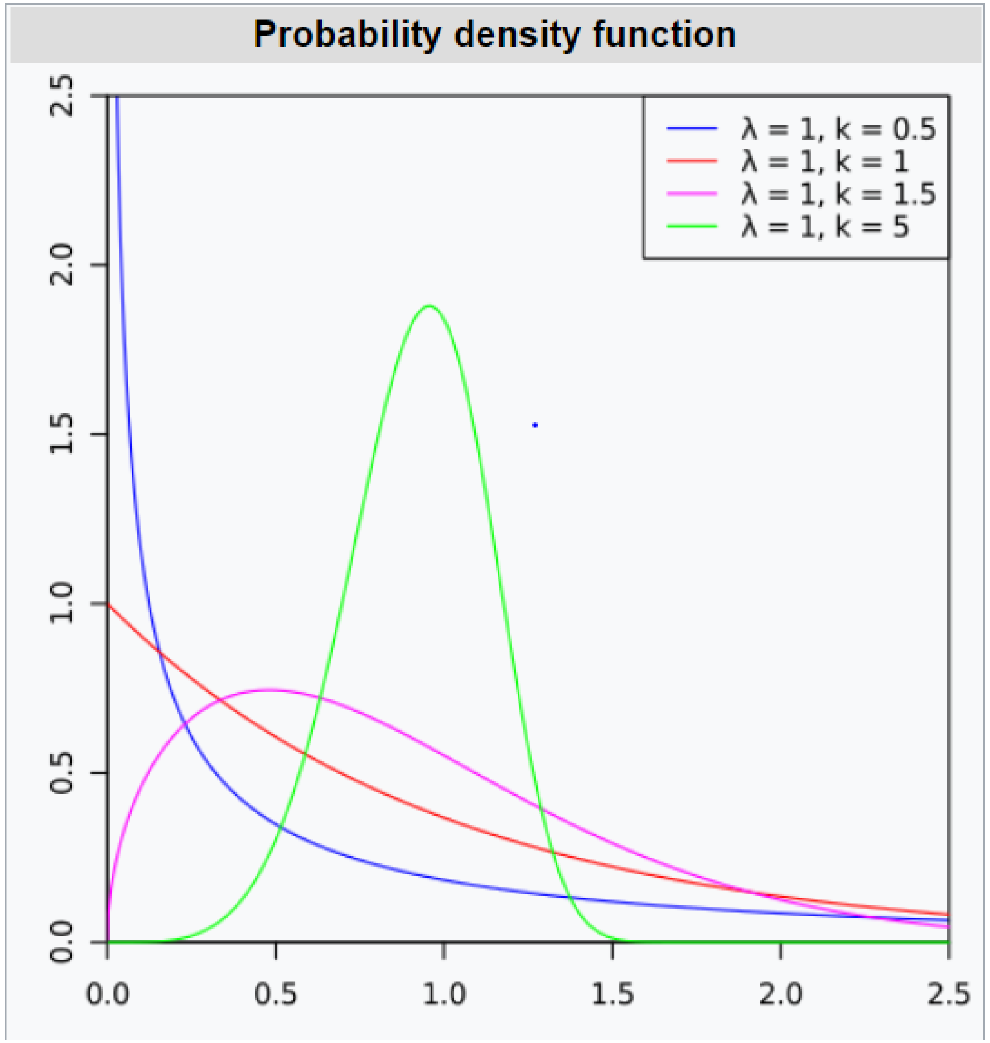
- Many of the mathematical tools developed at the time of the Comet aircraft and Liberty ships still dominate damage analysis in aerospace today
- Modeling damage and fracture is a challenging problem for many reasons: **failure behavior is very material-specific, fracture involves displacement continuities which traditional elasticity struggles to incorporate, damage initiation depends intrinsically on the material microstructure, failure is frequently stochastic, finite elasticity is required to capture extreme deformation states associated with failure, and auxiliary damage variables are often required to supplement elasticity models**
- It is not surprising that fracture mechanics has remain an active area of research, and a generally "nasty" problem!

Statistical Models

- Leonardo da Vinci (~1500) conducted very early fracture research by demonstrating that a wire's failure load was inversely proportional to its length
- Suggested that random "flaws" in the wire contributed to failure (longer wire, more flaws, lower failure load)
- When causes of failure are unknown or not controlled, they can be modeled as random and failure can be characterized statistically
- This is simplest possible approach to mathematically modeling damage and fracture
- Weibull survival analysis is a flexible framework to statistically characterize failure of an engineering component
- Weibull analysis can give qualitative insight into causes of failure, but does not illuminate any "physics" of the failure process

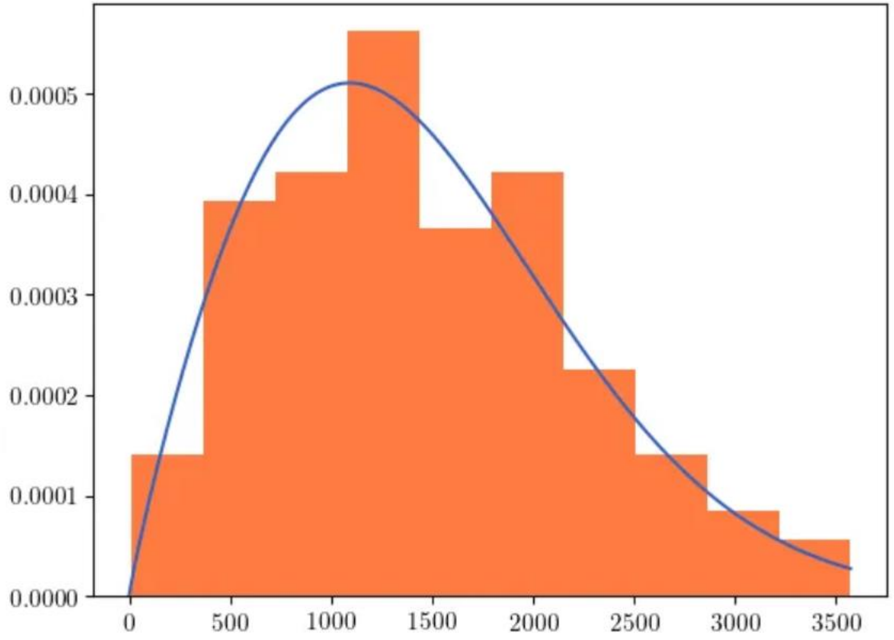
$$f(x;\lambda,k) = \begin{cases} \frac{k}{\lambda}\left(\frac{x}{\lambda}\right)^{k-1} e^{-(x/\lambda)^k}, & x \geq 0, \\ 0, & x < 0, \end{cases}$$

- Weibull distributions are specified by a shape parameter "k" and a scale parameter "λ"
- The horizontal axis is some measure of time (load cycles, months, etc.) and the vertical axis is failure probability
- k<1 indicates failure rate decreases with time, k=1 indicates constant failure rate, k>1 is increasing failure rate



Use of Data

- Data is gathered through experiments or field studies on when a particular engineering component fails
- A histogram for the component's lifetime is made, and a Weibull distribution is fit to the data by estimating the shape and scale parameters
- The Weibull distribution can be used to make estimates of a component's remaining lifetime, the number of in-service parts that will fail in a given time interval, and other useful things



Pros and Cons

- Because the parameters of the Weibull distribution are interpretable, a Weibull distribution for component survival can give some insight into causes of failure (increasing failure probability could indicate fatigue, whereas decreasing probability might suggest defects in raw material)
- It is a simple and intuitive analysis which aids in making practical decisions about planning, maintenance, and qualitative design interventions
- Weibull analysis does not provide detailed physical insight into the causes of failure, thus limiting its ability to inform design (failure is a black box with certain statistical characteristics)
- Because no attempt is made to explain precise causes of failure, Weibull analysis of one component may not generalize to another

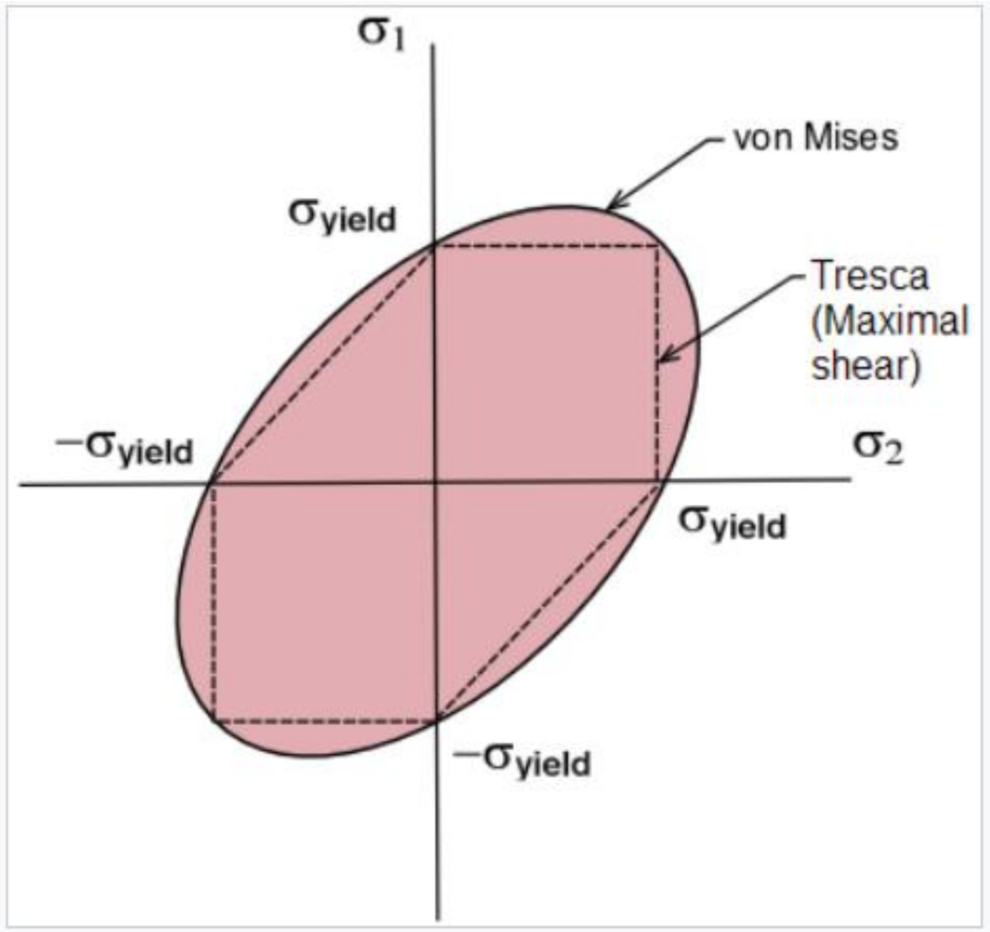
Typical Analysis

- Data on time to failure for a particular component is obtained, and a Weibull distribution is fit to the data
- The fit distribution can be used to gain some insight into the type of failures being observed, plan inventory and perform maintenance at appropriate intervals
- Weibull analysis can be used to assess the impact of interventions related to failure (comparing empirical distributions for failure probability vs. time before and after changing raw material suppliers, for example)

Stress-based Yield Criteria

- The elastic stress tensor characterizes the force intensity at each point in a body
- Though elasticity struggles to handle the opening and propagation of cracks, it is natural to think the stress tensor would govern the initiation of this process
- Yield criteria are attempts to explain the causes/mechanics of failure in materials in terms of the stress state
- Increase in sophistication from statistical approach with introduction of physics governing failure
- The post-yield behavior of the material is not modeled; the yield criteria acts as threshold after which character of material response differs

- Tresca and von Mises are two common yield criteria (~1850)
- The Tresca criterion states that the material yields when the maximum shear stress reaches a material specific (empirical) threshold
- The magnitude and orientation of the maximum shear stress can be computed from principal stresses/directions of the stress tensor
- The von Mises criterion states that the material fails when the energy associated with the deviatoric stresses reaches a measured threshold



Use of Data

- Tensile specimens are used to compute the critical Tresca and von Mises stresses
- Non-uniform stress state in test specimen, pinpointing precise yield force and position make this experimental characterization non-trivial
- Yield criteria calibrated on tensile specimen but verified on more complex stress states

Pros and Cons

- Gives some insight into mechanics of material failure, generalizes well one from part to the next (unlike Weibull analysis)
- Simple to use as design/analysis criteria, may act as useful and conservative proxy for avoiding failure-prone stress states
- Anisotropic material microstructures often not accounted for in stress-based yield criteria (failure tends to occurs along directions of weakness in microstructure)
- Provides no insight into what happens after yield/failure
- Cannot predict whether existing cracks are stable or will cause catastrophic failure

Typical Analysis

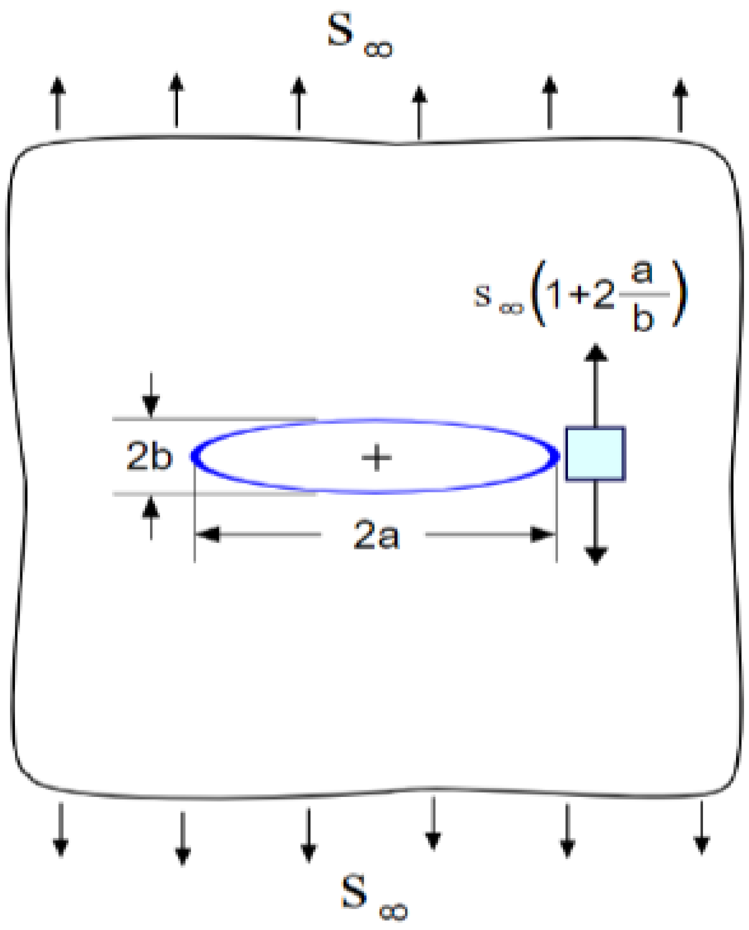
- With these methods, any candidate structural design should never see stress states which approach or exceed a given yield criteria (with some factor of safety)
- The stress-based yield criteria can be used as a constraint or objective to be minimized in structural design optimization process

Linear Elastic Fracture Mechanics

- Linear Elastic Fracture Mechanics (LEFM) represents another step forward in understanding structural failure
- Focuses exclusively on sharp cracks (not distributed damage)
- The early work of Inglis, Westergaard, Irwin, and Griffith (~1900) laid the groundwork for the field
- LEFM builds on traditional elasticity by introducing new fracture-related concepts, quantities, and material parameters
- LEFM primarily answers a question which is impossible within the framework of elasticity: under what conditions is a sharp crack stable?
- Classical fracture mechanics approaches do not model the initiation of cracks within the structure, only the stability and growth of pre-existent cracks
- In industry settings, pre-existing cracks are assumed to come from imperfections and defects in the raw material

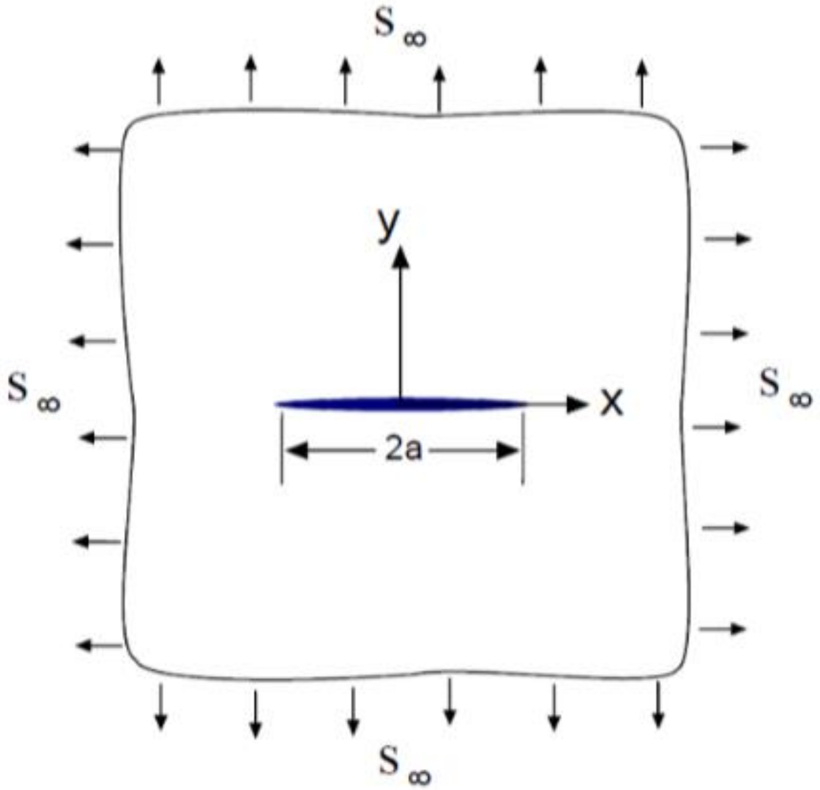
Inglis Solution

- In 1898, Kirsch found the solution for the stress field of an infinite plate with a circular hole pulled in tension
- Inglis extended this solution to elliptical holes, showing that the stress at the crack tip grew without bound as the aspect ratio of the ellipse was increased
- Via the Inglis solution, linear elasticity predicted material failure for any non-zero applied load due to the sharp crack stress singularity



Westergaard Solution

- Inglis modeled stress around sharp crack in a limiting sense, and the use of elliptical coordinates made the solution difficult to interpret
- Westergaard used complex-valued Airy stress function to model the stress field around a sharp crack in an infinite plate directly
- The plate is pulled in bi-axial tension in this case, but the use of Cartesian coordinates in obtaining the stress field proved fruitful



Irwin Stress Intensity Factor

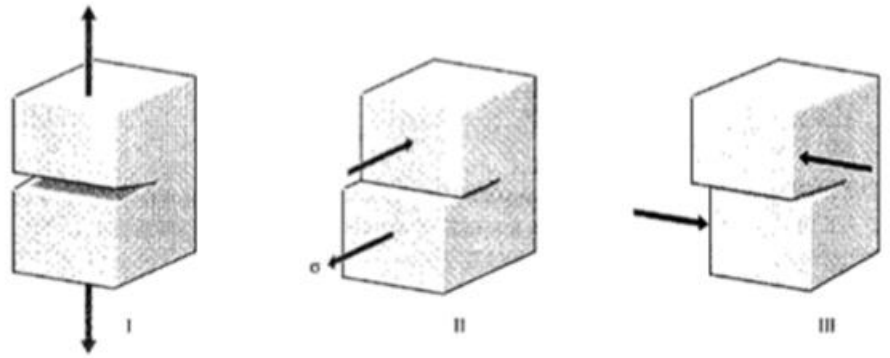
- Irwin suggested that attention be restricted to the stress field in a small vicinity of the crack tip
- This permits approximations which simplify the Westergaard solution
- Despite the stress singularity at the crack tip, a single parameter characterizes the stress field in this region
- Irwin called this parameter the "stress intensity"

$$K := \sigma_\infty \sqrt{\pi a}$$

$$\sigma_{ij} = \frac{K}{\sqrt{2\pi r}} f_{ij}(\theta)$$

Stress components are written in polar coordinates centered at crack tip. The stress intensity "K" fully characterizes the crack tip stress field, depending on the applied stress and crack length.

- Stress intensity fully defines stress state around crack tip, thus Irwin claimed that a crack grows when the stress intensity reaches an empirical, material-dependent critical value
- Different stress intensities for different types of loading
- The stress intensity framework, along with material parameter of critical stress intensity (or fracture toughness), permits predictions of crack stability based on its size, the applied loads, and the geometry of the structure
- The stress intensity for the cracked infinite plate is available analytically from the Westergaard solution, but more complex structural geometries require numerical or empirical stress intensity determination



$$K = \sigma_\infty F(a, d)$$

In general, the stress intensity depends linearly on the applied loads and is some function of the crack length "a" and the geometry of the structure, via a set of parameters "d"

Use of Data

- Irwin proposed the stress intensity model of fracture by noting that the linear elastic stress field in an infinite plate near a sharp crack tip was characterized by a single parameter
- Stress fields around sharp cracks in structures with other geometries should also be singular and described by a single parameter
- The fracture toughness is the only material parameter to be experimentally determined in this model
- Fracture toughness tests can be conducted for different materials
- Fracture toughness is shown experimentally to depend on material thickness
- Stress intensity factors for complex geometries can be empirically determined
- The accuracy of the stress intensity model gauged by comparison with data: is the fracture toughness truly a material parameter? how much ductility in the material can be neglected?

