

To the Graduate Council:

I am submitting herewith a thesis written by Giang D. Huynh entitled “Hyperbolic Phase Field Models for Dynamic Fracture and Fragmentation.” I have examined the final paper copy of this thesis for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Applied Mechanics.

Reza Abedi, Major Professor

We have read this thesis
and recommend its acceptance:

Stephanie Ter Maath

Timothy Truster

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Accepted for the Council:

Dixie L. Thompson

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(Original signatures are on file with official student records.)

Hyperbolic Phase Field Models for Dynamic Fracture and Fragmentation

A Dissertation Presented for the
Doctor of Philosophy
Degree
The University of Tennessee, Knoxville

Giang D. Huynh

December 2024

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"If there is one thing we try to teach our students, ready to learn to be physicists, it is that everyone gets confused and stuck. Very few people understand difficult concepts the first time they encounter them, and the way to a deeper understanding is to move forward with small steps. In the words of Douglas Adams: 'Don't panic!'"-by Theoretical physicist, Brian Cox.

Abstract

Fracture is a prevalent phenomenon in engineering structures, critically influencing their lifespan. Fragmentation has gained significant attention within engineering and academic communities, given its diverse application applications, such as in military armor and projectile design, as well as for its complex mechanisms. This process often occurs when a high-velocity impactor collides with a target object, breaking it into numerous smaller pieces called fragments. The formation of these fragments is triggered by micro-scale flaws or defects and gradually evolves into macrocracks. As a result, this phenomenon encompasses multiple scales and rate effects, making it challenging to model computationally.

Numerical models of fracture can be categorized into smeared and discrete approaches. The smeared approach regularizes a sharp crack using a continuous damage variable, and is favored over the discrete approach due to its simplicity in tracking evolving cracks without requiring additional criteria for crack kinking and branching. As a smeared approach, the phase field method has demonstrated success in engineering applications. Nonetheless, its application to fragmentation has remained limited, mainly due to its difficulty in cleanly resolving fragment boundaries, relative to sharp crack models. Additionally, the nonconvex nature of coupled governing equations necessitates the use of optimization solvers or complex numerical schemes, giving rise to increased computational costs.

This work aims to address these challenges. A phase field approach is proposed, adhering to a thermodynamically-consistent framework, applicable to both brittle and

ductile fracture. Particularly, the evolution equation is formulated using different types of partial differential equations (PDEs), enabling it to accommodate a wide range of strain rates while ensuring efficient, robust, and straightforward numerical solvers. An extensive mathematical analysis on low dimensions of the presented models is conducted to gain insight in rate-dependency of the phase field models on fragmentation response, in which analytical and numerical solutions are provided. As fragments are initiated from weak points within microstructures, material properties can be treated as random fields in the presented numerical models, reducing mesh dependency and accounting for realistic heterogeneity of materials in nature.

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Chapter 1

Introduction

Understanding the failure mechanisms of solids and structures is a fundamental concern in engineering design, driven by both economic imperatives and safety considerations. Among the primary failure mechanisms, fracture plays a crucial role in defining the lifespan of engineering products. Fracture occurs when a material's stress state exceeds a critical threshold, leading to the initiation and growth of cracks. Under high-rate loading, materials can undergo fragmentation, breaking into multiple smaller pieces due to significant energy input. Fragmentation occurs across a variety of applications, including military armor systems designed to withstand ballistic impacts [1], aerospace components subjected to high-velocity impacts [2], and oil and gas extraction where hydraulic fracturing is used to enhance resource recovery [3]. Despite the preference to prevent fracture and fragmentation, controlling these phenomena predictably and effectively is essential in cases where they are unavoidable.

1.1 Overview of the topic

1.1.1 Failure mechanisms at high rates

The fragmentation mechanism is inherently complex and involves multiple scales. It starts with microscale defects or voids that develop into macrocracks, ultimately leading to the disintegration of the material into fragments [4]. At lower loading rates, newly formed cracks release stress waves that unload the surrounding material, inhibiting further crack propagation—a phenomenon known as crack arrest. In contrast, at higher loading rates, the material does not have sufficient time to adjust to rapid loading, leading to chaotic stress wave interactions that accelerate crack propagation and drive the material toward complete fragmentation.

To predict the behavior of dynamic fragmentation, Grady [5] proposed an energy balance model, suggesting that newly created cracks result from the potential energy of cracked surfaces equilibrating with local kinetic energy. Glenn *et al.* [6] further refined this by incorporating the elastic energy of fragments into the balance.

Although these models provide insights into fragment size distribution, they often predict sizes larger than those observed in experiments. More advanced models, such as those proposed by Miller *et al.* [7] and Drugan [8], incorporate cohesive zone descriptions that account for time-dependent deformation and crack evolution.

1.1.2 Computational methods for fracture and fragmentation

Despite theoretical advancements, the complexity of dynamic fragmentation necessitates computational modeling to capture interactions among stress waves, crack initiation, propagation, and coalescence. Classical numerical models for fracture are broadly divided into smeared and discrete approaches. In discrete approaches, such as cohesive zone models (CZMs) [7, 9, 10, 11, 12], cracks are represented along element boundaries, with crack propagation governed by traction–separation laws. This approach, however, faces challenges related to mesh dependency and accurately modeling crack branching.

In contrast, smeared models, particularly phase field (PF) models, regularize sharp cracks using a continuous damage field. PF models offer significant advantages, such as seamless crack tracking and natural handling of crack initiation, propagation, and coalescence without requiring additional criteria for crack kinking and branching. Pioneered by Francfort and Marigo [13], PF models are derived based on the variational principle, where damage evolution is determined by minimizing the energy functional. Mathematical analysis for numerical solutions of phase field modeling was supported by the Gamma-convergence proof from Ambrosio and Tortorelli [14], demonstrating that discrete cracks can be approximated by a regularized representation as the internal length scale parameter decreases. Bourdin *et al.* [15] further facilitated the implementation of PF models by transforming the surface integral for fracture energy into a volume integral, enabling efficient integration within the finite element method. A key milestone in phase field modeling was achieved by

Miehe *et al.* [16], who introduced an alternative derivation rooted in thermodynamic principles, notably incorporating a local crack geometric function to represent the crack surface explicitly. This development has been extended to dynamic fracture by [17, 18].

Recently, Fischer *et al.* [19] utilized a phase field (PF) model to explore the mechanisms underlying dynamic fragmentation. However, this model is restricted to brittle fracture and does not account for tensile strength, a critical factor influencing crack propagation. Their findings indicated a linear increase in the number of fragments with decreasing length scale parameter, and the model neglected the associated energy dissipation, further limiting its comprehensive assessment. Furthermore, both the thick level set (TLS) method [20] and the PF model [19] lacked the incorporation of a micro-inertia term, which has been shown to be crucial in accurately modeling high strain-rate phenomenon [21, 22, 23].

1.1.3 Numerical challenges for nonconvex functionals

Phase field modeling, despite its theoretical simplicity, faces several numerical challenges. The nonconvex nature of the energy functional results in indefinite matrices after discretization, making the numerical system difficult to solve. Additionally, accurately capturing the characteristic length scale of the damage zone requires a highly refined mesh, leading to a high number of degrees of freedom and significant computational demands. Furthermore, to ensure thermodynamic consistency, the phase field must exhibit irreversibility, necessitating specific treatments during numerical implementation.

Phase field models are primarily categorized based on the local fracture energy term, which characterizes the homogeneous dissipative mechanism, and the degradation function, which reduces material stiffness during crack propagation. The selection of these functions can introduce additional numerical challenges, particularly depending on whether they are locally convex. Pham *et al.* [24, 25], referred to as

the AT1 model, employs a linear form for the local crack geometric function and a quadratic form for the degradation function. In contrast, Miehe’s proposed PF-AT2 model [16] utilizes quadratic forms for both functions. Lorentz introduced a rational form for the degradation function, enabling the model to approximate the behavior of a classical cohesive zone model (CZM) [26, 27, 26]. Recently, Wu [28] further generalized Lorentz’s model to replicate various traction-separation laws found in cohesive zone theory, including linear, exponential, Cornelissen, and hyperbolic forms, which are critical for representing quasi-brittle materials such as concrete.

However, Wu’s PF-CZM model presents significant numerical challenges compared to other phase field models. This complexity arises partly from its nonconvex local crack geometric function, in addition to the previously mentioned numerical complications [29]. As a result, it often necessitates the use of advanced solvers, such as the relaxed Newton method [28] or the Broyden-Fletcher-Goldfarb-Shanno (BFGS) scheme [30], which was first introduced by Lorentz to solve his PF-CZM model [31].

While the BFGS solver can address convergence issues, it still requires a substantial number of iterations to reach convergence; dozens of iterations may be needed during elastic or late post-peak regimes, while hundreds of iterations may be required during critical phases of rapid crack propagation. [30] also indicates that the standard Newton-Raphson scheme can require thousands of iterations in more severe scenarios. These factors limit the model’s capacity to accurately predict fracture behavior, particularly in highly nonlinear problems, such as ductile fracture under finite strain or in multi-physics fracture scenarios. Advanced solvers like BFGS generally build upon standard iterative methods, such as Newton-Raphson or fixed-point iteration schemes, or require reformulating the original discrete system, which further increases computational demands and numerical complexity.

1.2 Research objectives and thesis formatting

This dissertation aims to focus on both modeling perspective and numerical efficiency for dynamic fracture and fragmentation at high rates. The research is structured as follows:

- **Rate-Dependent Behavior of Phase Field Models** in §2: This chapter will explore the rate-dependent behavior of phase field models by analyzing the elliptic, parabolic, and hyperbolic formulations. Analytical solutions will be provided to validate numerical implementations and offer insights into the physical behavior of the models under different loading rates.
- **Efficient and Robust Solvers for Dynamic Fracture** in §3: A hyperbolic phase field-cohesive zone model will be developed to address the computational challenges associated with fast crack propagation. The chapter will focus on numerical schemes, including explicit time integration, parallel implementation, and adaptive mesh refinement to enhance solver efficiency.
- **Extension to Ductile Fracture at Finite Strain** in §4: The hyperbolic phase field model will be extended to simulate ductile fracture under finite strain. The theoretical framework will be presented along with numerical results to validate the model's application to complex fracture scenarios.

The dissertation concludes with a summary of contributions, findings and directions for future research in §5.

Chapter 2

Rate dependency and
fragmentation response of phase
field models with micro inertia and
micro viscosity terms

2.1 Abstract

We present elliptic, parabolic, and hyperbolic phase field (PF) equations, referred to as EPF, PPF, and HPF, for cohesive zone model (CZM) and Linear Elastic Fracture Mechanics (LEFM) PF models. The micro viscosity and micro inertia terms result in PPF and HPF, that can be solved explicitly in time. The additional advantage of the HPF is implying a finite damage propagation speed and a more favorable time advance limit. The desired micro-viscosity for the HPF is shown to correspond to a damping factor of one. The appropriate length and time scales, nondimensional equations, and (asymptotic) strain-stress solutions are provided for each differential equation. Two sources of rate sensitivity are discussed. First, when the fields are spatially uniform (0D solution) the rate effect arises from the form of differential equation. Asymptotic solutions show that at high loading rates, the energy dissipation has the rates of $2/3$ and 1 for the PPF and HPF, respectively, with the former matching Grady's rate-sensitivity. The dynamic strength and failure strain show half of this rate. The analysis is extended to damage models with stress-based and bounded driving forces. Second, the rate effect arises from the deviation of 1D from 0D solutions as the damage exceeds a critical value and fragments form. Since this critical value tends to zero for quasi-static loading, this rate-effect is mainly present for low loading rates. This results in lower- and upper-bound energy limits for the EPF at low and high loading rates, resembling some experimentally observed sigmoidal rate models for energy dissipation.

2.2 Introduction

There are many fracture problems where rate-dependency of response is of great importance. For example, in fragmentation problems the domain goes through pervasive fracture. The *Quantities of Interest* (QoIs) such as the distribution and average of fragment size, dynamic strength, and energy dissipation vary significantly

versus the loading rate. Some of foundational experimental and analytical fragment size studies are [32, 5, 6]. Beyond the military applications [33, 34], the fragmentation phenomenon is relevant in ice-sheet morphology [35, 36], geophysics [37, 38], fragmentation of asteroids and comets [39, 40], nuclear reactor fuels [41], just to name a few. A more detailed review of the fragmentation problem can be found in [42, 43].

The rate dependency of fracture QoIs can arise from two effects. First, bulk material inertia effects, finite speed of wave propagation and damage evolution, and fragment formation all result in rate-dependency. For example, most analytical and computational studies such as [5, 6, 11, 8] use rate-independent elastic and fracture models, yet recover rate-dependent macroscopic QoIs. Second, the material can be rate-dependent, either in the bulk, *e.g.*, rate-dependent fracture toughness and viscoelastic response in [44], or at an interface [45, 46]. This inherent rate dependency adds to the rate-dependency arising from the first effect. As for the second effect, while there are some studies [47, 48] that incorporate both bulk (*e.g.*, the form of viscoelasticity) and fracture rate-dependency, we will limit our attention only to rate-dependency of the fracture model. Accordingly, we will next discuss some relevant rate-dependent experimental observations and computational fracture models. This will be followed by the discussion of the role of fragmentation, first effect, on rate-dependent properties.

2.2.1 Rate dependency of fracture models

The discussion of rate-dependency of fracture model starts with interfacial models. *Traction Separation Relation* (TSR) *Cohesive Zone Models* (CZMs) are widely used to model the debonding of interfaces. For a rate-independent material, they require a rate-independent fracture toughness and a strength parameter. However, in many instances for example for polymers [49], adhesives [50, 46], asphalt concrete [51], and concrete [52], fracture toughness and strength show rate dependency. Except for a

few cases such as glassy materials, fracture toughness increases versus loading rate for these dependent materials. This rate dependency is handled in two ways for TSRs. In the first approach, the parameters of the TSR, *e.g.*, fracture toughness and strength, are changed subject to the instantaneous crack opening rate [53, 23, 46, 54, 55]. These models may suffer from convergence problems when the loading rate changes quickly. In the second approach, rate-dependency is built into the TSR by turning it into a differential equation [56, 57, 58, 59] or by having a loading rate correction factor [60].

The rate-dependency can also be built into continuum damage models. As a background, [61] showed the mesh dependency of local damage models. There are many approaches that introduce a length scale to the damage model to remedy this problem. Among them, we focus on gradient damage models due to their resemblance to the *Phase Field* (PF) model [62]. The gradient damage models were initially formulated for quasi-static problems and due to the presence of a Laplacian operator, they correspond to an elliptic *Partial Differential Equation* (PDE). By adding a first time derivative of the field of the PDE (damage or strain), referred to as adding a *micro-viscosity* term, the PDE turns parabolic. Adding a second time derivative turns it to a hyperbolic PDE; this corresponds to adding a micro-inertia term, associated with the damage PDE field, to the kinetic energy of the system. The micro-inertia term reflects the inertia at the micro-crack [63, 48]. This micro-inertia term is also motivated from the need to have a finite speed for damage propagation in [64, 47] among others. The micro-viscosity effect is argued to have a different source, corresponding to some micro viscosity-related damping effects, for example from the unhydrated inclusions in concrete [48]. Moreover, micro-viscosity allows to describe the differences in stress-strain softening response at low loading rates [65]. We refer the reader to [64] for a detailed discussion on all PDE types of the damage model. Regardless of the physical motivation and arguments, both parabolic and hyperbolic continuum damage models are rate-dependent. This is in contrast to the elliptic PDE that predicts a point-wise stress-strain response that is independent of the loading rate.

Phase field (PF) fracture models are derived from the smoothing of interfacial fracture models. The earlier works [15, 66, 67] applied to brittle fracture by smoothing the *Linear Elastic Fracture Mechanics* (LEFM) model, using a variation approach [13]. It has also been extended to quasi-brittle fracture by regularizing a CZM [27, 68, 28]. We refer to the latter set as the *Phase Field Cohesive Zone Models* (PF-CZMs). PF models are also applied to dynamic fracture problems, where in most cases, *e.g.*, [17, 19, 69], the elliptic PF equations are coupled with the elastodynamic equations. More recently, however, parabolic [70, 71, 48] and hyperbolic [72, 73, 73] PF formulations are also proposed. Similar to gradient damage models, the micro-viscosity and micro-inertia terms added for the parabolic and hyperbolic equations make the PF fracture models rate-dependent.

2.2.2 Rate dependency arising from fragmentation

In many fracture problems, the material breaks into fragments. As the loading rate increases the fragments get smaller so that the material can dissipate more energy at fracture interfaces (fragment boundaries). As mentioned earlier, the rate dependency in the (average) fragment size, energy dissipation, and dynamic strength has been studied by analytical [5, 6] and TSR CZM models [7, 9, 11, 8]. The fragmentation studies using the thick level set and Lip-field methods [20, 74] are also mentioned due to some of their similarities to the PF models.

Fragmentation instabilities in PF fracture were first analyzed in [25, 75]. Therein, the response of a homogeneous material undergoing a spatially uniform and temporally increasing loading (typical of fragmentation studies) was analyzed for a quasi-static problem. That is, the inertia effects were ignored, a reasonable assumption for very low loading rates. It was shown that as soon as the increasing stress reached the strength of the material, bifurcation occurred and the instability of response beyond this point was reflected in the formation of fragments. Unfortunately, this analysis does not apply to dynamic fragmentation, where material inertia must be

considered. As shown in [19] for PF fragmentation with inertia effects, the spatially uniform solution is valid up to a stress level beyond which any small perturbation to the solution will rapidly grow and fragments will form. For PF fragmentation with inertia effects, the spatially uniform solution remains valid until a critical stress level is reached. Beyond this point, small perturbations rapidly grow, leading to fragmentation [19]. The dynamic stability analysis identifies this stress threshold. It is noted that in all aforementioned studies the bulk and fracture models are rate-independent. We will comment on incorporating such inherent rate effects in fragmentation study below.

2.2.3 Scope of this study

In §2.2.1 and §2.2.2 rate-dependency of fracture QoIs were discussed from two perspectives: 1) inherent rate dependency of the fracture model; 2) rate-dependency arising from the formation of fragments. The goal of this study is to investigate both effects for the PF fracture models. We consider the response of a 1D homogeneous domain (a bar or a ring) undergoing a spatially uniform and temporally increasing stress field. To study the inherent rate-sensitivities of the fracture model, we consider a 0D idealization of this problem where the fragment formation is not considered. While this is a valid solution to the 1D problem, it is only stable before the formation of the fragments.

For the 0D PF solutions, we consider *Elliptic Phase Field* (EPF), *Parabolic Phase Field* (PPF), and *Hyperbolic Phase Field* (HPF) equations. The 0D strain-stress solutions reveal the rate sensitivity inherent to each equation by determining how QoIs such dynamic strength and dissipated energy vary versus the applied loading rate. In contrast to the rate-independent EPF equation, we show that the PPF and HPF equations are rate-dependent. Using analytical and computational solutions of the actual equations and their high rate asymptotic (HRA) solution, we determine the rate sensitivity of each PF equation. This analysis is extended to a broader set

of continuum damage models that have micro-inertial and/or micro-viscosity terms and when the damage evolution is driven by an energy, stress, or bounded (high rate asymptotic) damage force function. Examples of such damage models are provided from the literature.

The rate-sensitivity of PF fracture problem from instabilities and fragment formation is studied using 1D simulations. This is the extension of quasi-static [25, 75] and dynamic [19] fragmentation response of PF models discussed in §2.2.2 from the following perspectives. First, [19] applies to a form of brittle (LFEM-based) PF equation, whereas we investigate the fragmentation response of both brittle and quasi-brittle PF models. Second, in [19] and many fragmentation studies such as [5, 6, 11, 8] the key QoI is fragment size distribution, and specifically the dynamic strength is not studied. We consider dynamic strength and energy dissipation in addition to the (average) fragment size. Third, and perhaps the most important contribution, is investigating the interaction of the rate-sensitivities that arise from the fracture model and fragmentation process. For example, we show that the rate-insensitive EPF equation, is rate-sensitive in 1D mainly due to the fragmentation process. Two limiting lower- and upper-bound energy thresholds are determined at quasi-static and high loading rate limits. Interestingly, this sigmoidal energy dissipation curve versus loading rate mirrors experimental observations and rate-dependent CZM models (*cf.* §2.2.1) such as [46, 57, 58, 59, 60]. The PPF and HPF equations show the same fragmentation-based rate-sensitivity at quasi-static and low loading rates. In addition, we show that at high loading rates, the entire domain undergoes uniform damage up to late stages of damage accumulation. Thus, the 0D PPF and HPF solutions determined previously and their particular rate-dependency apply in 1D at the high loading rate limit.

To our knowledge the asymptotic investigation of rate-sensitivity of PPF and HPF equations, and the rate-dependency of EPF, PPF, and HPF equations for 1D PF equations are some of the new contributions of this work. The rate-sensitivity of HPF equation is studied for a different problem of macroscopic crack propagation in

[72, 73] and some other benchmark problems in [72, 76]. However, to our knowledge none of these studies consider the asymptotic analysis or rate-dependency of the fragmentation problem.

The remainder of the manuscript is organized as follows. The PF equations and various nondimensional forms of this equation for brittle and quasi-brittle fracture and different PF PDE types are provided in §2.3. The inherent rate sensitivity of EPF, PPF, and HPF and their high-rate asymptotic solutions are provided in §2.4. The process of fragmentation formation and the resulting rate-dependency in combination with 0D (fracture model) rate-sensitivity are discussed in §2.5. The summary and final conclusions are provided in §2.6.

2.3 Formulation

2.3.1 Coupled elastodynamics and phase field equations

The objective of this section is to provide the final PDEs for the elastodynamic and PF problems. For brevity, we do not provide all the intermediate steps of the PF formulation, particularly, the variational statement of the problem and taking the variation that results in the PDEs. We refer the reader to [15, 66, 67] for more details on the intermediate steps.

In PF models, the sharp crack $\mathcal{S}$ is smeared over a localization band in which the continuum phase field parameter $d \in [0, 1]$, defined over the entire domain $\mathcal{D}$, approximates the damage surface. The point-wise PF value of $d = 0$ represents an intact material and the upper-bound value of $d = 1$, represents a fully damaged point. For example, a sharp crack will be smeared to a region of finite width, in which the interior of the band takes the value of $d = 1$, and d tends to zero moving away from the interior of the smeared crack.

Least action, Hamilton's principle, and micro-force balance equations are some of the approaches proposed to formulate the PF problem; see for example [77, 78, 72, 79].

We begin by summarizing the derivation of the coupled elastodynamic-PF problem, omitting viscous terms, based on the Hamilton's principle from [79]. We simplify their derivation by neglecting higher gradient terms of the PF (resulting in a fourth order PDE for d) and considering the infinitesimal rather than finite strain gradient theory. Derived from D'Alembert's principle [80], the extended Hamilton principle states:

$$\int_{t_1}^{t_2} (\delta \mathcal{L} + \delta \mathcal{W}_{\text{ext}}) dt = 0, \quad \forall t_1, t_2 \in \mathbb{R}^+, \quad (2.1)$$

where the Lagrangian $\mathcal{L} := \mathcal{K} - \mathcal{E}$ is the difference between kinetic energy functional $\mathcal{K}$ and the potential energy functional $\mathcal{E}$ and $\mathcal{W}_{\text{ext}}$ is the external work. The first variation operator is denoted by δ .

The kinetic energy is defined as,

$$\mathcal{K} := \int_{\mathcal{D}} \frac{1}{2} \rho_u \frac{\partial \mathbf{u}}{\partial t} \cdot \frac{\partial \mathbf{u}}{\partial t} + \frac{1}{2} \rho_d \left(\frac{\partial d}{\partial t} \right)^2 dv, \quad (2.2)$$

where $\mathcal{D}$ is the spatial domain and ρ_u is the mass density. Here, $\mathbf{u}$ is the displacement vector and $\partial \mathbf{u} / \partial t$ is the velocity vector. The *micro-inertia phase field density* ρ_d accounts for the local inertia of material at the crack tip [64]. The external work of the body force vector $\mathbf{b}$ and applied traction $\mathbf{t}^*$ on the Neumann boundary $\partial \mathcal{D}_f$ is $\mathcal{W}_{\text{ext}} := \int_{\mathcal{D}} \rho_u \mathbf{u} \cdot \mathbf{b} dv + \int_{\partial \mathcal{D}_f} \mathbf{u} \cdot \mathbf{t}^* ds$. It is assumed that the potential energy functional $\mathcal{E} := \mathcal{E}_e + \mathcal{E}_d$ decomposes into an elastic strain functional $\mathcal{E}_e$ and surface energy (damage) functional $\mathcal{E}_d$,

$$\mathcal{E}_e := \int_{\mathcal{D}} \phi_{ed}(\boldsymbol{\epsilon}, d) dv, \quad (2.3a)$$

$$\mathcal{E}_d := G A_d(d), \quad \text{where} \quad A_d(d) := \int_{\mathcal{D}} \gamma(d) dv, \quad (2.3b)$$

G is the fracture toughness, and the integral $A_d(d)$ is discussed below. The *free energy density* function $\phi_{ed}(\boldsymbol{\epsilon}, d)$,

$$\phi_{ed}(\boldsymbol{\epsilon}, d) := \omega(d)\phi_e(\boldsymbol{\epsilon}), \quad \text{where} \quad \phi_e(\boldsymbol{\epsilon}) = \frac{1}{2}\boldsymbol{\epsilon} : \mathbf{C}\boldsymbol{\epsilon}. \quad (2.4)$$

is comprised of a contribution from the PF, $\omega(d)$ and the *elastic strain energy density* $\phi_e(\boldsymbol{\epsilon})$. The infinitesimal deformation theory strain is given by $\boldsymbol{\epsilon} = 0.5(\nabla_{\mathbf{x}}\mathbf{u} + \nabla_{\mathbf{x}}^T\mathbf{u})$, where $\nabla_{\mathbf{x}}$ is the spatial gradient operator, and T represents the transpose operator. In (2.4), $\mathbf{C}$ stands for the elasticity tensor. The degradation function $\omega(d)$ determines how the energy and stress decrease through the evolution of d . The functional forms of $\omega(d)$ will be provided in §2.3.2.

The integral $A_d(d) = \int_{\mathcal{D}} \gamma(d) \, dv$ approximates $\mathcal{A}_S$, the total surface area of all sharp cracks. The *crack surface density function* is expressed as $\gamma = (\alpha(d) + b^2\nabla d \cdot \nabla d)/bc_\alpha$. The important internal length scale of the PF model b characterizes the width of localization bands that approximate sharp cracks. The *geometric crack function* $\alpha(d) : [0, 1] \rightarrow [0, 1]$ characterizes damage (d) evolution. It is a monotonically increasing function, satisfying $\alpha(d = 0) = 0$ and $\alpha(d = 1) = 1$. The scaling parameter $c_\alpha > 0$ is determines such that the surface of a crack is recovered from the regularized volume integral, when the crack is fully developed, resulting in the formula $c_\alpha = 4 \int_0^1 \sqrt{\alpha(\beta)} \, d\beta$. The specific forms of $\alpha(d)$ and values of c_α are later provided in Table 2.1.

After the substitution of (2.2), (2.3), and $\mathcal{W}_{\text{ext}}$ in (2.1) and some algebraic manipulations, the terms multiplying $\delta\mathbf{u}$ and δd in the interior of the domain correspond to the elastodynamic and phase field PDEs, respectively,

$$\rho_u \frac{\partial^2 \mathbf{u}}{\partial t^2} - \nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma} = \rho_u \mathbf{b}, \quad (2.5a)$$

$$\rho_d \frac{\partial^2 d}{\partial t^2} - 2\nabla_{\mathbf{x}} \cdot \left(\frac{Gb}{c_\alpha} \nabla_{\mathbf{x}} d \right) = -\omega'(d)\phi_e(\boldsymbol{\epsilon}) - \frac{G}{c_\alpha b} \alpha'(d), \quad (2.5b)$$

where the stress tensor is given by,

$$\boldsymbol{\sigma} := \frac{\partial \phi_{ed}(\boldsymbol{\epsilon}, d)}{\partial \boldsymbol{\epsilon}} = \omega(d) \boldsymbol{\sigma}_e, \quad \boldsymbol{\sigma}_e = \mathbf{C} \boldsymbol{\epsilon}. \quad (2.6)$$

We observe that $\boldsymbol{\sigma}$ is equal to the elastic stress $\boldsymbol{\sigma}_e = \mathbf{C} \boldsymbol{\epsilon}$ times the degradation function $\omega(d)$. Another perspective is that the PF d degrades the elasticity stiffness $\mathbf{C}$ to $\omega(d)\mathbf{C}$, where the stiffness remains intact for $d = 0$ and tends to zero as $d \rightarrow 1$.

The Hamilton's principle cannot include damping effects due to their dissipative mechanism [79]. In [64] micro-inertia ($\rho_d(\partial d/\partial t)^2$ in (2.2)) and micro-viscosity are incorporated in a general damage PDE to model micro-forces that influence crack propagation. The micro inertia term reflects the inertia at the crack tip [63, 48] and is also motivated by requiring a finite speed of damage propagation; *cf. e.g.*, [64, 47]. The micro-viscosity term is related to micro-scale fracture damping effects, for example from unhydrated inclusions in concrete [48].

With the presence of micro-viscosity term, [48] takes an approach very similar to the one provided above with the difference of adding a micro-viscosity resistive force to the PF equation. Another approach to consider the viscous terms is postulating the balance of micro-forces and enforcing the dissipation inequality (second law of thermodynamics). This more involved approach reaches at the same equation (2.5) with the addition of a viscous term. We refer the reader to [79], section 2.2 for the formulation and comparison of the Hamiltonian and balance of force approaches. With the latter approach, (2.5) is extended to,

$$\rho_u \frac{\partial^2 \mathbf{u}}{\partial t^2} + \xi_u \frac{\partial \mathbf{u}}{\partial t} - \nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma} = \rho_u \mathbf{b} \quad \text{equation of motion, (2.7a)}$$

$$\rho_d \frac{\partial^2 d}{\partial t^2} + \xi_d \frac{\partial d}{\partial t} - b^2 \Delta_{\mathbf{x}} d = \left\langle -\frac{c_\alpha}{2} \omega'(d) \frac{\mathcal{H}(\phi_e(\boldsymbol{\epsilon})) b}{G} - \frac{\alpha'(d)}{2} \right\rangle_+ \quad \text{PF PDE, (2.7b)}$$

where $\mathcal{H}(\cdot)$ and $\langle \cdot \rangle_+$ denote the history and positive operators. That is, $\mathcal{H}(f)(t) = \max_{\tau \in (0, t)} f(\tau)$ for a time-dependent function f , and $\langle x \rangle_+ = x$ for $x \geq 0$ and zero otherwise. The damping force corresponding to the elastodynamic damping coefficient

ξ_u is the difference between (2.5a) and (2.7a). The PF equation has the same physical dimension of (2.5b) with the addition of a micro-viscosity term. However, by multiplying it with $c_\alpha b/2G$ we reach at (2.7b) which is physically dimensionless. The corresponding *scaled phase field density* $\varrho_d := \rho_d c_\alpha b/2G$ and *phase field damping time* ξ_d have physical dimensions of time squared $[T]^2$ and time $[T]$, respectively. Hence, we define the *time scale of the phase field* τ_d and *phase field damping factor* d_f through the relations,

$$\varrho_d := \tau_d^2, \quad \xi_d := d_f \tau_d. \quad (2.8)$$

Equation (2.7b) encompasses all PF PDE types. When $\varrho_d = 0$ and $\xi_d = 0$, we recover the common EPF equation. The PPF equation corresponds to $\varrho_d = 0$ and $\xi_d > 0$, whereas for the HPF equation $\varrho_d > 0$ and $\xi_d \geq 0$. τ_d is the inherent time scale associated with a HPF equation and corresponds to the time it takes for PF waves with *phase field speed* $c_d := \sqrt{b^2/\varrho_d} = b/\tau_d$ to traverse the distance b . The strength of the damping term (first order time derivative term) is represented by the value of the nondimensional *damping factor* $d_f = \xi/\tau_d \geq 0$ for the HPF equation. As the ratio of the damping to PF wave equation time scales, d_f greatly affects the response of a HPF equation. We will observe that low values ($d_f \ll 1$) can result in some numerical artifacts, whereas high values ($d_f \gg 1$) can provide solutions that are very close to the corresponding PPF equation.

Other differences of (2.5b) and (2.7b) are discussed next. First, we need to enforce the irreversibility of d . That is, no self-healing is allowed and $\partial d/\partial t \geq 0$. In addition, d should be bounded in the range $[0, 1]$. The history operator on $\phi_e(\mathbf{e})$ was proposed in [16, 67] and was shown to enforce all such conditions for an AT2 EPF equation (AT2 and other PF models are discussed in §2.3.2). While this history operator has been used in other PF models and even the HPF equation in [72], the reversibility condition is not guaranteed for non-AT2 and PPF or HPF equations. Similar to [81] and some other PF implementations, we directly enforce the irreversibility of d in numerical setting, cf. §2.5.1. Second, the positive operator prevents damage

evolution when the damage force, the *Right Hand Side* (RHS) of (2.7b), is negative. This condition happens in the early loading stages for certain PF models that have an elastic response.*

2.3.2 Degradation and geometric crack functions

We provide expressions for $\omega(d)$ and $\alpha(d)$ for various PF models. The degradation function satisfies the conditions,

$$\omega(0) = 1, \quad \omega(1) = 0, \text{ and } \omega'(d) < 0. \quad (2.9)$$

As mentioned earlier, the degradation function $\omega(d)$ degrades the ϕ_{ed} and elasticity stiffness (hence σ) as damage accumulates. The conditions in (3.35) represent no stiffness degradation at $d = 0$ and complete degradation at $d = 1$. The monotonically decreasing function ($\omega'(d) < 0$) ensures that the stiffness is further reduced as damage accumulates.

The PF models used in subsequent sections are summarized in Table 2.1. We adopt the AT1 and AT2 terminologies from [82]. The AT1 and AT2 phase field models were proposed by Pham *et al.* [24] and Miehe *et al.* [16] respectively. These models regularize the LEFM in that G is the only fracture properties and the models do not possess an intrinsic strength. The AT1 and AT2 models have a quadratic degradation function $\omega(d) = (1-d)^2$. This function satisfies (3.35) without additional arguments and requirements. In contrast, the *phase field cohesive zone models* (PF-CZMs), including CZM-L by E. Lorentz [27] and CZM-W by J.Y. Wu [28] require an additional strength parameter $\tilde{\sigma}$. The LEFM and CZM PF models are also referred to as PF models for brittle and quasi-brittle materials, respectively. The $\omega(d)$ for PF-CZMS is a rational function specified by the polynomial order p and the polynomial function $Q(d)$,

$$Q(d) = a_1 d(1 + a_2 d(1 + a_3 d)), \quad (2.10)$$

*This applies to all the PF models considered, except the AT2 model.

where the constants a_1 , a_2 , and a_3 define the softening curve of the PF model in accordance with the local crack geometric function $\alpha(d)$. The coefficients a_1 and a_2 need to satisfy certain conditions as further discussed below.

A few comments are provided on the properties and parameters of the PF models in Table 2.1. First, the nondimensional initiation strain $\bar{\epsilon}_i$, further discussed in §2.4.1, corresponds to a nondimensional strain level below which the strain-stress remains linear and $d = 0$. That is, it is the nondimensional elastic limit. As observed, except the AT2 model, all models possess an initial elastic response. Second, the condition for the phase field length scale b is discussed for AT and CZM models. For the AT models, b is a free parameter; as will be shown *cf.* §2.4.1, the smaller the b , the larger the maximum stress of the model. On the other hand, if the strength of the material $\tilde{\sigma}$ is known, to ensure that the PF model recovers it for quasi-static loading, AT2 and AT1 models require the *normalized phase field length scale by cohesive length scale*,

$$\bar{b}_c = b/\tilde{l}_c \quad (2.11)$$

to be equal to 27/256 and 3/8, respectively, where $\tilde{l}_c = GE/\tilde{\sigma}_c^2$ is the *cohesive length scale*. For the CZM models the condition,

$$a_1 = \frac{2\alpha'(0)}{c_\alpha \bar{b}_c}, \quad (2.12)$$

ensures that the maximum quasi-static loading is equal to $\tilde{\sigma}$; *cf.* the discussion in §2.4.1. Third, for the CZM models, an upper-bound is stipulated for $\bar{b}_c$ to ensure the well-posedness of the problem and a valid strain-stress response. These upper-bounds are provided for the two CZM models in the last column of the table. The equivalent lower-bounds for a_1 values are also provided.

The other parameters of the CZM models, pertained to (2.10) and the power p for $\omega(d)$, are provided in Table 2.2. The value for a_1 is obtained from (2.12) by using the corresponding c_α and $\alpha'(0)$ from Table 2.1. For the CZM-W model, other softening

curves such as exponential, hyperbolic, Cornelissen (concrete), and polynomial are also provided in [28] and in [83] using another approach. However, since we will only be using the linear softening model, the other softening curves are not shown in the table. For the CZM-L model, the stability conditions $a_2 \geq 1$ and $a_1 \geq a_2 + 2$ are provided in [27].[†] For the remainder of this manuscript, we will use the CZM-L model for $a_2 = 1$, resulting in conditions $a_1 \geq 3$ and $\bar{b}_c \leq 0.25$. We further use the limiting values of a_1 and $\bar{b}_c$ for the CZM-L model; that is, we use $a_2 = 1$ and $a_1 = 3 \Leftrightarrow \bar{b}_c = 0.25$.

For the CZM-W model, the condition $\omega'(d) \leq 0$ in (3.35) is fulfilled by demanding $a_1 \geq 2$. This condition is stricter than the value given in [28] requiring $a_1 \geq 1.5$ for the irreversibility of the damage value. Alongside the condition $\omega'(d) \leq 0$, we observed that the zero-dimensional, *i.e.*, spatially uniform, strain-stress response of the CZM-W model with linear softening curve will have a snap-back for $a_1 < 2$, showing the problem of the limit in [28]. That is, for $1.5 \leq a_1 < 2$ the strain at the zero stress point is smaller than the strain at the maximum stress point. We did not observe a major problem for quasi-problems with the more relaxed condition $a_1 = 1.5$. However, for dynamic loadings the zero-dimensional solution becomes more prevalent as further discussed in next sections and the solution demonstrates spurious damage field oscillations for $a_1 = 1.5$. We contribute this to the aforementioned snap-back problem. For the remainder of the manuscript, we use the linear CZM-W model with $a_1 = 4$ ($\bar{b}_c = 1/\pi$), unless otherwise specified. This corresponds to a normalized failure strain of 2, ($\epsilon_f = 2\tilde{\sigma}/E$) and a linear cohesive model with equal loading and unloading slopes.

[†]The stability conditions in [27] are expressed in terms of a phase field length that is twice that of b and the labels of a_1 and a_2 are different. Once expressed in our notation, they coincide with the conditions provided above.

2.3.3 Physical scales and nondimensionalization

Almost all the results will be presented in a nondimensional form. Since the only physical dimensions of length $[L]$, time $[T]$, and mass $[M]$ are involved in the coupled elastodynamic PF problem, we need three dimensional parameters to nondimensionalize the problem. These can naturally be some length, time, and mass scales. Alternatively quantities that have a clearer physical interpretation in the context of PF fracture can be used. Accordingly, instead of a mass scale, we use the fracture energy G as one of the scales of the problem. This, combined with the length scale $\tilde{l}$ and time scale $\tilde{\tau}$ completes the dimensional scales of the problem,

$$\tilde{G} = G \quad \text{fracture energy scale,} \quad (2.13a)$$

$$\tilde{l} = \begin{cases} \tilde{l}_c = \frac{GE}{\tilde{\sigma}_c^2} & \text{Cohesive length-scale (appropriate for PF-CZM)} \\ b & \text{PF length-scale (appropriate for AT1 \& AT2)} \\ L & \text{Domain length scale} \end{cases} \quad (2.13b)$$

$$\tilde{\tau} = \begin{cases} \tilde{\tau}_l := \frac{\tilde{l}}{c_u} & \text{Derived from } \tilde{l} \text{ and elastodynamic speed scale } c_u \\ \xi_d = d_f \tau_d & \text{PPF time scale} \\ \sqrt{\varrho_d} = \tau_d & \text{HPF time scale} \end{cases} \quad (2.13c)$$

The rationale for multiple choices for $\tilde{l}$ and $\tilde{\tau}$ is discussed next. The appropriate $\tilde{l}$ mainly depends whether the PF model uses a separate strength parameter. The internal length scale of the PF model b is one choice for all PF models. For the PF-CZM models, the cohesive (Griffith's or Irwin's) length scale, $\tilde{l}_c = GE/\tilde{\sigma}_c^2$ is the more natural length scale. In the remainder of the manuscript, whenever the results are presented only for AT2 and AT1 models, $\tilde{l} = b$ used. Otherwise, when only the PF-CZM results are presented or AT2 and AT1 results are compared with CZM ones, for objective comparison we use $\tilde{l} = \tilde{l}_c$. Since we refer to the results in [19] in §2.5.2, we additionally reference their selected length scale $\tilde{l} = L$ in (2.13b). Although, as

will be seen in that section, the nondimensionalization can more naturally be done with respect to $\tilde{l} = b$.

The appropriate time scale $\tilde{\tau}$ mainly depends on the PF PDE type. As will become evident later, many results of PPF and HPF equations collapse to one curve for different ξ_d and/or τ_d , if $\tilde{\tau} = \xi_d$ and $\tilde{\tau} = \tau_d$ is used for the PPF and HPF equations, respectively. For the quasi-static loading condition, the solutions of the PPF and HPF equation tend to the solution of the EPF equation. For this condition no time scale is required. This also holds true for some other EPF results presented below, including the so-called 0D solutions in §2.4.1. Still, the time scale $\tilde{\tau}_l = \tilde{l}/c_u$, derived from the length scale $\tilde{l}$ and the elastodynamic wave speed scale, is not only the natural choice for many transient responses of the EPF equation, but also is another choice for the PPF and HPF equations. c_u can be chosen as $\sqrt{E/\rho_u}$ for 1D problems. Other choices of c_u such as (the directionally maximum of) longitudinal or shear wave speed can be used for 2D and 3D problems.

Since all these length and time scales will be interchangeably used, we specify the choices for $\tilde{l}$ and $\tilde{\tau}$ whenever there is room for ambiguity. For example, mentioning that the spacetime scale is $[b, \xi_d]$ means $\tilde{l} = b$ and $\tilde{\tau} = \xi_d$. As will be seen in §2.4.2, this is the scaling of choice for the AT1 and AT2 PPF equations. Once the choices of $\tilde{l}$ and $\tilde{\tau}$ are made, the scales of other dimensional quantities can be derived as follows

[84],

$$\tilde{\sigma} = \sqrt{\frac{GE}{\tilde{l}}} \quad \text{strength \& stress scale,} \quad (2.14a)$$

$$\tilde{\epsilon} = \frac{\tilde{\sigma}}{E} = \sqrt{\frac{G}{\tilde{l}E}} \quad \text{strain scale,} \quad (2.14b)$$

$$\tilde{u} = \tilde{\epsilon}\tilde{l} = \frac{G}{\tilde{\sigma}} = \sqrt{\frac{G\tilde{l}}{E}} \quad \text{displacement \& separation scale,} \quad (2.14c)$$

$$\tilde{\phi} = \tilde{\sigma}\tilde{\epsilon} = \frac{G}{\tilde{l}} \quad \text{strain energy density \& energy per volume scale,} \quad (2.14d)$$

$$\tilde{c} = \frac{\tilde{l}}{\tilde{\tau}} \quad \text{wave speed scale,} \quad (2.14e)$$

$$\tilde{\dot{\epsilon}} = \frac{\tilde{\epsilon}}{\tilde{\tau}} = \frac{\tilde{\sigma}}{E\tilde{\tau}} = \frac{1}{\tilde{\tau}} \sqrt{\frac{G}{\tilde{l}E}} \quad \text{strain rate scale,} \quad (2.14f)$$

$$\tilde{v} = \frac{\tilde{u}}{\tilde{\tau}} = \tilde{\epsilon}\tilde{c} = \frac{\tilde{\sigma}\tilde{c}}{E} = \frac{1}{\tilde{\tau}} \sqrt{\frac{G\tilde{l}}{E}} \quad \text{velocity scale,} \quad (2.14g)$$

$$\tilde{a} = \frac{\tilde{v}}{\tilde{\tau}} = \frac{\tilde{u}}{\tilde{\tau}^2} = \tilde{\dot{\epsilon}}\tilde{c} = \frac{\tilde{\sigma}^3\tilde{c}^2}{GE^2} = \frac{1}{\tilde{\tau}^2} \sqrt{\frac{G\tilde{l}}{E}} \quad \text{acceleration scale.} \quad (2.14h)$$

We note that the tilde decoration is used for the scales presented in (2.13) and (2.14). The nondimensional form of a quantity q is decorated by an overbar, and is expressed as,

$$\bar{q} = \frac{q}{\tilde{q}}. \quad (2.15)$$

Some of these scales will be frequently used. For example, $\tilde{\sigma}$, $\tilde{\epsilon}$, and $\tilde{\phi}$ will be used to normalize the dynamic strength, failure strain, and energy dissipation per volume. For CZM models, since generally $\tilde{l} = \tilde{l}_c$, we recover $\tilde{\sigma} = \tilde{\sigma}_c$. Another important scale is $\tilde{\dot{\epsilon}}$, as it normalizes the applied strain rate for fragmentation problems. Finally, $\tilde{u}$, $\tilde{v}$, and $\tilde{a}$ scale the material displacement, velocity, and acceleration of fracture problems. For example, in the context of a TSR-CZM study, we have demonstrated that the maximum material velocity around a propagating crack is proportional to $\tilde{v}$ [85]. While we do not use $\tilde{u}$, $\tilde{v}$, and $\tilde{a}$ herein, they can be used in other PF problems to nondimensionalize displacement, velocity, and acceleration QoIs.

2.3.4 Nondimensionalized coupled equations

Next, we present the elastodynamic and PF equations in terms of the nondimensional parameters. The nondimensional forms of (2.6), (2.7a), and displacement-strain relation are given by,

$$\bar{\rho}_u \frac{\partial^2 \bar{\mathbf{u}}}{\partial \bar{t}^2} + \bar{\xi}_u \frac{\partial \bar{\mathbf{u}}}{\partial \bar{t}} - \nabla_{\bar{\mathbf{x}}} \cdot \bar{\boldsymbol{\sigma}} = \bar{\rho}_u \bar{\mathbf{b}} \quad \text{equation of motion,} \quad (2.16a)$$

$$\bar{\boldsymbol{\sigma}} = \omega(d) \bar{\boldsymbol{\sigma}}_e, \quad \bar{\boldsymbol{\sigma}}_e = \bar{\mathbf{C}} \bar{\boldsymbol{\epsilon}} \quad \text{constitutive equation,} \quad (2.16b)$$

$$\bar{\boldsymbol{\epsilon}} = \frac{\nabla_{\bar{\mathbf{x}}} \bar{\mathbf{u}} + \nabla_{\bar{\mathbf{x}}}^T \bar{\mathbf{u}}}{2} \quad \text{compatibility equation,} \quad (2.16c)$$

where the *nondimensional mass density* is $\bar{\rho}_u = (\tilde{\tau}_l/\tilde{\tau})^2$ for $\tilde{\tau}_l$ given in (2.13c). If $\tilde{\tau}$ is chosen to be $\tilde{\tau}_l$, as expected, $\bar{\rho}_u = 1$. The *nondimensional solid damping coefficient* is $\bar{\xi}_u = f_u(\tilde{\tau}_l/\tilde{\tau})$, where f_u is the *nondimensional solid damping factor*, denoting the strength of the damping parameter for the elastodynamic problem. One can compare its role to d_f in (2.8). This damping factor is defined as the ratio of two time scales, $f_u := \tilde{\tau}_l/\tilde{\tau}_u^\xi$, where $\tilde{\tau}_u^\xi = \rho_u/\xi_u$ is a time scale defined by the values of mass density and damping coefficient in (2.7a). Finally, the *nondimensional elasticity stiffness* is $\bar{\mathbf{C}} = \mathbf{C}/E$. As mentioned earlier, for 2D and 3D problem E can stand for elastic modulus for an isotropic material or a more general measure of stiffness for anisotropic materials.

The PF PDE, expressed in terms of nondimensional parameters, is derived from (2.7b) as,

$$\bar{\rho}_d \frac{\partial^2 d}{\partial \bar{t}^2} + \bar{\xi}_d \frac{\partial d}{\partial \bar{t}} - \bar{b}^2 \Delta_{\bar{\mathbf{x}}} d = \left\langle -F\omega'(d)\mathcal{H}(\bar{\phi}_e) - \frac{\alpha'(d)}{2} \right\rangle_+, \quad (2.17)$$

where $\bar{\rho}_d = (\tau_d/\tilde{\tau})^2$ is the *nondimensional micro-inertia phase field density* and $\bar{\xi}_d = d_f(\tau_d/\tilde{\tau})$ is the *nondimensional phase field damping coefficient*. For the PPF equation $\bar{\rho}_d = 0$ and for EPF equation $\bar{\rho}_d = \bar{\xi}_d = 0$. The *nondimensional elastic strain energy density* $\bar{\phi}_e = \phi_e/\tilde{\phi}$ is the nondimensional form of ϕ_e . The source term factor

$$F := \frac{c_\alpha \bar{b}}{2} \quad (2.18)$$

is introduced to streamline calculations. Note that when $\tilde{l} = b$, which is a common choice for AT1 and AT2 models, $\bar{b} = 1$. As mentioned earlier, even for the AT1 and AT2 models, one may use the cohesive length scale $\tilde{l}_c$, in which case to avoid the need to mention the length scale for normalization, we introduced $\bar{b}_c = b/\tilde{l}_c$ in (2.11). In fact, any nondimensional parameter that has a subscript c uses the length scale $\tilde{l} = \tilde{l}_c$. The specific values of F for the AT2 and AT1 models for the two choices of length scale b and $\tilde{l}_c$ are provided in Table 2.3, as they will be frequently used in forthcoming sections.

We note the resemble between the nondimensional elastodynamic and PF equations. In both cases, the density terms are the squares of the ratios of the time scale of the given problem to $\tilde{\tau}$ and the damping coefficients are the same time ratio times the corresponding damping factor. The damping factor plays a key role in the behavior of each of the damped hyperbolic equations. [‡]

2.3.5 1D fragmentation problem

After a general nondimensional form of the PF problem was presented in §2.3.3, we focus on 1D and 0D problems, the latter having no spatial coordinates. Additionally, we assume that the damping coefficient and body force are both zero for the elastodynamic problem. Accordingly, (2.16) is simplified to,

$$\bar{\rho}_u \frac{\partial^2 \bar{u}}{\partial \bar{t}^2} - \frac{\partial \bar{\sigma}}{\partial \bar{x}} = 0 \quad \text{equation of motion,} \quad (2.19a)$$

$$\bar{\sigma} = \omega(d) \bar{\sigma}_e, \quad \bar{\sigma}_e = \bar{\epsilon} = \frac{\partial \bar{u}}{\partial \bar{x}} \quad \text{constitutive and compatibility equations.} \quad (2.19b)$$

Moreover, in (2.17) $\Delta_{\bar{x}} d$ changes to $\frac{\partial^2 d}{\partial \bar{x}^2}$.

[‡]In this manuscript, we limit our focus to rate-effects that arise from the temporal partial derivatives of the PF PDE. Beyond this, one can study the rate-dependency of fracture from the dispersive nature of the elastodynamic problem; see for example [86] where the rate-dependency of a viscoelastic material in combination with an EPF equation is studied. Equation (2.16a) paves the way to investigate the effect of material damping, through f_u , on fracture QoIs in future works.

We consider the fracture of a bar of length L with the nondimensional coordinates $\bar{x} = [-L/2\tilde{l}, L/2\tilde{l}]$, subject to a spatially uniform strain rate $\bar{\epsilon}_o$. That is, up to the time that no fracture occurs ($d = 0$), the exact solution matches the function below,

$$\bar{u}_{\text{icbc}} = \bar{\epsilon}_o \bar{x} \bar{t}, \quad (2.20)$$

This function specifies the *Initial Conditions* (ICs) and the *Boundary Conditions* (BCs),

$$\bar{u}(\bar{x}, 0) = 0, \quad \bar{v}(\bar{x}, 0) = \bar{\epsilon}_o \bar{x}, \quad \text{initial conditions}, \quad (2.21a)$$

$$\bar{v}(\bar{x}, \bar{t}) = \bar{\epsilon}_o \bar{x}, \quad \text{for} \quad \bar{x} = \mp \frac{L}{2\tilde{l}} \quad \text{boundary conditions.} \quad (2.21b)$$

2.3.6 0D fragmentation problem

By referencing (2.17), (2.19), (2.20), and the ICs/BCs, we note that (2.20) is already a solution of the 1D fragmentation problem, for a spatially uniform strain $\bar{\epsilon}(\bar{x}, \bar{t}) = \bar{\epsilon}(\bar{t}) = \bar{\epsilon}_o \bar{t}$, phase field $d(\bar{x}, \bar{t}) = d(t)$, and stress $\bar{\sigma}(\bar{t}) = \omega(d(\bar{t}))\bar{\epsilon}(\bar{t})$ solutions. We refer to this spatially uniform solution as a *0D* solution, because it only depends on time. Noting that $\partial^2 d / \partial \bar{x}^2 = 0$ and $\mathcal{H}(\bar{\phi}_e) = 0.5\bar{\epsilon}^2$ in (2.17), and the change of differentiation variable from $\bar{t}$ to $\bar{\epsilon}$, we derive the following *Ordinary Differential Equation* (ODE) for d in terms of $\bar{\epsilon}$,

$$\bar{\epsilon}_{oH}^2 \frac{d^2 d}{d\bar{\epsilon}^2} + \bar{\epsilon}_{oP} \frac{dd}{d\bar{\epsilon}} = \bar{\epsilon}_{oH}^2 \frac{d^2 d}{d\bar{\epsilon}^2} + d_f \bar{\epsilon}_{oH} \frac{dd}{d\bar{\epsilon}} = \left\langle -\frac{F}{2} \omega'(d) \bar{\epsilon}^2 - \frac{\alpha'(d)}{2} \right\rangle_+, \quad (2.22)$$

where

$$\tilde{\epsilon}_P = \frac{\tilde{\epsilon}}{\xi_d} \Rightarrow \quad \bar{\epsilon}_{oP} = \frac{\dot{\epsilon}_o}{\tilde{\epsilon}_P} = \bar{\epsilon}_{oH} d_f, \quad (2.23a)$$

$$\tilde{\epsilon}_H = \frac{\tilde{\epsilon}}{\tau_d} \Rightarrow \quad \bar{\epsilon}_{oH} = \frac{\dot{\epsilon}_o}{\tilde{\epsilon}_H} = \frac{\bar{\epsilon}_{oP}}{d_f}. \quad (2.23b)$$

The strain rate scales $\tilde{\epsilon}_P$ and $\tilde{\epsilon}_H$ use the PPF and HPF specific time scales of ξ_d and τ_d from (2.13c). They are the appropriate nondimensional forms of strain rate for the PPF and HPF equations, respectively. That is, the *Left Hand Side* (LHS) of (2.22) will be expressed as $\bar{\epsilon}_{oP} dd/d\bar{\epsilon}$ and $\bar{\epsilon}_{oH}^2 d^2d/d\bar{\epsilon}^2 + d_f \bar{\epsilon}_{oH} dd/d\bar{\epsilon}$ for the PPF and HPF equations. For the EPF equation, the LHS will be zero. In the next section we will study this 0D solution for different PF PDEs, whereas in §2.5 we will show that this 0D solution is not stable beyond a certain damage threshold, resulting in genuinely spatially nonuniform 1D solutions.