Pros and Cons

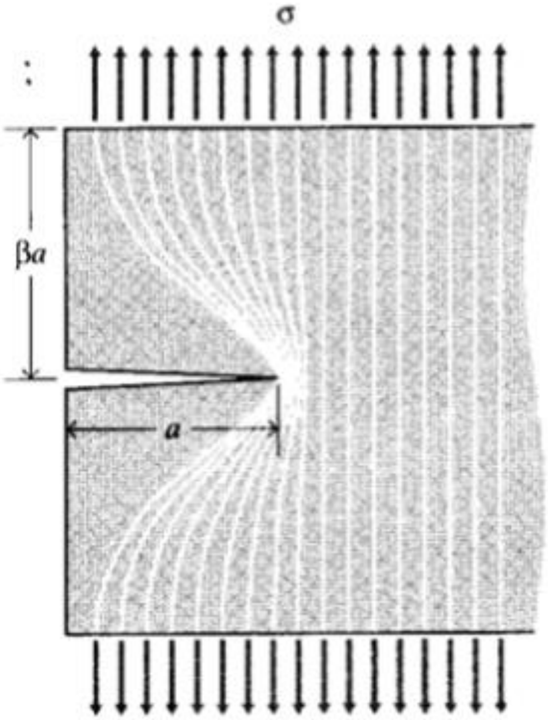
- The stress intensity approach deals with the problem of singular stress fields, and provides a method to analyze the stability of pre-existing cracks
- Simple and practical analysis framework which can easily be tabulated and used by non-experts
- Whereas stress-based yield criteria gives insight into physics of damage initiation, stress intensities describe basic physics of crack growth
- Typically restricted to isotropic materials (decent approximation for metals) and does not account for multiscale effects
- The formation of cracks is not modeled, and LEFM is mostly applicable to brittle failures where a crack grows suddenly without bound
- Bounded crack growth and varying propagation directions not accounted for
- Emphasis on "local" stress criteria do not explain global phenomena such as the size effect (discussed in the following)

Typical Analysis

- Determine the loads a structural component will support throughout its life, and the locations of the maximum stresses
- Determine the maximum crack size which would go undetected by non-destructive inspection techniques
- Assume that a crack of this size occurs in the locations of maximum stress with the worst orientation
- Compute/obtain the stress intensity factor for this crack and the fracture toughness of the material
- Ensure that the stress intensity is below the critical value (with some factor of safety) throughout the lifespan of the component
- Ongoing inspection and maintenance can be employed to ensure the health of the structure as well

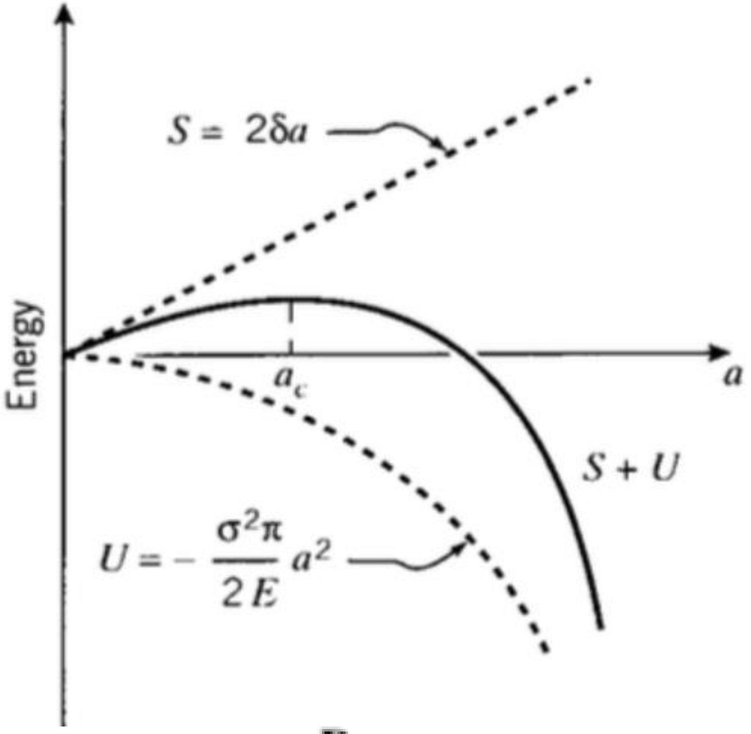
Griffith's Approach to LEFM

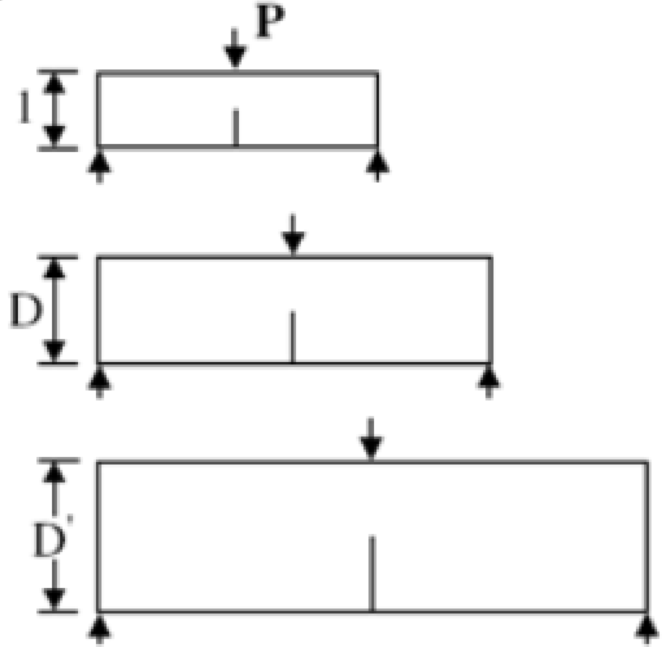
- Griffith conceptualized the fracture problem from the standpoint of energy
- In the context of a semi-infinite plate with an edge crack in tension, he argued that strain energy was liberated from a triangular region around the crack
- The reduction in the structure's strain energy as a result of crack growth was compensated by dissipated energy required to advance the crack, controlled by a material parameter G_c
- The crack grows when the increasing the crack length decreases the total energy U
- The fracture process is seen as a competition between liberated strain energy and energy required to advance the crack



$$U = G_c a - \frac{1}{2E}\sigma^2 \beta a^2$$

- The critical crack length is a function of the applied stress and marks the point at which the structure becomes unstable
- The material parameter G_c is called the "energy release rate" and can be empirically determined
- This analysis is applicable to brittle materials for which plasticity at the crack tip is minimal
- Griffith's most significant contribution was to conceptualize the fracture process in terms of energies
- Because the released strain energy is proportional to the square of the structure's size, whereas the energy associated with the crack has linear dependence, larger structures fail at lower stresses
- This is the size effect, which is explained by the Griffith's solution and is an important consideration in engineering design
- Note that the energy release rate and stress intensities are related





Use of Data

- The model is constructed from the first principles of linear elasticity and leaves only one material parameter to be measured
- The energy release measures the energy required to advance a crack in a given material and can be obtained experimentally
- Original Griffith's solution seems to have functioned more as a "thought experiment," as there were not many predictions it could make beyond the example problem

Pros and Cons

- Griffith's solution provides a different and intuitively appealing way of conceptualizing the fracture problem which sidesteps the problem of stress singularities
- Explains the size effect unlike stress-based failure criteria
- Blazes trail for powerful energy-based computational methods
- Still does not model the initiation of cracks, or their stable growth
- Not usable in most realistic situations because analytical expressions for the energy as a function of crack length are not available

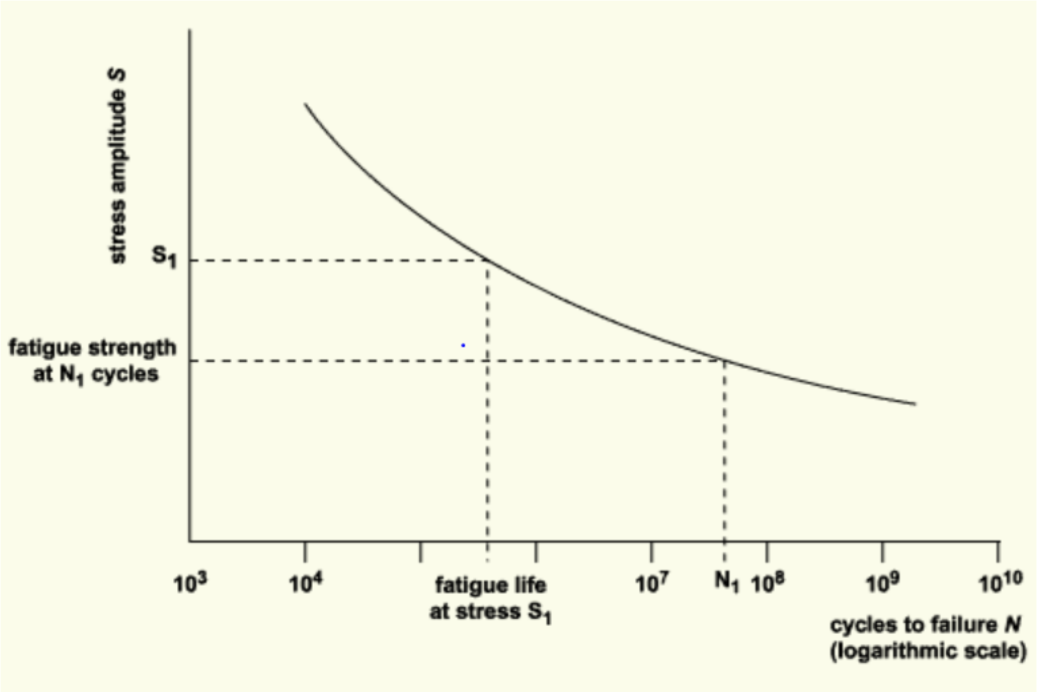
Typical Analysis

- If an expression for the energy of a fracturing solid as function of crack length is available, the energy release rate for the given material can be substituted and the critical crack length computed as a function of the applied stress
- Alternatively, the critical stress as a function of a given crack length can be found
- Much like the stress intensity approach, this analysis can only be used to determine if cracks in a structure are stable

Fatigue Models

- When a component is subjected to a fluctuating stress state "there is progressive, localized, permanent microstructural change which occurs in the material. This microstructural change may culminate in the initiation of cracks and their subsequent growth to a size which causes final fracture after a sufficient number of stress or strain fluctuations" [31]
- Fatigue cracks steadily grow as a function of load cycles, as opposed to the catastrophic crack growth modeled in brittle fractures of LEFM
- Quantities from fracture mechanics such as stress intensity should still govern the fatigue cracking process, but relationships are fit to empirical data
- Fatigue models are made for each material and are typically interested in cyclic loading, where stresses oscillate sinusoidally between two levels
- With increasing demands placed on metal structures, fatigue research became active in the mid 20th century

- Classical fatigue models rely primarily on experiments and are very costly to produce
- The simplest approach is to cyclically load specimens of a given material at a range of stress amplitudes until failure and plot the results
- There is significant stochastic effect, thus each data-point is an average of many tests
- There can be a mean effect to the stress, thus it may be necessary to produce S-N curves for stress reversal amplitude and mean stress
- Experiments can also be used to fit average rate of crack growth in a material as a function of the stress intensity amplitude



S-N curves are experimentally determined relationships between the amplitude of the stress cycle and the life of the component

$$\frac{da}{dN} = A\Delta K^m$$

The Paris Law is an empirical relationship between the rate of crack growth and the fluctuation in the stress intensity

Use of Data

- Classical fatigue models such as S-N curves and the Paris Law (standards in industry) do not model the physics of progressive damage formation
- Fatigue modeling almost entirely data driven, mostly through "curve fitting"
- Quantities from elasticity and fracture mechanics used in experimental characterization of fatigue cracking
- Fracture mechanics suggests what variables are relevant in characterizing fatigue behavior

Pros and Cons

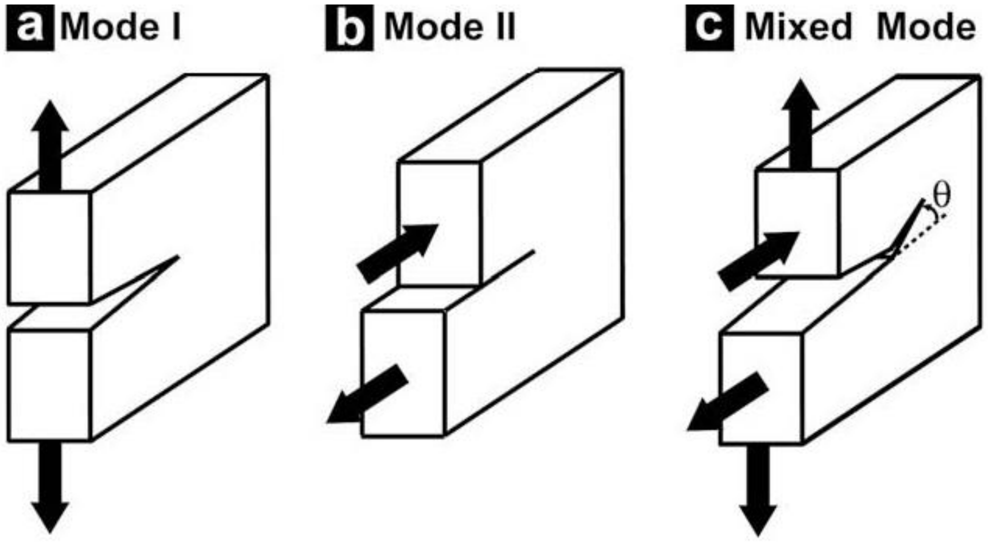
- Experimental characterization of fatigue in materials has proven suitable for use in industry
- Fatigue models provide qualitative insight into the mechanics of progressive damage formation (not explained by LEFM), and a framework for how to integrate this into typical fracture mechanics analysis
- Experiments extremely expensive, time consuming, and do not generalize from one material to the next
- Without physical model of microstructural damage formation, there is little insight into methods to design against fatigue cracking

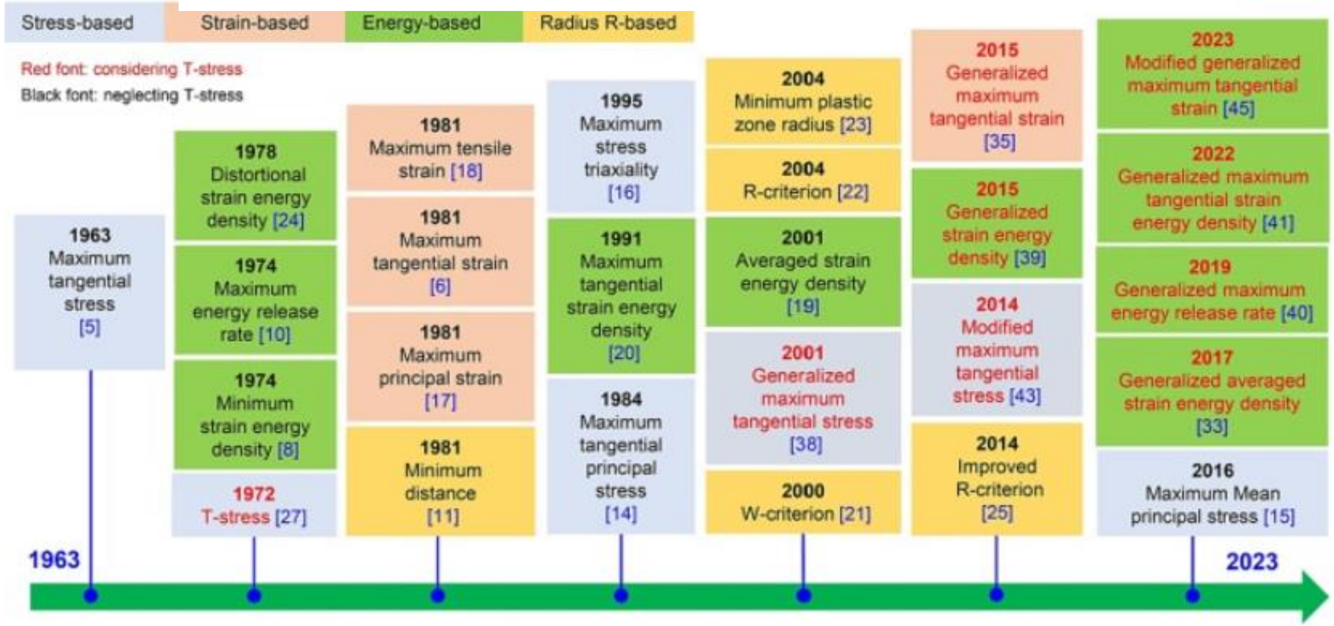
Typical Analysis

- Because fatigue cracking occurs at sub-critical stress levels, fatigue analysis is conducted in addition to LEFM to ensure that cracks do not grow to critical sizes
- S-N curves can be used to ensure that the operating conditions of a structure are safe from the standpoint of fatigue cracking
- Paris Law used to model time periods in which undetected fatigue cracks could grow to critical sizes
- Empirical fatigue models are used to plan inspection, maintenance, and the maximum service life of a cyclically loaded structure

Mixed Mode Fracture Models

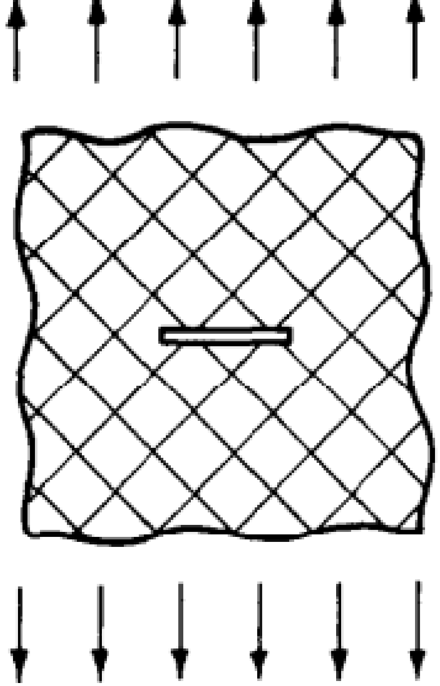
- When the load are not aligned with the crack or multiple loads are present, mixed mode fracture occurs
- Fracture toughness criteria does not directly apply
- A simple approach would be to claim that fracture occurs when an experimental-determined function of the respestive stress intensities reaches a critical value
- There are a multitude of stress, strain, and energy-based mixed mode fracture criteria [30]





Anisotropic LEFM

- The traditional stress intensity approach relies on isotropy of the underlying material (no reference is made to material properties)
- The stress intensity factor can be extended to anisotropic materials, so that in addition to the loading, crack length, and structural geometry, K depends on the orientation of the crack w.r.t. the material symmetry planes [18]
- This analysis is much more complex, and requires additional experimental characterization of anisotropic fracture toughness parameters



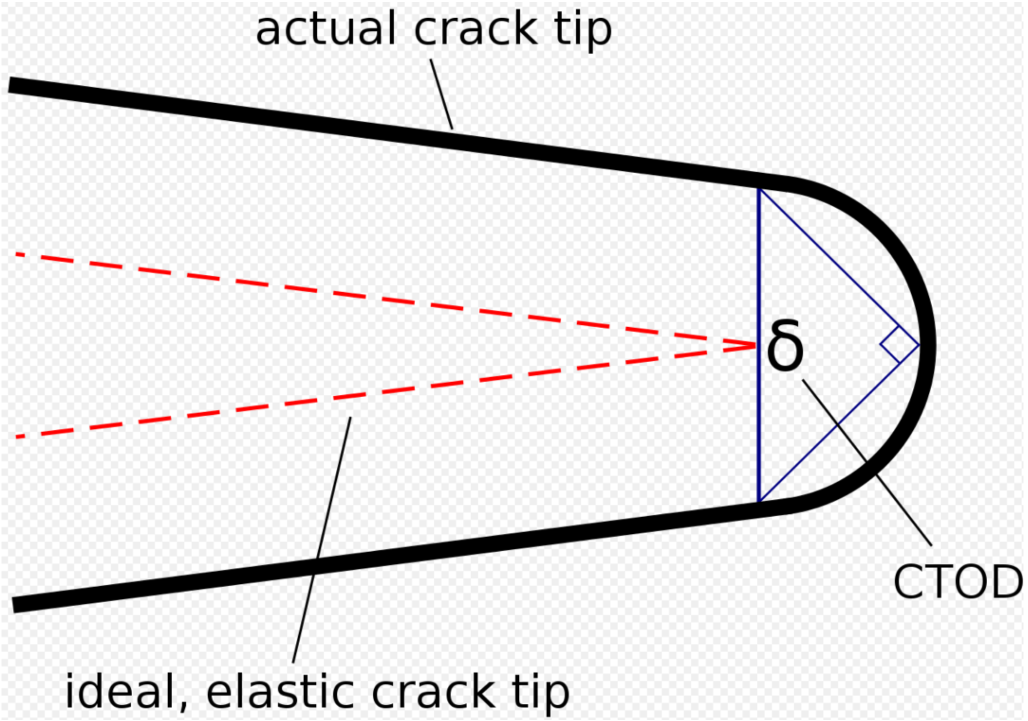
Dynamic Fracture & Other Effects

- Only static fracture models have been discussed, but the rate of load application influences the fracture behavior of a material
- This can be seen in impact and viscoelastic phenomena
- Dynamic fracture an important topic for many engineering applications (sports equipment, crash-worthy structures, etc.)
- Damage and fracture can be strongly influenced by other "physics" such as temperature
- Environmental effects such as corrosion or water absorption can play important role in the constitutive behavior of some materials