2.4 0D fragmentation analysis

2.4.1 Elliptic Phase Field (EPF) equation

The relation between damage d and strain $\bar{\epsilon}_i$ is obtained by setting the RHS of (2.22) equal to zero. That is,

$$\bar{\epsilon}(d) = \sqrt{\frac{\alpha'(d)}{-F\omega'(d)}}, \quad \text{for } \bar{\epsilon} > \bar{\epsilon}_i, \quad \text{where } \bar{\epsilon}_i = \sqrt{\frac{\alpha'(0)}{-F\omega'(0)}}. \quad (2.24)$$

The values of $\bar{\epsilon}_i$, computed from the equation above, are provided in Table 2.1. Only the AT2 model with $\bar{\epsilon}_i = 0$ does not have an elastic response. For the AT1 model, if $\tilde{l} = \tilde{l}_c$, $F = 0.5$ in Table 2.3 and the normalized initiation strain (and stress) will be one. This explains the condition $\bar{b}_c = 3/8$ in Table 2.1, when the quasi-static strength of the model is required to match the material strength. We provide the strain, stress, and damage solutions corresponding to (2.24), past the initiation point. Prior to the initiation point, the normalized stress is equal to the normalized strain; that is, $\bar{\sigma} = \bar{\epsilon}$ for $\bar{\epsilon} \leq \bar{\epsilon}_i$. For the AT2 model we have,

$$\bar{\epsilon}(d) = \frac{d}{\bar{b}(1-d)} \quad \Rightarrow \quad \begin{cases} d(\bar{\epsilon}) = \frac{\bar{b}\bar{\epsilon}^2}{1+\bar{b}\bar{\epsilon}^2} \\ \bar{\sigma}(\bar{\epsilon}) = \frac{\bar{\epsilon}}{(1+\bar{b}\bar{\epsilon}^2)^2} \end{cases} \quad (2.25)$$

For the AT1 model, (2.24) yields,

$$\bar{\epsilon}(d) = \frac{\bar{\epsilon}_i}{\sqrt{1-d}} \quad \Rightarrow \quad \begin{cases} d(\bar{\epsilon}) = 1 - \left(\frac{\bar{\epsilon}}{\bar{\epsilon}_i}\right)^{-2} \\ \bar{\sigma}(\bar{\epsilon}) = \bar{\epsilon}_i \left(\frac{\bar{\epsilon}}{\bar{\epsilon}_i}\right)^{-3} \end{cases}, \quad \text{all for } \bar{\epsilon} \geq \bar{\epsilon}_i = \sqrt{\frac{3}{8b}}. \quad (2.26)$$

Finally, for the linear CZM-W model, we have,

$$\bar{\sigma}(\bar{\epsilon}) = \begin{cases} \bar{\epsilon} & \bar{\epsilon} \leq \bar{\epsilon}_i \\ \bar{\epsilon}_i \frac{\bar{\epsilon}_f - \bar{\epsilon}}{\bar{\epsilon}_f - \bar{\epsilon}_i} & \bar{\epsilon}_i < \bar{\epsilon} < \bar{\epsilon}_f \\ 0 & \bar{\epsilon}_f \leq \bar{\epsilon} \end{cases}, \quad \text{where } \bar{\epsilon}_i = 1, \text{ and } \bar{\epsilon}_f = \frac{a_1}{2} = \frac{2}{\pi \bar{b}_c}. \quad (2.27)$$

The failure (or final) strain, $\bar{\epsilon}_f$ corresponds to the strain beyond with $d = 1$ and $\bar{\sigma} = 0$. To prevent snap-back of the strain-stress response, we require $\bar{\epsilon}_f \geq \bar{\epsilon}_i$, which results in the condition $a_1 \geq 2 \Leftrightarrow \bar{b}_c \leq 2/\pi$ provided in Table (2.1) for the CZM-W model with the linear degradation function. Finally, it is noted that for CZM models the length scale is $\tilde{l}_c$, thus $\bar{b} = \bar{b}_c = b/\tilde{l}_c$.

Figure 2.1 compares the EPF strain-stress response of the four PF models considered. The solutions for AT2, AT1, and CZM-W linear model are provided in (2.25), (2.26), and (2.27), respectively and for the CZM-L model solution is numerically obtained from (2.24). To objectively compare different PF models, all maximum stress values are made equal to one. This corresponds to $\bar{b}_c = 27/256$ and $3/8$ for the AT2 and AT1 models as shown in Table 2.4 and obtained from (2.25) and (2.26), respectively. The normalization length-scale is $\tilde{l} = \tilde{l}_c$. For the CZM-W model, we choose $a_1 = 4$ ($\bar{b}_c = 1/\pi$) to obtain $\bar{\epsilon}_f = 2$; that is, the same loading and unloading slopes as shown in (2.1). As mentioned in (2.3.2), we choose the stability limit values for the CZM-L model, that is, $a_2 = 1$ and $a_1 = 3 \Leftrightarrow \bar{b}_c = 0.25$. The same values of a_1 and a_2 will be used for all PF-CZM results, unless otherwise mentioned.

In fig. 2.1, we observe two stages of loading. In the maximum stage, the stress takes its maximum value. This corresponds to $\bar{\sigma}_i = \bar{\epsilon}_i$ for the models that possess an elastic response; that is, AT1, CZM-W, and CZM-L models. For the AT2 model,

the maximum stress of $\bar{\sigma}_M = 3\sqrt{3}/16\sqrt{\bar{b}}$ is obtained for $\bar{\epsilon}_M = 1/\sqrt{3\bar{b}}$. It is evident that for $\bar{b} = 27/256$, $\bar{\sigma}_M = 1$. The quantities associated with the maximum stage are denoted by the subscript M . The failure (or final) stage corresponds to the stage where $d = 1$ and $\bar{\sigma} = 0$. This condition can be achieved for CZM-W model at a finite $\bar{\epsilon}_f$. In contrast, all the other models only asymptotically tend to the $d = 1$ condition. However, if a user-specified final damage such as $D_f = 0.99$ or 0.999 is chosen, the corresponding $\bar{\epsilon}_f$ can be obtained from (2.25) and (2.26) for AT2 and AT1 models.

The energy densities per volume defined as,

$$\bar{\phi}_d = \int_0^\infty \bar{\sigma}(\bar{\epsilon})d\bar{\epsilon}, \quad \bar{\phi}_M = \int_0^{\bar{\epsilon}_M} \bar{\sigma}(\bar{\epsilon})d\bar{\epsilon}, \quad \bar{\phi}_f = \int_{\bar{\epsilon}_M}^\infty \bar{\sigma}(\bar{\epsilon})d\bar{\epsilon} \quad (2.28)$$

correspond to total dissipated energy, and densities up to maximum stage and past the maximum stage, respectively. Clearly, $\bar{\phi}_d = \bar{\phi}_M + \bar{\phi}_f$. Finally, following [87], we use the *brittleness indicator*,

$$B_\phi = \frac{\bar{\phi}_M}{\bar{\phi}_d} \quad (2.29)$$

to measure the brittleness of the strain-stress response. When, $B_\phi = 1$, there is no energy dissipation reserve past the maximum stage, whereas for $B_\phi \rightarrow 0$, the response becomes more ductile by having a higher energy dissipation reserve past the maximum stress.

Table 2.4 compares the QoIs extracted from the EPF responses of the four PF models. For the AT1, AT2, and CZM-W linear models, the results are presented for a general $\bar{b}$, whereas for the CZM-L model the previously mentioned values of $a_2 = 1$ and $a_1 = 1$ ($\bar{b}_c = 0.25$) are used.

2.4.2 Parabolic Phase Field (PPF) equation

The parabolic PF equation corresponds to the equation (2.22) without the second time derivative of d . By choosing the time scale $\tilde{\tau} = \xi_d$, *cf.* (2.13c), the solution of

the 0D PPF equation is obtained from,

$$\bar{\epsilon}_{oP} \frac{dd}{d\bar{\epsilon}} = -\frac{F}{2} \omega'(d) \bar{\epsilon}^2 - \frac{\alpha'(d)}{2}, \quad \text{for } \bar{\epsilon} \geq \bar{\epsilon}_i \quad (\tilde{\tau} = \xi_d). \quad (2.30)$$

2.4.2.1 Analytical solution for AT1

We obtained an analytical solution for this ODE only for the AT1 model. The PPF equation for the AT1 model can be written as,

$$\bar{\epsilon}_{oP} \frac{dd}{d\bar{\epsilon}} = \frac{1}{2} \left((1-d) \left(\frac{\bar{\epsilon}}{\bar{\epsilon}_i} \right)^2 - 1 \right), \quad \text{for } \bar{\epsilon} \geq \bar{\epsilon}_i \quad (2.31)$$

This equation can be solved by the change of variable $z = z_i(\bar{\epsilon}/\bar{\epsilon}_i)^3$, where the initial condition $\bar{\epsilon} = \bar{\epsilon}_i = \sqrt{3/8b}$ corresponds to $z = z_i = \bar{\epsilon}_i/6\bar{\epsilon}_{oP}$. The ODE (2.31) cast in terms of z is $dd/dz = 1 - d - (z/z_i)^{-2/3}$. The solution to this ODE is $d(z) = e^{-z} \left\{ e^{-z_i} + z_i^{2/3} [\Gamma(1/3, -z_i) - \Gamma(1/3, -z)] \right\} - 1$. The incomplete upper and lower Gamma functions are,

$$\Gamma(s, x) = \int_x^\infty t^{s-1} e^{-t} dt, \quad \gamma(s, x) = \int_0^x t^{s-1} e^{-t} dt.$$

Other Gamma function expressions that will be used later are, the (complete) Gamma function $\Gamma(s) = \int_0^\infty t^{s-1} e^{-t} dt$, that is $\Gamma(s) = \Gamma(s, 0)$, and normalized incomplete gamma functions $\bar{\gamma}(s, x) = \gamma(s, x)/\Gamma(s)$ and $\bar{\Gamma}(s, x) = \Gamma(s, x)/\Gamma(s)$. The analytical solution of 0D AT1 PPE (2.31) recast from z in terms of $\bar{\epsilon}$ is,

$$d(\bar{\epsilon}) = 1 - e^{-\frac{\bar{\epsilon}^3 - \bar{\epsilon}_i^3}{6\bar{\epsilon}_{oP}\bar{\epsilon}_i^2}} - \frac{1}{2\bar{\epsilon}_{oP}} \int_{\bar{\epsilon}_i}^{\bar{\epsilon}} e^{-\frac{\bar{\epsilon}^3 - s^3}{6\bar{\epsilon}_{oP}\bar{\epsilon}_i^2}} ds, \quad \text{for } \bar{\epsilon} \geq \bar{\epsilon}_i. \quad (2.32)$$

2.4.2.2 High Rate Asymptotic (HRA) PPF solutions

2.4.2.2.1 Formulation of the asymptotic solution Generally, a numerical integration scheme is needed for the solution of (2.30). Aside from such solutions, one is interested in the asymptotic behavior of this 0D PPF problem as the loading rate

tends to zero or large values. The limiting solution of the solution as $\bar{\epsilon}_{oP} \rightarrow 0$ is the EPF solution provided in (2.4.1). The problem of obtaining the difference between the PPF solution at low $\bar{\epsilon}_{oP}$ and the EPF solution is a singular-perturbation problem as $\bar{\epsilon}_{oP}$, the coefficient of the leading term $\bar{\epsilon}_{oP} dd/d\bar{\epsilon}$ in (2.30), tends to zero. While there are applications where finding such low loading rate asymptotic solutions is of interest, in this work we focus on the *High Rate Asymptotic* (HRA) solution.

In §2.4.2.3 the solutions to (2.30) are provided for a range of loading rates. As will become evident, for high rates, the maximum stress, failure strain, and dissipated energy increase. To derive the HRA behavior of these QoIs and the solution of the ODE, we introduce a scaled nondimensional strain for the HRA solution,

$$\hat{\epsilon} := \varepsilon(\bar{\epsilon} - \bar{\epsilon}_i). \quad (2.33)$$

The solution at high rates can now be expressed in terms of $\hat{\epsilon}$, and a nondimensional scaled stress $\hat{\sigma}$ that are independent of the loading rate. The asymptotic scaling ε will be chosen such that the highest order terms on the left and right sides of the equation are of the same order of magnitude. The subtraction by $\bar{\epsilon}_i$ in (2.33) ensures that the solution is sought from the instant that damage starts to accumulate.

By choosing $\varepsilon = \bar{\epsilon}_{oP}^{-1/3}$, and recalling (2.33),

$$\frac{dd}{d\hat{\epsilon}} = -\frac{F}{2}\omega'(d) \left(\hat{\epsilon}^2 + \varepsilon\bar{\epsilon}_i + \varepsilon^2\bar{\epsilon}_i^2 \right) - \varepsilon^2 \frac{\alpha'(d)}{2}, \quad \text{for } \hat{\epsilon} \geq 0 \quad (2.34)$$

the highest order terms on the LHS ($dd/d\hat{\epsilon}$ and RHS ($0.5F\omega'(d)\hat{\epsilon}^2$) are now of the same order of magnitude and we can seek an asymptotic solution in the form $d(\hat{\epsilon}) = d_0(\hat{\epsilon}) + \varepsilon d_1(\hat{\epsilon}) + \varepsilon^2 d_2(\hat{\epsilon}) + \dots$. By using the Taylor's expansion of $\omega'(d)$ around $d = 0$, and collecting the highest order terms, the zeroth order term d_0 is obtained from the solution of,

$$\frac{dd_0}{d\hat{\epsilon}} = -\frac{F}{2}\omega'(d_0)\hat{\epsilon}^2, \quad \text{for } \hat{\epsilon} \geq 0, \text{ and initial condition } d_0(\hat{\epsilon} = 0) = 0. \quad (2.35)$$

Next, we express the zeroth order expansion terms for nondimensional strain, stress, and energy density. From (2.33), we have $\bar{\epsilon} = \hat{\epsilon}/\varepsilon + \bar{\epsilon}_i$. That is, the highest order strain term is $\hat{\epsilon}$ multiplied by the factor $1/\varepsilon$. This justifies the notation of $\hat{\epsilon}$ with the hat accent as the high order strain measure. The accent decoration will be used to denote other leading higher order terms as well. Using the expansion of d , the stress is expressed as $\bar{\sigma} = \omega(d)\bar{\epsilon} = \omega(d_0 + \varepsilon d_1 + \varepsilon^2 d_2 + \dots)(\hat{\epsilon}/\varepsilon + \bar{\epsilon}_i)$. The highest order term (HOT) of this expansion is $\omega(d_0)\hat{\epsilon}/\varepsilon$, leading to the expression of the zeroth order stress term $\hat{\sigma}_0 = \omega(d_0)\hat{\epsilon}$ and $\bar{\sigma} = \hat{\sigma}_0/\varepsilon + \text{HOTs}$. Similarly, the energy density per volume, as the integral of stress versus strain, will have a zeroth order energy term computed from the integral of $\hat{\sigma}_0(\hat{\epsilon})$ versus $\hat{\epsilon}$, divided by ε^2 . In short, we have,

$$\bar{\epsilon} = \hat{\epsilon}/\varepsilon + \bar{\epsilon}_i, \quad (2.36a)$$

$$\bar{\sigma} = \hat{\sigma}_0/\varepsilon + \text{HOTs}, \quad \text{where} \quad \hat{\sigma}_0 = \omega(d_0)\hat{\epsilon}, \quad (2.36b)$$

$$\bar{\phi}_d(\bar{\epsilon}) = \int_0^{\bar{\epsilon}} \bar{\sigma}(e)de = \hat{\phi}_0/\varepsilon^2 + \text{HOTs}, \quad \text{where} \quad \hat{\phi}_0 = \int_0^{\hat{\epsilon}} \hat{\sigma}_0(\hat{e})d\hat{e}. \quad (2.36c)$$

The HRA-PPF solutions of different PF models are compared in fig. 2.2a. As will be further discussed below, we have closed-form solution for this HRA solution for AT1 and AT2 solutions, whereas for CZM-W and CZM-L models, we numerically integrated (2.35), using the Runge-Kutta 4 (RK4) method. To make the models comparable, the length scale of $\tilde{l}_c$ with $\bar{b}_c$ values from Table 2.1 are used such that the nondimensional quasi-static maximum stress of each model is 1. Furthermore, ξ_d is the time scale for PPF solutions.

We observe that the asymptotic zeroth stress solution starts at zero and reaches a maximum value, before only asymptotically tending to zero as $\hat{\epsilon} \rightarrow \infty$. Similar to the definitions in §2.4.1, the maximum and failure stages correspond to points that $\hat{\sigma}_0$ attains its maximum value and $d_0 = D_f$, where D_f is a damage threshold close to one. We denote the maximum stage HRA strain and zeroth stress values by $\hat{\epsilon}_M$ and

$\hat{\sigma}_M$, respectively. The HRA energies and brittleness indicator are defined similar to (2.28) and (2.29). That is,

$$\hat{\phi}_M = \int_0^{\hat{\epsilon}_M} \hat{\sigma}_0(\hat{\epsilon}) d\hat{\epsilon}, \quad \hat{\phi}_f = \int_{\hat{\epsilon}_M}^{\infty} \hat{\sigma}_0(\hat{\epsilon}) d\hat{\epsilon}, \quad \Rightarrow \quad \hat{\phi} = \hat{\phi}_M + \hat{\phi}_f, \quad \text{and} \quad B_\phi = \frac{\hat{\phi}_M}{\hat{\phi}}. \quad (2.37)$$

2.4.2.2.2 HRA-PPF solution for AT1 and AT2 models The zeroth term of HRA-PPF equation (2.35) can be analytically solved for AT1 and AT2 models. The ODE and the corresponding solutions are,

$$\frac{dd_0}{d\hat{\epsilon}} = F(1 - d_0)\hat{\epsilon}^2, \quad \Rightarrow \quad d_0(\hat{\epsilon}) = 1 - e^{-F\hat{\epsilon}^3/3}, \quad \text{for} \quad \hat{\epsilon} \geq 0, \quad (2.38)$$

where the IC in (2.35) is used to derive the solution. The value of F provided in (2.18) depends on $\bar{b}$.

Recalling (2.36b) and (2.37) the zeroth HRA stress, and maximum and final stage solutions are obtained as,

$$\hat{\sigma}_0 = \hat{\epsilon} e^{-2F\hat{\epsilon}^3/3} \quad \Rightarrow \quad \begin{cases} \hat{\epsilon}_M = \frac{1}{\sqrt[3]{2F}} \\ \hat{\sigma}_M = \frac{1}{\sqrt[3]{2F}} e^{-1/3} \\ \hat{\phi}_M = \frac{1}{\sqrt[3]{12F^2}} \gamma\left(\frac{2}{3}, \frac{1}{3}\right) \\ \hat{\phi}_f = \frac{1}{\sqrt[3]{12F^2}} \Gamma\left(\frac{2}{3}\right) \end{cases}, \quad \text{and} \quad B_\phi = \bar{\gamma}\left(\frac{2}{3}, \frac{1}{3}\right). \quad (2.39)$$

2.4.2.2.3 Summary of HRA-PPF solutions Table 2.5 summarizes the QoIs of HRA-PPF solutions for all the PF models. For the first rows of AT1 and AT2 models the expressions are obtained for an arbitrary $\bar{b}$ from (2.39) and Table 2.3. The QoIs in the other rows correspond to the solutions in fig. 2.2a and the CZM length scale $\tilde{l} = \tilde{l}_c$, such that quasi-static $\bar{\sigma}_M = 1$.

For none of the models d_0 reaches zero at a finite $\hat{\epsilon}$. This is evident from the asymptotic decay of $\hat{\sigma}_0$ in fig. 2.2a. For the AT2 and AT1 models, the terminal HRA strain is computed from (2.38) for $d_0(\hat{\epsilon}_f) = D_f$. For the CZM models, $\hat{\epsilon}_f$ is computed

for $D_f = 0.99$. We also observe that while all the models have a normalized strength of one for quasi-static loading, the AT2 and AT1 have a higher maximum stress for the zeroth asymptotic expansion. Moreover the CZM models have a more ductile response by having a larger post-peak energy dissipation capacity. This is reflected in their lower B_ϕ values.

2.4.2.3 Numerical solutions for 0D PPF equation

Figure 2.3 shows the 0D PPF solutions for different loading rates. The AT1 and CZM-W models are used as representatives of LEFM- and CZM-based PF models. The solutions (colored solid lines) are obtained by numerical integration of (2.30) using the RK4 method. Even for the AT1 model this equation is used, as the exact solution (2.32) involves an integral that cannot be cumulatively updated for successive $\bar{\epsilon}$ if $\exp(-\bar{\epsilon}^3/6\bar{\epsilon}_{oP}\bar{\epsilon}_i^2)$ is kept in the integrand; otherwise the solution blows up quickly.[§] The asymptotic solutions, shown by the dashed lines, is computed from (2.38) for the AT1 model and RK4 integration of (2.35) for the CZM-W model. The HRA strain and stress $(\hat{\epsilon}, \hat{\sigma}_0)$ and nondimensional strain and stress $(\bar{\epsilon}, \bar{\sigma})$ are related through (2.36a) and (2.36b). Alternatively, one can integrate the pull-back of (2.35), $\bar{\epsilon}_{oP} d\bar{\sigma}/d\Delta\bar{\epsilon} = -F\omega'(d)(\Delta\bar{\epsilon})^2/2$ using the RK4 method for $\Delta\bar{\epsilon} = \bar{\epsilon} - \bar{\epsilon}_i \geq 0$.

As expected, the results of both models tend to the EPF solution (shown by solid black line) as the loading rate tends to zero. For higher loading rates, the HRA-PPF solutions provide a relatively good estimate of the solution, albeit overestimating the maximum stress $\bar{\sigma}_M$. Furthermore, we observe that as the loading rate increases, $\bar{\epsilon}_M$ and failure strain $\bar{\epsilon}_f$ increase. From the HRA analysis, that is the definitions (2.36a), (2.36b), and $\varepsilon = \bar{\epsilon}_{oP}^{-1/3}$, $\bar{\epsilon}_M$ and $\bar{\epsilon}_f$ are expected to grow asymptotically as $\bar{\epsilon}_{oP}^{1/3}$ for high loading rates. This claim will be further investigated for the actual values of $\bar{\sigma}_M$ and $\bar{\epsilon}_f$ in §2.4.5.

[§]The blow-up is related to the difference of two incomplete gamma functions in terms of z in §2.4.2.1 with negative z arguments.

2.4.3 Hyperbolic Phase Field (HPF) equation

Referring to (2.13c), the natural time scale for the HPF equation is $\tilde{\tau} = \sqrt{\varrho_d} = \tau_d$. By choosing this time scale, $\bar{\rho}_d = 1$ and $\bar{\xi}_d = d_f$, and the solution of (2.22) for inelastic regime is obtained form,

$$\bar{\epsilon}_{oH}^2 \frac{d^2 d}{d\bar{\epsilon}^2} + \bar{\epsilon}_{oH} d_f \frac{dd}{d\bar{\epsilon}} = -\frac{F}{2} \omega'(d) \bar{\epsilon}^2 - \frac{\alpha'(d)}{2}, \quad \text{for } \bar{\epsilon} \geq \bar{\epsilon}_i \quad (\tilde{\tau} = \tau_d). \quad (2.40)$$

2.4.3.1 High Rate Asymptotic (HRA) HPF solution

2.4.3.1.1 Formulation of the asymptotic solution Similar to the PPF equation, we only limit the asymptotic analysis of the HPF equation to high loading rates and for the zeroth term of the expansion. The rationale is that such analysis determines the loading rate dependency of maximum stress, failure strain, and dissipated energy of the 0D model.

At high loading rates, $\bar{\epsilon}_{oH}^2 d^2 d / d\bar{\epsilon}^2$ is the dominant term on the LHS. By the change of strain variable (2.36a) and choosing $\varepsilon = \bar{\epsilon}_{oH}^{-1/2}$, and recalling (2.33),

$$\frac{d^2 d}{d\hat{\epsilon}^2} + \varepsilon d_f \frac{dd}{d\hat{\epsilon}} = -\frac{F}{2} \omega'(d) \left(\hat{\epsilon}^2 + \varepsilon \bar{\epsilon}_i + \varepsilon^2 \bar{\epsilon}_i^2 \right) - \varepsilon^2 \frac{\alpha'(d)}{2}, \quad \text{for } \hat{\epsilon} \geq 0. \quad (2.41)$$

The solution can be expanded as $d(\hat{\epsilon}) = d_0(\hat{\epsilon}) + \varepsilon d_1(\hat{\epsilon}) + \varepsilon^2 d_2(\hat{\epsilon}) + \dots$. By using the Taylor's expansion of $\omega'(d)$ around $d = 0$, and collecting the highest order terms, the zeroth order term d_0 is obtained from the solution of,

$$\frac{d^2 d_0}{d\hat{\epsilon}^2} = -\frac{F}{2} \omega'(d_0) \hat{\epsilon}^2, \text{ for } \hat{\epsilon} \geq 0, \text{ and } d_0(\hat{\epsilon} = 0) = 0, \text{ and } \frac{dd_0}{d\hat{\epsilon}}(\hat{\epsilon} = 0) = 0, \quad (2.42)$$

where the initial conditions correspond to zero damage and continuity of slope of strain-stress response ($d\bar{\sigma}/d\bar{\epsilon} = 1$) at the start of the HRA-HPF solution. The only difference between (2.42) and (2.35) is the appearance of the second order derivative on the LHS of (2.42). The zeroth order stress and energies are computed following the same process detailed in §2.4.2.2.2. Specifically, the zeroth order stress and its

relation to $\bar{\sigma}$ is provided in (2.36b). The definition of HRA energy and stage value energies follows (2.36c) and (2.37), respectively.

2.4.3.1.2 HRA-HPF solution for AT1 and AT2 models Similar to the HRA-PPF, we do not have a closed-form solution of (2.42) for the CZM models. The zeroth term of HRA-HPF equation (2.42) can be analytically solved for AT1 and AT2 models. The ODE and the corresponding solutions are, [¶]

$$\frac{d^2 d_0}{d\hat{\epsilon}^2} = F(1 - d_0)\hat{\epsilon}^2, \Rightarrow d_0(\hat{\epsilon}) = 1 - \sqrt[8]{F} \frac{\Gamma(0.75)}{\sqrt{2}} J_{-0.25}(\sqrt{F} \frac{\hat{\epsilon}^2}{2}), \text{ for } \hat{\epsilon} \geq 0, \quad (2.43)$$

where $J_{-0.25}$ is the Bessel function of the first kind of order -0.25. Recalling (2.36b) and (2.37) the zeroth HRA stress and HRA-HPF QoIs are obtained as,

$$\hat{\sigma}_0 = \hat{\epsilon} \sqrt[4]{F} \frac{\Gamma^2(0.75)}{2} J_{-0.25}^2(\sqrt{F} \frac{\hat{\epsilon}^2}{2}) \Rightarrow \begin{cases} \hat{\epsilon}_M = \frac{1.0874}{\sqrt[4]{F}} \\ \hat{\sigma}_M = \frac{0.8543}{\sqrt[4]{F}} \\ \hat{\phi}_M = \frac{0.5475}{\sqrt{F}} \\ \hat{\epsilon}_f = \frac{2.0031}{\sqrt[4]{F}} \\ \hat{\phi}_f = \frac{0.9752}{\sqrt{F}} \end{cases}, \text{ and } B_\phi = 0.5615, \quad (2.44)$$

where unlike the HRA-PPF solution, $\hat{\epsilon}_f$ is finite and is obtained from the first zero of $J_{-0.25}$.

2.4.3.1.3 Summary of HRA-HPF solutions Figure 2.2b compares the HRA-HPF solutions for all PF models for $d_f = 1$. All solutions are obtained by the RK4 method and expressing (2.42) as a system of two first order differential equations. As mentioned earlier, τ_d is the time scale of choice for the HPF equation. The cohesive length scale $\tilde{l}_c$ ensures that all the models have a quasi-static maximum stress of one. Although as can be seen, the ordering of maximum stresses of the asymptotic solution

[¶]The general solution for the ODE $d^2 y/dx^2 - ax^n y = 0$ is provided in [88], section 2.1.2-1 (7). By using $y = d_0$, $x = 1 - d_0$, $n = 2$, and employing the ICs from (2.42), the solution (2.43) is derived.

is similar to that of the HRA-PPF solution; *cf.* fig. 2.2a. That is, the AT2 and AT1 models have a higher $\hat{\sigma}_M$ than the CZM models.

The QoIs extracted from these simulations are presented in Table 2.6. For the first rows of AT1 and AT2 models the expressions are obtained for an arbitrary $\bar{b}$ from (2.44) and Table 2.3. The QoIs in the other rows correspond to the solutions in fig. 2.2b and the CZM length scale $\tilde{l} = \tilde{l}_c$, such that quasi-static $\bar{\sigma}_M = 1$. There are two differences when these QoIs are compared to HRA-PPF ones in Table 2.5. First, for the HPF equation, there a finite strain at which d reaches zero, and there is no need to compute $\hat{\epsilon}_f$ for a $D_f < 1$. Second, while the response of CZM models is still more ductile, the difference between B_ϕ of different models is much smaller than those observed for the HRA-PPF in Table 2.5. The rather symmetric loading and unloading strain-stress curves in fig. 2.2b correspond to B_ϕ values close to 0.5 in Table 2.6.

2.4.3.2 Numerical solutions for 0D HPF equation

The 0D HPF solutions are shown for different loading rates and AT1 and CZM-W models in fig. 2.4. All the solutions, (2.40) for the solid lines and (2.42) for the dashed lines, are obtained by the RK4 method. Another way to solve the HRA-HPF equation is to pull back (2.42) to nondimensional strain, using (2.36a). This corresponds to $\bar{\epsilon}_{oH}^2 d^2 d/d\Delta\bar{\epsilon}^2 = -c_\alpha/4\omega'(d)(\Delta\bar{\epsilon})^2\bar{b}$. That is, the HRA-HPF problems solves the HPF problem for the difference in strain and a zero damping factor d_f .

Similar to the PPF equation, the results tend the EPF solutions (black solid lines) as the loading rate tends to zero. For the higher loading rates, the solutions are generally close to the asymptotic ones (dashed lines). In fact, the relative error between the actual and HRA solutions seems to be smaller for the HPF equation than the PPF equation. From the asymptotic analysis in §2.4.3.1, $\varepsilon = \bar{\epsilon}_{oH}^{-1/2}$, and strain (2.36a) and stress (2.36b) relations, we know that for the zeroth order HRA solutions, $\bar{\sigma}_M$ and $\bar{\epsilon}_f$ grow as $\bar{\epsilon}_{oH}^{1/2}$. In §2.4.5, we investigate how accurately the actual values of $\bar{\sigma}_M$ and $\bar{\epsilon}_f$ vary versus for $\bar{\epsilon}_{oH}$ for the HPF equation.

2.4.4 Behavior of failure strain $\bar{\epsilon}_f$ for 0D PF solutions

We will investigate the trend at which damage reaches zero for different PF models and differential equations. Understanding this trend is important in labeling certain regions of solution as fully damaged in 0D to 3D setting. In addition, we believe that it also impacts the response of regions close to full damage in PF simulations. The summary of the behavior of failure strain $\bar{\epsilon}_f$ is provided in Table 2.7. The EPF row corresponds to the values of $\bar{\epsilon}_f$ from Table 2.1. We observe that except the CZM-W model that has a finite strain, $\bar{\epsilon}_f$ is inversely proportional to $1 - D_f$. The power of -1 means that damage for AT2 model tends to one much slower than AT1 and CZM-L models with the power of $-1/2$.

The behavior for dynamic PF equations is more complicated. For this, we refer to fig. 2.5, where damage evolution versus $\bar{\epsilon}$ is depicted for the PPF and HPF equations. Results are only presented for the AT1 model as for moderate to high loading rates, the other models behave similarly. While we have not performed an asymptotic analysis for the low loading regime, the response of $\bar{\epsilon}_f$ is expected to tend to that of the EPF equations discussed above. For moderate to high loading rate in general we have observed that damage only asymptotically reaches one for the PPF equation and $\bar{\epsilon}_f$ takes finite values for the HPF equation.

The high loading rate results for the PPF equation in fig. 2.5a and Table 2.7 show that while d still only asymptotically reaches one, it has a faster convergence than the EPF equation. This can be explained by logarithmic dependence of $\bar{\epsilon}_f$ on $1 - D_f$ for the former case versus power dependence on $1 - D_f$ in the latter case. Still, to explain why $\bar{\epsilon}_f$ is not finite (for $D_f = 1$ and high loading rates), we refer to (2.38) and observe that as $d \rightarrow 1^-$, the RHS tends to zero. This implies that $dd/d\bar{\epsilon} \rightarrow 0$ as $d \rightarrow 1^-$, hence d only asymptotically converges to one. This behavior can be observed in fig. 2.5a.

The results for the HPF equation are shown in fig. 2.5b. In this case for moderate to high loading rates, d approaches unity with an almost constant slope versus $\bar{\epsilon}$ as

$D_f \rightarrow 1$, explaining the finiteness of $\bar{\epsilon}_f$ for $D_f = 1$. From the HRA-HPF equation (2.42) we observe that as d tends to one, the RHS and hence the second derivative on the LHS tend to zero. This explains the rather constant slope of D_f versus $\bar{\epsilon}$ in the figure. There is also another difference between the PPF and HPF equations in terms of $\bar{\epsilon}_f$. Once a $D_f < 1$ is set for the PPF equation, we observe that $\bar{\epsilon}_f$ grows faster for the HPF equation; that is, $\mathcal{O}(\bar{\epsilon}_o^{1/2})$ versus $\mathcal{O}(\bar{\epsilon}_o^{1/3})$ for the PPF equation. This is an outcome of value of ε in their corresponding asymptotic solutions.

2.4.5 Rate-dependency of PF and some continuum damage models

In this section we examine the rate dependency of QoIs such as energy dissipation density, maximum stress, and failure strain for the PF models discussed and a slightly more general form of a damage evolution model.

2.4.5.1 Verification of rate-dependency of PPF and HPF equations

The asymptotic analysis of PPF and HPF solutions at high loading rates in §2.4.2.2 and §2.4.3.1 showed that the maximum stress $\bar{\sigma}_M$ and failure strain $\bar{\epsilon}_f$ scaled as ε^{-1} ; cf. (2.36a) and (2.36b). As the integral of stress versus strain, the energy dissipation density $\bar{\phi}_f$ scales as ε^{-2} . Since, $\varepsilon = \bar{\epsilon}_o^{-1/3}$ and $\bar{\epsilon}_o^{-1/2}$ for the PPF and HPF equations, respectively, we expect $\bar{\sigma}_M, \bar{\epsilon}_f = \mathcal{O}(\bar{\epsilon}_o^{1/3})$, $\bar{\phi}_f = \mathcal{O}(\bar{\epsilon}_o^{2/3})$ for the former and $\bar{\sigma}_M, \bar{\epsilon}_f = \mathcal{O}(\bar{\epsilon}_o^{1/2})$, $\bar{\phi}_f = \mathcal{O}(\bar{\epsilon}_o^1)$ for the latter. The objective is to verify such rate dependency and determine the loading rates beyond which they apply.

The strain stress response of AT1 and CZM-W models are provided in fig. 2.3 and fig. 2.4 for PPF and HPF equations. The aforementioned QoIs are determined from the simulation of a wider range of loading rates for all four PF models. To determine the dependency of QoIs on the loading rate at high values, the log-log plots of $\bar{\sigma}_M$ and $\bar{\phi}_f$ versus $\bar{\epsilon}_o$ are presented in fig. 2.6 for the PPF and HPF equations. As expected, QoIs converge to the quasi-static QoIs determined by EPF equation (solid dashed

lines) as $\bar{\epsilon}_o$ tends to zero. Dashed lines correspond to the solutions of HRA equations (2.35) and (2.42). Their slopes are $p/2$ and p for $\bar{\sigma}_M$ and $\bar{\phi}_f$, respectively, where $p = 1/3$ for the PPF and $p = 1/2$ for the HPF equation.[†] We observe that the slopes of the results of both QoIs match the predicted asymptotic rates. In fact, the QoIs associated with the exact solutions follow the power energy rate dependencies even earlier than the HRA solutions; *e.g.*, *cf.* fig. 2.6a. In general, we observe that the values determined from the HRA,

$$\bar{\sigma}_M = \hat{\sigma}_M \bar{\epsilon}_o^{\frac{p}{2}}, \quad \bar{\epsilon}_f = \hat{\epsilon}_f \bar{\epsilon}_o^{\frac{p}{2}}, \quad \bar{\phi}_f = \hat{\phi}_f \bar{\epsilon}_o^p \quad (2.45)$$

are very accurate for $\log_{10}(\bar{\epsilon}_o) \gtrsim 0.5$ to 1 ($\bar{\epsilon}_o \gtrsim 3$ to 10). $\hat{\sigma}_M$, $\hat{\epsilon}_f$, $\hat{\phi}_f$, and other relevant factors are provided in Table 2.5 and Table 2.6.

2.4.5.2 Rate dependency of a more general set of continuum damage and PF models

As mentioned in §2.2.1, the gradient continuum damage models are one of the approaches that by incorporating a length scale resolve the mesh sensitivity of earlier local damage models. The elliptic form of these equations involves the Laplacian of either a parameter that acts as the driving force of the damage parameter (for example a strain field as in [89, 90]) or the actual damage parameter. We restrict the remainder of discussion to the latter set, where the PDE of the fracture problem is directly expressed in terms of the damage parameter d . In this case, [64] provides a very general thermodynamic framework to derive elliptic, parabolic, and hyperbolic PDEs for d . After some relabeling and simplifying the equations in section 3.2.4 of [64], one subclass of scalar damage models can be expressed in the form $\varrho_d \partial^2 d / \partial t^2 + \xi_d \partial d / \partial t - b^2 \Delta_{\mathbf{x}} d$ equal to the RHS damage driving force. We note

[†]These slopes are exact for the AT2 model, whereas for the models with nonzero $\bar{\epsilon}_i$ the addition of initiation stress and energy results in some discrepancies for lower $\bar{\epsilon}_o$ values.

the resemblance to the PF PDE (2.7b), with the difference that for the continuum damage models the driving force takes different and more flexible forms.

Time-delay and time-dependent damage models are other sets of continuum damage models that are relevant to subsequent discussion. In [91, 92, 93], instead of a characteristic length, a characteristic time is introduced in the damage equation to resolve the mesh sensitivity of local damage models ^{**} and model some fracture rate effects. For example, in [93, 96, 97], the damage rate is bounded by $1/\tau_d$, where τ_d is the relaxation time. These damage models do not include a Laplacian and can be expressed as $\tau_d \partial d / \partial t$ equal to a RHS that is a function of the difference between the target local damage and instantaneous damage values.

The following differential equation,

$$\tau_d^n \frac{d^n d}{dt^n} + f_{d,n-1} \tau_d^{n-1} \frac{d^{n-1} d}{dt^{n-1}} + \dots + f_{d,1} \tau_d \frac{dd}{dt} = G(d) \epsilon^m + \text{strain independent terms} \quad (2.46)$$

captures the transient part of many of continuum damage and PF models, where n is the temporal order of the differential equation and m the highest power by which the damage driving force (the RHS) grows versus strain. For example, for gradient damage models expressed in d (e.g., [64]) and PF equation (2.22), $n = 2$ and 1 for hyperbolic and parabolic PDEs. Furthermore, the time-delay damage models [93, 96, 97] can be cast in the form above for $n = 1$. The spatial derivatives of the damage equation (e.g., the Laplacian for gradient damage and PF equations) are eliminated in (2.46) as we seek the 0D solution. For ODE-type time-delay models such as [97, 96], the damage equation is already in the form (2.46) as the equation does not include any spatial derivatives. While (2.46) is written for an arbitrary n to facilitate the discussion of its role, we are going to only consider $n = 1$ (same as PPF equation) and $n = 2$ (same as HPF equation). ^{††}

^{**}These models do not fully eliminate the mesh dependency for example at low loading rates; cf. see the results and discussion in [94, 95].

^{††}The challenges in formulating well-posed PDEs with a higher than 2 temporal order is discussed in [98] (pages 205-211), quoting “The equations of order greater than 2 must be of very special form if they are to have well-posed initial value problems.”.

The term $G(d)$ plays the role of $-\omega'(d)$ for the PF models and determines how the driving force is affected by d . We assume that $G(d)$ and the degradation function of stress versus d satisfy the usual damage mechanics conditions. The order m determines the nature of driving force. In most PF formulations, d is driven by the elastic energy density ϕ_e , *cf.* (2.7b). As in (2.22), this results in $m = 2$ for the 0D analysis considered. On the other hand, for a phenomenological damage model, d can be driven by a strain measure such as Mazars equivalent strain [99], the modified von-Mises strain [89] or a variety of stress measures computed from strain. In such cases, $m = 1$.^{‡‡} Finally, there are models for which the damage evolution force is bounded from above. For example, for all the time-delay models in [93, 96, 97, 100, 101], the stipulation of a maximum damage rate of $1/\tau_d$ implies that the RHS is $\mathcal{O}(1)$ ($m = 0$) at high strain rates.

The HRA analysis of (2.46) follows the same process detailed in §2.4.2.2 and §2.4.3.1. From $\epsilon = \dot{\epsilon}_0 t$, nondimensionalization of the equation, and change of variable to the nondimensional strain $\bar{\epsilon}$, the terms on the LHS are in the form $f_{d,i} \bar{\epsilon}_0^i d^i d/d\bar{\epsilon}^i$ for $i = 1$ to n ($f_{d,n} = 1$). For constant $f_{d,i}$ and large enough strain rate $\bar{\epsilon}_0$ the leading term $\bar{\epsilon}_0^n d^n d/d\bar{\epsilon}^n$ dominates the LHS. The dominant term on the RHS is $\bar{\epsilon}^m$. A change of variable of the form (2.33), results in $(\bar{\epsilon}_0 \epsilon)^n \frac{d^n d}{d\bar{\epsilon}^m}$ and $1/\epsilon^m \bar{\epsilon}^m$ leading terms on the LHS and RHS of equation, respectively. For the solution of the zeroth term of the asymptotic solution, ϵ is determined by equating the factors of these terms, resulting in $\epsilon = -p/2$, where,

$$p = \frac{2n}{n+m} \quad (2.47)$$

determines the rate dependency of (2.46). Equations of the form (2.36a), (2.36b), and the fact that energy density is the integral of strain versus stress, results in (2.45) where now p for the more general differential equation (2.46) is provided in (2.47).

^{‡‡}In [62] different forms of damage and PF formulations are compared. One continuum damage formulation is written in terms of the damage field d and can have a strain-based driving force. While [62] focuses on quasi-static fracture, one can easily add the temporal derivative terms in (2.46) to this particular formulation and have the sample formulations listed in the Table.

The rate-dependency of some realistic models are provided in Table 2.8. The PPF and HPF equations presented correspond to $m = 2$ row of the table. For a strain/stress driven damage force (second row), the rate dependency of (2.46) is higher. This can be justified by the fact that when the damage force is driven by energy ($m = 2$), it grows faster than for $m = 1$. This results in a more rapid accumulation of d to unity and explains the milder rate sensitivity of the corresponding QoIs. The same more delayed damage evolution argument can be applied from $m = 1$ to $m = 0$ row as in the latter case, no matter how large the strain gets, the driving force is bounded. In fact, in [97] damage rate is bounded by the inverse of a relaxation time τ_d , resulting in a very high rate-sensitivity of 2 for energy. The results in [97] confirm this rate dependency. In §2.5.5, we will discuss how the rate p for energy dissipation compares with fragmentation models such as Grady's model [5].

Finally, we note that the differential equations of the form (2.46) can explain the rate-dependencies of some interfacial damage models by replacing strain with displacement jump and stress with traction. For example, the rate-dependent models proposed in [102, 103] have the same functional form as the time-delay damage model [93, 96, 97] with $n = 1$ and $m = 0$. Not surprisingly, they exhibit the same rate dependency of p and $p/2$ for the energy dissipation and maximum traction.

2.4.6 Effect of damping factor

In this section, we use the time scale $\tilde{\tau} = \tau_d$ to examine the effect of d_f on the response of PPF and HPF equations. The study for the PPF case is more nuanced; recalling (2.13c), $\tilde{\tau} = \xi_d = d_f \tau_d$ is the time scale of choice for the PPF equation. This results in the use of $\bar{\epsilon}_{oP}$ for the nondimensional strain rate in the entire §2.4.2. Clearly, with this time scale, the strain-stress response only depends on $\bar{\epsilon}_{oP}$ in fig. 2.3. The effect of d_f is already incorporated in the value that $\bar{\epsilon}_{oP}$ takes, given a dimensional strain rate $\dot{\epsilon}_o$. However, there are many instances where $\tilde{\tau} = \tau_d$ is the time scale of choice

even for the PPF equation; for example in 1D to 3D problems, the interaction of elastic waves and PF solution becomes important. The time scale, $\tilde{\tau} = \tau_d = b/c_u$ better represents these interactions. By using $\tilde{\tau} = \tau_d$ and noting $\bar{\epsilon}_{oP} = \bar{\epsilon}_{oH}d_f$, we will investigate how the response of the PPF equation for a given $\bar{\epsilon}_{oH}$ depends on the damping factor d_f . For the HPF equation, the d_f has a more fundamental impact; as it will be discussed later under some conditions low d_f values results in a nonphysical response and high d_f values provide solutions that are too close to the corresponding PPF equation.

2.4.6.1 Strain stress response

Figure 2.7 shows the effect of d_f on PPF and HPF solutions for the loading rate $\bar{\epsilon}_{oH} = 10$ and the AT1 model. In fig. 2.7a, we observe that as d_f decreases the solution tends to the EPF solution, shown by solid black line. This is expected, because the relevant loading rate $\bar{\epsilon}_{oP} = \bar{\epsilon}_{oH}d_f$ that determines the response of the PPF equation decreases as d_f tends to zero for a fixed $\bar{\epsilon}_{oH}$. The dashed lines display the HRA-PPF solution (2.38) which similar to fig. 2.3a overestimate the exact PPF stress values.

Two aspects pertaining to the effect of d_f for the HPF equation will be discussed referring to fig. 2.7b. First, as d_f tends to zero, the solution converges to an undamped HPF solution; unlike the PPF case, this limiting solution is distinct from the EPF solution as it solves (2.40) for $d_f = 0$, that is $\bar{\epsilon}_{oH}^2 d^2 d / d\bar{\epsilon}^2 = -c_\alpha \omega'(d) \bar{\epsilon}^2 \bar{b} / 4 - \alpha'(d) / 2$. As discussed in §2.4.3.2, the HRA-HPF solution also solves this equation for a zero damping term. For comparison the HRA-HPF solution is shown by the dashed black line. §§

The second aspect is the convergence of the HPF (solid colored lines) to PPF (dotted colored lines) solution as d_f increases. In the nondimensional PF equation

§§ The difference between HPF solution as $d_f \rightarrow 0$ and this HRA-HPF solution is contributed to the fact that the latter solves for the difference in strain, as explained in §2.4.3.2, and the former solved so the strain.

(2.22), the ratio of the coefficients of the first order ($dd/d\bar{\epsilon}$) to second order ($d^2d/d\bar{\epsilon}^2$) derivatives is,

$$r_{PH} = \frac{\bar{\epsilon}_{oP}}{\bar{\epsilon}_{oH}^2} = \frac{d_f}{\bar{\epsilon}_{oH}} = \frac{1}{\bar{\epsilon}} \frac{d_f \tau_d E}{\tilde{\sigma}}. \quad (2.48)$$

When $r_{PH} \gg 1$ the contributions from the second order time derivative term is negligible compared to the first one and the PPF solution is very close to the HPF solution. We observe this for $d_f = 100$ for which $r_{PH} = 10$. As r_{PH} gets smaller than the transition value of one, the solution of the PPF starts to deviate from the HPF solution. This transition corresponds to $d_f = 10$ (green lines) for the loading rate used in this example and holds true for other loading rates considered (not shown for brevity). In short, in general the larger the nondimensional parameter r_{PH} the closer the PPF and HPF solutions and for $r_{PH} \lesssim 1$ the solutions significantly deviate.

2.4.6.2 Rate-dependency

Figure 2.8 shows the effect of d_f on rate dependency of PPF and HPF equations for the AT1 model. The results for the PPF equation match the AT1 results presented in fig. 2.6a and fig. 2.6b with the difference that now the employed loading rate is $\bar{\epsilon}_{oH}$. Noting that $\bar{\epsilon}_{oP} = \bar{\epsilon}_{oH} d_f$, it is evident that for $\bar{\epsilon}_{oH} \lesssim 1/d_f$ ($\bar{\epsilon}_{oP} \lesssim 1$), the PPF solution tends to EPF solution and shows no rate-dependency. The effect of d_f is more interesting for the HPF equation. For all d_f , we observe that for large enough $\bar{\epsilon}_{oH}$, $\bar{\sigma}_M$ and $\bar{\phi}_f$ reach the HPF dependency versus the loading rate for powers of 0.5 and 1 discussed in §2.4.5.1. On the other hand, for small enough $\bar{\epsilon}_{oH}$, the QoIs tend to their rate-independent EPF limits. The response in the intermediate loading rates depend on d_f ; for $d_f \geq 10$, a transition region can clearly be observed between the EPF solution and HPF asymptotic solution. In this range the solution is close to the PPF solution (that is, by dropping the second derivative term). For $d_f < 1$, on the other hand, we do not have this transition region and there are some numerical artifacts, where for a range of loading rates $\bar{\phi}_f$ takes values smaller than that from

the EPF equation. This artifact and the intermediate transition region for $d_f > 1$ will be further discussed next.

2.4.6.3 Problem of low d_f for HPF equation

We will first discuss the presence of a transition region for the HPF equation and $d_f > 1$. From §2.4.6.1, we recall that for $r_{PH} \gtrsim 1$, the HPF solution is close to the corresponding PPF solution. In fig. 2.8c and fig. 2.8d, we observe this transition for $r_{PH} \approx 1$ ($\bar{\epsilon}_{oH} \approx d_f$); in fact for $\bar{\epsilon}_{oH} \gtrsim 10d_f$ to $100d_f$ ($r_{PH} = 0.01$ to 0.1), the HPF solution is already matching HRA-HPF asymptotic rate dependencies. The PPF solution itself converges to the EPF solution as its relevant loading rate $\bar{\epsilon}_{oP} = d_f \bar{\epsilon}_{oH}$ gets smaller than one. Thus, for $d_f > 1$, for the loading rate range $1/d_f \lesssim \bar{\epsilon}_{oH} \lesssim d_f$ the solution is close to the PPF solution and the rate dependencies powers are around $1/3$ and $2/3$ for $\bar{\sigma}_M$ and $\bar{\phi}_f$, respectively. For $\bar{\epsilon}_{oH} \lesssim 1/d_f$, the response approaches the EPF solution. In contrast, for $\bar{\epsilon}_{oH} \gtrsim d_f$ the HPF and PPF solutions deviate (cf. fig. 2.7b) and the rate dependency powers tend to HPF rates of $1/2$ and 1 for $\bar{\sigma}_M$ and $\bar{\phi}_f$, respectively. These ranges are shown in fig. 2.8d for $d_f = 10$ and 100 by the vertical dashed lines.

In contrast, when $d_f < 1$, there does not exist a transition region for which the PPF solution provides an accurate representation of the HPF solution. It is exactly for these low d_f values and the transition loading rates between HPF and EPF solutions that we observe some artifacts in $\bar{\phi}_f$. For example, for $d_f = 0.01$, we observe that the HPF equation predicts a smaller $\bar{\phi}_f$ for $0.001 \lesssim \bar{\epsilon}_{oH} \lesssim 0.1$ than the EPF equation. To better understand this effect, the strain-stress response of the AT1 model in the middle of this range, that is for $\bar{\epsilon}_{oH} = 0.01$, is shown in fig. 2.9a. While the HPF equation captures the correct maximum stress of $\bar{\sigma}_M \approx 1$, the unloading branch is very sharp and full damage is realized at $\bar{\epsilon}_f = 1.30$, a much smaller value than that of the EPF equation. For comparison, the solutions of the CZM-W model are also provided for the same $\bar{\epsilon}_{oH}$ and d_f in fig. 2.9b. Again, $\bar{\sigma}_M$ is reasonable, but the unloading path covers a smaller area, corresponding to a smaller $\bar{\phi}_f$ for the HPF equation.