Non-linear Fracture Mechanics

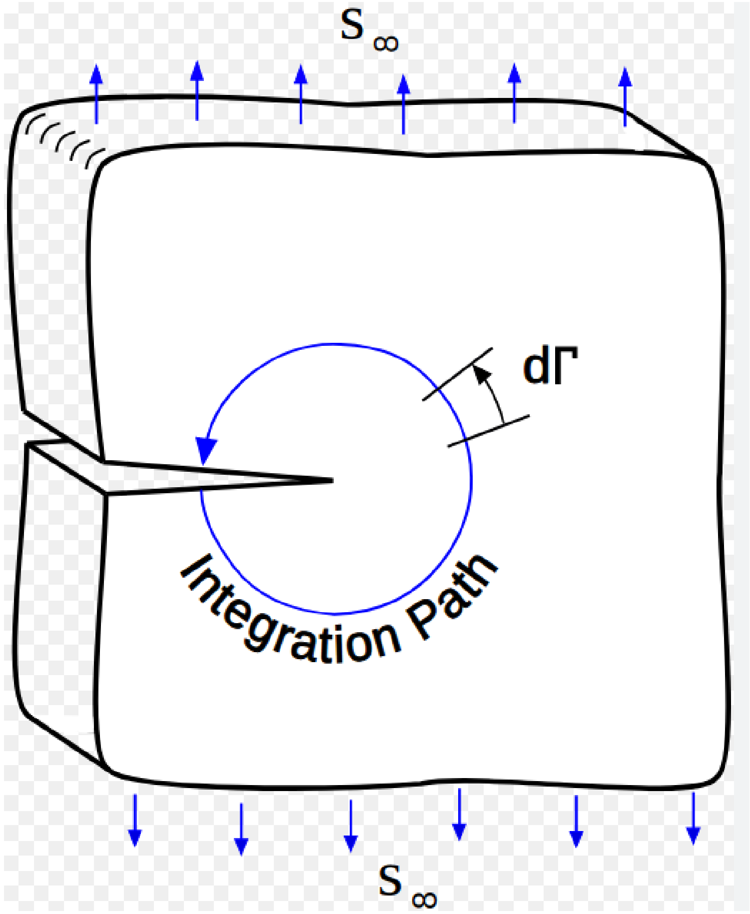
Crack Tip Opening Displacement

- The separation of the two faces of the crack at the tip was identified as a way to characterize fracture in ductile materials (~1960)
- In ductile materials, plastic deformation blunts the crack tip resulting in a measurable at the original crack tip
- Empirical protocols were devised to use this parameter as a method to analyze fracture of materials for which LEFM did not apply [32]



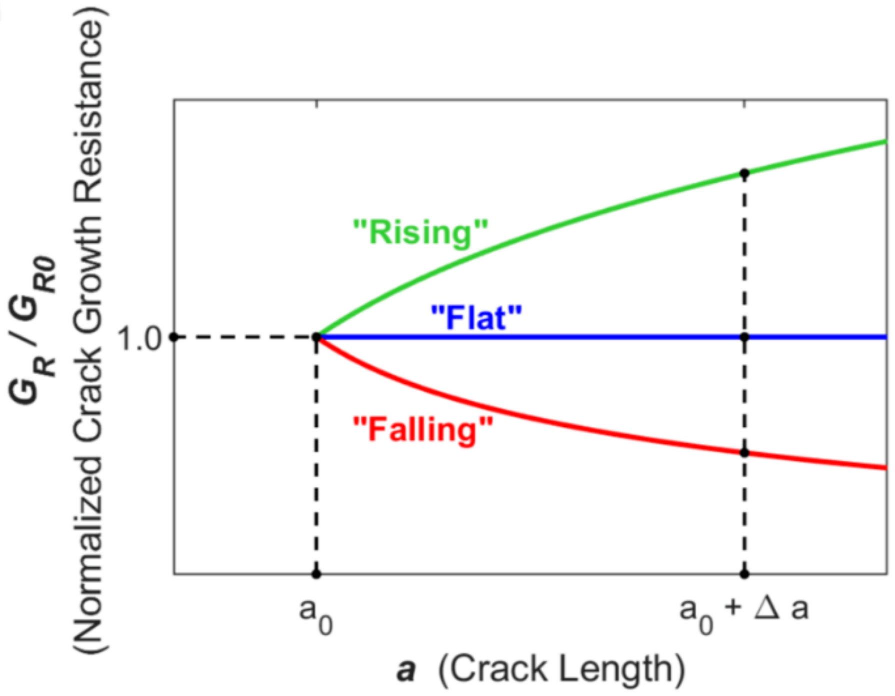
J-Integral

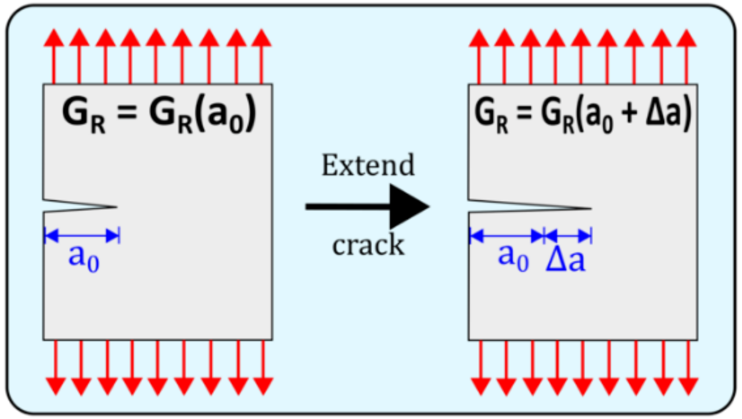
- The J-integral (~1970) provides a means of computing the rate at which energy is released from the structure as a function crack extension [32]
- When stresses are monotonically increasing, non-linear elasticity and plasticity can be viewed as equivalent
- Involves computing contour integral of stress response around crack tip
- J parameter acts as generalized energy release rate for non-linear deformations
- The J parameter can also be used to characterize the stress field around the crack tip, thus acting as a stress intensity or energy parameter



Crack Growth Resistance Curves

- In some ductile materials, the resistance to crack growth (analogue of energy release rate in LEFM) changes as a function of the crack length [32]
- This challenges the notion that the crack growth resistance is a material parameter
- Flat and rising crack growth resistance curves are the most common
- This can be a more accurate but complex failure criteria than a constant, material-specific critical crack resistance value





Use of Data

- CTOD measured directly from notched specimens, material characterized by the crack tip displacement at which the crack grows
- J-integral is a mathematical technique which is as good as the empirical characterization of the constitutive properties of the elastic body
- Crack growth resistance curve needs to be empirically determined, motivated by inadequacy of treating fracture resistance as a constant material parameter

Pros and Cons

- J-integral computations can be carried out for arbitrary material laws and crack/solid geometries in computational setting
- Along with a crack growth resistance curve for a given material, the J-integral can make predictions about crack growth in the presence of significant plastic deformation
- As before, the location and path of the crack are specified a priori
- No connection between material microstructure and its resistance to crack growth

Typical Analysis

- Using the J-integral and crack growth resistance curve to analyze ductile fracture is very similar to LEFM but slightly more complex
- For a given structure, initial crack, and set of loads, the J-integral the rate at which energy is dissipated per unit crack length
- The critical energy release rate is read off the crack growth resistance curve for the given initial crack length
- The crack is considered to be unstable if the rate of energy dissipation computed from the J-integral exceeds the critical value

Computational Fracture Mechanics

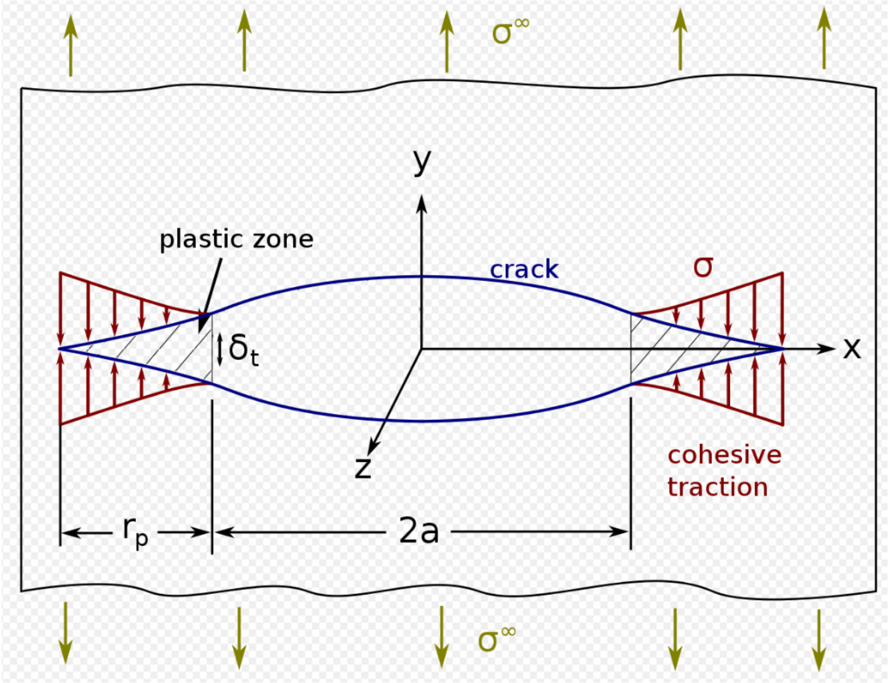
Common Numerical Methods

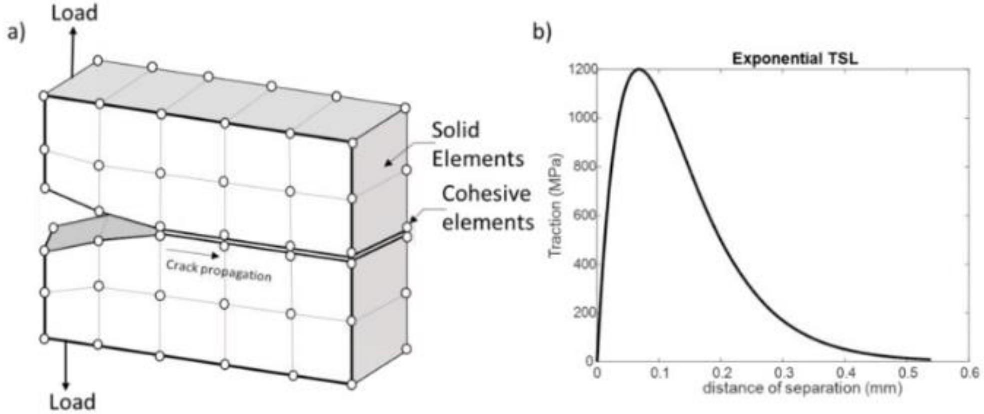
- Finite Element Method (FEM)
- eXtended Finite Element Method (XFEM)
- Boundary Element Method (BEM)
- Finite Difference Method (FD)
- Element-free Galerkin Method
- Material Point Method
- Level Set Method

- Numerical methods must be distinguished from a physical damage or fracture model
- Numerical methods provide framework for implementing solutions to an underlying physical model, usually in the form of partial differential equations
- Though numerical methods can make certain models seem convenient or natural, a numerical method is only as good as the physics it describes
- FEM and XFEM are most common methods for general fracture problems
- Element-free Galerkin and Material Point method come from class of "mesh-free" methods, which can be useful for modeling the evolving geometry of a crack (no re-meshing required) or very extreme deformation states (meshes do not become "tangled")

Cohesive Zone Model

- CZM related to strip yield model from Dugdale and Barenblatt [29]
- Seeks to model constitutive response of fracture process zone ahead of crack tip, where microcracks form and damage accumulates in the absence of complete material separation
- Traction-separation law relates displacement discontinuity across crack face to a cohesive stress
- Traction initially increases with separation, then decays to zero indicating the crack has fully formed
- The work required for total separation (integral of traction-separation law) must equal the energy release rate of the material





(a) Cohesive zone model;(b) Exponential traction separation law

Use of Data

- Traction-separation law can be calibrated with experiments [42]
- Different fracture modes require their own cohesive constitutive relation
- Calibration of traction-separation on simple experimental specimen should predict fracture of a body with more complex loading and geometry
- Sensitivity of fracture process to exact cohesive law, location of cohesive elements, etc. should be studied

Pros and Cons

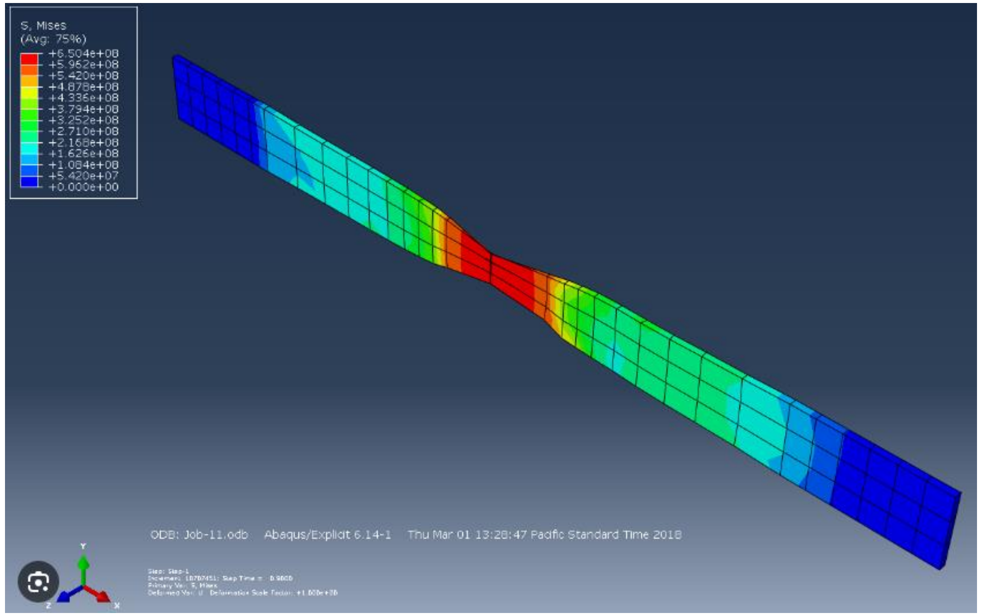
- Can model effects of plasticity and general non-linear material behavior
- Naturally describes bounded crack growth
- Good for adhesively bonded materials where failure occurs in predictable locations
- Straightforward to implement in general computational framework (typically FEM)
- Requires assumptions on where cracks initiate and in which direction they grow
- Can struggle with mixed mode fracture

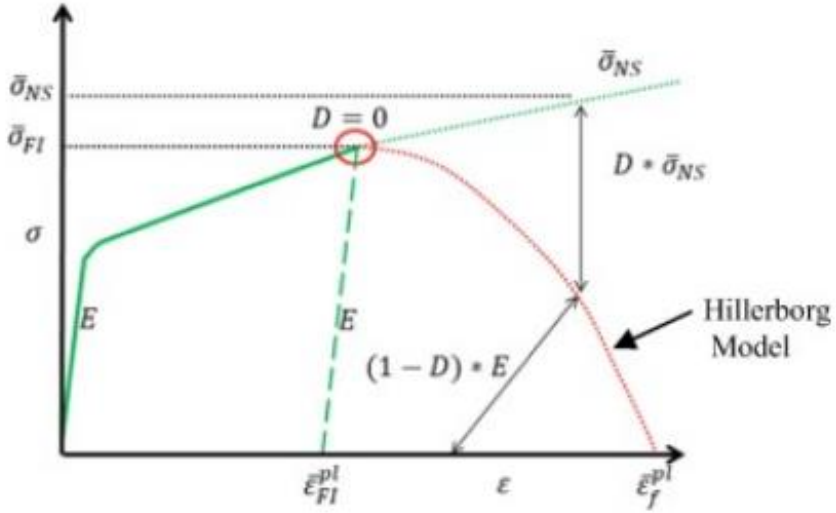
Typical Analysis

- Cohesive elements with a given traction-separation law are introduced into the finite element mesh of a structure
- The location and orientation of the cohesive elements must be specified and should be based on a priori knowledge of the structure and its potential failure modes
- The system of equations for static equilibrium is solved to find the response of the structure, and the formation of cracks is studied by observing the separation across cohesive elements

Element Deletion Method

- Strongly grounded in FEM framework
- The stiffness of elements is reduced as a function of their stress/strain
- This models ongoing process of damage formation leading to total loss of stiffness
- First method we have seen which does not require assumptions about where and how damage/cracks grow [13]
- But, no explicit representation of crack surface
- Results can be highly mesh dependent
- Similar to eigen-erosion damage model [88]





Use of Data

- Damage constitutive relation of elements needs to be calibrated against existing damage models or data in some way
- Numerical studies conducted to ensure approximate objectivity of damage predictions
- Overall force-displacement curves and spatial damage distribution from element deletion analysis can be compared to experiments for a number of mesh sizes
- Predictions of damage initiation sites, crack paths, and overall load-displacement curves compared to experiments

Pros and Cons

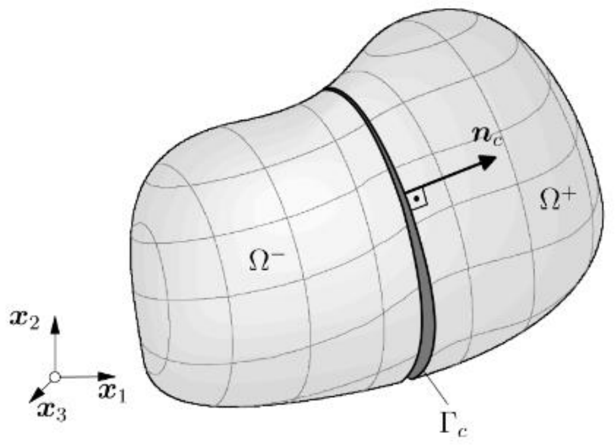
- Conceptually straightforward extension to traditional finite element method
- Allows the representation of damage via continuous material stiffness degradation
- Requires no assumptions about the initial location of cracks and how they grow
- Necessary to combat mesh dependency
- No explicit representation of crack surface
- Does not explain microstructural mechanics of damage formation (stiffness degradation law not connected to specific failure modes and/or material microstructure)

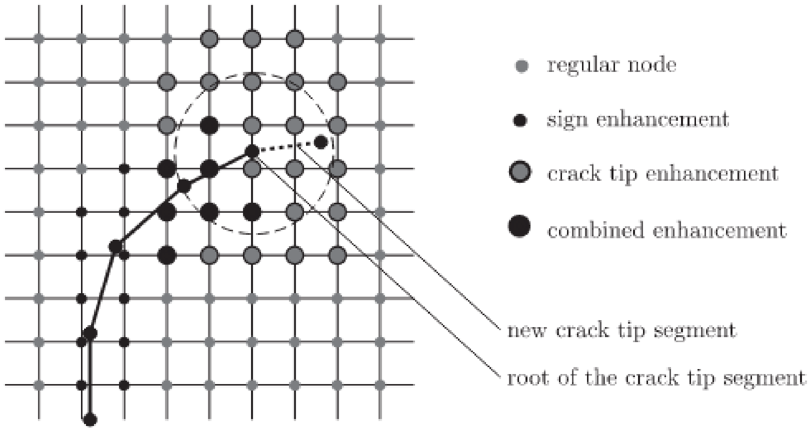
Typical Analysis

- Similar to cohesive zone analysis, except a priori knowledge of crack locations and paths is not required
- Stiffness degradation law specified, and load stepping analysis is performed to model the onset and growth of damage in the structure
- Crack paths can be approximated from zones of significant stiffness loss
- Mesh study should be conducted to ensure approximate objectivity of damage predictions
- This analysis is the first (in our timeline) to give insight into how stress redistributes around damaging zones of the structure
- Analyst can use material degradation law as design criteria, determine whether damage in the structure for given loads is acceptable/stable, use estimates of crack locations and paths as basis for a cohesive zone analysis, etc.