In summary, d_f is a critical parameter for the HPF equation. If $d_f < 1$, the HPF equation lacks the intermediate loading rate range of $1/d_f \lesssim \bar{\epsilon}_{oH} \lesssim d_f$ for which the solution is close to the corresponding PPF solution. This sharp transition of the HPF to EPF solution can result in various numerical artifacts, with the example of low $\bar{\phi}_f$ for the 0D results reported above. For reference, the need for a lower-bound for the damping value of the HPF equation is motivated by avoiding an “underdamped” problem in [72]. However, to turn a PDE to a single degree of freedom (SDOF) oscillator, one needs to consider a wavelength. Our attempts to derive the critical damping value of the HPF equation by using reasonable wavelengths such as b have not been as successful as the nondimensional analysis and results provided above. We believe the lack of the PPF transition region for $d_f < 1$ is a better measure to determine and avoid the “underdamped” HPF solution. Finally, it is emphasized that this analysis did not involve the Laplacian operator in the PF equation. Hence rather than actually dealing with a parabolic or hyperbolic PDE, it is the damping factor d_f that affects the quality of the second order ODE (labeled as HPF) solution.

2.4.7 Effect of wave speed ratio for HPF equation

For the HPF equation, the PF wave speed $c_d = b/\tau_d$ can be different from the elastodynamic wave speed c_u . The ratio of these wave speeds $k = c_d/c_u$ will play a crucial role on the HPF solution. If we enforce the rationale of [64, 47, 72] that the damage wave speed should be smaller than the maximum elastic wave speed for a hyperbolic damage / PF model, we require $k \leq 1$. However, in this study we consider $k > 1$ because it demonstrates the tendency of the HPF to EPF solution when k increases. In fact, the EPF solution corresponds to the HPF solution in the limit of infinitely fast damage speed $k \rightarrow \infty$. When the interaction of the PF with elastodynamics waves is concerned, for example in 1D to 3D problems, $\tilde{\tau}_l := c_u \tilde{l}$ is a reasonable time scale to the problem. Referring to $\tau_d = \tilde{\tau}_l \bar{b}/k$, we observe $\bar{\epsilon}_{oH} = \bar{\epsilon}_o \bar{b}/k$, where $\bar{\epsilon}_o = \dot{\epsilon}_o \tilde{\tau}_l E / \tilde{\sigma}$ is the normalized strain rate using the time scale $\tilde{\tau}_l$.

Figure 2.10 shows the effect of k on the HPF strain stress response for $\bar{\epsilon}_o = 10$. The loading rate that determines the form of HPF strain-stress response is $\bar{\epsilon}_{oH}$; cf. §2.4.3 and fig. 2.4a. Accordingly, as k increases, $\bar{\epsilon}_{oH}$ decreases and as shown in fig. 2.10, the response tends to that of the EPF equation. This confirms the expected influence of k in the beginning of the section.

Another very important effect of k is on the (limiting) speed of propagating cracks in 2D and 3D. Many experimental results show that in contrast to the LEFM predictions, crack speed does not reach a material's Rayleigh wave speed c_R . Gradient damage and PF models that incorporate micro-inertia and micro-viscosity effects are capable of reproducing experimentally observed limiting crack speeds. Some examples of these models with micro-inertia and micro-viscosity terms are [63, 72, 73] and [104, 48], respectively. Our preliminary results show that the value of k can directly be related to the ratio of terminal crack speed to c_R . We will discuss these effects in more details in forthcoming publications.

2.5 1D fragmentation analysis

2.5.1 PF finite element formulation and implementation

A brief overview of the implementation is provided. The formulas for the weak statements, time marching schemes, and solution of the resulting nonlinear equations are not provided for brevity. We use a continuous finite element method for the formulation of both elastodynamic and PF equations. The weak statements corresponding to (2.7a) and (2.7b) are implemented in Deal.II [105]. We discretize $\mathbf{u}$ and d by first order elements.

The inertia term of elastodynamics and PF (only for HPF equation) contributes to the mass matrix, whereas the damping (micro viscosity) term of the PF (for PPF and HPF equations) contributes to the damping matrix. The elastodynamic equations are coupled to the PF equation from the stress relation (2.6), whereas the reverse

coupling arises from the presence of strain elastic energy density in (2.4). Instead of solving these equations with a monolithic approach, the staggered scheme proposed by Miehe *et al.* [16] is employed, where at each time step the elastodynamic and PF equations are solved separately and successively. The hyperbolic PDEs including the elastodynamic and HPF equation are discretized in time using the implicit Newmark method [106], due to its second order accuracy. The generalized trapezoidal method [107] is employed for the time integration of the PPF equation. The solution of the EPF equation is updated by the standard Newton-Raphson method. We enforce the irreversibility condition by taking the maximum of the computed d at a finite element node from the PF PDE (2.7b) and its corresponding previous time step value. The boundedness condition $d \in [0, 1]$ is also enforced in a similar manner at the node level.

2.5.2 QoIs of fragmentation problem in 1D

We will first elaborate on an instability that results in the formation of fragments in §2.5.2.1. This will be followed by providing the details of the calculation of fragmentation QoIs from 1D simulations in §2.5.2.2. For all numerical results in §2.5.3 and §2.5.4, we consider the fragmentation response of a 1D ring of length $L = 1$ and properties $G = 1$, $\rho_u = 1$, $E = 1$, $b = 0.01$, and $k = 1$, using the AT1 model. The damping factor is set to one except in §2.5.4. A uniform mesh containing $2^{10} = 1024$ elements is used. The corresponding mesh size $h = L/2^{10}$ satisfies the recommended condition of $h \leq b/4$ [19]. All results are presented in terms of nondimensional parameters from §2.3.3. Spacetime scales are (b, τ_d) , unless otherwise noted.

2.5.2.1 Critical damage value and fragmentation in 1D

The problem of dynamic fragmentation is analytically and numerically studied in [19] for a 1D EPF equation that resembles the AT1 formulation from Table 2.1. The spatially uniform solutions persist until a critical time t^* with the corresponding critical damage value d^* . Beyond this time, fragments of average size s_{ave} are formed

in a ring of length L and the spatially uniform solutions (labeled as 0D solutions here) are no longer valid. The stability analysis involves finding the time beyond which a harmonic perturbation in the solution will grow. The asymptotic parameter of the problem is,

$$\eta := \bar{\epsilon}_o \bar{b} = \dot{\epsilon}_o b / c_u \bar{\epsilon} = \dot{\epsilon}_o \sqrt{b^3 \rho_u / G}, \quad (2.49)$$

where in [19] the space scale is chosen as $\tilde{l} = L$ and the time scale is derived from $\tilde{l}$ and elastodynamic wave speed as $\tilde{\tau} = \tilde{\tau}_l = \tilde{l} / c_u$; cf. (2.13b) and (2.13c). The nondimensional strain rate $\bar{\epsilon}_o$ and PF length are derived from the corresponding scales in (2.13). For example, $\bar{b} = b / L$. The last two expressions of η are derived by expanding $\bar{\epsilon}_o \bar{b}$. After slightly reworking equations 58 to 60 in [19], the associated QoIs with this instability are expressed as,

$$d^* = 1 - \frac{1}{(1 + \eta \ln S + 0.5 \eta^2 \ln S \ln(S - 1))^2}, \quad (2.50a)$$

$$\bar{t}^* = \frac{1}{\bar{\epsilon}_o \sqrt{1 - d^*}}, \quad (2.50b)$$

$$\bar{s}_{\text{ave}} = \pi \bar{b} (2 - (\ln S - 1) \eta), \quad (2.50c)$$

for $\eta \ll 1$. In (2.50), $\bar{t}^* = t^* / \tilde{\tau}$ is the normalized time of fragmentation, and $\bar{s}_{\text{ave}} = s_{\text{ave}} / \tilde{l}$ is the normalized fragment size. The user-specified parameter S denotes the ratio of target perturbation magnitude that defines the onset of perturbation to the first computationally detectable perturbation magnitude. By choosing 10^{-3} for the former and machine-epsilon of 10^{-16} for the latter, [19] suggests using the value of $S = 10^{13}$.

A few comments are made regarding (2.50) and the analysis in [19]. First, referring to (2.49) and requiring $\eta \ll 1$, (2.50) provides accurate estimates for the critical values when $\dot{\epsilon}_o$ and/or b are small enough. Second, the asymptotic expansion using the length scale $\tilde{l} = L$ results in the specific form of asymptotic parameter η . Once this parameter is computed from (2.49), other time and space scales can be used in (2.50b) and (2.50c), respectively. We believe $\tilde{l} = b$ is a more appropriate length scale

for this AT1-like PF model, and $\tilde{l} = \tilde{l}_c$ is more appropriate when the results of this model are compared with TSR-CZM and PF-CZM models. Third, the PF in [19] is not identical to the AT1 model due to a factor of 0.5 difference form of PF energy function of the AT1 model. This results in $\alpha'(d) = 2d$ and $c_\alpha = 8\sqrt{2}/3$ for the model in [19].

Figure 2.11 shows the initiation of instabilities for a ring problem. This serves two purposes. First, by using the AT1-like model from [19] we verify (2.50). Second, from a more qualitative perspective, this example demonstrates how 1D solutions differ from 0D spatially uniform solutions from the inception of fragmentation instabilities. For consistency with the results in [19], the same nondimensional quantities are used for this examples. That is, $\tilde{l} = L$, and $\tilde{\tau} = L/c_u$. The results are presented for the nondimensional strain rate $\bar{\epsilon}_o = 1$ and $\bar{b} = 0.01$ ($b = 0.01L$). Since $\eta = \bar{\epsilon}_o \bar{b} = 0.01 \ll 1$, (2.50) provides accurate values for the fragmentation instability QoIs. As can be seen in fig. 2.11a, damage grows uniformly from $\bar{t} = 1$, where the stress exceeds the strength of one. This persist until $\bar{t}^* = 1.345$ when damage perturbations start to grow quickly. The spatially uniform and temporally increasing stress solution up to $\bar{t}^*$ and its oscillation and overall tendency to zero after the formation of fragments can be seen in fig. 2.11b. Figure 2.11c shows damage profiles at three instants, including $\bar{t}^*$. The zoomed-in view of the solution at $\bar{t}^*$ is shown in fig. 2.11d. Damage oscillates around the mean value of $d^* = 0.455$ on a small part of the left side and most part of the right side. These oscillations gradually develop to fragments, noting that for this particular example fragments in the middle part form a bit later due to higher initial damage oscillations on the two sides. This confirms that small perturbations at the early instability time $\bar{t}^*$ lead to fully formed fragments at a later time.

This example was used to verify our PF implementation for 1D fragmentation problems and to demonstrate how the instabilities initiate and evolve. The numerically derived $\bar{t}^* = 1.345$ and $d^* = 0.455$ are close to $\bar{t}^* = 1.3441$ and $d^* = 0.4465$ obtained from (2.50). The small differences in $\bar{t}^*$ and d^* are attributed on how

these values are computed. The solutions from [19] depend on the user-specified parameter S , whereas we use numerical results to determine such fragmentation QoIs. Specifically, t^* refers to the earliest time when the span of variation of damage, $\Delta d = \max_{x \in \mathcal{D}}(d(x)) - \min_{x \in \mathcal{D}}(d(x))$, exceeds a user-specified threshold. In the remainder of this manuscript, we extend the 1D fragmentation analysis to CZM-W and AT1 models as well as PPF and HPF equations. The use of AT1 model rather than the one in [19] is motivated by the fact that this form of the PF equation is more common and the solutions in the preceding sections were derived for the AT1 model. Finally, it is reiterated that $\tilde{l} = L$ is only used for this comparative study and $\tilde{l} = b$ or $\tilde{l}_c$ are used in the following sections.

2.5.2.2 Computation of fragmentation QoIs from 1D simulations

The nondimensional average strain for the 1D fragmentation problem is obtained from the imposed nondimensional strain rate, $\bar{\epsilon}(\bar{t}) = \bar{\epsilon}_0 \bar{t}$; cf. (2.21). We consider three volumetric energy densities that are obtained from the strain and stress history for an arbitrary point x in the spatial domain $\mathcal{D} := (-0.5L, 0.5L)$,

$$\phi_{xt}(x, t) = \int_0^{\epsilon(x, t)} \sigma(x, \epsilon) \, d\epsilon = \int_0^t \sigma(x, t) \dot{\epsilon}(x, t) \, dt \quad \text{Internal energy density,} \quad (2.51a)$$

$$\phi_{xt,r}(x, t) = 0.5\sigma(x, t)\epsilon(x, t) \quad \text{Recoverable internal energy density,} \quad (2.51b)$$

$$\phi_{xt,d}(x, t) = \phi_{xt}(x, t) - \phi_{xt,r}(x, t) \quad \text{Dissipated internal energy density.} \quad (2.51c)$$

$\phi_{xt}(x, t)$ is the entire area under the strain-stress curve up to the strain $\epsilon(x, t)$ at time t . Upon unloading, stress radially returns to 0. This results in the recoverable energy density $\phi_{xt,r}(x, t)$. Finally, the dissipated energy density is the difference of the two in (2.51c). At any given point beyond the time that d reaches one, $\sigma(x, t)$ and $\phi_{xt,r}(x, t)$ remain zero, and $\phi_{xt,d}(x, t) = \phi_{xt}(x, t)$.

Each of these energy densities can be integrated over the spatial domain to calculate the corresponding total value at a given time t . We are mainly interested

in the total energy dissipation given by,^{¶¶}

$$\phi_{t,d}(t) = \int_{\mathcal{D}} \phi_{xt,d}(x, t) \, dx, \quad (2.52)$$

The energy dissipation $\phi_{t,d}(t)$ is a non-negative and monotonically increasing function, taking a zero value before any point experiences damage. Our 1D simulations show that once damage accumulation starts, $\phi_{t,d}(t)$ gradually increases, even often well beyond the instants that maximum dynamic stress is experienced and fragment count stabilizes. However, $\phi_{t,d}(t)$ asymptotically tends to a terminal value. For all the results for which energy results are provided, the simulations are run to a *final time* t_f for which a nondimensional rate of change of $\phi_{t,d}(t)$ is below a user-specified tolerance.

To calculate the nondimensional energy dissipation density from 1D simulations, we first divide $\phi_{t,d}(t_f)$ by L to calculate the spatially averaged energy density. Next, this value is normalized by the energy per volume scale $G/\tilde{l}$ from (2.14d). The other two nondimensional values are calculated in a similar manner. The maximum average stress (labeled as dynamic strength) is taken as the maximum of spatially averaged stress from time zero to t_f . This is nondimensionalized by dividing it by strength and stress scale $\tilde{\sigma}$ from (2.14a). Finally, the fragment count $N_f(t)$ for a given time t is computed as the number of segments formed between damaged regions. A damaged region corresponds to a spatial span for which at all points d is greater than the user specified *fragmentation damage threshold* d_{frag} . In all the simulations, the value of $d_{\text{frag}} = 0.95$ is used. Similar to $\phi_{t,d}(t)$, $N_f(t)$ increases in time beyond its initial value of one, once fragments start to form. N_f reaches its terminal value earlier than the energy dissipation. The formulas for the discussed nondimensional QoIs are as

^{¶¶}The energy dissipation of PF simulations is often expressed as $GA_d(d) \approx G \int_{\mathcal{D}} \gamma(d) dv$. However, the presence of the time derivatives of d in (2.7b) results in phase-field kinetic and damping energy terms that differentiate the two energy dissipation formulas. We will use (2.52) to calculate the energy dissipation due to its applicability to the rate-dependent PF equations.

follows,

$$\bar{\phi}_f := \frac{\phi_f}{\tilde{\phi}} = \frac{\phi_{t_f,d}}{G} \frac{\tilde{l}}{L}, \quad \text{where} \quad \phi_f = \frac{\phi_{t_f,d}}{L} \quad \text{Energy dissipation density,} \quad (2.53a)$$

$$\bar{\sigma}_M := \frac{1}{\tilde{\sigma}} \max_{t \in (0, t_f)} \frac{\int_{\mathcal{D}} \sigma(x, t) dx}{L} \quad \text{Maximum stress (dynamic strength),} \quad (2.53b)$$

$$\bar{s}_{\text{ave}} := \frac{s_{\text{ave}}(t = t_f)}{\tilde{l}} = \frac{L}{N_f(t = t_f) \tilde{l}} \quad \text{Fragment size,} \quad (2.53c)$$

where the length scale $\tilde{l}$ can be any of the choices given in (2.13b). The 0D $\bar{\phi}_f$ provides an upper limit for the corresponding 1D value in (2.53a), since the uniform damage evolution in the domain corresponds to the maximum energy dissipation; cf. fig. 2.11. As will become apparent in the remainder of the manuscript, $\bar{\phi}_f$ and $\bar{\sigma}_M$ tend to their 0D counterparts from §2.4 as the loading rate increases. Finally, there is no counterpart for $\bar{s}_{\text{ave}}$ from 0D results.

2.5.3 Comparison of 0D and 1D strain-stress response

We investigate how the instability of the uniform stress solution and fragmentation formation, discussed in §2.5.1, affects the average strain-stress response. Figure 2.12 compares the 0D and 1D strain-stress responses. For up to a critical strain value, corresponding to the damage value d^* , the 1D solution remains spatially uniform; accordingly the 0D and 1D average stresses match up to this stage. However, once the instability is initiated and fragments are formed, the average stresses of the 0D and 1D solutions deviate. This is what we observe for the results of the two low loading rates shown. For the 1D solution, the stress is released around the cracks, explaining its sharper drop of stress beyond the instability initiation point. For the higher loading rates, the damage level at which the instability initiates increases and the 0D and 1D solutions start to deviate much closer to the failure stage (average

zero stress). In fact, since for the higher loading rates, the 0D and 1D strain-stress solutions were visually indistinguishable, we did not include them in the figure.

These results demonstrate the rate dependency that simply arises from fragmentation, even when the PF model is rate independent. The identical 0D EPF strain-stress response of all loading rates in fig. 2.12 signifies the rate-independent behavior of the EPF. However, the 1D EPF strain stress results match the 0D result only for high loading rates; for the low loading rates, the unloading gets sharper for lower loading rates. The earlier unloading of stress results in a decrease in the normalized energy dissipation density. The inspection of fig. 2.12 reveals that for the same loading rate, the fragmentation and unloading of models occurs first for the EPF solution, followed in order by the PPF and HPF solutions. That is, the fragmentation-based rate sensitivity has the highest effect for the EPF equation, followed by the PPF and HPF equations at low loading rates. For the PPF and HPF equations, not only the 0D model is inherently rate-dependent, *cf.* fig. 2.6, but also the fragmentation too contributes to the rate-dependency of the PF results in 1D-3D problems. The inherent model rate-dependencies are more pronounced at high loading rates; for example, in fig. 2.12 all 0D EPF, PPF, and HPF solutions are almost indistinguishable for the low loading rates considered. The two sources of rate-dependency are further discussed in §2.5.5.

2.5.4 Effect of damping factor and loading rate on 1D fragmentation QoIs

We will quantitatively analyze the effect of loading rate and d_f on fragmentation QoIs in 1D. For the damping factor effect, this section naturally continues the investigation of §2.4.6.2, now for the 1D ring problem. We first study how the fragmentation changes the 0D $\bar{\sigma}_M$ and $\bar{\phi}_f$, shown earlier in fig. 2.8. This is followed by discussing the effect of loading rate and d_f on QoIs that only apply to 1D fragmentation, namely the critical damage value d^* (*cf.* §2.5.2.1) and fragment count.

2.5.4.1 Comparison of 0D and 1D results for $\bar{\sigma}_M$ and $\bar{\phi}_f$

The effect of d_f on $\bar{\sigma}_M$ and $\bar{\phi}_f$ is shown in fig. 2.13 for 1D AT1 HPF results. The EPH results are also shown for comparison. For brevity, the 1D PPF results are not included as the 0D results in fig. 2.8a and fig. 2.8b did not have the complex effect of d_f for the HPF equation. Moreover, the only difference of 0D and 1D results is the decrease of $\bar{\phi}_f$ of 1D results relative to 0D ones. Since the same reasoning contributes to this behavior for PPF and HPF equations, we only focus on the latter in the discussion below.

The HPF solutions should be compared with the corresponding 0D solutions in fig. 2.8c and fig. 2.8d. The largest difference between 0D and 1D results appear for low loading rates $\bar{\epsilon}_{oH} \lesssim 1$. As explained in §2.5.3, such large differences at low loading rates is attributed to the instabilities starting at smaller d^* values. The sharper stress unloading of 1D solutions, *cf.* fig. 2.12, explains why $\bar{\phi}_f$ is smaller than 0D energy for $\bar{\epsilon}_{oH} \lesssim 1$. In fact, this decay of $\bar{\phi}_f$ for the rate-independent EPF equation very clearly demonstrates the second source of rate-dependency of PF results, the instability and formation of fragments. We also observe that the energy dissipation tends to a threshold smaller than the 0D EPF value. As explained in §2.4.6.2, the HPF solutions with higher d_f tend to their quasi-static limit at smaller $\bar{\epsilon}_{oH}$ values, *cf.* fig. 2.8d. This explains the quicker tendency of HPF $\bar{\phi}_f$ to this limit for smaller d_f . The nature of this lower threshold will be further discussed in §2.5.5. In contrast to $\bar{\phi}_f$, $\bar{\sigma}_M$ does not exhibit rate-dependency at low loading rates for the 1D results in fig. 2.13a. This can be explained by the fact that the maximum stress state generally precedes the initiation of instabilities and fragmentation; *cf.* fig. 2.12. Accordingly, the added rate-dependency from the fragmentation process has a much more pronounced contribution to $\bar{\phi}_f$ than $\bar{\sigma}_M$.

2.5.4.2 Critical damping and fragment count in 1D

The process of fragmentation was discussed in detail in §2.5.2.1. Referring to fig. 2.11, the quantities associated with deviation from 0D solution and formation of fragments were denoted by the superscript *. Figure 2.14 shows the effect of $\bar{\epsilon}_{oH}$ and d_f on d^* and N_f for the PPF and HPF equations. The solid black lines show the reference EPF solutions.

2.5.4.2.1 Effect of loading rate Some loading rate effects, shared by all PF equations, are,

1. Monotonic increase of d^* versus $\bar{\epsilon}_{oH}$: Referring to fig. 2.14a and fig. 2.14c we observe that d^* tends to zero as $\bar{\epsilon}_{oH} \rightarrow 0$. This is consistent with the asymptotic analysis in [19] and the reworked equation (2.50a) from that reference. The limiting value of $d^* = 0$ for quasi-static loading is also consistent with immediate formation of fragments when the stress reaches the damage initiation threshold in quasi-static fracture [25, 75]. The almost linear increase of d^* in the log-log plots up to $d^* \approx 0.4$ to 0.9 for different d_f values corresponds to a power relation of the form $d^* \propto \bar{\epsilon}_{oH}^{p^*}$ for $p^* = 1$ for low to intermediate loading rates. In fact, the asymptotic expansion of (2.50a) yields $d^* = (0.5\bar{b} \ln S)\bar{\epsilon}_o + \mathcal{O}(\eta^2)$ for $\eta \propto \bar{\epsilon}_o \rightarrow 0$ and the EPF equation. Given that PPF and HPF solutions tend to the EPF solution for $\bar{\epsilon}_{oH} \rightarrow 0$, obtaining the power $p^* = 1$ for all PDE types was expected from (2.50a). Finally, d^* tends to unity at a slower rate for intermediate to high loading rates.
2. Failure of PF to form fragments at high loading rates: As observed in fig. 2.14b and fig. 2.14d, for the highest loading rate range discussed above, the fragment count precipitously decreases and is even equal to one (*i.e.*, no fragmentation) for the highest d_f . As will be shown in §2.5.5, PF models are capable of accurately predicting fragmentation QoIs such as $\bar{\sigma}_M$ and $\bar{\phi}_f$. However as shown here, PF models are incapable of capturing the right fragment

count for intermediate to high loading rates. This is in contrast to TSR-CZM fragmentation studies such as [11].

3. The combined effect of d^* and N_f on energy dissipation density $\bar{\phi}_f$: The differences between 1D (fig. 2.13b) and 0D (fig. 2.8d) energy dissipation can be explained by the interaction of two effects depicted in fig. 2.13. The first effect is the energy dissipation in the interior of fragments, which is a function of d^* . If d^* tends to zero (quasi-static loading), the interior regions of fragments dissipate almost no energy, as the strain stress response is mainly linear up to fragment formation. The second effect is the energy dissipation at the fragment boundaries, which is a function of N_f . We will explain how from high to quasi-static loading rates, d^* and N_f differentiate between 1D and 0D energy dissipation values.

For high loading rates, almost the entire domain reaches full damage since $d^* \rightarrow 1$. In this limit N_f has a minor effect on $\bar{\phi}_f$ as all points dissipated almost the same energy. Hence, 1D and 0D energy dissipation densities match in fig. 2.13b and fig. 2.8d. For intermediate to low loading rates, fig. 2.14 shows that N_f relatively quickly tends to a terminal value, whereas d^* keeps decreasing. Consequently, it is d^* that mainly drives the decrease of $\bar{\phi}_f$ from the high loading rate values to the quasi-static limit. Finally, at quasi-static and low loading rates, $\bar{\phi}_f$ is directly proportional to N_f (as almost no energy is dissipated within the fragments due to $d^* \rightarrow 0$). This is in contrast to high loading rate response where N_f has almost no effect on $\bar{\phi}_f$.

For the EPF equation, the deviation of 0D and 1D energy dissipations at low loading rates results in lower and upper limiting values for $\bar{\phi}_f$. In §2.5.5, it will be demonstrated that N_f reaches a terminal lower-bound as $\bar{\epsilon}_{oH} \rightarrow 0$, resulting in the appearance of a “lower-bound” energy dissipation density limit in fig. 2.13b. As mentioned, in the intermediate loading rate range, $\bar{\phi}_f$ mainly increases from the increase of N_f . Eventually, the energy dissipation density of

the EPF equation is saturated by the rate-independent 0D $\bar{\phi}_f$ at high loading rates. This limit is referred to as the “upper-bound” value. It shall be noted that the PPF and HPF equations share the same low rate response, but have the rate-dependent 0D $\bar{\phi}_f$ behavior at high rates.

2.5.4.2.2 Effect of damping factor on fragmentation QoIs Referring to fig. 2.14a and fig. 2.14c, we observe that for both PPF and HPF equations, d^* monotonically increases by increasing d_f . For low loading rates, the general observation from fig. 2.14b and fig. 2.14d is that the fragment count counteracts the effect of d^* for energy dissipation. That is, for $\bar{\epsilon}_{oH} \lesssim 10^{-3.5}$, if the change to d_f increases d^* , N_f decreases, thus decreasing the energy dissipation from fully damaged fragmented regions; *cf.* regions with $d \approx 1$ in fig. 2.11.

The effect of d_f on d^* is further discussed referring to fig. 2.15. For the PPF equation, as $d_f \rightarrow 0$, d^* tends to that of the EPF equation. This is expected as the PPF solution tends to the EPF solution in this limit. For $d_f \geq 1$, on the other hand, increasing d_f noticeably increases d^* . This can be explained by noting that for the 0D PPF solutions, it was $\bar{\epsilon}_{oP}$ rather than $\bar{\epsilon}_{oH}$ that unified strain stress responses for different d_f ; *cf.* fig. 2.3. Given that $\bar{\epsilon}_{oP} = \bar{\epsilon}_{oH}d_f$, the increase of d^* versus d_f for $d_f \geq 1$ is expected; although the implied linear proportionality of d^* versus d_f only hold for the lowest loading rate considered (a slope close to one for $\log_{10}(\bar{\epsilon}_{oH}) = -5$ and $d_f \geq 1$ in fig. 2.15). The deviation from such dependence of d^* on d_f for other cases is attributed to the more complicated interactions of the time scale $\tilde{\tau}_l$ implied by elastodynamic wave propagation and the PPF time scale ξ_d ; *cf.* (2.13c). The effect of d_f on d^* for the HPF equation is similar to the PPF equation from two perspectives. First, the effect of d_f on d^* is again more pronounced for $d_f \geq 1$. In fact, the tendency of HPF d^* to that of PPF equation at high loading rate is justified as for high d_f (more precisely for high r_{PH}) the HPF solution tends to the PPF solution; *cf.* §2.4.6.1 and fig. 2.7b. Second, the HPF d^* also has a milder dependency on d_f at low d_f . The difference is that unlike the PPF equation, the limiting case of the HPF equation for $d_f \rightarrow 0$ is

an undamped hyperbolic equation. This contributes to slightly higher d^* values for the HPF solution than the PPF solution in fig. 2.15.

2.5.4.2.3 Summary of 0D and 1D studies on choosing the damping factor for the HPF equation The key finding from 0D and 1D studies is that $d_f \approx 1$ is the best choice for the HPF equation. For smaller d_f values and $0.001 \lesssim \bar{\epsilon}_{oH} \lesssim 0.1$, we observed nonphysical unloading in 0D (*cf.* fig. 2.9) resulting in artifacts in fig. 2.8d. On the other hand, for high d_f values, the HPF solutions resemble the PPF solutions for a wide range of loading rates ($\bar{\epsilon}_{oH} \leq d_f$), undermining the rationale of using a HPF equation in the first place. More importantly, a high d_f value prevents the formation of fragments for high loading rates, *cf.* fig. 2.14d. Even if the HPF equation can accurately predict $\bar{\sigma}_M$ and $\bar{\phi}_f$ at high loading rates, this inability to form fragments is an undesirable outcome as the statistics of fragments is important in dynamic fracture.

2.5.5 Causes of rate dependency for the fragmentation problem: PF versus CZM and analytical models

In this section, we will further elaborate on the two sources of rate-dependency of PF results, the differential equation and fragment formation. In addition, we will compare key QoIs of the fragmentation problem (energy dissipation, dynamic strength, and average fragment size) obtained from PF, CZM, and some semi-analytical models.

2.5.5.1 CZM and semi-analytical models

Fragment size statistics is the most studied aspect with several existing models for the shape of the distribution [108], and the rate-dependency of the average fragment size $\bar{s}_{ave}$. It is the latter that is the focus of this section. We will compare the rate-dependency of $\bar{s}_{ave}$ with some of the most popular models [5, 11, 6]. The Grady's model [5] is based on an energy argument and only provides reasonable fragment size

estimates at high loading rates. For more detailed review of these models, we refer the reader to [11]. In addition to $\bar{s}_{\text{ave}}$, we study the rate dependency of $\bar{\phi}_f$ and $\bar{\sigma}_M$ from (2.53).

TSR-CZM models are a popular choice for fragmentation studies. These models require the value of (cohesive) strength $\tilde{\sigma}$ in addition to G . Moreover, often a linear softening curve is used for these TSR-CZM studies; see for example [10, 11]. Accordingly, as will be further discussed in §2.5.5.2, we will use the PF CZM-W model with linear softening curve to have the best comparison possible with the results provided in [11]. Given the comparison of CZM TSR and PF results, we need to use the CZM-based length and time scales from (2.13b) and (2.13c) and the corresponding strain rate scale from (2.14f). These CZM-based scales are,

$$\tilde{l} = \tilde{l}_c = \frac{GE}{\tilde{\sigma}_c^2}, \quad \tilde{\tau} = \tilde{\tau}_c = \frac{\tilde{l}_c}{c_u}, \quad \Rightarrow \quad \tilde{\epsilon} = \tilde{\epsilon}_c = \frac{\tilde{\sigma}_c^3 c_u}{GE^2} \quad (2.54)$$

where the subscript c stands for *cohesive*. To clarify that $\tilde{\epsilon}_c$ is used to normalize the strain rate, we use the subscript c for the nondimensional strain loading rate too $\bar{\epsilon}_{\text{oc}} = \dot{\epsilon}_o / \tilde{\epsilon}_c$. The equations for nondimensional average fragment size for the comparison models [5, 11, 6] are,

$$\bar{s}_{\text{ave}}(\bar{\epsilon}_{\text{oc}}) = \frac{\sqrt[3]{24}}{\bar{\epsilon}_{\text{oc}}^{\frac{2}{3}}} \quad \text{Grady [5],} \quad (2.55a)$$

$$\bar{s}_{\text{ave}}(\bar{\epsilon}_{\text{oc}}) = \frac{4}{\bar{\epsilon}_{\text{oc}}} \sinh \left[\frac{1}{3} \sinh^{-1} \left(\frac{3}{2} \bar{\epsilon}_{\text{oc}} \right) \right] \quad \text{Glenn-Chudnovsky (GC) [6],} \quad (2.55b)$$

$$\bar{s}_{\text{ave}}(\bar{\epsilon}_{\text{oc}}) = 4.5 \left[1 + 0.77 \bar{\epsilon}_{\text{oc}}^{\frac{1}{4}} + 5.4 \bar{\epsilon}_{\text{oc}}^{\frac{3}{4}} \right]^{-1} \quad \text{Zhou-Molinari-Ramesh (ZMR) [11].} \quad (2.55c)$$

The nondimensional energy dissipation is not directly provided for the TSR-CZM models. However following [20], we can determine a lower-bound for $\bar{\phi}_f$ from the equations above. For a TSR-CZM model, the total energy dissipation is $\phi_{t,d}(t) = N_f G$, thus $\bar{\phi}_f = 1/\bar{s}_{\text{ave}}$. For this argument, we have used equations (2.52), (2.53a),

and (2.53c) that apply to TSR-CZM fracture too, and have only considered the energy dissipation that occurs at fully debonded TSR interfaces. Hence, the value $\bar{\phi}_f(\bar{\epsilon}_{oc}) = 1/\bar{s}_{ave}(\bar{\epsilon}_{oc})$ provides a lower-bound for the normalized energy dissipation of the three models above.

For $\bar{\sigma}_M$, the Grady's model does not provide an estimate for the maximum stress (dynamic strength), as the only input to the model is G . The TSR used in [11] is rate-independent, meaning that $\bar{\sigma}_M$ is always one independent of the loading rate.***

There is also no maximum stress provided in [6]. Considering all these aspects, $\bar{s}_{ave}$ from (2.55) and its inverse (as a CZM-based lower-bound energy) will be compared to PF $\bar{s}_{ave}$ and $\bar{\phi}_f$ in §2.5.5.2, and there will be no comparison model for $\bar{\sigma}_M$.

2.5.5.2 Problem set-up and nondimensionalization

We consider the same fragmentation problem setup in [20], solved by a thick level set method therein. Instead of a ring, a bar of length $L = 2$ mm made of Alumina (AlO₃) is considered. While [20] simulates only half the domain invoking the symmetry with respect of center point, our computational domain is the entire length $L = 2$ mm. The material properties are the elastic modulus $E = 610$ GPa, mass density $\rho_u = 3900$ kg/m³, fracture energy $G = 83.13$ N/m, and tensile strength $\tilde{\sigma}_c = 1$ GPa. Accordingly, the fracture length scale is $\tilde{l}_c = GE/\tilde{\sigma}_c^2 = 50.7$ μ m. The computational domain is discretized to 2^{14} elements resulting in $h = 122.07$ nm. The nondimensional phase field length scale is chosen as $\bar{b}_c = b/\tilde{l}_c = 1/32\pi$ resulting in $b = 504$ nm. Similar to [20], we treat the strength as a random field with a point-wise Weibull distribution and no spatial correlation (*i.e.*, a white noise field) to facilitate the formation of fragments at high loading rates, as further discussed in §2.5.5.3. For the Weibull model, a shape parameter of 2 and a coefficient of variation of 0.01 are used. We will present the results both in nondimensional and dimensional forms. The former facilitates the comparison with nondimensional results in the literature, whereas the

***Our results in [109] show that if in addition to TSR interfaces, one examines the stress within the fragments, $\bar{\sigma}_M$ can exceed one even for a rate-independent TSR-CZM.

latter provides the actual strain rate limit at which the responses of different PF equations start to deviate for this material and PF parameters.

We note some differences between the forthcoming study and the results in [20]. First, we present results both for the rate-independent EPF equation that is comparable to the thick level set model in [20] and the rate-dependent PPF and HPF equations. Second, in addition to $\bar{s}_{\text{ave}}$ and $\bar{\phi}_f$ in [20], we include the QoIs of $\bar{\sigma}_M$ and d^* . Third, the highest loading rate considered is about four orders of magnitude higher than [20]. This enables to more clearly see the differences between different PF equations. Fourth, we will present all the results in the nondimensional form, using the cohesive scales (2.54) and equations (2.14) and (2.15). This representation make the comparison with other fragmentation result easier.

The rate-dependency of the three QoIs and d^* are presented in fig. 2.16 in terms of dimensional and nondimensional values. The bottom and top axes show the nondimensional $\bar{\epsilon}$ and dimensional $\dot{\epsilon}$ strain rates related by $\dot{\epsilon} = \bar{\epsilon}_{\text{oc}} \tilde{\epsilon}_c$ for $\tilde{\epsilon}_c = 404310/\text{s}$. In fig. 2.16a, the left and right axes show the nondimensional $\bar{s}_{\text{ave}}$ and dimensional s_{ave} fragment sizes related by $s_{\text{ave}} = \bar{s}_{\text{ave}} \tilde{l}_c$. The nondimensional dynamic strength $\bar{\sigma}_M$ and its dimensional value are related by $\sigma_M = \bar{\sigma}_M \tilde{\sigma}_c$ for $\tilde{\sigma}_c = 1 \text{ GPa}$ in fig. 2.16c. Finally, the energy dissipation per volume ϕ_f and its nondimensional form $\bar{\phi}_f$ are related by $\phi_f = \bar{\phi}_f \tilde{\phi}_c$ for $\tilde{\phi}_c = 1.64 \text{ MPa}$ in fig. 2.16d.

2.5.5.3 Fragmentation

Figure 2.16a shows the fragment size results, only up to $\bar{\epsilon}_{\text{oc}} \approx 100$, as for higher values the fragments cannot be counted due to the tendency of d^* to one. This tendency of d^* to one is shown in fig. 2.16b. A disadvantage of using a heterogeneous strength field is the algorithmic determination of d^* values much smaller than those for a homogeneous domain at low loading rates; *cf.* figs. 2.14(a,c) and fig. 2.16b. The inhomogeneity also has a stronger effect on d^* and $\bar{s}_{\text{ave}}$ than the PDE type, because almost equal values are observed for the three PDEs in figs. 2.16(a,b). In fact, all $\bar{s}_{\text{ave}}$ values very closely follow the ZMR curve, the TSR-CZM best fit from [11]. This is

contrast to the results for the homogeneous domain. For example in fig. 2.15, d^* of the EPF solution is noticeably smaller than that of the PPF and HPF solutions at the damping factor used for these results ($d_f = 1$). However, the introduction of such minute heterogeneities has enabled us to extend the loading rates at which fragments can be formed by about 1 to 2 orders of magnitude compared to the homogeneous strength fields used in §2.5.4.2 and figs. 2.14(b,d). Given the physical importance of mean fragment size and following [20], we believe that introducing small perturbations to the strength field has a net positive impact. One very important aspect of these fragmentation models is the value of $\bar{s}_{\text{ave,qs}}$, the non-dimensional fragment size in the limit of $\bar{\epsilon}_{\text{oc}} \rightarrow 0$. Noting that the solution for the Grady's model is applicable only to high loading rates, such values are provided for GC, ZMR, and PF solutions in Table 2.9. As will become apparent, $\bar{s}_{\text{ave,qs}}$ plays a crucial role in energy dissipation behavior of the PF model.

2.5.5.4 Dynamic strength

The results for $\bar{\sigma}_M$ in fig. 2.16c, demonstrate that 1D results follow the same trends observed in 0D in fig. 2.6a and fig. 2.6c. That is, the asymptotic rate of $\bar{\sigma}_M$ versus $\bar{\epsilon}_{\text{oc}}$ is 1/3 and 1/2 for the PPF and HPF equations, respectively. The fact that at high loading rates, $d^* \rightarrow 1$ implies that the entire domain undergoes the 0D (spatially uniform) strain-stress response up to late stages of unloading. This explains matching the 0D solutions at high rates. For low loading rates, the formation of fragments does not affect $\bar{\sigma}_M$, as the stress level needs to first reach $\bar{\sigma}_c$ for damage to start to accumulate. For the quasi-static loading, the instability and fragmentation occurs almost immediately after this stage (see fig. 2.14a and fig. 2.14c) resulting in $\bar{\sigma}_M = 1$ even in 1D setting.

2.5.5.5 Energy Dissipation

Figure 2.16d shows the rate-dependency of energy dissipation per volume for the PF equations and comparison models. As mentioned in §2.5.5.1 for GC and ZMR comparison models, similar to [20] we calculate the lower-bound energy dissipated only at the boundaries of fully debonded fragments. We will discuss the two sources of rate-dependency of energy dissipation in 1D.

2.5.5.5.1 Rate-effect from fragmentation: Lower- and upper-bounds for the EPF equation

Referring to the EPF results in fig. 2.16d, we observe different limiting values at quasi-static and high loading rates. In the limit of quasi-static loading rate, the average fragment size tends to $\bar{s}_{\text{ave,qs}} \approx 4$ for the PF results. At this quasi-static limit, stress increases uniformly in the domain until it reaches the strength of the material σ_M . This is followed almost immediately by the instability and formation of fragments, as in the quasi-static limit $d^* \rightarrow 0$. Accordingly, almost no energy is dissipated within the fragments and $G/s_{\text{ave,qs}}$ provides a very accurate lower-bound estimate for the energy dissipation. This expressed in the nondimensional form is $\bar{\phi}_f = 1/\bar{s}_{\text{ave,qs}}$. This lower-bound energy dissipation density is labeled as *lower-bound* energy dissipation and is denoted by $\bar{\phi}_f^L := 1/\bar{s}_{\text{ave,qs}}$.

The energy dissipation of EPF and ZMR solutions are still decreasing for the lowest loading rates considered. The same can be observed in fig. 2.16a where the fragment size for both solutions is still decreasing. However, referring to (2.55c) the limiting value of $\bar{s}_{\text{ave,qs}} = 4.5$ is evident for the ZMR model. We did not solve the PF problem for loading rates $\bar{\epsilon}_{\text{oc}} \leq 0.01$ as reaching the failure stage takes a long time. Still, we expect the PF solutions to tend to a limiting lower-bound energy value similar to the ZMR (and GC) model(s), given the proximity of PF and ZMR solutions at lower loading rates.

The energy dissipation limit of the EPF model at the high loading rate is discussed next. For high loading rate $d^* \rightarrow 1$. Accordingly, the entire domain experiences a uniform solution from the initiation of damage accumulation up to a d^* very

close to one. Thus, as also pointed out in §2.5.5.4, the 0D solution provides an accurate estimation of the 1D solution for high loading rates. Accordingly, the energy dissipation densities provided for the EPF equation in Table 2.4 are the limiting values for $\bar{\phi}_f$ at high loading rates. This upper-bound energy dissipation density is labeled as *upper-bound* energy dissipation and is denoted by $\bar{\phi}_f^U$, equal to 0D EPF $\bar{\phi}_f$.

This sigmoidal form of energy dissipation versus loading rate for the EPF equation resembles the experimental results from [46, 58] for the energy dissipation rate-dependency of bonded interfaces. Various TSR cohesive models [46, 57, 58, 59, 60] are designed to capture such a sigmoidal shape, and as discussed in [59, 60] the sigmoidal shape of energy rate sensitivity is expected to apply to many fracture problems. Interestingly, by tuning some parameters of the EPF equation, *e.g.*, $\bar{b}_c$ and potentially modifying the equation, one may be able to adjust the lower- and upper-bound values based on experimental observations, a topic that is beyond the scope of this work.

The explanation and values of $\bar{\phi}_f^L$ and $\bar{\phi}_f^U$ are provided in Table 2.10. Referring to Table 2.4, the ratio of the upper- to lower-bound energy densities is,

$$\frac{\phi_f^U}{\phi_f^L} = \frac{\bar{\phi}_f^U}{\bar{\phi}_f^L} = \begin{cases} \frac{\bar{s}_{\text{ave,qs}}(\bar{b}_c)}{2\bar{b}_c} \geq \frac{128}{27} \bar{s}_{\text{ave,qs}}(\bar{b}_c) & \text{AT2} \\ \frac{3\bar{s}_{\text{ave,qs}}(\bar{b}_c)}{8\bar{b}_c} \geq \bar{s}_{\text{ave,qs}}(\bar{b}_c) & \text{AT1} \\ \frac{\bar{s}_{\text{ave,qs}}}{\pi\bar{b}_c} \geq 0.5\bar{s}_{\text{ave,qs}} & \text{CZM-W (linear softening)} \end{cases} \quad (2.56)$$

for AT2, AT1, and CZM-W model. The inequality conditions are deduced from the upper-bounds of b in Table 2.1. A few comments on provided regarding these lower- and upper-bound values and their ratios:

1. **Mesh bias of PF models in quasi-static loading condition:** For quasi-static regime, all PF models along with many other continuum damage models that have an internal length scale are shown to have no “mesh bias”; *cf.* §2.2.1 and §2.4.5.2. That is, once the discretization (finite element mesh) is fine enough, QoIs such as dissipated energy are mostly mesh-size independent.

The fact that continuum damage models without such an internal length scale exhibit mesh bias is well documented; *cf.* for example [61]. PF models do not exhibit this problem due to the presence of b in (2.7b).

2. Length-scale dependency of PF models in quasi-static loading condition:

The dependency of fracture QoIs to the internal length scale of a fracture model is called the “length-scale” dependency of the model. The length-scale dependency of the PF models in quasi-static regime is studied in detail in [82] for AT2, AT1, and CZM-W models. While as expected all the models do not exhibit any mesh bias, only the CZM-W model is shown to be length-scale independent for several quasi-static benchmark problems where damage propagates from pre-existing cracks. For fragmentation problems, [19] shows that AT1 model is length-scale dependent for low-loading rates, in that $\bar{s}_{\text{ave}}$ is inversely proportional to b . Our results, not included for brevity, show that similar to [82] the CZM-W model is length-scale independent for low loading rates. For example, for b smaller than the bound provided in Table 2.1, $\bar{s}_{\text{ave,qs}} \approx 4$ (close to the ZMR value) is obtained. The differences in the length-scale dependency of PF models in quasi-static loading regime, explains the treatment of $\bar{s}_{\text{ave,qs}}$ as a function of $\bar{b}_c$ for AT2 and AT1 models in Table 2.10 and (2.56).

3. Length-scale dependency of PF models in dynamic loading condition:

For all the PF models the upper-bound value $\bar{\phi}_f^U$ is inversely proportional to $\bar{b}_c$. As the phase field length scale decreases, dynamic energy dissipation is expected to increase with the same factor. From this perspective, the EPF energy dissipation is length-scale dependent at high loading rates.

4. $\bar{\phi}_f^U / \bar{\phi}_f^L$ **for the CZM-W model:** We limit the discussion to the CZM-W model, given that it is the model used for the numerical results in fig. 2.16. In this case, as b decreases, $\bar{\phi}_f^U$ increases inversely proportional to b whereas $\bar{\phi}_f^L$ stays close to 4. Hence, this ratio increases as b decreases. In fact, our motivation in choosing

$\bar{b}_c = 0.0035$ well below the upper-bound of $1/\pi$ in Table 2.1 is to better highlight the ratio of $\phi_f^U/\phi_f^L \approx 410$ in fig. 2.16d; for $\bar{b}_c = 1/\pi$ in fig. 2.1, this ratio would have been $\phi_f^U/\phi_f^L \approx 4$.

We conclude this section by re-emphasizing the role of local fragmentation and uniform (0D) damage accumulation on $\bar{\phi}_f^L$ and $\bar{\phi}_f^U$, respectively. A more thorough understanding of length-scale dependency of PF models in dynamic setting requires independent studies such as [82]. Given that the primary focus of this manuscript is on rate-dependency of the PF fracture problem, we limit the discussion of the length-scale dependency to the points mentioned above for the CZM-W model. The length-scale dependency of the PF model for fragmentation problems at different loading rates with the inclusion of AT2 and AT1 models will be pursued in future publications.

2.5.5.5.2 Rate-effect from the PDE type In this section, we will discuss the second source of rate-dependency of PF models, *i.e.*, the PDE type of the equations. Referring to fig. 2.16d, we observe that at high loading rates, the PPF and HPF equations exhibit the same rate-dependencies we observed for the 0D studies. As mentioned several times already, the fact that $d^* \rightarrow 1$ for high loading rate explains the match between 0D and 1D solutions for $\bar{\epsilon}_{oc} \gtrsim 100$. The PPF and HPF equations exhibit the rate-dependencies of $p = 2/3$ and $p = 1$ for $\bar{\phi}_f$ at high loading rates; *cf.* Table 2.8.

There are a few interesting observations on the rate-dependencies of PPF and HPF equations. First, the PPF rate of $p = 2/3$ matches that of the Grady and GC models in (2.55). We observe that for this material, for $\dot{\epsilon} \gtrsim 10^8/\text{s}$ ($\bar{\epsilon}_{oc} \gtrsim 10^4$) $\bar{\phi}_f$ the energy of the EPF equation saturated. Second, pertained to this, the EPF energy dissipation is bounded from above by $\bar{\phi}_f^U$. Third, the HPF equation exhibits a higher rate sensitivity than Grady and GC models. In fact, for this material for $\dot{\epsilon} \gtrsim 10^{12}/\text{s}$ ($\bar{\epsilon}_{oc} \gtrsim 10^8$) $\bar{\phi}_f$, the energy of the HPF model is expected to exceed that of the Grady and GC models. In short, the PPF and HPF equations are more suitable for

high-strain rate fracture as they capture the dynamic toughening of (semi)analytical models. The PPF is favored from this perspective, as it exactly matches the rate sensitivity of the Grady’s model. Beyond the behavior of $\bar{\phi}_f$ in this figure, we have observed significant differences in the responses of different PF PDEs, for example in the dynamics of propagating cracks. These aspects will be discussed in future works.

2.6 Summary and conclusions

We presented elliptic, parabolic, and hyperbolic forms of the PF equation. The exact and high loading rate asymptotic solutions of these equations facilitates the derivation of QoIs such as dynamic strength $\bar{\sigma}_M$, energy dissipation $\bar{\phi}_f$, failure strain $\bar{\epsilon}_f$, and a brittleness indicator for different PF models and differential equations. The high loading rate asymptotic analysis showed that $\bar{\phi}_f$ scales as $\bar{\epsilon}^p$ and both $\bar{\sigma}_M$ and $\bar{\epsilon}_f$ as $\bar{\epsilon}^{p/2}$ for a 0D solution, that is when the entire spatial domain undergoes the same strain versus stress solution. For the PF equation with only the micro-viscosity term ($n = 1$), $p = 2/3, 1$, and 2 when the damage driving force has the scale of (elastic) energy ($m = 2$), stress ($m = 1$), and is asymptotically bounded ($m = 0$), respectively. When the micro-inertia term is present ($n = 2$), the p values for the same three driving force cases are $p = 1, 4/3$, and 2 , respectively. In short, a higher temporal order n and a slower increasing driving force (smaller m) increases the rate sensitivity of the fracture model. Specifically, the HPF equation with $p = 1$ is more rate-dependent than the PPF equation with $p = 2/3$.

The second source of the rate-dependency of the PF models is the initiation of instability and fragmentation as the stress level increases. Once damage reaches the critical value d^* , the 0D solution is no longer energetically favorable and fragments are formed. The lower d^* , the higher this rate effect is. Given that $d^* \rightarrow 0$ and 1 in quasi-static and high loading rate regimes, the rate effect from fragmentation is mainly observed at low loading rates. This is in contrast to the rate effect from the form of PF differential equation which applies to high loading rates.

In terms of energy dissipation, the minimum value occurs in quasi-static loading conditions where G is dissipated at all fragment interfaces that are in average $s_{\text{ave,qs}}$ apart. This results in the lower-bound value of $\bar{\phi}_f^L = 1/\bar{s}_{\text{ave,qs}}(\bar{b}_c)$. The upper-bound value $\bar{\phi}_f^U$ corresponds to the maximum energy a PF differential equation can dissipate, that is when the entire spatial domain uniformly undergoes full damage. This corresponds to $\bar{\phi}_f$ of 0D models, which is inversely proportional to b . Accordingly, the energy dissipation of PF models is length-scale dependent at high loading rates.

The effect of d_f is discussed next. For the PPF equation, d_f simply scales the effective loading rate for 0D studies, see the collapse of responses in terms of $\bar{\epsilon}_{oP} = \bar{\epsilon}_{oH}d_f$ in fig. 2.3. In 1D, the interaction of the PF with elastodynamic wave propagation makes the effect of d_f non-trivial (see for example fig. 2.14a, fig. 2.14b, and fig. 2.15) and $\bar{\epsilon}_{oP}$ alone can no longer represent the solution. For the HPF equation, we concluded that a value of $d_f \approx 1$ should be used. For high d_f values, the HPF solution tends to the PPF solution for the wide range of loading rates $\bar{\epsilon}_{oH} \leq d_f$. Moreover, high damping values prevent the formation of fragments. On the other hand, $d_f \ll 1$ results in other problems such as rapid unloading of the stress response for moderate-to-low loading rates and the corresponding lower than quasi-static energy dissipation. We attribute these nonphysical responses to the lack of existence of an intermediate loading rate at which the damping-driven solution (corresponding to first order time derivative in the PF equation) accurately represents the solution of the PF equation. This is another perspective on having a damping factor of unity; in the first proposed HPF equation, [72] used the analogy with a damped harmonic oscillator to show that by adding just enough damping, corresponding to a critically damped system, unphysical vibrations of the damage field can be precluded.

The PDE form of the PF equation can be analyzed from other perspectives too. The EPF and PPF equations lack the finite speed of propagation of damage discussed in [64, 47]. For time marching of these schemes, at the very least the PF part of the equation must be solved implicitly for the EPF equation. The nonlinearity of the

equation, and non-negativity and irreversibility of damage have resulted in complex solution algorithms to advance the solution in time; see for example [110, 111, 30]. In contrast, both PPF and HPF equations can be solved explicitly. This not only simplifies the implementation and addressing the damage value constraints, but also can result in a more efficient computational model for medium to high loading rates. The HPF equation is favored from this perspective for fine discretization sizes h , as the time step scales a h/c_d and h^2/ξ_d for the HPF and PPF equation, respectively. Finally, the PPF and HPF equations better match the (semi-)analytical fragmentation models; unlike the EPF equation, they can capture the increase of energy dissipation at high loading rates. Specifically, the energy rate-dependency of $p = 2/3$ exactly matches the Grady and GC models at high loading rates, favoring the PPF equation from the rate-dependency perspective. However, if the bulk material exhibit other forms of rate-dependency, other PDEs may need to be considered. For example, we showed that the EPF equation can capture the sigmoidal energy rate sensitivity experimentally observed in [46, 58].