Stress-based LEFM in Computational Setting

- Generalization of stress intensity framework
- XFEM allows cracks to be represented inside an arbitrary body without remeshing [21]
- Classical solutions for displacement field around crack tip can be used as enriched basis functions in finite element displacement approximation
- Crack is advanced at (small) fixed lengths in a load stepping analysis using mixed-mode fracture criteria [22]
- Many different criteria exist to determine the direction of crack propagation (maximum circumferential stress, minimum strain energy density, maximum energy release rate, etc.) [23]
- Initial cracks can exist in the structure, or cracks can be opened with yield-type criteria





Energy-based LEFM in Computational Setting

- Generalization of Griffith's approach to fracture
- Total potential energy for fracturing solid written in terms of the unknown displacement field, propagation direction, and increment in crack length then minimized [20]
- Load stepping analysis performed to model crack progression
- XFEM is useful to represent cracks without re-meshing in the implementation of this approach
- Cohesion and other phenomena are straightforward to introduce in the variational setting [19]

Use of Data

- Extension of concepts from LEFM, no additional empirical parameters required
- However, there are not unique choices of finite element mesh size, crack length increment, or crack propagation criteria
- Numerical studies should be conducted to indicate crack path is not heavily dependent on these parameters
- Computational implement of LEFM permits more sophisticated comparison to experiments—global force-displacement curves and full crack paths can be predicted, whereas classical LEFM only predicts the point at which growth initiates

Pros and Cons

- Unifies many concepts from fracture mechanics into a general computational framework
- Makes no assumptions on the direction of crack propagation
- Griffith's model becomes practical approach to general fracture problem
- Arbitrariness in the length of crack advancement per load step and the size of cracks opened from yield criteria
- Crack initiation and advancement are modeled independently
- XFEM struggles in modeling branching and 3D cracks
- Does not incorporate progressive damage, though this could be accounted for by applying the same methods to the microstructure
- In many practical situations, it is more important to precisely model the initiation of cracks of cracks than their growth leading up to catastrophic failure—computational LEFM seems better suited to the latter

Typical Analysis

- These approaches are useful to determine the overall force-displacement response of a cracking structure or the path a crack follows as it grows
- The geometry and material of a structure are specified, loads are prescribed, and a finite element mesh generated
- The structure is often given initial cracks, though yield criteria could be used to seat cracks
- Load stepping analysis is performed along with a crack initiation and growth direction criteria
- At each load step, the crack is advanced by fixed increments until it becomes stable, then loads are increased
- Numerical studies with different mixed-mode fracture criteria, crack increment lengths, mesh sizes, etc. should indicate objectivity of the results

Interlude: What is the motivation for increasingly sophisticated computational models?

Case Study 1: Original vs. Generalized Griffith's Model

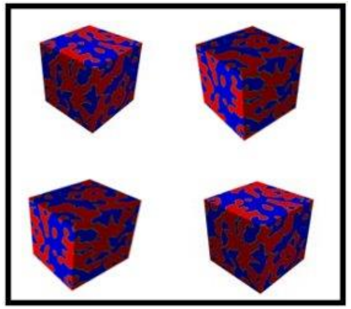
- Original Griffith's model assumes that the released strain energy has a simple form, and that the crack grows in a known direction
- For a given crack, length it predicts a stress level at which unstable crack growth will initiate
- A generalized Griffith's approach can model bounded crack growth, and whether cracks will arrest (especially if plasticity is present in a material with rising fracture resistance curve)
- Whereas the simple model necessarily predicts all cracking is catastrophic, the energy-based computational model could demonstrate the initial growth but subsequent arresting of cracks
- Stable cracking could be acceptable in some structures—thus the more sophisticated model facilitates more "aggressive" (efficient) design

Case Study 2: Conservative Approaches to Stochasticity

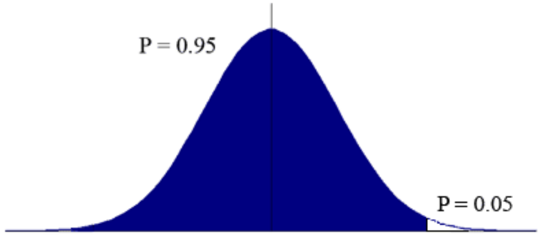
- Material fracture parameters such as the energy release rate and stress intensity influenced by the composition and geometry of the microstructure
- Material microstructures vary spatially and between samples
- This variation does not arise from known causal influences, so it is typically treated as random (though in principle it might be modeled by considering how the material is prepared)
- Measured fracture parameters depend on the microstructure and will thus exhibit variability
- In the interest of safety, reported values will be an "extreme" statistic such as the maximum or minimum of the experimental sample

- This amounts to arguing the material is in the worst possible state at each point
- By summarizing the stochasticity with a conservative parameter choice, we do not account for effects of random spatially varying fracture parameter
- Stochasticity should be carried through models to avoid overly conservative designs
- If statistical distributions of microstructures is known, the variation in experimental data could be explained by simulating microstructural mechanics for range of configurations
- The multiscale model with stochastic microstructure allows for more aggressive design than summarizing the stochastic microstructural response beforehand
- See the following two slides for a summary of these approaches

Approach 1: Summarizing Away Randomness



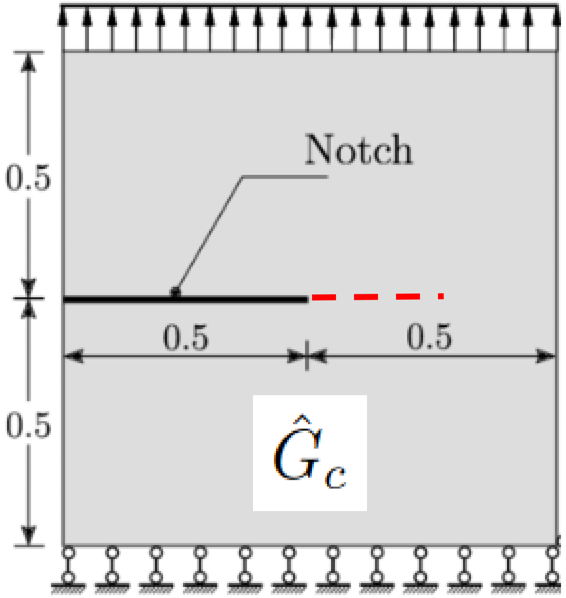
Unknown and variable material microstructure



Experiments show random distribution of fracture parameters

$$\hat{G}_c$$

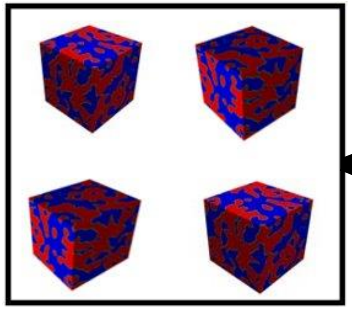
Reported material parameter comes from one-tailed confidence interval on experimental distribution of values, acting as conservative bound for possible material behavior in service



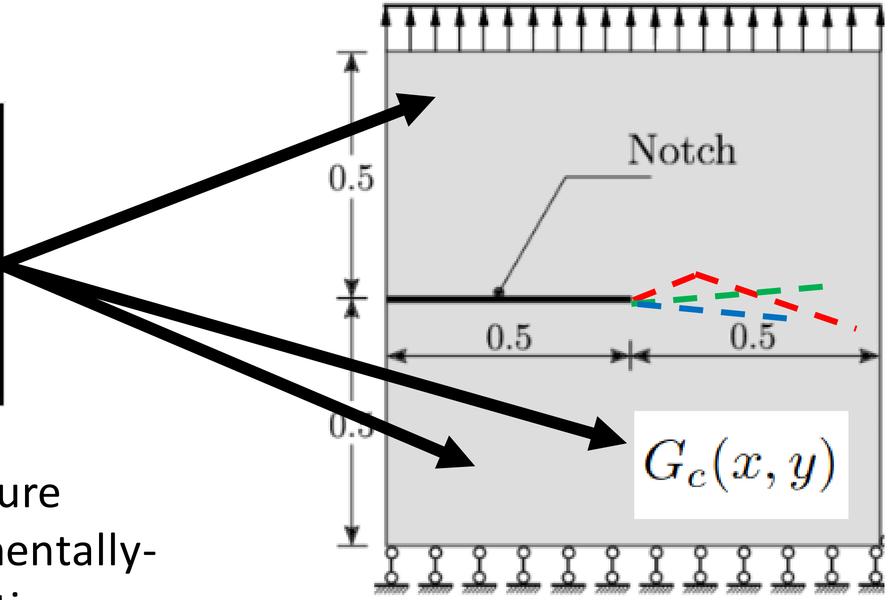
Constant material parameter applied to analysis of cracked structure, assuming that "worst case" microstructure exists everywhere

Overly conservative and potentially unrealistic predictions on the structure's response are obtained

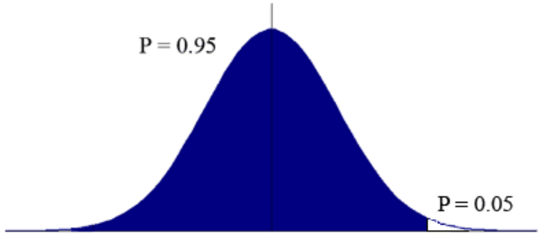
Approach 2: Uncertainty Quantification



Variable microstructure arising from experimentally-determined distribution



Structure populated randomly with sampled microstructure, fracture parameter computed from microstructure



UQ techniques used to obtain stochastic response of structure. Using a one-tailed confidence interval at the level of the response leads to more realistic predictions and more efficient designs

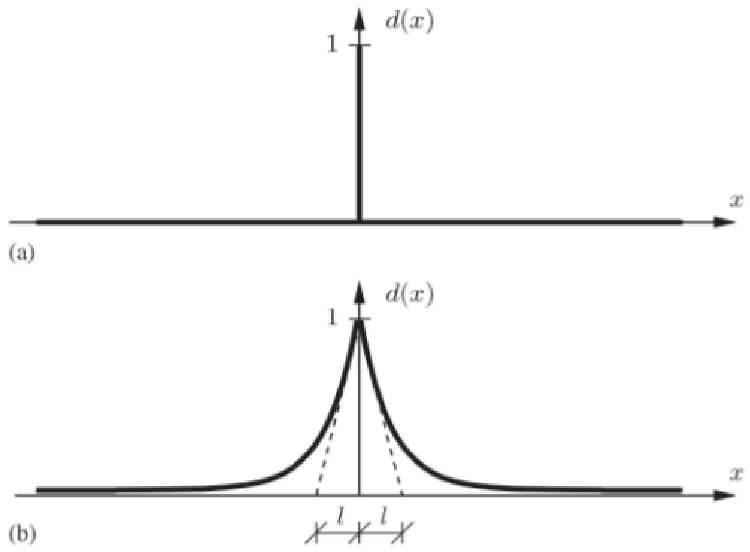
Computational Approaches Beyond Traditional Fracture Mechanics

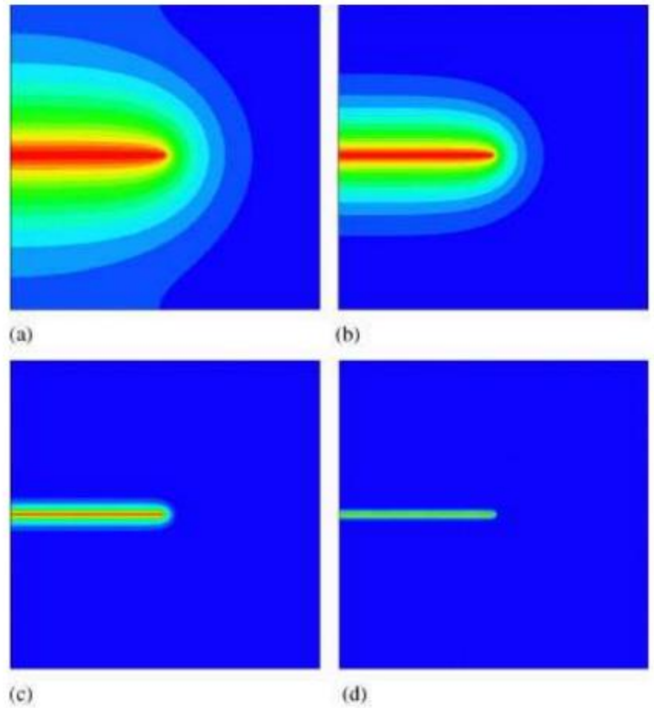
Before proceeding…Some Features of the Ideal Computational Damage Model

- Models both damage and cracking
- Initiation, growth, and branching should all be described by same framework
- Calibration on simple experimental tests has good predictive power in a wide range of different scenarios
- Informed by data in sophisticated ways
- Multiscale material behavior and stochasticity can be incorporated
- Computational cost is not prohibitively high
- Models brittle and ductile fracture as well as failure mechanisms for a breadth of materials
- Objective with respective to mesh size and any other numerical parameters
- **Emphasizes needs of practitioners—informed by material stochasticity, excels at modeling early onset of damage as opposed to full history of crack, does not require supercomputer to run, can be incorporated into design optimization, small number material parameters are feasible to determine experimentally, machine learning is used in a manner appropriate for safety-critical applications**

Phase Field Methods

- Analogous to generalized Griffith's model, except the fracture energy is written as a volume integral over a continuous crack density [28, 33, 34]
- This fracture energy term is such it can model continuous formation of damage, but also gives rise to sharp crack-like damage bands
- Introduction of scalar damage field which degrades the energy storage capacity of the material
- Multi-field variational minimization problem
- Energy degradation can be defined in such a way that damage does not occur in compression





Phase Field Extensions

- Original phase field papers give indications of how to partition energy to prevent compression fracture (anisotropic phase field methods)
- Phase field methods can be used in the finite strain setting, with 3D heterogeneous materials [54], to model fatigue [38], and with cohesive crack forces [39]
- Because of the variational formulation of the problem, it is straightforward to introduce coupled physics such as thermoelasticity or environmental effects
- The phase field model has also been used for ductile fracture [48]
- Some research in multiscale phase field approaches (see below)

Application to Different Materials

- Phase field models have been used to model fracture in concrete, 3D printed metals, ductile materials such as aluminum, fiber-reinforced composites, rubber-type hyperelastic materials, and brittle materials such as mortar [76-81]
- The phase field model is validated by comparing theoretical and experimental load-displacement curves for these materials
- There are is not currently experimental validation of phase field fracture in porous materials
- Materials which have been successfully modeled with gradient damage methods are likely to fit within phase field framework
- PSAAP for fracture modeling of granular materials?

Use of Data

- Phase field model makes use of the empirical constitutive relations of elasticity and the energy release rate from fracture mechanics
- There are some specific relationships and parameters which are phase field "hyperparameters"
- These include: the length scale (occasionally interpreted as material rather than numerical parameter), the partition of strain energy (form of anisotropy), and the energy degradation law (how the material softens with increasing damage)
- These are frequently chosen without rationale, but could be fit to data
- Phase field model should predict the locations of onset of damage, the damage pattern, and overall force-displacement curve
- Thus, very precise predictions can be compared to experimental results

Pros and Cons

- Naturally models crack branching, easy extension to 3D
- Makes use of traditional finite element framework
- Variational formulation facilitates coupling with other physics
- Crack/damage initiation and propagation modeled within same framework
- Scalar damage variable does not allow for multiple mechanisms of failure
- Length scale parameter arbitrary and introduces mesh dependency
- High degree of mesh refinement required in vicinity of the crack
- Questionable agreement with experiments [46]
- But, lots of freedom to fine tune the model

Typical Analysis

- Typical elastic material model supplemented by energy release rate from fracture mechanics (these are assumed to be known already)
- Length scale parameter, energy degradation function, mesh size (or adaptive meshing scheme), and tension-compression split (or more generally, crack constitutive behavior) must be chosen
- As proposed above, these could be informed by or fit to data on the material
- Load stepping analysis performed along with crack irreversibility condition
- It is also possible to include non-zero initial conditions on the damage field
- Damage initiation sites, crack paths, and load-displacement curve for structure determined from phase field analysis
- There is not extensive work in integrating phase field methods with structural design optimization, but computational models for damage initiation could be incorporated as constraints or objectives in optimization [49, 50, 51]

Gradient Damage

- Gradient damage distinct from gradient-enhanced damage; the former can be considered a special case of phase field methods (consistent with thermodynamic principles, can be interpreted through global energy principle)
- Continuous damage variable used for strain softening
- Damage is smeared over crack front of non-zero width—non-local damage criterion introduced to avoid loss of well-posedness
- Non-locality governed by length scale parameter analogous to that of phase fields
- Gradient damage evolution equations similar to strong form of phase field model
- Gradient damage came before phase fields, and the latter seems to be a generalization and refinement [47]

Gradient-enhanced Damage

- Scalar damage variable softens stress response of material
- Damage is function of effective "non-local" strain, which is governed by a PDE forced by a scalar measure of the usual strain tensor [90-92]
- Not consistent with thermodynamic principles; boundary conditions on damage are ad hoc
- Driving force for damage field governing equation does not decay to zero when crack is fully formed leading to unphysical damage growth orthogonal to crack surface
- Predicts different shape of damage band than phase fields (less sharp profile)
- GED has more constitutive relations to fit—model is more complex but potentially has more freedom to fit real material behavior
- Effectively same model as phase field method up to how the damage evolution is computed

	Gradient-enhanced damage model	Phase-field fracture model
stress–strain relation	$\boldsymbol{\sigma} = (1-\phi)\mathbb{E}_0 : \boldsymbol{\epsilon}; \quad \phi = h(\bar{\epsilon}_{\text{eq}})$	$\boldsymbol{\sigma} = g(\phi)\mathbb{E}_0 : \boldsymbol{\epsilon}$
extra PDE	$\bar{\epsilon}_{\text{eq}} - c_0 \Delta \bar{\epsilon}_{\text{eq}} = \epsilon_{\text{eq}}(\boldsymbol{\epsilon})$	$\phi - l_0^2 \Delta\phi = -g'(\phi)\bar{Y} l_0 / G_c$
boundary conditions	$\nabla \bar{\epsilon}_{\text{eq}} \cdot \boldsymbol{n} = 0$	$\nabla \phi \cdot \boldsymbol{n} = 0$

Table 4: Main equations of the isotropic gradient-enhanced damage (GED) and the standard PFMs. The local equivalent strain, a scalar measure of the strain tensor, is denoted by ϵ_{eq}, its nonlocal counterpart is designated by $\bar{\epsilon}_{\text{eq}}$ on which the damage variable ϕ depends.

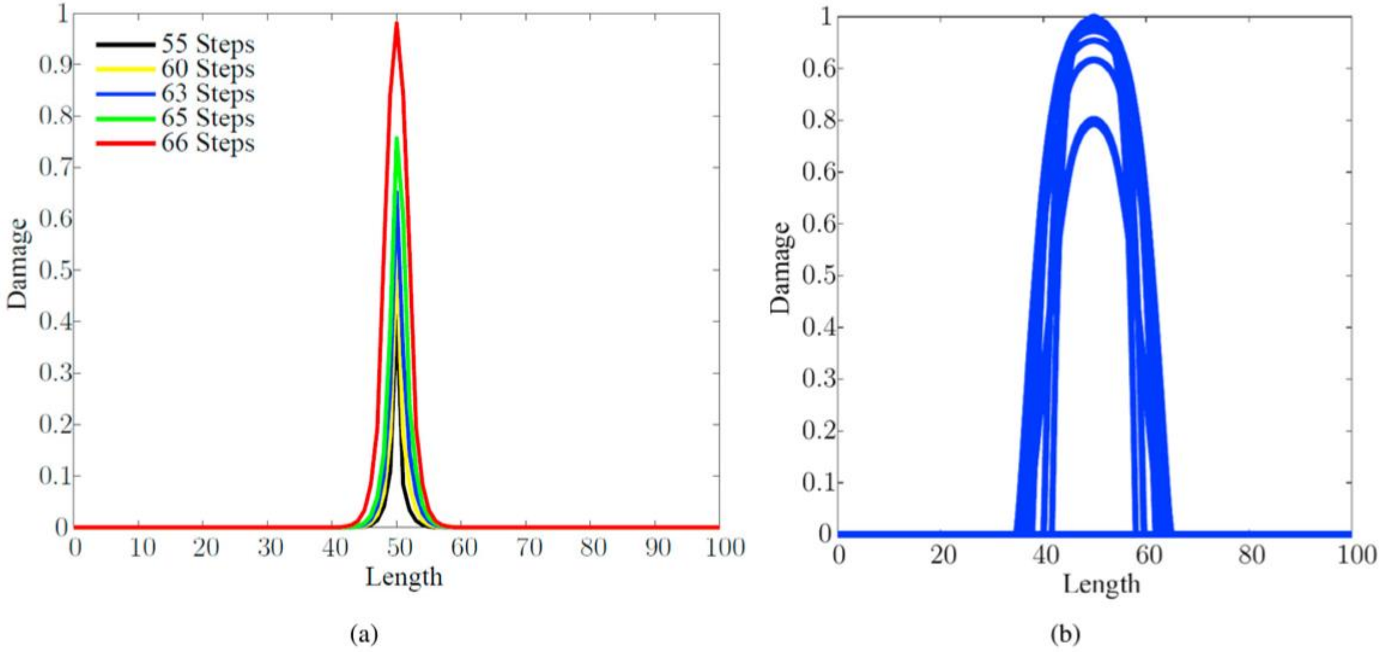
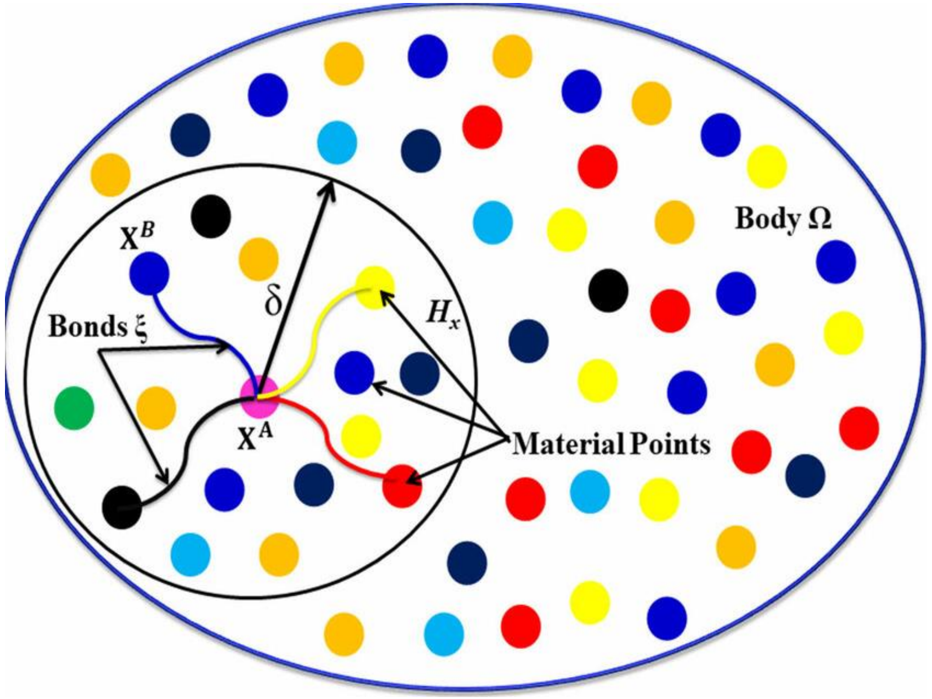


Fig. 7. Damage parameter evolution: (a) PFM; (b) GED.