We conclude by mentioning some extensions of this work. First, the study of the length-scale sensitivity of different PF models can be extended from the quasi-static loading condition [82] to the dynamic condition. While the crack-band model is deemed to be length scale insensitive, [112] shows that this only holds in the quasi-static loading conditions. Supported by our analysis above and [112], we believe the PF equation suffers from the same problem at high loading rates. Second, the effect of PF differential equation can be studied for 2D/3D problems. Especially, our preliminary results show how the parameters of HPF and PPF equations affect the dynamics of propagating cracks, especially the limiting crack speed.

Appendix

Tables

Table 2.1: Definitions of crack geometric and degradation functions in phase field models.

PF model	$\bar{\epsilon}_i$	$\omega(d)$	$\alpha(d)$	c_α	PF length-scale ($\bar{b}_c = b/\tilde{l}_c$)
AT2	0	$(1-d)^2$	d^2	2	$\bar{b}_c = \frac{27}{256}$
AT1	$\sqrt{\frac{3}{8b_c}}$		d	$\frac{8}{3}$	$\bar{b}_c = \frac{3}{8}$
CZM-W	1	$\frac{(1-d)^p}{(1-d)^p + Q(d)}$	$2d - d^2$	π	$\bar{b}_c \leq \frac{2}{\pi} (a_1 \geq 2)$ for linear softening $\bar{b}_c \leq \frac{3}{4(a_2+2)} (a_1 \geq a_2 + 2)$
CZM-L	1		d	$\frac{8}{3}$	

Table 2.2: Parameters for the polynomial function $Q(d)$ in Eq. 2.10.

PF model	Softening curve	p	a_1	a_2	a_3
CZM-W, [28]	Linear	2	$\frac{4}{\pi b_c}$	-0.5	0
CZM-L, [27]	Exponential	2	$\frac{3}{4b_c}$	$a_2 \geq 1$	0

Table 2.3: Common values of $F = c_\alpha \bar{b}/2$ in (2.17) for AT2 and AT1 models. The second column presents the values corresponding to PF length scale normalization, that is when $\bar{b} = 1$. The third column uses the values that make the AT2 and AT1 models comparable with CZM models with a normalized quasistatic strength of one. That is, $\bar{b} = \bar{b}_c$, where $\bar{b}_c$ is provided in the sixth column of Table 2.1.

Model	$\tilde{l} = b$	$\tilde{l} = \tilde{l}_c$
AT2	1	$\frac{27}{256}$
AT1	$\frac{4}{3}$	$\frac{1}{2}$

Table 2.4: QoIs associated with different stages of loading for the EPF solutions. The reference length for CZM models is $\tilde{l}_c$. For all models except CZM-W, stress asymptotically approaches zero and $\bar{\epsilon}_f$ corresponds to the user-specified failure damage $D_f \approx 1$.

Model	$\bar{\epsilon}_M$	$\bar{\sigma}_M$	$\bar{\phi}_M$	$\bar{\epsilon}_f$	$\bar{\phi}_f$	B_ϕ
AT2	$\frac{1}{\sqrt{3b}}$	$\frac{3\sqrt{3}}{16} \frac{1}{\sqrt{b}}$	$\frac{1}{8b}$	$\frac{D_f}{b(1-D_f)}$	$\frac{1}{2b}$	0.25
AT1	$\sqrt{\frac{3}{8b}}$	$\bar{\epsilon}_M = \sqrt{\frac{3}{8b}}$	$\frac{3}{16b}$	$\frac{\bar{\epsilon}_M}{\sqrt{1-D_f}}$	$\frac{3}{8b}$	0.5
CZM-W (linear)	1	1	0.5	$\frac{a_1}{2} = \frac{2}{\pi b_c}$	$\frac{a_1}{4} = \frac{1}{\pi b_c}$	$\frac{2}{a_1} = \frac{\pi \bar{b}_c}{2}$
CZM-L ($a_1 = 3, a_2 = 1$)	1	1	0.5	$\approx \frac{2.9376}{\sqrt{1-D_f}}$	1.4999	0.3333

Table 2.5: QoIs associated with different stages of loading for the PPF-HRA solutions. The first lines of AT1 and AT2 models provide expressions for general $\bar{b}$ (for example $\bar{b} = 1$ for $\tilde{l} = b$). For the other rows, $\tilde{l} = \tilde{l}_c$, corresponding to $\bar{\sigma}_M = 1$ in quasi-static loading and $\bar{b}_c$ equal to 27/256, 3/8, $1/\pi$, and 0.25 for AT2, AT1, CZM-W, and CZM-L models respectively. The time scale is $\tilde{\tau} = \xi_d$. For all models stress asymptotically approaches zero and $\bar{\epsilon}_f$ corresponds to $D_f = 0.99$ when D_f does not explicitly appear in the QoI values.

Model	$\hat{\epsilon}_M$	$\hat{\sigma}_M$	$\hat{\phi}_M$	$\hat{\epsilon}_f$	$\hat{\phi}_f$	B_ϕ
AT2	$\frac{1}{\sqrt[3]{2b}}$ 1.6800	$e^{-\frac{1}{3}} \frac{1}{\sqrt[3]{2b}}$ 1.2037	$\frac{1}{\sqrt[3]{12b^2}} \gamma(\frac{2}{3}, \frac{1}{3})$ 1.2409	$\sqrt[3]{\frac{-3 \log(1-D_f)}{b}}$ 5.0786	$\frac{1}{\sqrt[3]{12b^2}} \Gamma(\frac{2}{3})$ 2.6496	$\bar{\gamma}(\frac{2}{3}, \frac{1}{3})$ 0.4684
AT1	$\frac{1}{2} \sqrt[3]{\frac{3}{b}}$ 1.0000	$\frac{e^{-\frac{1}{3}}}{2} \sqrt[3]{\frac{3}{b}}$ 0.7165	$\frac{1}{4} \sqrt[3]{\frac{3}{b^2}} \gamma(\frac{2}{3}, \frac{1}{3})$ 0.4398	$\sqrt[3]{\frac{-9 \log(1-D_f)}{4b}}$ 3.0232	$\frac{1}{4} \sqrt[3]{\frac{3}{b^2}} \Gamma(\frac{2}{3})$ 0.9388	$\bar{\gamma}(\frac{2}{3}, \frac{1}{3})$ 0.4684
CZM-W	0.7647	0.4952	0.2431	3.6844	0.7017	0.3465
CZM-L	0.8360	0.6071	0.3098	5.5350	0.8349	0.3711

Table 2.6: QoIs associated with different stages of loading for the HPF-HRA solutions. The first lines of AT1 and AT2 models provide expressions for general $\bar{b}$ (for example $\bar{b} = 1$ for $\tilde{l} = b$). For the other rows, $\tilde{l} = \tilde{l}_c$, corresponding to $\bar{\sigma}_M = 1$ in quasi-static loading and $\bar{b}_c$ equal to 27/256, 3/8, $1/\pi$, and 0.25 for AT2, AT1, CZM-W, and CZM-L models respectively. The time scale is $\tilde{\tau} = \tau_d$ and the damping factor is $d_f = 1$. For all models stress reaches zero at a final strain.

Model	$\hat{\epsilon}_M$	$\hat{\sigma}_M$	$\hat{\phi}_M$	$\hat{\epsilon}_f$	$\hat{\phi}_f$	B_ϕ
AT2	$\frac{1.0874}{\sqrt[4]{b}}$ 1.9082	$\frac{0.8543}{\sqrt[4]{b}}$ 1.4991	$\frac{0.5475}{\sqrt{b}}$ 1.6860	$\frac{2.0031}{\sqrt[4]{b}}$ 3.5150	$\frac{0.9752}{\sqrt{b}}$ 3.0028	0.5615
AT1	$\frac{1.0120}{\sqrt[4]{b}}$ 1.2932	$\frac{0.7950}{\sqrt[4]{b}}$ 1.0160	$\frac{0.4742}{\sqrt{b}}$ 0.7743	$\frac{1.8641}{\sqrt[4]{b}}$ 2.3822	$\frac{0.8445}{\sqrt{b}}$ 1.3791	0.5615
CZM-W	0.9779	0.7429	0.4362	2.3131	0.9133	0.4776
CZM-L	1.1417	0.9049	0.6061	2.5449	1.1349	0.5340

Table 2.7: Behavior of the failure strain $\bar{\epsilon}_f$ for different PF differential equations. For the cases that d only asymptotically reaches zero, the order of $\bar{\epsilon}_f$ is expressed in terms of user-defined failure damage D_f .

Differential equation	Behavior of $\bar{\epsilon}_f$
EPF	AT2: $\mathcal{O}(\frac{1}{1-D_f})$; AT1 and CZM-L: $\mathcal{O}(\frac{1}{\sqrt{1-D_f}})$; CZM-W: finite $\bar{\epsilon}_f = \frac{a_1}{2} = \frac{2}{\pi b_c}$
PPF	infinite; $\mathcal{O}(\bar{\epsilon}_o^{1/3})$ for HRA-PPF; $\mathcal{O}(\bar{\epsilon}_o^{1/3} \sqrt[3]{-\log(1-D_f)})$ for HRA-AT1 and HRA-AT2
HPF	finite; $\mathcal{O}(\bar{\epsilon}_o^{1/2})$ for HRA-HPF

Table 2.8: Power p in (2.47); the rate dependency of the damage evolution equation (2.46) in terms of the order of differential equation n and order of strain in the damage driving force m . The asymptotic behaviors of energy dissipation density, maximum stress, and failure strain are $\bar{\phi}_f = \mathcal{O}(\bar{\epsilon}_o^p)$, $\bar{\sigma}_M, \bar{\epsilon}_f = \mathcal{O}(\bar{\epsilon}_o^{p/2})$ for high loading rate and $p = 2n/n + m$.

m	$n = 1$	$n = 2$
2 (energy driving force)	$\frac{2}{3}$ (PPF)	1 (HPF)
1 (strain/stress driving force)	1	$\frac{4}{3}$
0 (bounded driving force)	2	2

Table 2.9: Nondimensional quasi-static fragment size from different fragmentation models and the CZM-PF model.

Fragmentation model	GC	ZMR	PF
	[6]	[11]	PF
$\bar{s}_{\text{ave,qs}}$	2	4.5	≈ 4

Table 2.10: Lower-shelf (quasi-static) and Upper-shelf (dynamic limit) normalized energy dissipation densities for the EPF equation, referring to fig. 2.16d.

Energy	Loading rate	Formula	Energy dissipation mechanism
$\bar{\phi}_f^L$	Quasi-static $\bar{\epsilon}_{\text{oc}} \rightarrow 0$	$1/\bar{s}_{\text{ave,qs}}(\bar{b}_c)$	G dissipated at fragments in average s_{ave} apart; negligible energy dissipation within the fragments
$\bar{\phi}_f^U$	High loading rate $\bar{\epsilon}_{\text{oc}} \gtrsim 100$	0D EPF (Table 2.4)	Maximum possible energy dissipation by every point going through full damage (0D response)

Figures

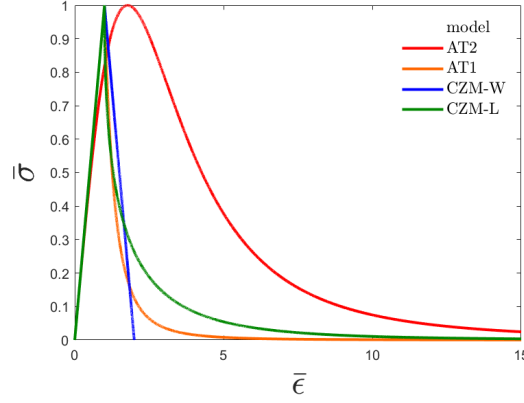


Figure 2.1: Normalized strain versus normalized stress for the EPF equation. The reference length for all four models is $\tilde{l}_c$, resulting in $\bar{\sigma}_M = 1$; *cf.* Table 2.4. For the linear CZM-W model $a_1 = 4$ ($\bar{b}_c\pi = 1 \Rightarrow \bar{\epsilon}_f = 2$). For the CZM-L model the parameters are $a_1 = 3, a_2 = 1$.

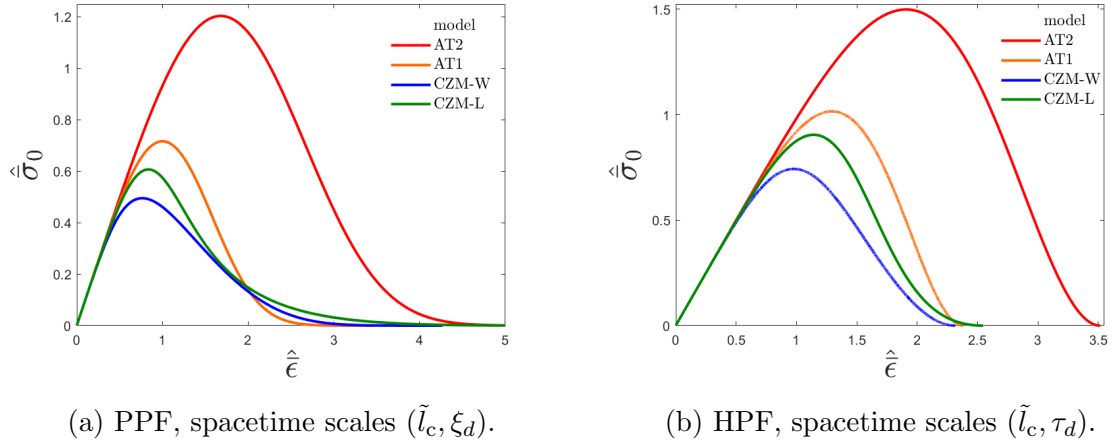
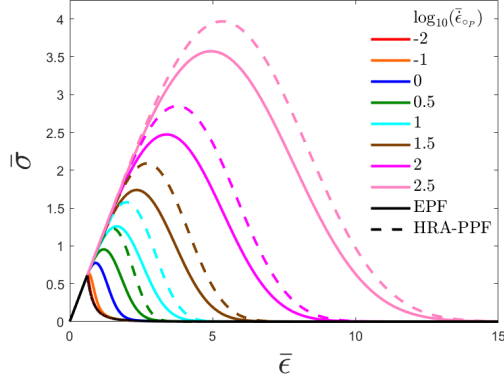
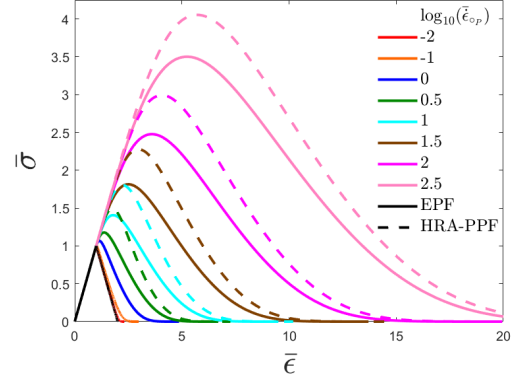


Figure 2.2: Normalized high rate asymptotic (HRA) strain versus zeroth term stress for PPF and HPF equations for $d_f = 1$. $\bar{b}_c$ is set to $27/256$, $3/8$, $1/\pi$, and 0.25 for AT2, AT1, CZM-W, and CZM-L, respectively, resulting in $\bar{\sigma}_M = 1$ for quasi-static loading.

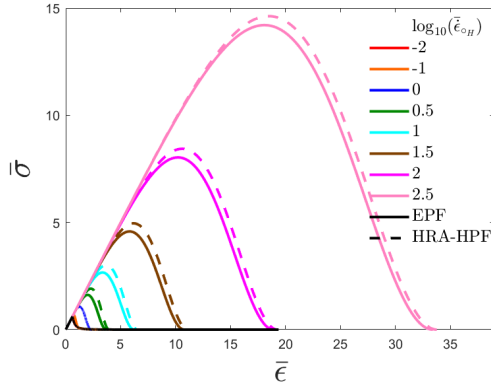


(a) AT1, spacetime scales (b, ξ_d) .

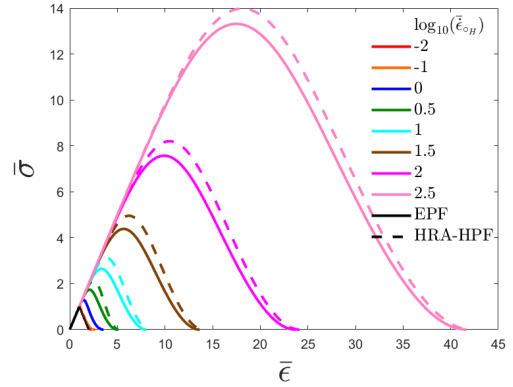


(b) HPF, spacetime scales $(\tilde{l}_c, \xi_d)$.

Figure 2.3: Normalized strain versus normalized stress for different loading rates $\dot{\epsilon}_o$ and PPF equation. The reference length scale $\tilde{l}$ for the AT1 and CZM-W models are b and $\tilde{l}_c$, respectively. The time scale of ξ_d is used, resulting in $\xi_d = 1$. For the linear CZM-W model $a_1 = 4$ ($\bar{b}_c \pi = 1 \Rightarrow \bar{\epsilon}_f = 2$). The dashed lines show the HRA-PPF solutions from (2.35) (specifically (2.38) for the AT1 model.)

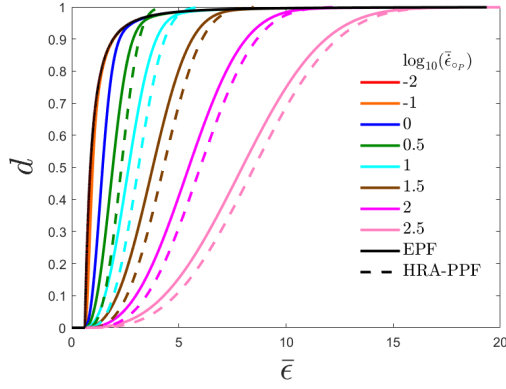


(a) AT1, spacetime scales (b, τ_d) .

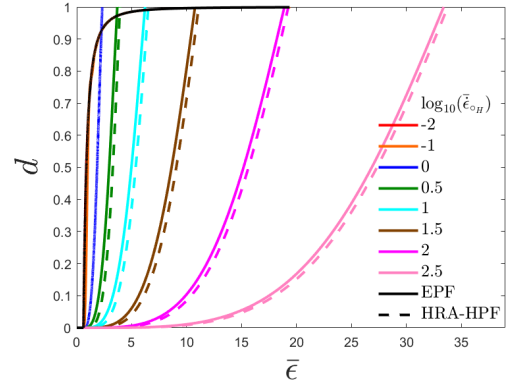


(b) HPF, spacetime scales $(\tilde{l}_c, \tau_d)$.

Figure 2.4: Normalized strain versus normalized stress for the HPF equation for different loading rates $\dot{\epsilon}_o$ and $d_f = 1$. The reference length scales for the AT1 and CZM-W models are b and $\tilde{l}_c$, respectively. The time scale of $\sqrt{\varrho_d} = \tau_d$ is used, resulting in $\bar{\rho}_d = 1$. For the linear CZM-W model $a_1 = 4$ ($\bar{b}_c \pi = 1 \Rightarrow \bar{\epsilon}_f = 2$). The dashed lines show the HPF-HRA solutions from (2.42).



(a) PPF, time scale $\tilde{\tau} = \xi_d$.



(b) HPF, time scale $\tilde{\tau} = \sqrt{\varrho_d} = \tau_d$.

Figure 2.5: The accumulation of d versus $\bar{\epsilon}$ for the AT1 model for PPF and HPF equations. The solid black line shows the EPF solution and dashed lines correspond to HRA solutions. $d_f = 1$ for the HPF equation and the phase field length scale is $\tilde{l} = b$ ($\bar{b} = 1$).

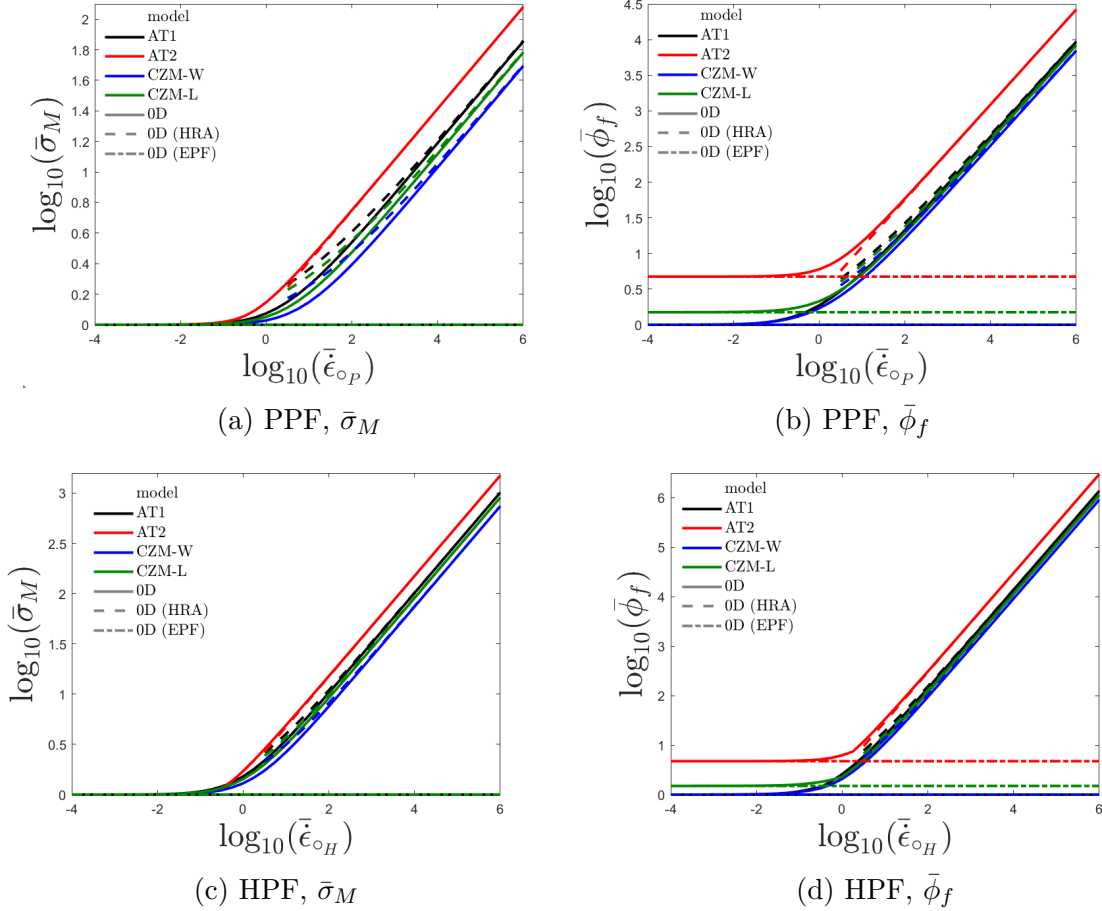
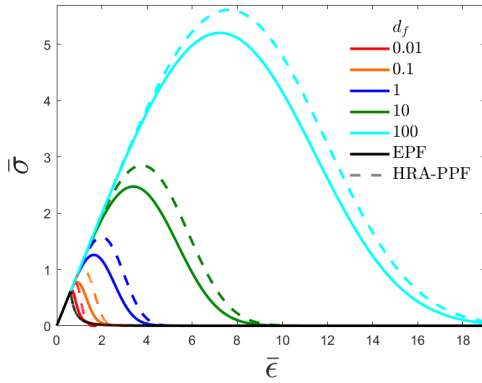
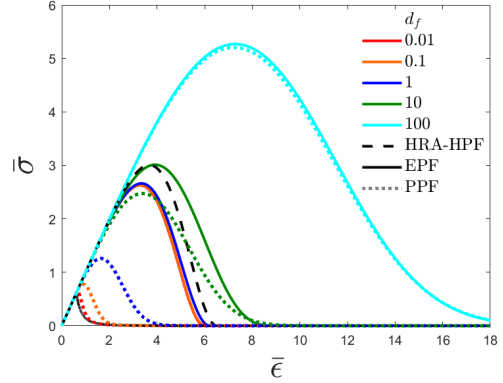


Figure 2.6: Rate-dependency of normalized maximum (dynamic) stress $\bar{\sigma}_M$ and energy dissipation density $\bar{\phi}_f$ for PPF (a,b) and HPF (c,d) equations. Time scales are ξ_d and $\sqrt{\varrho_d} = \tau_d$ for the PPF and HPF equations. The length scale $\tilde{l} = \tilde{l}_c$ results in $\bar{\sigma}_M = 1$ as $\bar{\epsilon}_o \rightarrow 0$; *cf.* column 6 of Table 2.1 for AT1 and AT2 models. The damping factor is $d_f = 1$ for the HPF equation. The constant y-axis value dot-dashed lines, corresponding to the EPF solutions, limit and match the PPF and HPF solutions at low loading rates. The dashed lines correspond to asymptotic results from (2.35) and (2.42). The asymptotic slopes of lines from a) to d) are 1/3, 2/3, 1/2, and 1, respectively.



(a) PPF



(b) HPF

Figure 2.7: The effect of damping factor d_f on strain-stress response of the PPF and HPF equations for $\bar{\epsilon}_{oH} = 10$ and the AT1 model. Spacetime scales are (b, τ_d) . For both solutions, the solid black curve shows the EPF solution. For the PPF solutions, dashed lines, show the HRA-PPF solutions corresponding to the same color solid line PPF solutions. For the HPF solutions, the single black dashed line shows the HRA-HPF solution (high rate approximation with effective $d_f = 0$), whereas the dotted color lines show the PPF solutions corresponding to the same color solid line HPF solutions.