Peridynamics

- Novel approach to model the mechanics of continua where governing equations do not incorporate spatial derivatives
- Material comprises particles which interact through "bonds"
- In original peridynamics paper, the force at a point was the integral over all particles within a fixed "horizon" of some function of the bond stretch [26]
- Non-zero horizon gives peridynamics non-local character
- The horizon and relationship between bond stretc and force are seen as material constitutive parameters
- It was shown that this model restricted the type of materials which could be modeled, so in a subsequent extension, the force at a point became dependent on the overall deformation state of the particles in the horizon [27]



$$\rho\ddot{u}(x,t) = L(u,x,t) + b(x,t)$$

$$L(x,t) = \int f\Big(u(x',t) - u(x,t), x' - x\Big) dV_{x'}$$

Use of Data

- Constitutive parameters and functions in peridynamics can be determined from empirical material models in elasticity
- If a true atomistic simulation is being conducted, the horizon radius might follow from theoretical considerations
- Most of the time, however, the choice of the horizon radius is somewhat arbitrary, and could be fit to optimize agreement with experiments [45]
- Peridynamic model should predict global load-displacement curves of damaging structure and precise crack path—this should be compared to experiments

Pros and Cons

- Shows that the same problem can be conceptualized in totally different ways
- Fracture and damage are incorporated naturally into material constitutive relation
- Crack/damage initiation and growth are governed by same mechanism
- Ductile fracture can be modeled with dissipative mechanisms in bond-force relationship
- Dispenses with tools of traditional elasticity, but subsequently calibrates model on elastic parameters
- Boundary conditions take unusual form
- Requires new numerical methods to solve integral equations
- Particles do not have rotational degrees of freedom
- Constitutive parameters have strange and seemingly unphysical units
- Questionable agreement with experiments [46]
- Struggles in multi-material settings

Typical Analysis

- Peridynamic constitutive relations for a given material determined from comparison to elasticity
- Horizon radius specified, load boundary conditions implemented in peridynamic-specific framework
- The structure is discretized but does not have a mesh in the finite element sense
- Force equilibrium used to determine the deformation and damage state of the structure
- Crack paths are determined based on the locations of damaged or broken bonds

Other Damage Models

- Microplane M7 Model [3]—complex damage model from Bazant which incorporates a large number of distinct failure modes and shows good agreement with experimental results
- Reddy GraFEA Model [1]—incorporates existing non-local damage criteria into finite element framework
- Micromorphic damage theories [4, 72]—an inherently multiscale approach to damage where the microstructure of the material is included explicitly in the kinematics of the body
- Bonded Particle Method [2]—approach to damage more popular in geomechanics in which materials are modeled as collections of irregularly sized spheres with breakable bonds at their contact points

Multiscale Damage

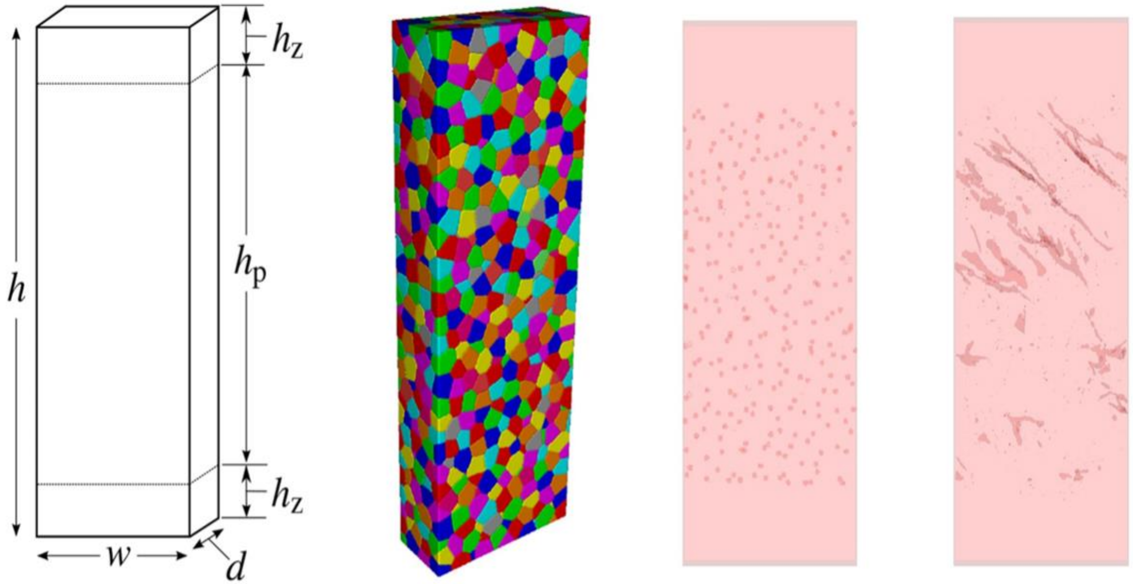
Common Multiscale Methods

- Direct Numerical Simulation
- Asymptotic (periodic) Homogenization
- FE2 Method
- Multiscale Aggregating Discontinuities Method
- Multiscale Finite Elements
- Variational Multiscale Method
- Variationally Consistent Homogenization
- Multiscale Projection

- Damage and fracture exhibit intrinsic multiscale behavior—damage forms first at the level of the microstructure around regions of localized stress, and propagates through regions of weakness
- Damage or cracks initiate on the small scale, but then grow to be macroscopic
- Multiscale damage is a hard problem because scales cannot be "sealed off" from one another
- This differs from traditional elasticity, where the only role of the microstructure is to determine the effective macroscopic constitutive relation (less information "passed up" from micro to macro)
- Direct numerical simulation of multiscale damage is prohibitively expensive

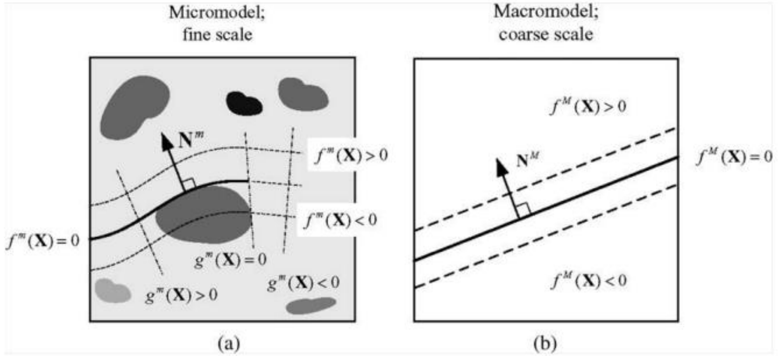
Direct Numerical Simulation of Fracture in Magnesium

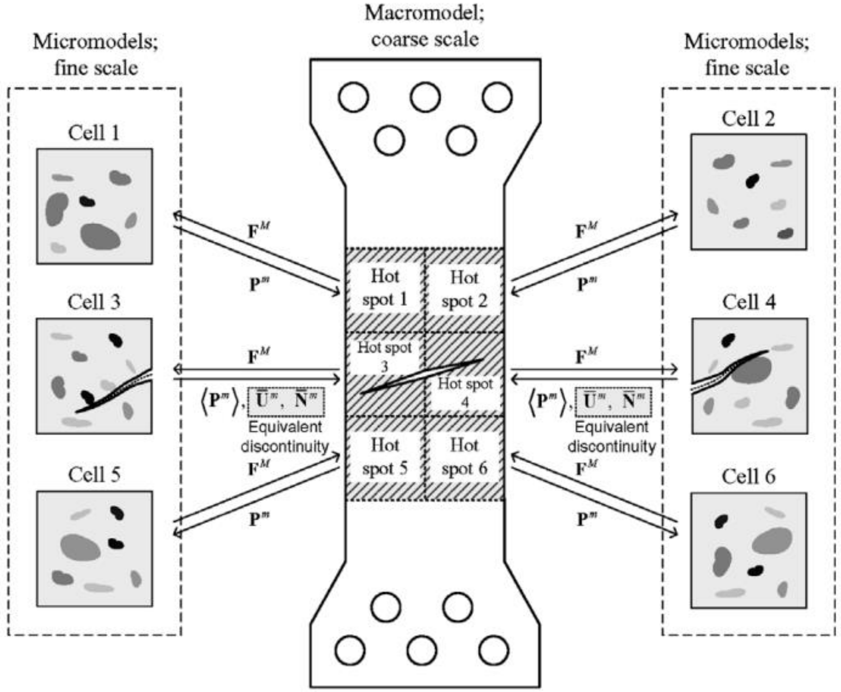
- Simple maximum tensile stress criteria used to reduce stress to zero within elements [82]
- Plasticity model used for material response leading up to failure
- Material microstructure resolved directly; possible to accurately model failure of material with simple criteria when material is modeled precisely



Multiscale Aggregating Discontinuities Method

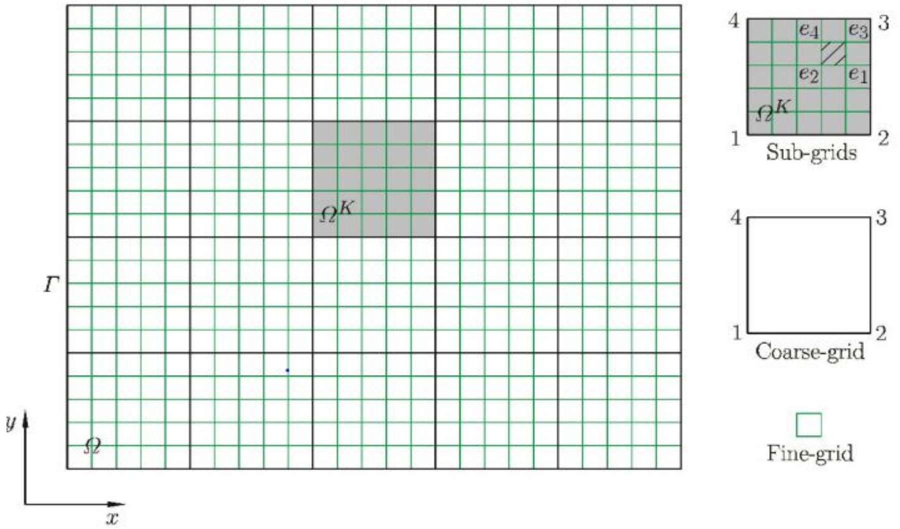
- In order to model the multiscale characteristics of damage, regions surrounding macroscopic discontinuity are termed "hot spots" and are given a microstructure [17]
- Sharp cracks on the micro and macro scales are represented with XFEM
- The average stress response of a cracked RVE is computed as a function of the macroscopic deformation
- Additionally, a coarse-grained displacement discontinuity (crack) is computed from the RVE and passed up to the macroscale
- Traditional homogenization boundary conditions on RVE are inadequate to capture deformation in presence of crack, thus "hourglass" modes are added
- Critical energy release rate and tensile strain fracture criteria used
- By computing the effective macroscopic damage from the microstructure, this method seeks to model the progression of damage from small to large scales

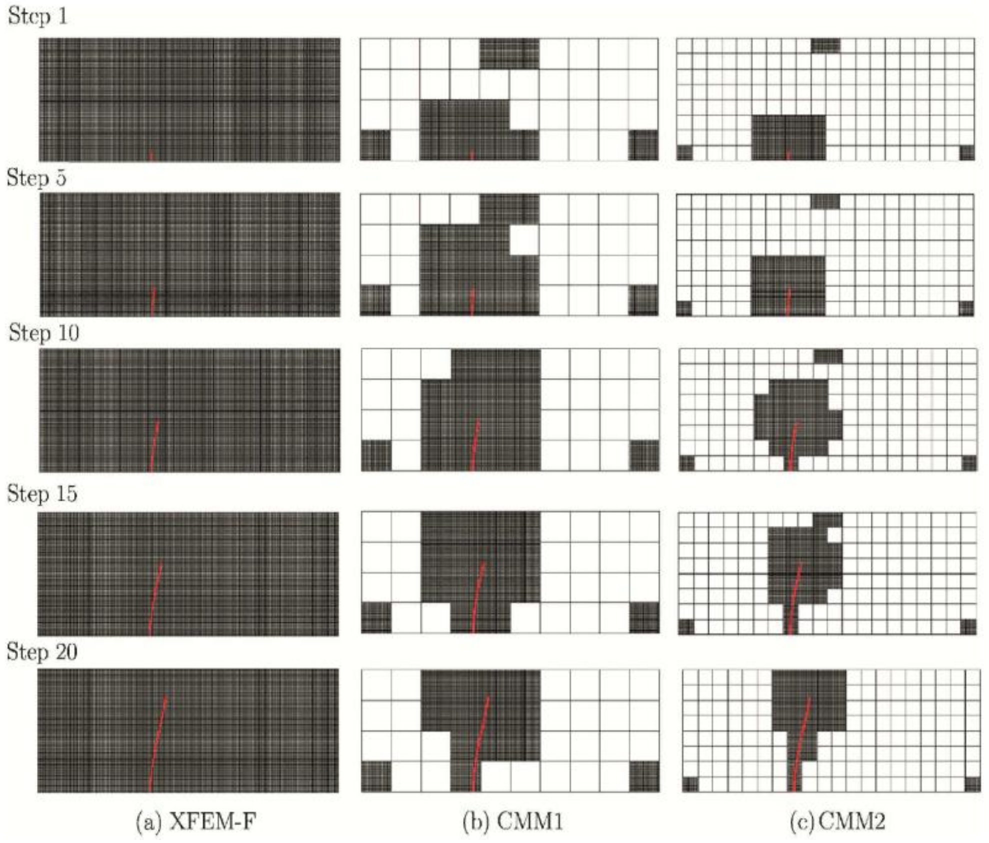




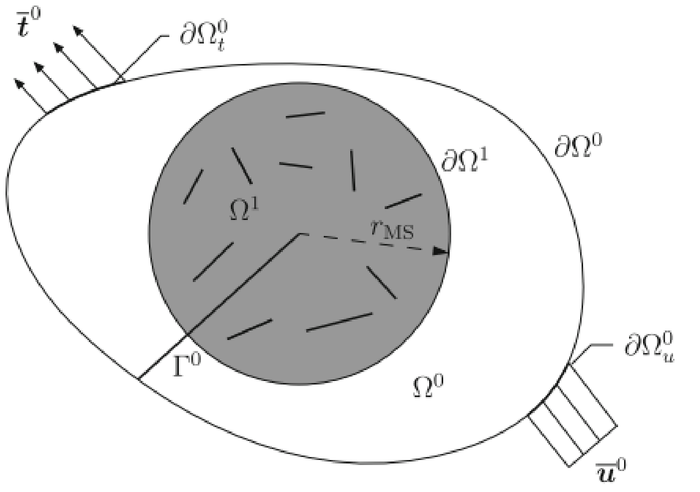
Multiscale Finite Element Method

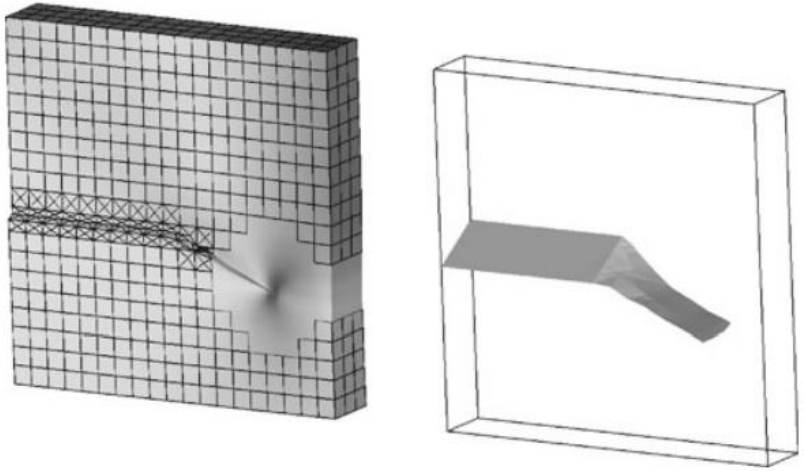
- Finite element basis functions with multiscale behavior can be constructed by solving BVP's on coarse elements [43]
- Level sets and XFEM used to track and represent crack
- Multiscale basis functions are used in vicinity of the crack, coarse mesh is used elsewhere
- Multiscale basis functions used as mesh refinement strategy rather than representation of material heterogeneity
- Crack advanced in fixed increments in the direction of maximum circumferential stress





3D Multiscale XFEM





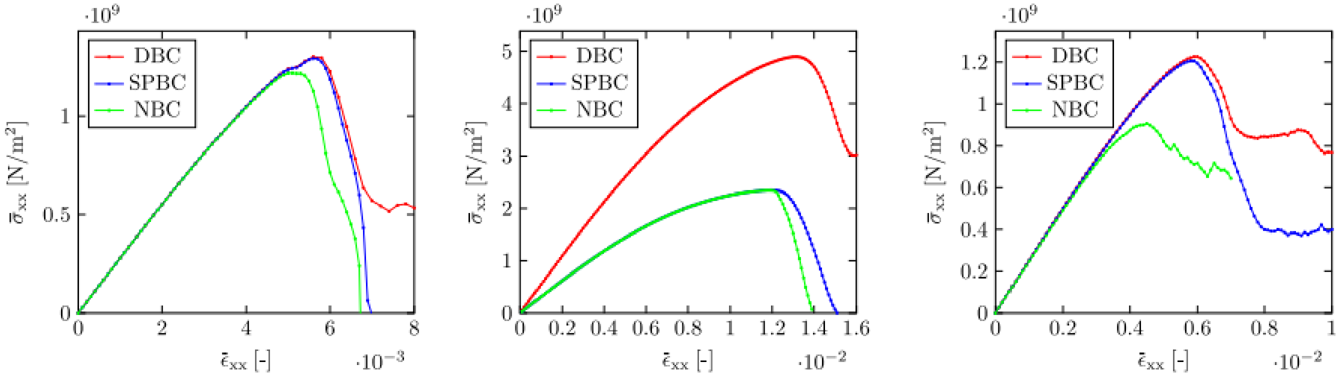
- Model brittle crack growth/progression in 3D solids using J-integral to compute stress intensity growth criterion, maximum hoop stress for growth direction, and level sets to track the crack [58]
- The influence of sub-grid microcracks is accounted for—this assumes finite scale separation but avoids costly single scale analysis of microcracks
- Mesh adaptively refined around the crack tip
- Primary original contribution is using XFEM in 3D, and the multiscale projection technique for upscaling influence of microcracks [59, 60]
- Fatigue analysis performed on model for gas turbine blade

Multiscale Phase Field 1

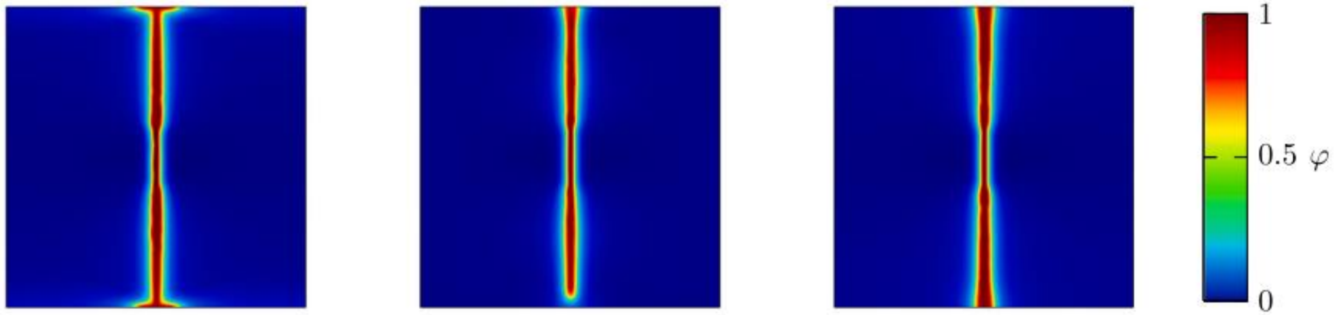
- Molecular dynamics simulations used on porous material to determine the energy release rate used in the phase field model from first principles [14]
- The calibrated phase field model is then used to model brittle fracture in heterogeneous material
- Interesting to determine constitutive parameter from microscale simulation, but this only seems interesting if used for the sake of uncertainty quantification (otherwise it can just be measured and forgotten about)

Multiscale Phase Field 2

- Phase field methods used to determine stress-strain response of damaging periodic RVE's [15]
- FE2 multiscale scheme used whereby each integration point in macroscopic structure has associated microstructure
- Scale coupling scheme specific to phase fields developed
- Average stress comes from damaged RVE driven by macroscopic strains
- Future work in comparison to experiment, different RVE boundary conditions, determination of length scale, more complex macroscopic structure and load case



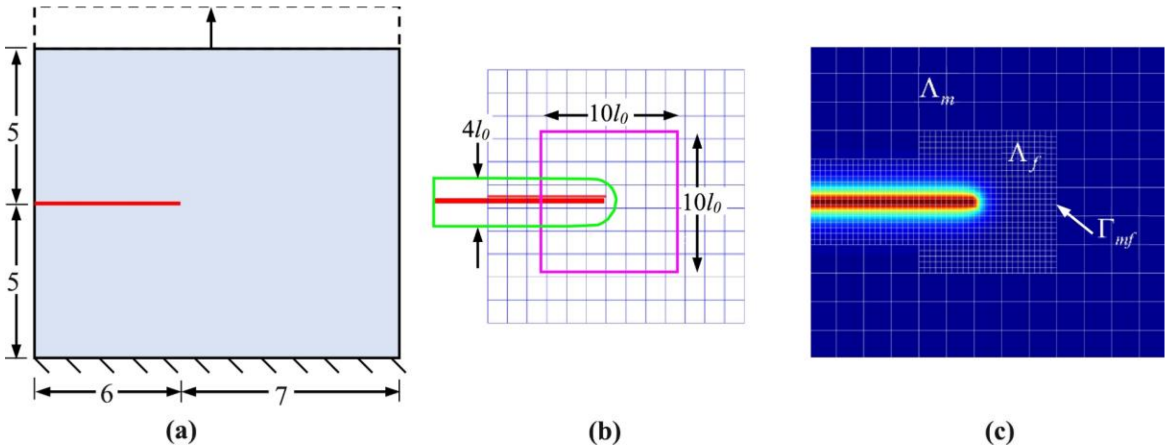
(a) RVE with single fracture (b) RVE with stiff inclusions (c) RVE with random fractures

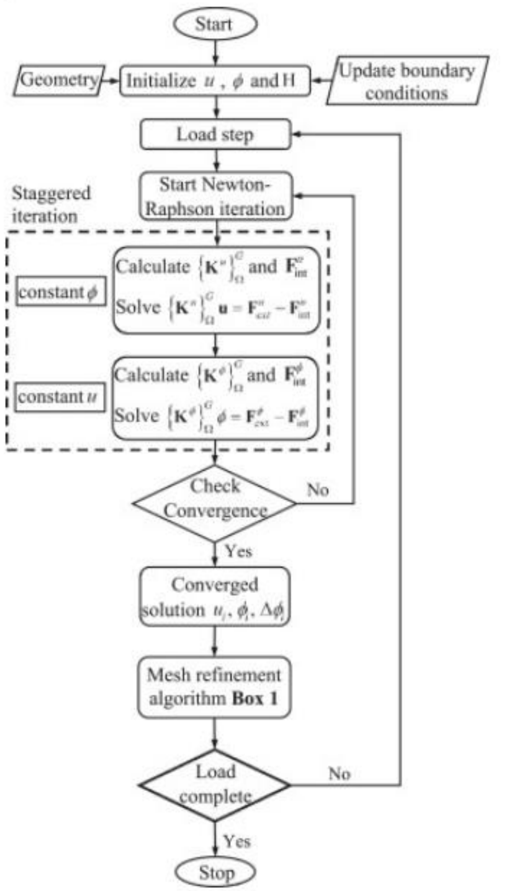


(a) DBC (b) NBC (c) SPBC

Multiscale Phase Field 3

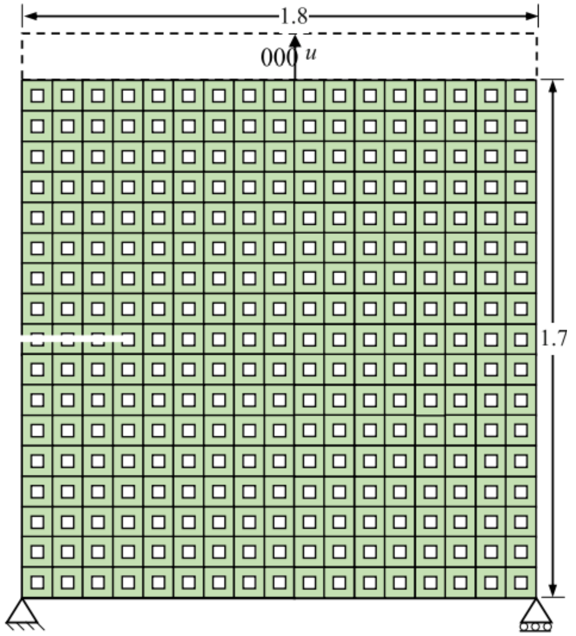
- Multiscale finite elements used as mesh refinement strategy near the crack [16]
- Analogous to use of multiscale finite elements with XFEM in [43]
- This reduces high computational cost of phase field method by refining mesh in efficient way in the vicinity of crack
- Does not incorporate multiscale heterogeneities of the material, though bi-material structures are analyzed

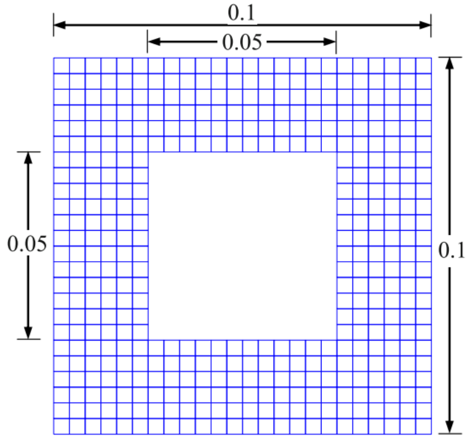


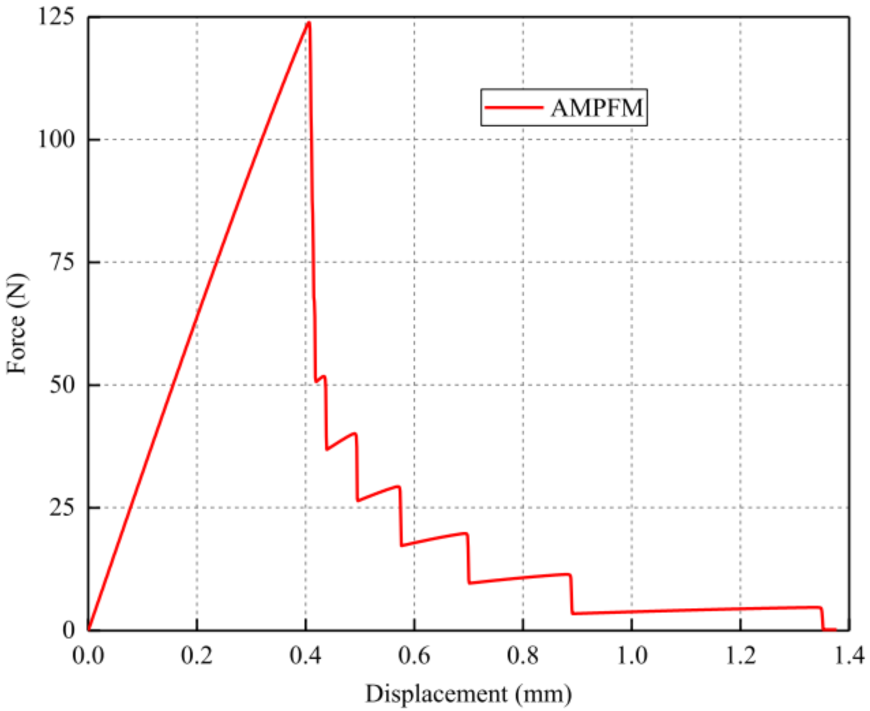


Multiscale Phase Field 4

- Multiscale finite elements used for adaptive mesh refinement near crack similar to [16] except that microscale heterogeneities are modeled in the area of refined mesh [53]
- XFEM is used in fine scale region in representing material boundaries, voids, and other discontinuities in the displacement field
- Phase field variable is continuous throughout domain
- Influence of periodic sub-grid heterogeneities are captured with multiscale finite element basis functions
- Load-displacement curves exhibit some sharp oscillations due to sub-grid voids



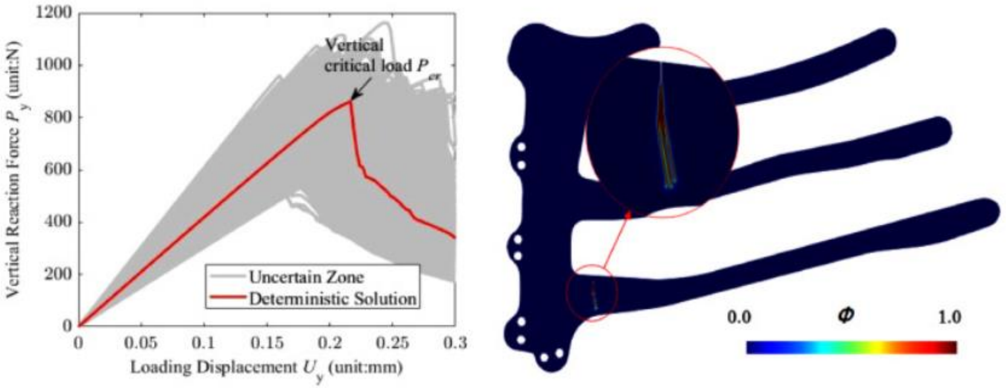




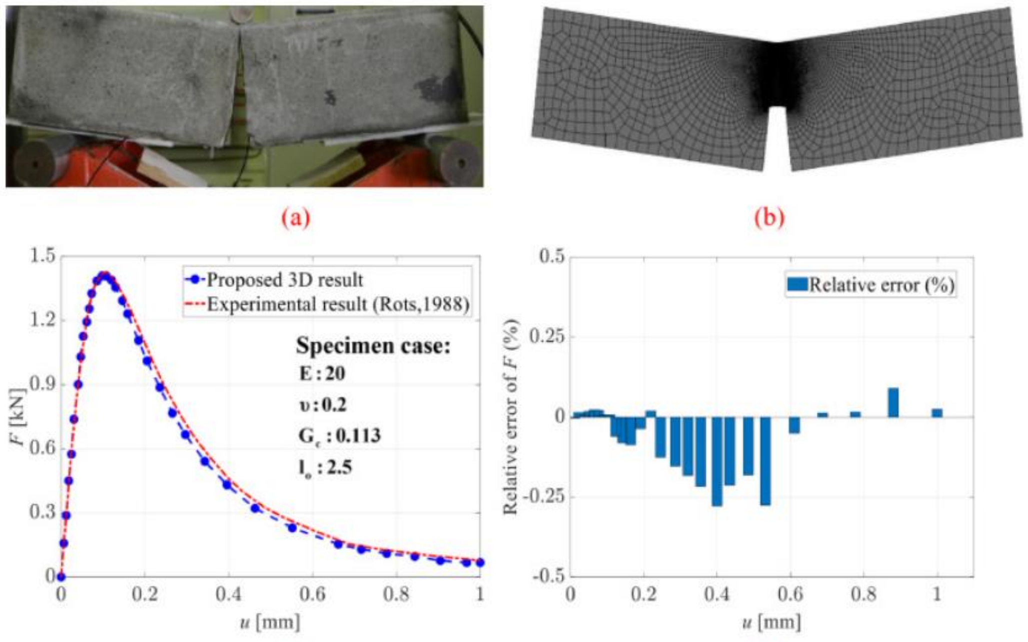
Stochastic Damage and Fracture Mechanics

Uncertainty Quantification with Phase Field Surrogate Model

- Data-driven surrogate model takes in sample of uncertain material and fracture parameters and predicts crack growth and force displacement curve [56]
- Training data generated Monte Carlo style with phase field fracture model
- Extended Support Vector Regression used to construct surrogate model
- Goal is facilitate to facilitate real-time safety assessment of cracked structures
- Stochastic surrogate model only as good as training data set, training data extremely expensive to produce



(a) (b)



(a) (b) (c) (d)

Phase Field Fracture Properties as Random Field

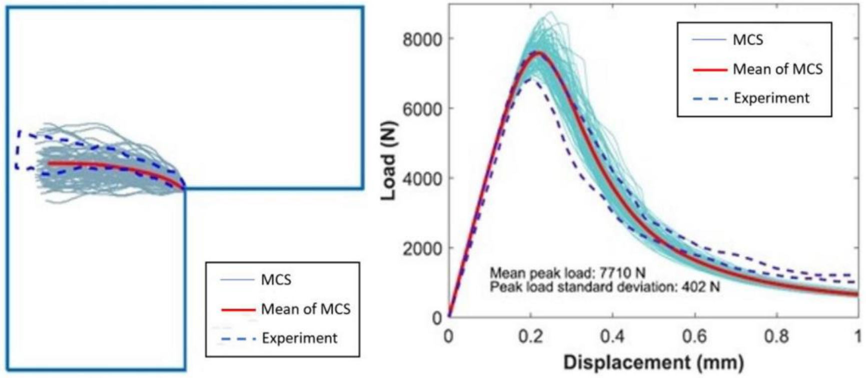
- Phase field model used with energy partition that enforces frictionless contact in compression of crack surfaces [63]
- Random field model fit to energy release rate parameter, impact of the assumed random field model (through its covariance) on fracture morphology studied
- Different covariance functions can lead to very different fracture properties
- A statistical inverse is problem to fit a phase field parameter to experimental data (brute force approach)
- Random fields must be sampled and then deterministic forward analysis performed, so this does not offer robust UQ framework

Sensitivity Analysis on Random RVE Properties

- Phase field model used to determine macroscopic energy release rate for double-notched RVE two-phase composite with random material properties [65]
- RVE fracture toughness evaluated for a variety of samples of random properties and fit with regression model
- Sensitivity analysis performed on regression model to determine which microscale properties have largest influence on overall fracture toughness
- No explicit UQ carried out, only deterministic solves at sampled values of random parameters
- Not clear that rigorous multiscale analysis is conducted here

Non-deterministic Fracture Mechanics

- Review paper for predicting fracture and damage arising from random materials and loading [57]
- In one example, Monte Carlo analysis used to predict distribution of crack paths and load-displacement curves for random field material properties
- Higher correlation length lead to greater variance in the output
- Data-driven surrogate models for UQ identified as future research direction
- Design of experiment recognized as important first step in construction of surrogate models



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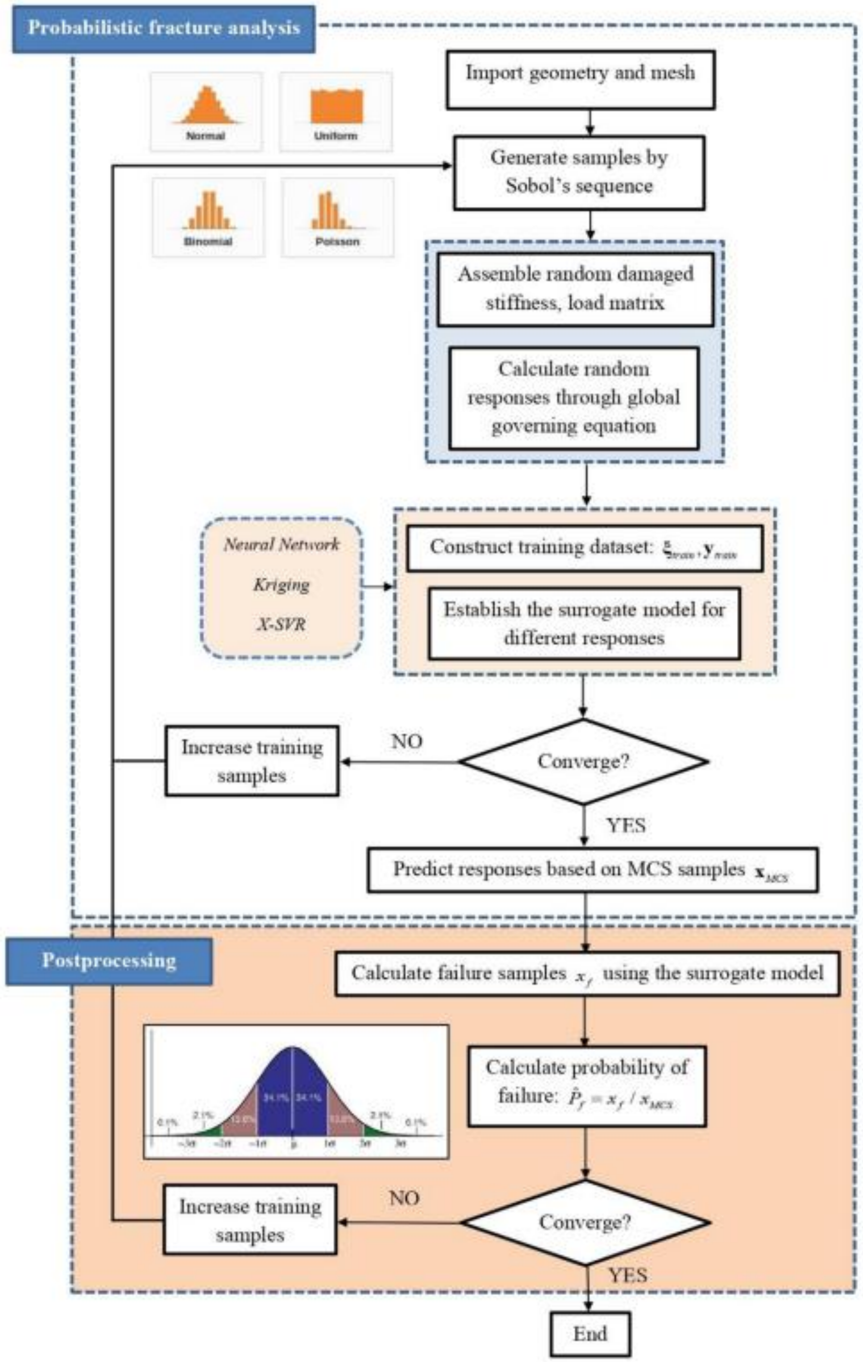
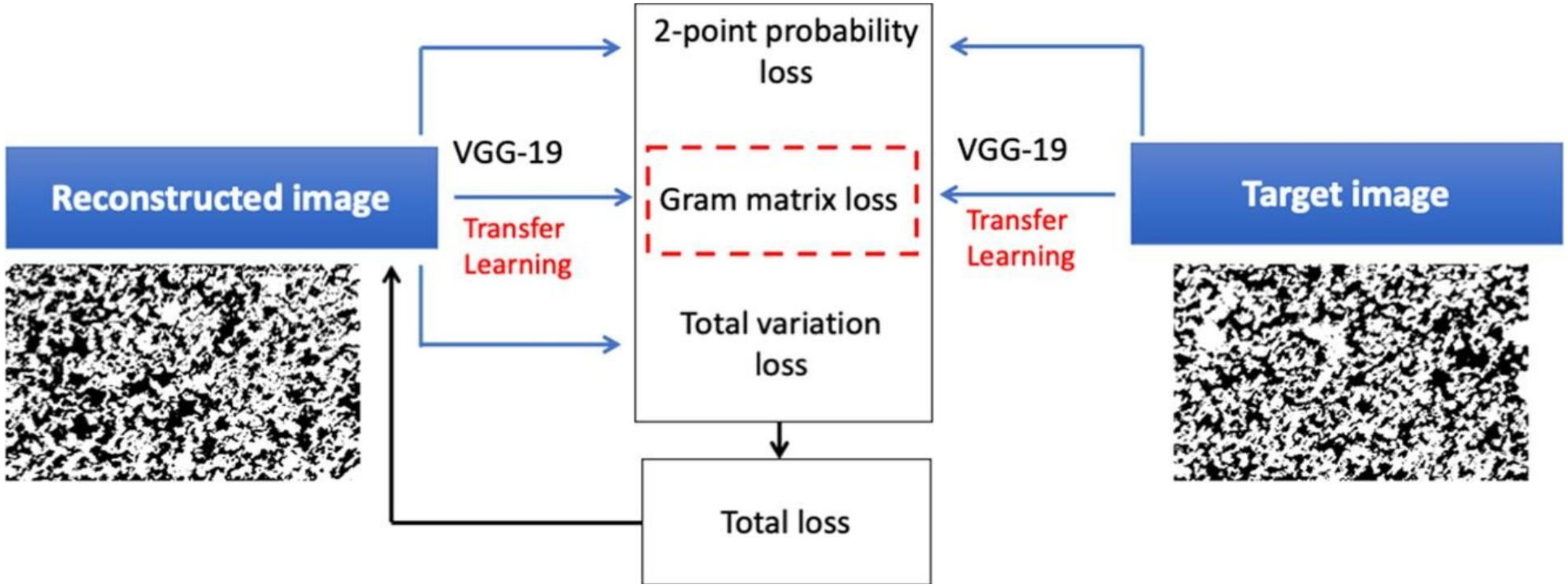


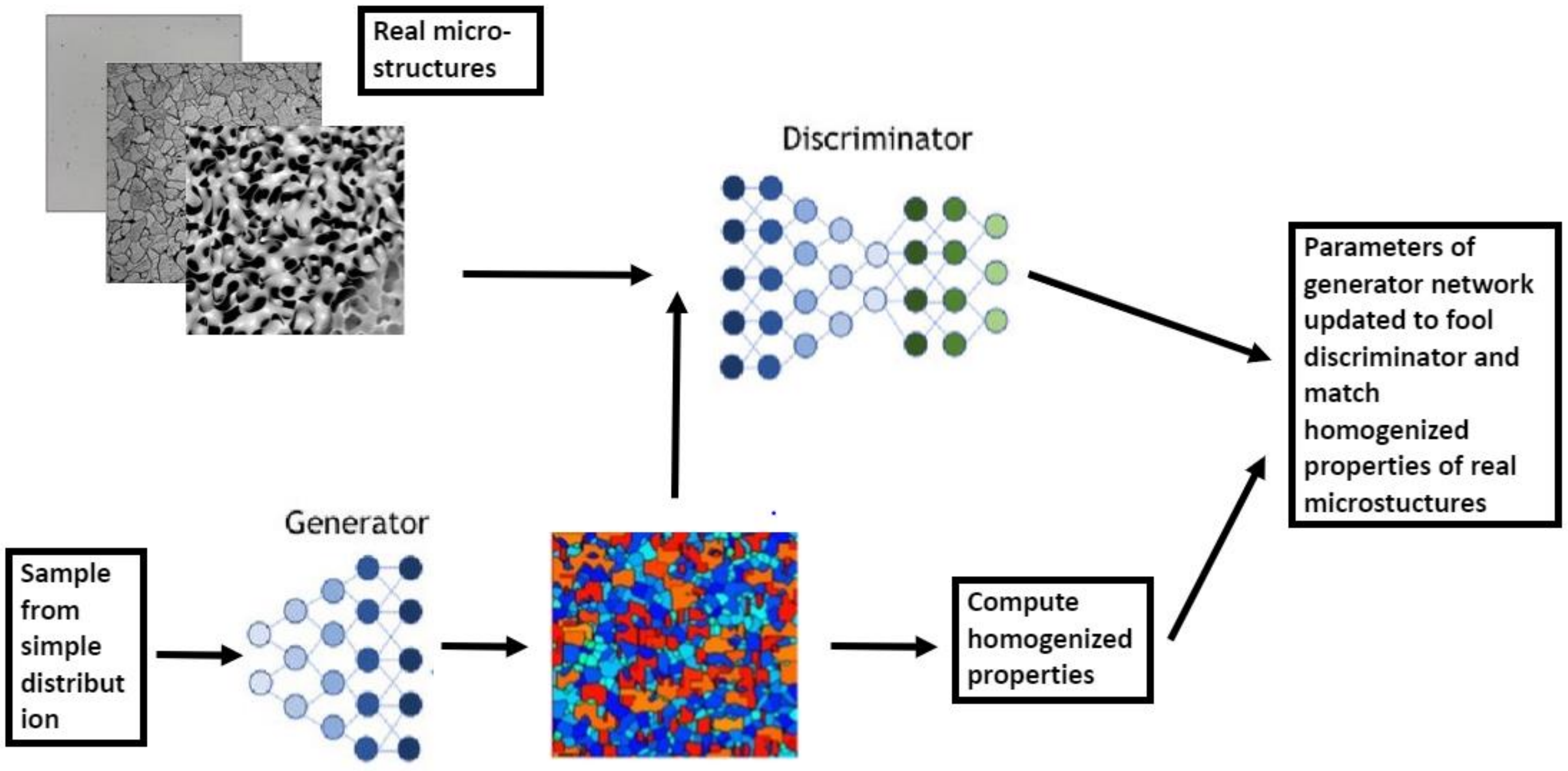
Machine Learning and Data-Driven Methods

Generative Models

- Data-driven generative models are useful for material reconstruction problems
- Novel material microstructures can be generated which are statistically equivalent to a training data set of real microstructures [10]
- Novel microstructures are useful in multiscale simulations and for uncertainty quantification



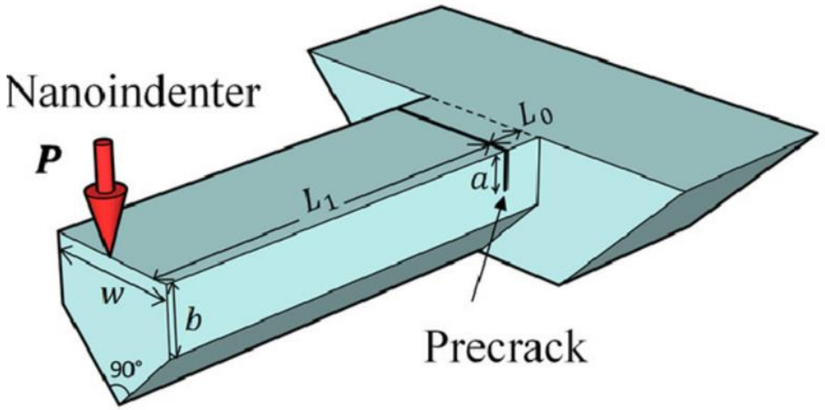
An idea for data-driven material reconstruction which leads to statistically and mechanically equivalent microstructures...



Glorified Curve Fitting

- For given class of structures J-integral used to find stress intensity as a function of geometry and load parameters [9]
- Large training data set generated by repeatedly running this analysis
- Neural network fit to training data and used to interpolate in training data set
- No physics or problem-specific knowledge incorporated here, neural network used simply as tool for non-linear regression
- Unimaginative and ceases to work when inputs/outputs are high-dimensional

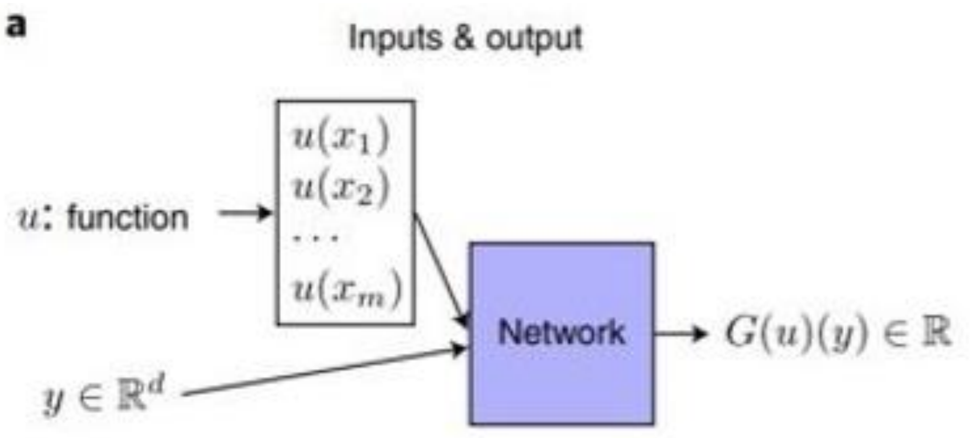
Fracture toughness measurement

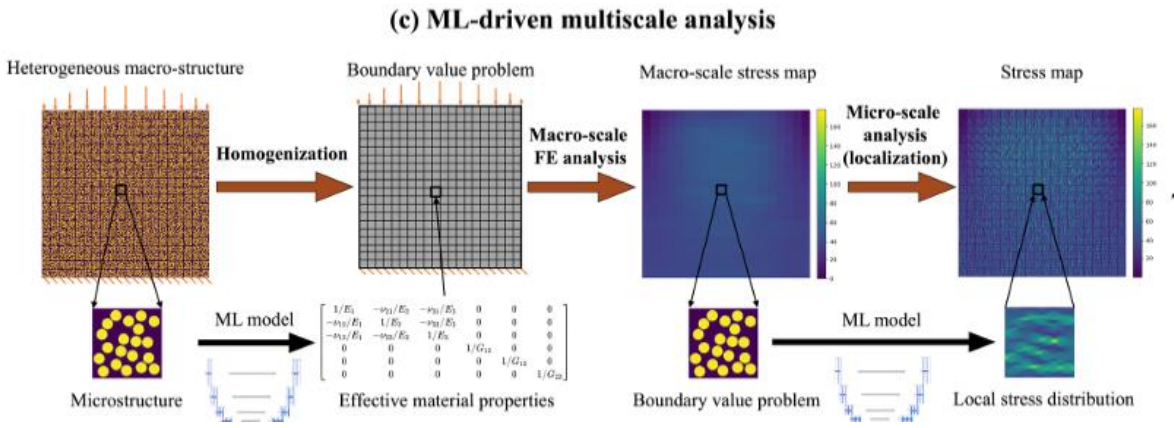


$$K_I = \Gamma(P, w, b, a, L_0, L_1)$$

Surrogate Models and Operator Learning

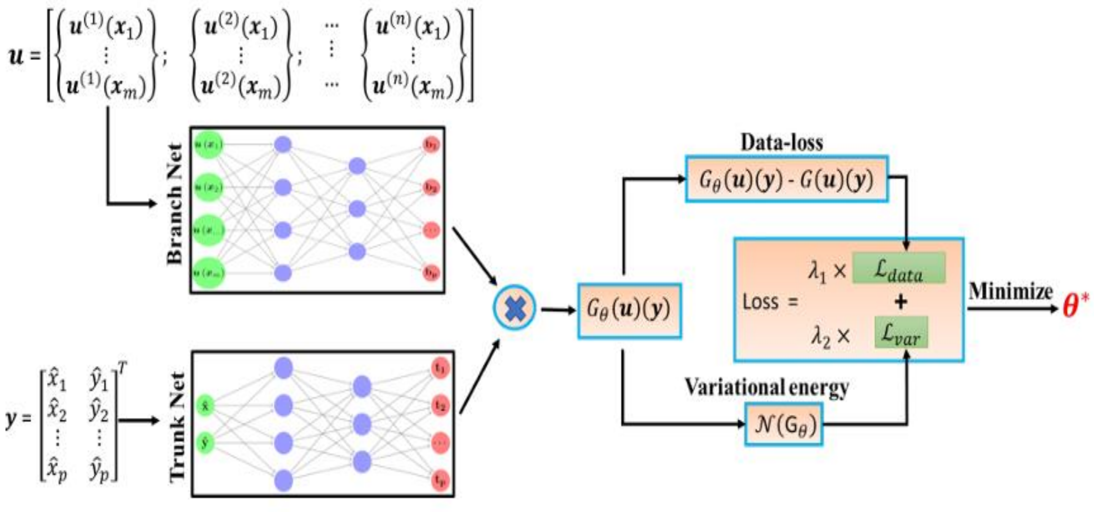
- Operator takes input in space of functions to output in space functions, often interpreted as a PDE (boundary data -> solution field) [8]
- DeepOnet learns the operator taking an input function to the solution field from data
- Inputs are sampled functions and therefore much higher dimensional
- Neural networks for operator learning are structured in a particular way (i.e. not classical fully-connected network)
- Surrogate model replaces solution of differential equations with forward pass through pre-trained network and can be used to expedite computational models [12]
- As a result of their reduced cost, surrogate models can facilitate uncertainty quantification through Monte Carlo methods—accuracy of surrogate model less important on run-by-run basis when distribution of output is quantity of interest





Physics-informed Networks

- Neural network surrogate model for predicting the crack path for given initial defects and applied displacement [7]
- Energy associated with phase field model used in addition to data loss in objective function
- This selects for models which respect physics of fracture problem while matching training data
- Experimental data can be used for training, but phase field model is still assumed as representative of underlying physics
- If no parameters of the phase field model are learned in training, its not clear why data is used
- Seems that this acts as a more efficient solution method for phase field problems which is informed in some way by data
- Simultaneously respecting known physics and fitting data is a powerful idea
- Note that neural networks can be used to solve PDE's with collocation methods in the absence of data



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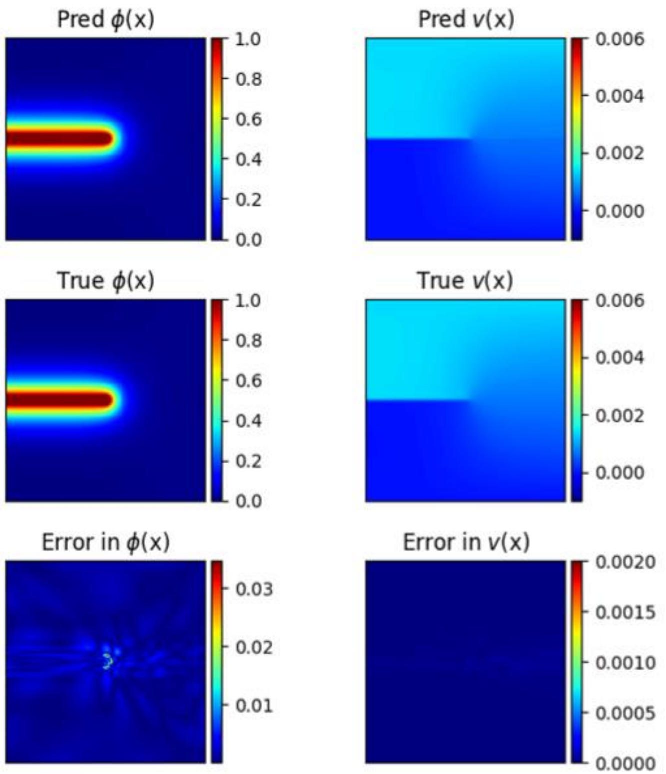


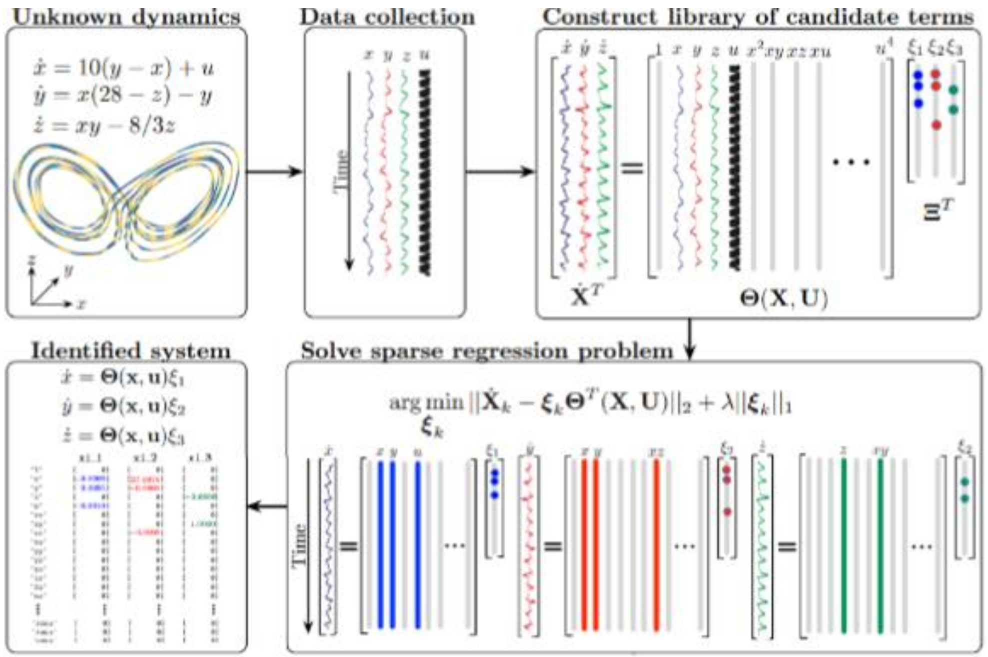
Partial Model Construction and Correction

- Neural networks can be used to represent empirical constitutive relationships within computational models
- Parameters of the network can be optimized so that solutions from the computational model match training data set [6]
- This departs from classical approaches to experimental characterization of constitutive models where simple tests are designed to isolate unknown parameters defining the constitutive relation
- Complex load states and component geometries can be used to determine constitutive relation; this is called "indirect' data
- Machine learning can also be used to learn corrections to simplified computational models by comparing against high-fidelity simulations or empirical data [5]

Model Discovery

$$\frac{\partial u}{\partial t} = \mathcal{N}(x, u, u_x, u_{xx}, \ldots; \theta)$$

- Governing differential equations for a system can be learned from data alone
- This can be done in the strong or weak form, with more or less assumptions on the underlying differential equation [24, 25]
- Derivatives compound adverse effects of noise in the data, making the model discovery problem difficult in practice
- Powerful and interesting idea—that the "rules" for the evolution of a system can be learned from data alone
- When the learned dynamics are used to make predictions, this departs from traditional "black box" conception of machine learning models



More Examples: Model-Free Fracture Mechanics

- Instead of fitting a function to an empirical constitutive relationship, the discrete measurement points are used so that the structure can only take on states that were experimentally observed [62]
- This is the general "model-free" framework, and it is applied to fracture mechanics problem
- Equilibrium is satisfied approximately by searching over discrete points in the data set
- Claims to reduce uncertainty induced by curve fitting by using the data directly—doesn't account for the fact that the data itself is uncertain...
- Novel and somewhat thought-provoking, but not informed by the important form of uncertainty which is that the experiments used to generate constitutive relations do not replicate

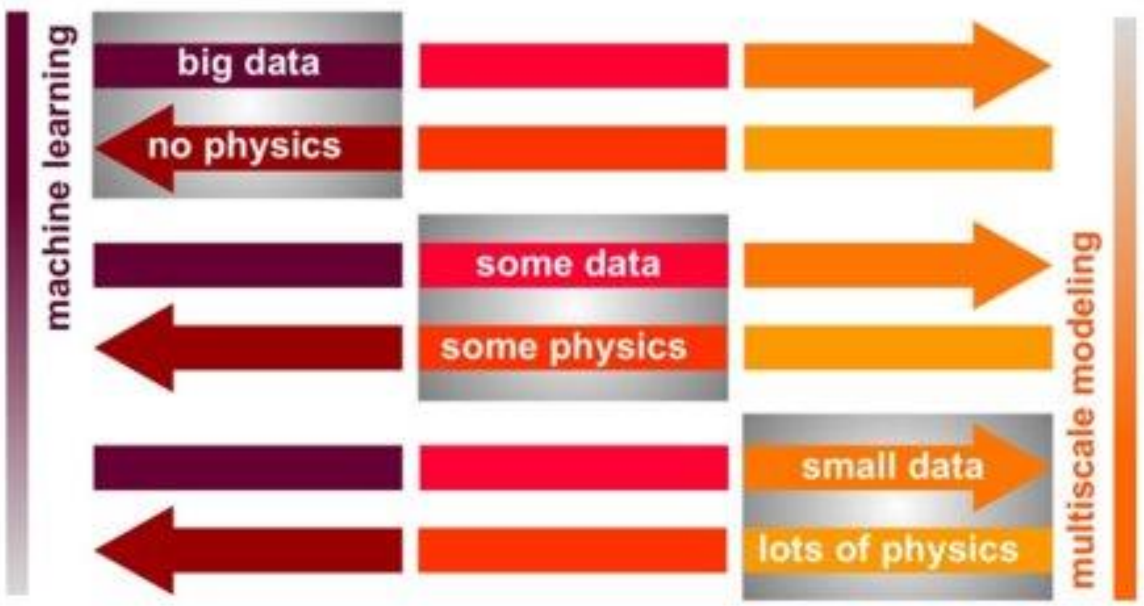
More Examples: Phase Field Parameter Estimation

- Bayesian approach used to calibrate elastic and fracture parameters of a material by comparing to experimental load-deflection curve of specimen [61]
- This a simple example of a model discovery framework, where a small-strain phase field model is assumed, and statistical estimation techniques are used to back out empirical constants from test data
- Minimizing distance between model prediction and experimental results can be ill-posed; Bayesian framework naturally incorporates prior knowledge of material parameters
- Prior probability distributions must be specified for the uncertain parameters to be estimated, polynomial chaos expansion can be used to estimate them
- Only one test specimen used for parameter estimation problem—could be interesting to use a variety of specimens and estimate the probability distributions on the uncertain material and fracture parameters
- Another parameter estimation approach is used where mean-squared error between model and experiment is the objective and surrogate models are used to grid search for a minimum over the length scale, Young's Modulus, and energy release rate [64]

Thoughts on Future Directions from the Literature

- "Future lines in integration of classical physics based with machine learning methods" [35]
- Promising use cases identified are: accelerating multiscale simulations with microstructural surrogate models, using neural networks to solve PDE's with and without data, invertible structure-property maps
- "Now it becomes possible to make predictions without this type of mechanistic [interpretable] 'understanding'—and 'understanding' is something may be redefined in the process" [37]
- Recommended future work: neural networks which better incorporate high-frequency (multiscale) characteristics of solution, standardization of meaningful benchmarks for data-driven physics problems, development of new mathematics for training convergence and error control of ML models

- "Most existing machine learning techniques identify correlations but are agnostic as to causality. In that sense, multiscale modeling complements machine learning: Where machine learning identifies a correlation, multiscale modeling can find causal mechanisms" [36]
- Recommended future work: use ML to identify missing information (do a set of input variables fully explain the output?), surrogate models for expensive simulations, supplementing data-driven models with physics to improve generalizability, formulating interpretable models which discover causal relationships

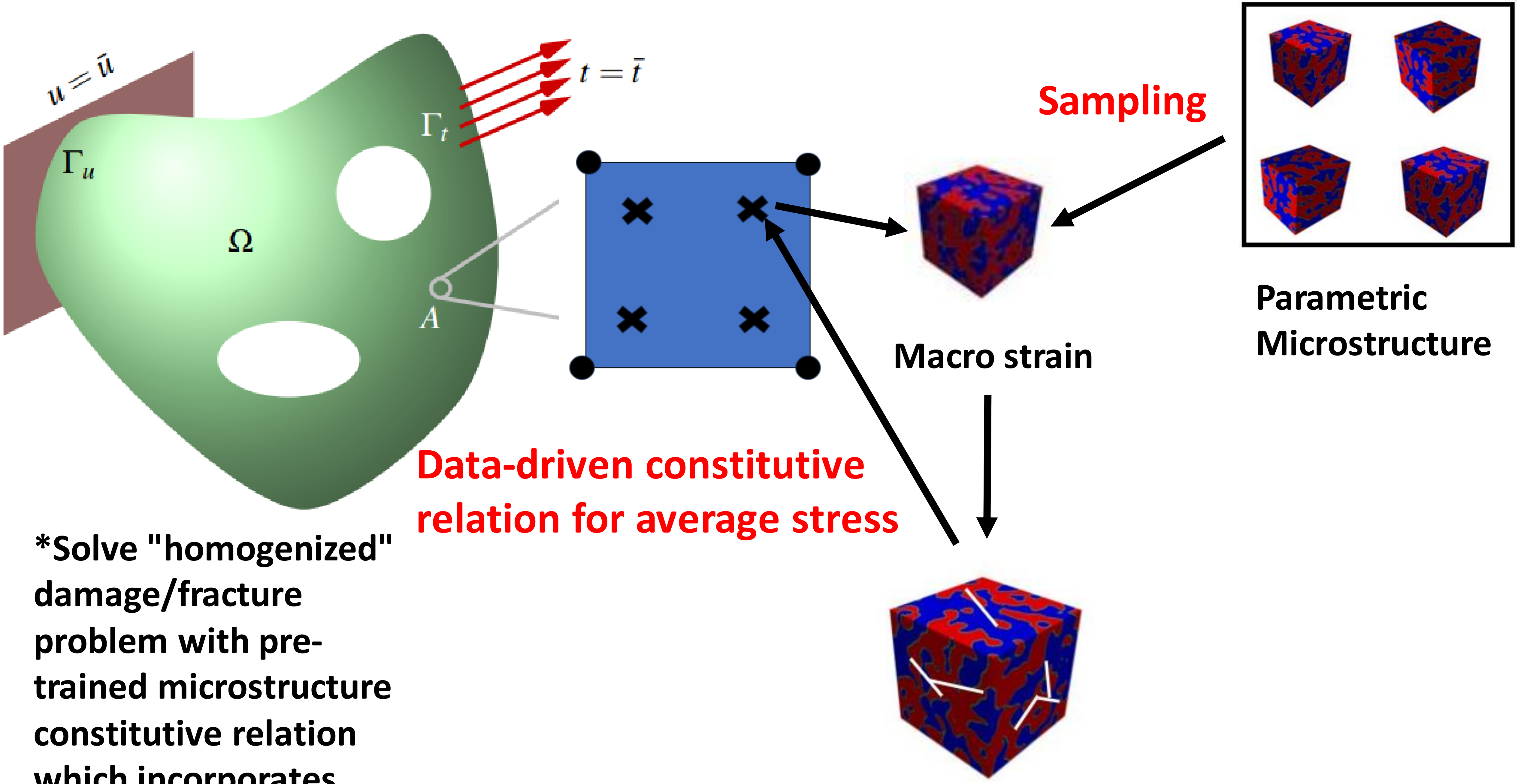


- Despite ML being the recurring theme in recommendations for future work, there is little serious discussion on two important sets of questions for machine learning in the context of computational mechanics
- First: can we enumerate general conditions which lead to success of ML models? These conditions help identify promising uses of ML in computational mechanics
- Second: what barriers exist for machine learning models to be implemented in industry and safety-critical settings? How can they be overcome or avoided?
- The second question requires insight into 1) how physics-based models are created and validated 2) how machine learning models differ from these classical approaches and 3) the industrial/legal context in which data-driven models will be introduced
- It seems that safety-critical applications of machine learning (autonomous vehicles) have lagged significantly behind other uses (chatGPT)—what does this mean for computational mechanics?

My Reflections on Open Problems and Future Directions

Offline Training of Stress-strain Relation of Damaging Microstructure

- In order to incorporate multiscale effects, the stress-strain response of a damaging stochastic microstructure could be simulated and fit
- Existing work on neural networks which incorporate physical constraints could be used to fit microstructural simulation data [11]
- Minimal effort has been made to do this in the case of damage or in stochastic setting
- Once trained, the constitutive response of the damaging microstructure could be incorporated into a macroscopic damage simulation
- The computational burden is transferred to generating data for the microstructure model, which is done offline
- Multiscale damage analysis can be conducted without real-time coupling of scales



Solve "homogenized" damage/fracture problem with pre-trained microstructure constitutive relation which incorporates damage

Explicit Uncertainty Quantification for Damage and Fracture Problems

- Predict a distribution of damage states in solids whose constitutive behavior is uncertain
- Need to understand how sensitive the state of the damage is with respect to the random heterogeneity of the material
- The stress-strain relation and damage/fracture behavior will depend on the microstructure, which varies in space and between parts
- Capturing probability distributions on damage fields for a component would allow designers to explicitly estimate the reliability of the part and design more aggressively
- Monte Carlo simulations probably too expensive for most realistic problems

Data-driven Damage Model Construction

- Use simulation or experimental data to estimate empirical parameters in a damage model (horizon in peridynamics, length scale in phase field methods, etc.)
- Represent empirical constitutive functions with neural networks in a given model and learn their form from data (energy degradation function and tension/compression split in phase fields, force function in peridynamics, etc.)
- Might multiple damage variables in phase fields representing different failure modes aid in fitting experimental data?
- Can progressively make fewer assumptions about the form of the model—is it possible to learn the entire damage model from data?
- Concern: models are severely underdetermined from data...how can damage even be identified in multifield problem when not explicitly observable? How can it be distinguished from hyperelastic constitutive relation? (Identifiability problem)
- As first step, data from simulations can be selectively used to mirror what is available from experiments (only measuring displacements on the surface, for example)
- Question: what is the right amount of structure to give a model before learning parameters from data?

Integrating Computational Damage Models with Topology Optimization

- There has not been extensive research in using phase fields or peridynamics in design optimization settings [49, 50, 51]
- These methods seem to offer an advantage over LEFM in practice because of the ability to model progressive damage and superior initiation criteria for damage
- A deterministic design problem might be: find a design which minimizes mass and for which the damage variable does not exceed a given threshold
- A stochastic design problem might be: find a design using an uncertain material which minimizes the mass and for which there is a certain probability that the damage variable does not exceed a given threshold
- These appear to be challenging but practical problems for which fracture mechanics is not particularly well-suited

Strong Emphasis on Needs of Practitioners

- Many researchers in the field do not motivate or constrain their work by a deep understanding of the needs of industry
- In practice, structures often do not need to be analyzed to the point of catastrophic failure
- Super high-fidelity damage models will be too expensive, complex, and material-specific to be practical in industry
- Uncertainty is an important consideration, as structural analysis is not performed on a part-by-part basis
- There is a trade-off between the complexity of the model, and its usability in practice—a balance must be struck
- Researchers using machine learning do not seem to think about practical barriers to its use in industry—error control, validation, liability, uninterpretability, etc.

Maybe: Bringing Renormalization Theory into Mechanics

- Mathematical tool from theoretical physics used to extract effective properties of a system
- Potentially furnishes continuous dependence of the effective response on the size of the domain over which effective properties are sought
- This could reduce need for assumptions on infinite scale separation coming from asymptotic homogenization, which is state-of-the-art in mechanics
- Minimal exploration of renormalization in solid mechanics [40, 41]
- Would be useful to know if it can be extended to multiscale solid mechanics problems

Others

- Multiscale enriched finite elements
- Machine Learning and VMS
- Stochastic Constitutive Models
- Learning Numerics

References

- [1]GraFEA https://paginas.fe.up.pt/~irf/Proceedings_IRF2020/data/papers/16004.pdf
- [2] Bonded Particle Method https://www.sciencedirect.com/science/article/pii/S1365160904002874
- [3] Microplane M7 Model https://www.semanticscholar.org/paper/Microplane-model-M7-for-plain-concrete.-I%3A-Caner-Ba%C5%BEant/4163a6d08aa326ddcaff83e3a062e15f3a2168e6
- [4] Micromorphic Damage https://www.sciencedirect.com/science/article/pii/S0020722511000644
- [5] ML Model Correction https://agupubs.onlinelibrary.wiley.com/doi/10.1029/2021MS002794
- [6] Learning Constitutive Relations from Indirect Data https://arxiv.org/abs/1905.12530
- [7] Variational DeepOnet for fracture https://arxiv.org/abs/2108.06905
- [8] DeepOnet paper https://arxiv.org/abs/1910.03193
- [9] Stress Intensity ML https://www.sciencedirect.com/science/article/pii/S1359645420302032

- [10] Material Reconstruction with Generative Models https://www.sciencedirect.com/science/article/abs/pii/S0927025621004365
- [11] Data-driven Hyperelastic Potential Function https://arxiv.org/abs/2302.02403
- [12] Microstructural Surrogate Model https://arxiv.org/abs/2212.14601
- [13] Element Deletion Method https://www.sciencedirect.com/science/article/abs/pii/S0141029617318217
- [14] Atomistic Phase Field https://www.osti.gov/servlets/purl/1251417
- [15] Periodic Multiscale Phase Field https://www.sciencedirect.com/science/article/pii/S0997753821000346
- [16] Other Multiscale Phase Field https://www.sciencedirect.com/science/article/pii/S0965997818305210#bib0052
- [17] Multiscale Aggregating Discontinuities https://www.sciencedirect.com/science/article/pii/S135983680900095X

- [18] Anisotropic LEFM https://www.sciencedirect.com/science/article/pii/0013794487901664
- [19] Generalized Griffith's Model with Cohesion https://www.sciencedirect.com/science/article/pii/S0045782507000230
- [20] Variational Approach to Fracture https://www.sciencedirect.com/science/article/pii/S0022509698000349
- [21] Computational LEFM with XFEM https://www.researchgate.net/publication/51992357_A_Finite_Element_Method_for_Crack_Growth_without_Remeshing
- [22] Computational LEFM (Fatigue) https://www.sciencedirect.com/science/article/pii/S0013794406000257
- [23] Computational LEFM with XFEM and Crack Growth Criteria https://onlinelibrary.wiley.com/doi/epdf/10.1002/nag.560
- [24] SINDy https://arxiv.org/abs/1711.05501
- [25] Weak SINDy https://arxiv.org/abs/2007.02848

- [26] Bond-based Peridynamics https://www.sciencedirect.com/science/article/pii/S0022509699000290
- [27] State-based Peridynamics https://www.sciencedirect.com/science/article/pii/S0020768308004496
- [28] Phase Field Review https://www.sciencedirect.com/science/article/pii/S0065215619300134
- [29] Cohesive Zone Model https://www.sciencedirect.com/science/article/pii/0022509660900132
- [30] Mixed-mode Fracture Criteria https://www.sciencedirect.com/science/article/pii/S0167844222004906
- [31] Lallit Anand "Mechanics of Solid Materials"
- [32] T.L. Anderson "Fracture Mechanics"
- [33] Thermodynamically Consistent Phase Field https://onlinelibrary.wiley.com/doi/10.1002/nme.2861

- [34] JH Song Phase Field https://www.sciencedirect.com/science/article/pii/B9780128141069000164
- [35] Machine Learning and Computational Mechanics https://link.springer.com/chapter/10.1007/978-3-030-87312-7_27
- [36] Machine Learning and Multiscale Modeling https://link.springer.com/article/10.1007/s11831-020-09405-5
- [37] Physics Informed Learning Review https://www.nature.com/articles/s42254-021-00314-5
- [38] Phase Field Fatigue https://link.springer.com/chapter/10.1007/978-3-030-87312-7_2
- [39] Thermoelastic Phase Field https://www.sciencedirect.com/science/article/pii/S0045782520308331
- [40] Renormalization in Mechanics 1 https://www.sciencedirect.com/science/article/abs/pii/S0045782512000242
- [41] Renormalization in Mechanics 2 https://www.sciencedirect.com/science/article/abs/pii/0020768394901074

- [42] Calibrating traction-separation law https://www.veryst.com/case-studies/cohesive-zone-model-czm-calibration
- [43] Multiscale finite element method crack propagation https://www.sciencedirect.com/science/article/pii/S0894916615300112
- [44] Variational multiscale method
- [45] Peridynamic horizon https://link.springer.com/article/10.1007/s00161-020-00896-y
- [46] Bazant comparison https://www.semanticscholar.org/paper/Critical-Comparison-of-Phase-Field%2C-Peridynamics-M7-Ba%C5%BEant-Nguyen/e0a5fba6eb44902e86a5f058b3092448ada4c3f2
- [47] Gradient Damage https://pure.tue.nl/ws/files/1428273/605429.pdf
- [48] Phase field ductile fracture https://www.sciencedirect.com/science/article/pii/S2352492823003173

- [49] Phase field design optimization https://onlinelibrary.wiley.com/doi/full/10.1002/nme.6340
- [50] Phase field design optimization ductile fracture https://arxiv.org/abs/2302.12583
- [51] SIMP phase field design optimization https://hal.science/hal-03225114/file/%5B88%5DPP.pdf
- [52] Multiscale phase field (no access) https://ui.adsabs.harvard.edu/abs/2018AGUFM.H21P1925H/abstract
- [53] Phase fields with microstructure https://www.sciencedirect.com/science/article/pii/S0045782517306515#:~:text=Adaptive%20multiscale%20phase%20field%20method%20(AMPFM)%20is,proposed%20to%20simulate%20brittle%20fracture.&text=Refined%20mesh%20in%20vicinity%20of,coarse%20mesh%20and%20vice%20versa.&text=Use%20of%20AMPFM%20leads%20to,as%20compared%20to%20standard%20PFM.
- [54] Heterogeneous materials and 3D example https://www.sciencedirect.com/science/article/pii/S0013794415001332
- [55] Phase fields with experimental testing in 3D concrete (dissertation) https://www.researchgate.net/publication/294219030_Modeling_of_complex_microcracking_in_cement_based_materials_by_combining_numerical_simulations_based_on_a_phase-field_method_and_experimental_3D_imaging

- [56] Machine learning, uncertainty quantification, phase fields https://www.sciencedirect.com/science/article/pii/S0020722521001294
- [57] Non-deterministic fracture mechanics review https://www.sciencedirect.com/science/article/pii/S0045782523002268
- [58] 3D multiscale XFEM turbine blade https://link.springer.com/article/10.1007/s00466-013-0900-5
- [59] Original multiscale projection method (Belytschko, no access) https://onlinelibrary.wiley.com/doi/10.1002/nme.2001
- [60] Multiscale methods for fracturing solids (book with multiscale projection chapter) https://link.springer.com/chapter/10.1007/978-1-4020-9090-5_7
- [61] Bayesian parameter estimation phase fields https://link.springer.com/article/10.1007/s00466-020-01942-x
- [62] Ortiz model-free fracture mechanics https://www.sciencedirect.com/science/article/pii/S0022509621002131

- [63] Phase field with frictionless contact and stochastic energy release rate https://www.sciencedirect.com/science/article/pii/S0045782520302905#b47
- [64] MSE Phase field and XFEM parameter estimation https://link.springer.com/chapter/10.1007/978-3-030-47638-0_13
- [65] Random RVE proprties to determine energy release rate using phase fields https://www.sciencedirect.com/science/article/pii/S0263822315007345
- [66] Effective toughness for heterogeneous media (not read) https://www.sciencedirect.com/science/article/pii/S0022509614001215?via%3Dihub
- [67] Stochastic multiscale crack modeling (contains good multiscale damage references) https://onlinelibrary.wiley.com/doi/10.1002/nme.6093
- [68] RVE different boundary conditions (not read) https://www.sciencedirect.com/science/article/pii/S0045782510001908?via%3Dihub
- [69] Failure zone averaging, existence of RVE's in softening materials (not read) https://www.sciencedirect.com/science/article/pii/S0045782510001854?via%3Dihub

- [70] Information bottleneck principle for deep networks 1 https://arxiv.org/abs/1503.02406
- [71] Information bottleneck review (tradeoff between compression and prediction, different perspective on deep learning) https://arxiv.org/abs/1904.03743
- [72] Micromorphic reference (Regueiro) https://onlinelibrary.wiley.com/doi/10.1002/nme.6991
- [73] Christan Linder research group (Stanford, multiscale fracture, phase fields) https://cm2.stanford.edu/research
- [74] Learning plastic constitutive relations https://www.sciencedirect.com/science/article/pii/S2352431622000244
- [75] Learning traction-separation laws with reinforcement learning (Steve Sun, "game" framework) https://www.sciencedirect.com/science/article/pii/S0045782518305851
- [76] Phase fields with concrete (experimental validation) https://www.sciencedirect.com/science/article/pii/S0045782522003413#sec4

- [77] Phase fields with additively manufactured metals (experimental validation) https://www.sciencedirect.com/science/article/pii/S0020740323002266#sec0013
- [78] Phase fields with aluminum (experimental validation) https://www.sciencedirect.com/science/article/pii/S0045782522000068#sec5
- [79] Phase fields with composites (decent experimental agreement) https://www.sciencedirect.com/science/article/pii/S0997753823001274
- [80] Phase fields with hyperelastic materials (experimental validation) https://www.sciencedirect.com/science/article/pii/S001379442030816X
- [81] Phase fields with brittle mortar material (experimental validation) https://www.sciencedirect.com/science/article/pii/S0013794417301169#s0035
- [82] DNS of magnesium fracture https://www.sciencedirect.com/science/article/pii/S0749641918303243
- [83] Microstructural patches and "handshake" regions https://www.sciencedirect.com/science/article/pii/S0021999105003608

- [84] 1D "handshake" coupling of particle model and finite element https://www.emerald.com/insight/content/doi/10.1108/EC-09-2014-0184/full/html
- [85] Jacob Fish—Practical Multiscaling
- [86] Neural networks and topology optimization (learning design sensitivities) https://www.sciencedirect.com/science/article/pii/S0045782519306292#b28
- [87] Neural networks and topology optimization (learning optimized design, using it to initialize) https://www.tandfonline.com/doi/full/10.1080/21681163.2015.1030775
- [88] Eigen-erosion damage model https://www.sciencedirect.com/science/article/pii/S0013794417302989
- [89] Multiscale strain-softening (has "homogenized" damage parameter) https://www.sciencedirect.com/science/article/pii/S004578251730710 7
- [90] Phase field and gradient-enhanced damage comparison 1 https://www.sciencedirect.com/science/article/abs/pii/S0013794418311986

- [91] Gradient-enhanced damage https://www.sciencedirect.com/science/article/abs/pii/S0045782517301275#b57
- [92] Phase field and gradient-enhanced damage comparison 2 https://www.sciencedirect.com/science/article/pii/S2452321621003097

Appendices

What is learnable in phase field model?

Crack density

General anisotropic phase field model

$$\Pi(u,\phi) = \int_\Omega \frac{1}{2}\Big[g(\phi)\Psi^+(x,u(x)) + \Psi^-(x,u(x))\Big]d\Omega + \int_\Omega \frac{G_c(x)}{2\ell}\Big(\phi^2 + \ell^2\nabla^2\phi\Big)d\Omega - \int_\Omega b\cdot u\,d\Omega - \int_{\partial\Omega} t\cdot u\,dS$$

Energy degradation

Tensile energy

Anisotropic phase field model with learnable energy degradation, energy partition, and length scale

$$\Pi(u,\phi;\theta_1,\theta_2,\theta_3,\ell) = \int_\Omega \frac{1}{2}\Big[\mathcal{N}_1(\phi;\theta_1)\mathcal{N}_2(x,u(x);\theta_2) + \mathcal{N}_3(x,u(x);\theta_3)\Big]d\Omega + \int_\Omega \frac{G_c(x)}{2\ell}\Big(\phi^2 + \ell^2\nabla^2\phi\Big)d\Omega - \int_\Omega b\cdot u\,d\Omega - \int_{\partial\Omega} t\cdot u\,dS$$

Anisotropic phase field model with learnable energy degradation, energy partition, length scale, and correlation length of random variation in energy release rate

$$\Pi(u,\phi;\theta_1,\theta_2,\theta_3,\lambda,\ell) = \int_\Omega \frac{1}{2}\Big[\mathcal{N}_1(\phi;\theta_1)\mathcal{N}_2(x,u(x);\theta_2) + \mathcal{N}_3(x,u(x);\theta_3)\Big]d\Omega + \int_\Omega \frac{\sum_i g_i(\xi) f_i(x;\lambda)}{2\ell}\left(\phi^2 + \ell^2\nabla^2\phi\right)d\Omega - \int_\Omega b\cdot u d\Omega - \int_{\partial\Omega} t\cdot u dS$$

- Neural networks and learned parameters must satisfy physical constraints
- Might reasonably think of length scale and correlation length as material parameters
- Allowing for stochastic energy release rate (and potentially stress-strain relation) is first pass at multiscale damage model
- Can calibrate directly on simulation data as proof of concept
- Question: can multiple damage fields better match data? Is this necessary? If so, under what conditions?