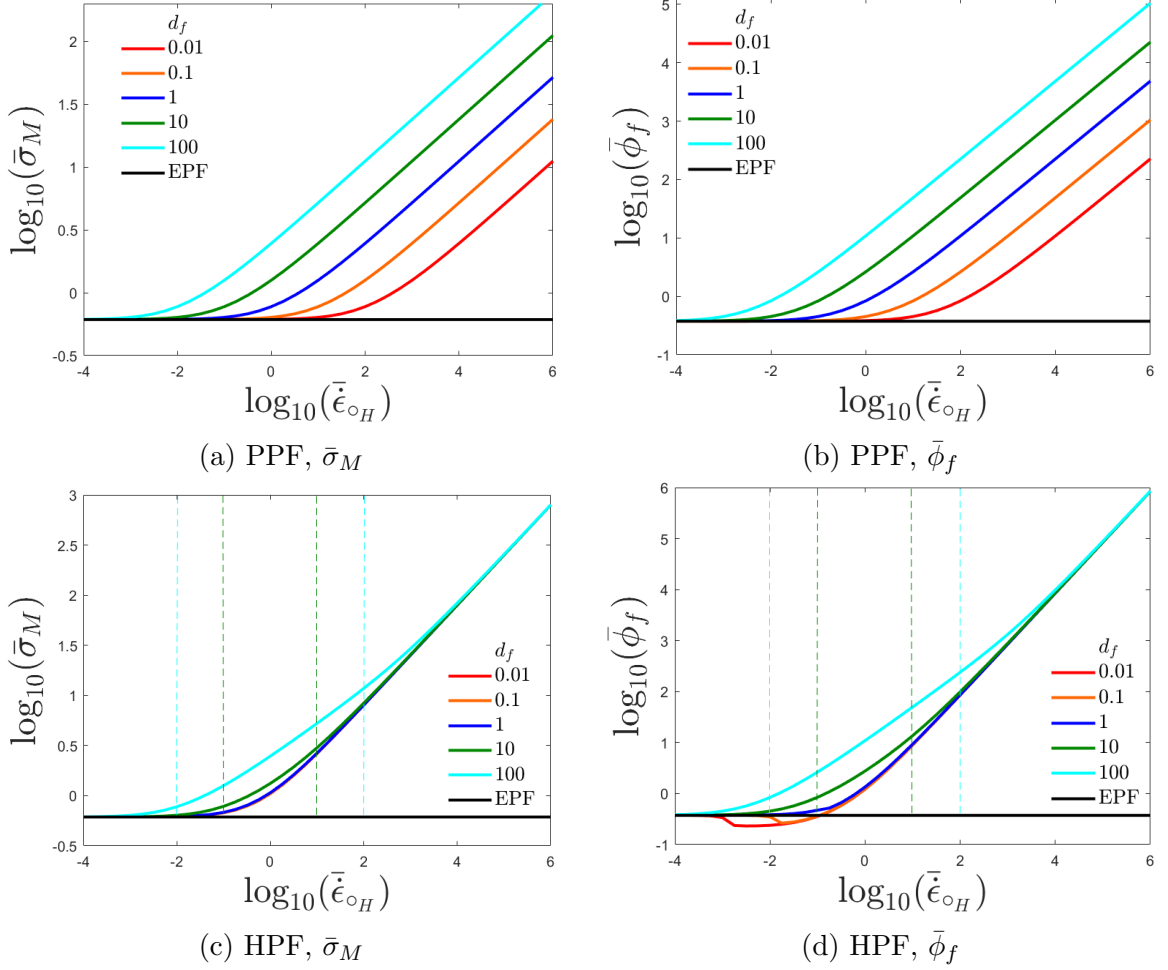


Figure 2.8: The effect of damping factor d_f on $\bar{\sigma}_M$ and $\bar{\phi}_f$ for the PPF (a,b) and HPF (c,d) equations and the AT1 model. Spacetime scales are (b, τ_d) . The reference EPF constant solutions are shown by solid black lines. In subfigure (d), we observe that $\bar{\phi}_f$ gets smaller than the quasi-static limit for low damping factors and a range of loading rates. In subfigures (c, d), the vertical dashed lines show the limits of the transitioning region between quasi-static EPF and high rate HPF solutions $1/d_f \leq \bar{\epsilon}_{oH} \leq d_f$ for $d_f > 1$; that is, $d_f = 10$ (orange) and $d_f = 100$ (cyan). In this region the HPF solution is close to the corresponding PPF solution.

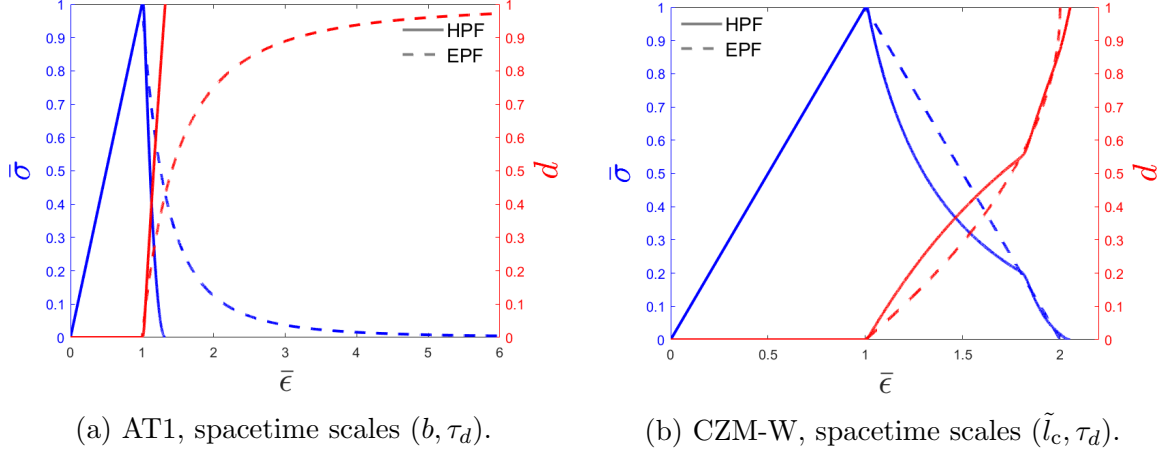


Figure 2.9: Explanation of the smaller than EPF energy dissipation of the HPF equation for a low to medium loading rate and a low damping factor. Strain-stress responses are shown for $\bar{\epsilon}_{oH} = 0.01$ and $d_f = 0.01$. Regions in the HPF solution where the stress is lower than that of the EPF solution, for the same strain value, demonstrate the lower energy dissipation problem.

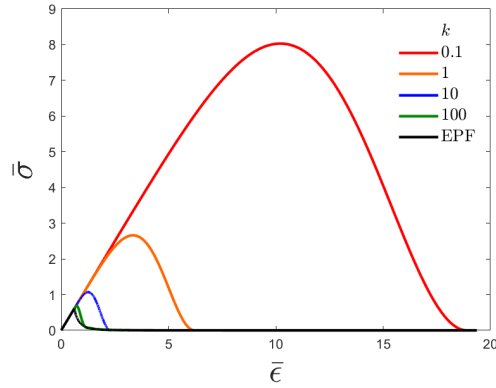


Figure 2.10: The effect of wave speed ratio $k = c_d/c_u$ on HPF strain-stress response for $\bar{\epsilon}_o = \dot{\epsilon}_o \tilde{\tau}_l E / \tilde{\sigma} = 10$ and the AT1 model. Spacetime scales are (b, τ_d) . The solid black curve shows the EPF solution.

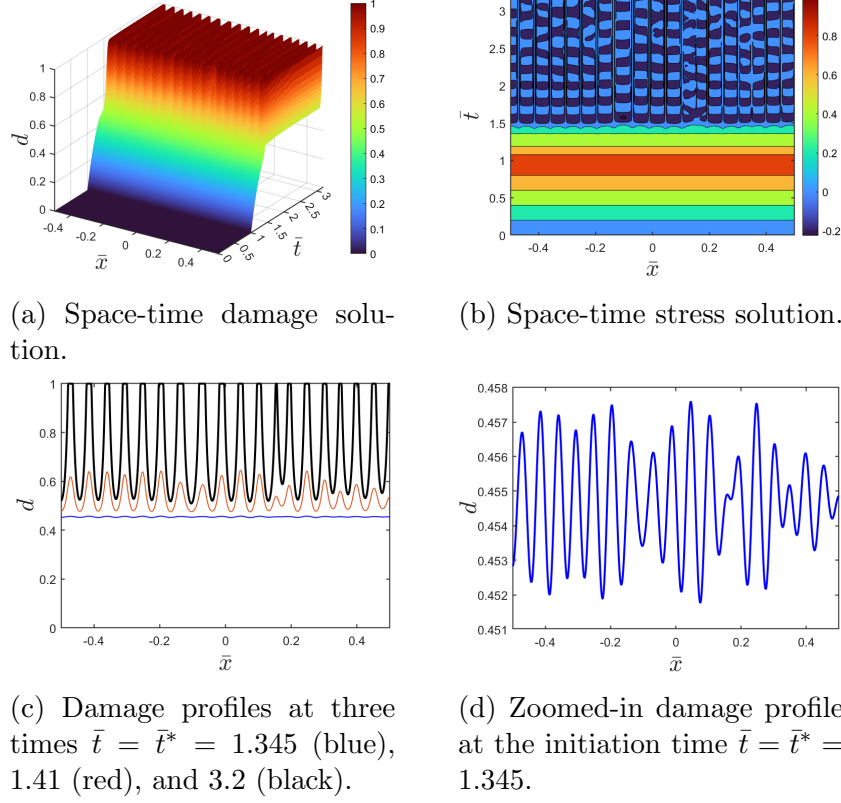


Figure 2.11: The transition from uniform strain, stress, and damage values (0D solution) to instability and formation of fragments in 1D.

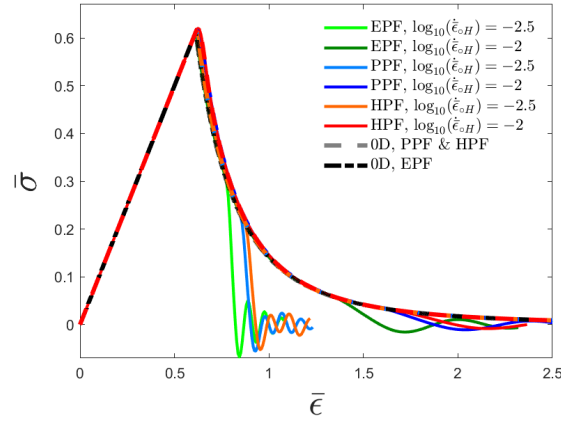


Figure 2.12: Comparison of the strain stress responses of 0D and 1D solutions for the AT1 model. The sharper unloading of the 1D models, especially for the lowest loading rate $\dot{\bar{\epsilon}}_{oH} = 10^{-2.5}$, is a result of instabilities and fragmentation formation discussed in §2.5.2.1. Otherwise, the 0D and 1D results for all higher loading rates (not shown) are visually indistinguishable. For the HPF and PPF solutions, dashed color lines correspond to the 0D solutions of the same 1D solutions shown. The dashed black line corresponds to the 0D EPF solution.

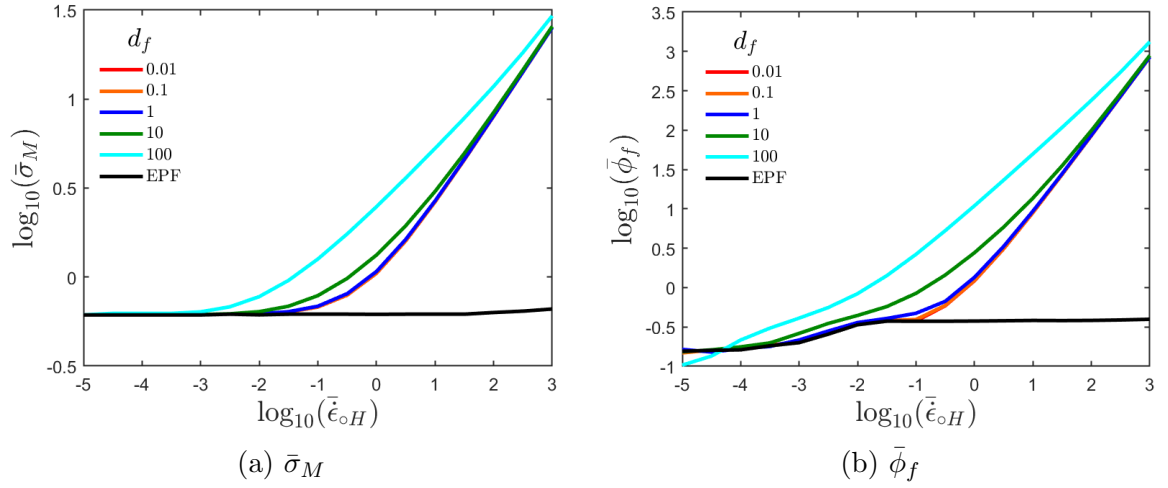


Figure 2.13: The effect of damping factor d_f on $\bar{\sigma}_M$ and $\bar{\phi}_f$ for the 1D ring fragmentation problem, HPF equation, and AT1 model. Spacetime scales are (b, τ_d) . The reference EPF solutions are shown by solid black lines.

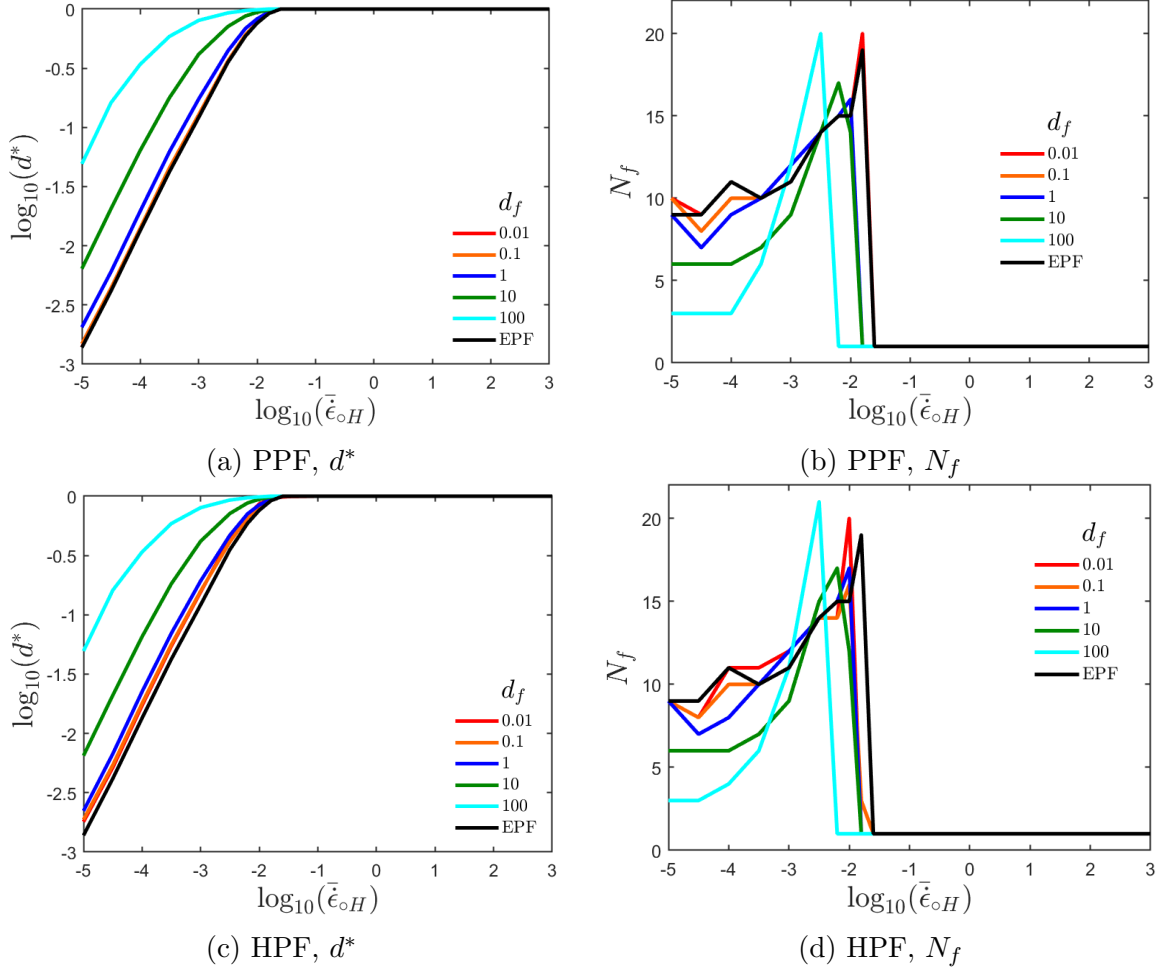


Figure 2.14: The effect of $\bar{\epsilon}_{oH}$ and damping factor d_f on critical damage value d^* and fragment count N_f for the PPF (a,b) and HPF (c,d) equations, the 1D ring fragmentation problem, and the AT1 model. Spacetime scales are (b, τ_d) . The reference EPF solutions are shown by solid black lines.

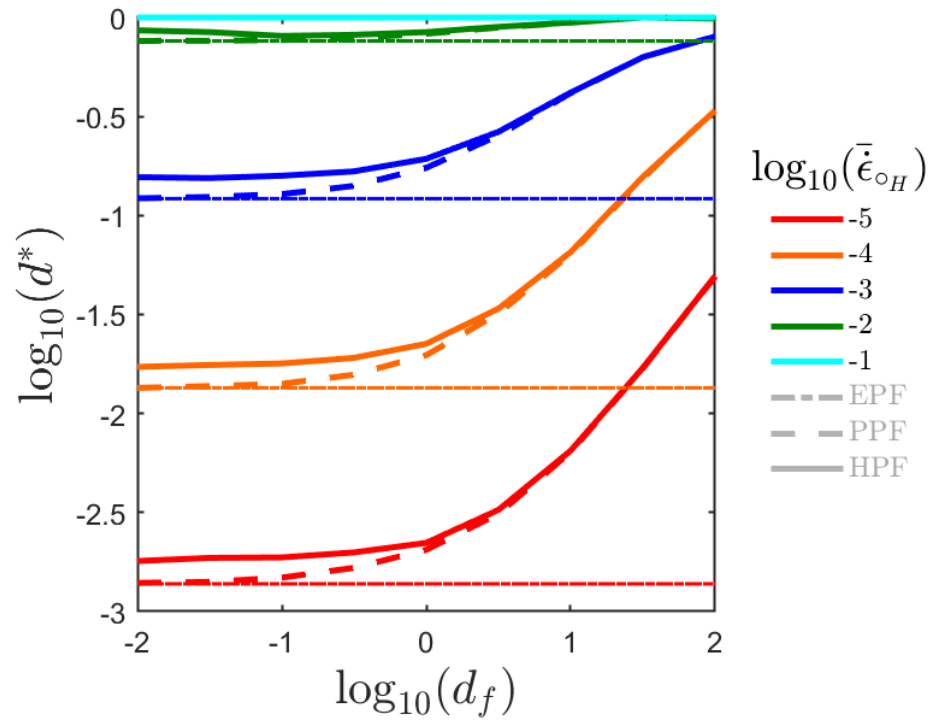


Figure 2.15: The effect of d_f on d^* for the three PF differential equations.

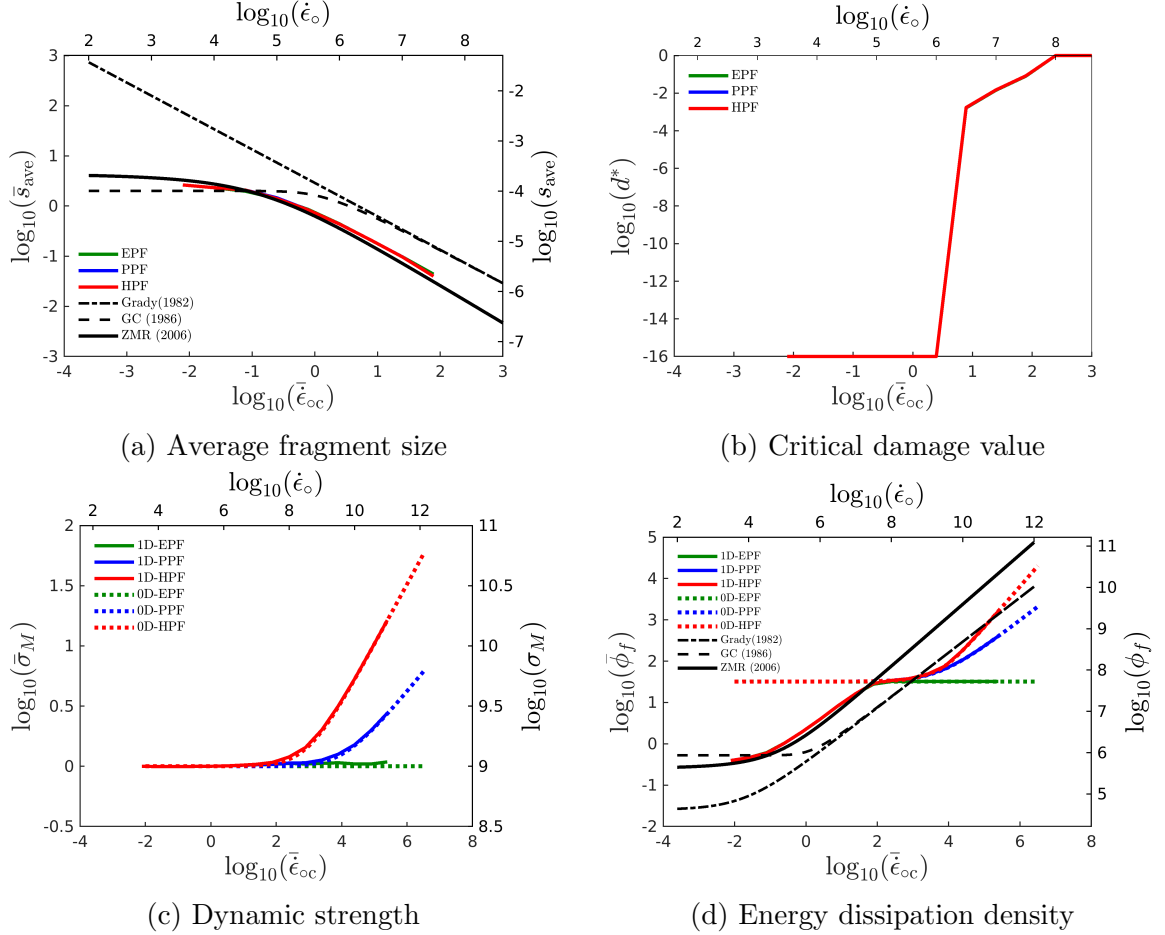


Figure 2.16: The rate-dependency of $\bar{s}_{ave}$, d^* , $\bar{\sigma}_M$, and $\bar{\phi}_f$ for EPF, PPF, and HPF equations and CZM-W model. The nondimensional and dimensional quantities are related by $\dot{\epsilon} = \bar{\epsilon}_{oc}\tilde{\epsilon}_c$, $s_{ave} = \bar{s}_{ave}\tilde{l}_c$, $\sigma_M = \bar{\sigma}_M\tilde{\sigma}_c$, and $\phi_f = \bar{\phi}_f\tilde{\phi}_c$ for $\tilde{\epsilon}_c = 404310/\text{s}$, $\tilde{l}_c = 50.7\mu\text{m}$, $\tilde{\sigma}_c = 1\text{ GPa}$, and $\tilde{\phi}_c = 1.64\text{ MPa}$. The values of $\dot{\epsilon}$, s_{ave} , and σ_M , ϕ_f are expressed in units of $1/\text{s}$, m , and Pa , respectively. At high loading rates, the rate dependency arises from the time derivatives of the PF, that is the 0D rate-dependency. This is evident from the colored dashed lines, showing the 0D solutions in c) and d). The fragment formation, especially at lower loading rates is the other cause of rate-dependency of QoIs. Grady, GC, and ZMR correspond to the fragmentation models [5], [6], and [11], respectively.

Chapter 3

**A hyperbolic phase field-cohesive
zone model: an efficient and robust
solver, and applications to fast
crack propagation**

3.1 Abstract

Elliptic phase field (EPF) models have proven to be attractive for simulating dynamic fracture at low loading rates. However, they suffer from high computational costs due to the need for small elements in cracked regions. Consequently, advanced solvers with optimal preconditioners are required to efficiently handle large systems of equations. Additionally, EPF models allow cracks to propagate at infinite speeds, leading to overestimated crack velocities and unrealistic patterns at high loading rates. In this work, we present a hyperbolic cohesive-zone phase field model that aims to address these limitations. The model is built on a thermodynamically consistent framework, systematically incorporating micro-inertia and viscous damping terms that are absent in elliptic models. A crucial feature of this framework is the introduction of a pseudo-dissipative potential that quantifies the rate of energy loss, effectively separating micro- and macro-stresses into elastic and dissipative components. The hyperbolic form of the evolution equation, combined with elastodynamics, enables the development of a fully explicit time integration scheme, which directly solves the coupled equations without iterative steps. This explicit solver demonstrates sublinear scaling for the entire algorithm and superlinear scaling in the solution phase, as verified through strong scaling analysis in parallel computing. An adaptive mesh refinement strategy is also developed, automatically refining the mesh as cracks evolve, which significantly reduces computational costs. The robustness and efficiency of the proposed solver are tested through applications to crack instability in polymethyl methacrylate (PMMA) under varying load rates, achieving both quantitative and qualitative accuracy that was not attainable with previous models.

3.2 Introduction

Fracture plays a crucial role in engineering applications, as effective and safe designs must account for fracture constraints, either by resisting catastrophic failure or

allowing failure modes to occur in a controlled manner. Predicting the post-peak behavior of materials requires computational models that can capture various stages of cracking, including initiation, coalescence, propagation, and branching [11]. These nonlinear mechanisms become more complex under extreme events with high loading rates, where existing microcracks and defects coalesce into larger macrocracks that propagate and branch. The rapid nature of crack propagation, coupled with its complex mechanisms, poses significant challenges for both numerical modeling and algorithm development, making accurate and efficient simulations difficult to achieve.

The PMMA model has been widely studied in the literature to understand crack propagation instability across different loading rates. Experimental results by [23] demonstrate that crack branching occurs when the crack speed reaches a certain threshold, preventing further acceleration beyond an upper limit of approximately 60% of the Rayleigh wave speed. Additionally, as the crack speed increases, the fracture surface becomes rougher due to complex phenomena around the crack tip, such as microcrack nucleation, heat generation, thermal softening, and high-rate plasticity. The high crack speeds make inertial effects, resulting from damage processes at the microscale and mechanical deformation, critical in influencing the fracture response.

Rate-independent fracture models struggle to accurately capture both crack paths and velocities when influenced by the level of applied loading, despite their effectiveness at lower rates. The rate-dependent toughening mechanism has been incorporated into models in several ways. One approach modifies the evolution equation, transforming it into a hyperbolic form of a non-local damage model [63], or phase field models [72] [73]. Alternatively, the rate-dependent effect can be introduced to constitutive equation of the bulk or fracture models. Typical examples include viscoelastic or rate-dependent plasticity models of a rate-independent cohesive zone model [10] [22] [113]. Additionally, rate-dependent cohesive models with linear or nonlinear bulk materials [114][115] are also investigated. In these models, one or

more parameters are incorporated to control the degree of rate effects on the fracture process.

Fracture models can be classified into two broad categories: discrete and continuum approaches. In discrete approaches, such as cohesive zone models [116] or extended finite element methods (XFEM) [117], cracks are embedded as discontinuities in the displacement field, necessitating tracking strategies for crack progression. This becomes more complex in three-dimensional problems with multiple cracks. In contrast, continuum approaches, such as nonlocal damage models and phase field methods, approximate cracks with a scalar continuous damage variable that ranges from 0 to 1, representing intact and fully broken states, respectively. The damage variable evolves continuously with crack growth, eliminating the need for additional tracking techniques. Due to this advantage, this work focuses on a hyperbolic phase field cohesive zone model. This model extends Wu’s original elliptic phase field model [28] to a hyperbolic form, serving not only to model rate dependency but also to improve numerical efficiency.

Although phase field modeling has gained significant attention over the past two decades due to its simplicity in simulating complex fracture patterns and its applications in dynamic fracture [17] [18] [78], [118] [119], it suffers from high computational costs. In the phase field approach, the width of the damage zone is controlled by a characteristic length scale, necessitating sufficiently small elements within crack regions. This becomes more challenging as the number of cracks increases, particularly under high-rate loading conditions. To address this limitation, several strategies have been proposed, which can be categorized into three main groups: 1) advanced solvers, 2) parallel techniques, and 3) mesh adaptivity. In the first category, D. Jodlbauer *et al.* [120] developed a geometric multigrid method as a preconditioner for a generalized minimal residual solver (GMRES), achieving linear speedup in strong scaling analyses. In the second category, overlapping and non-overlapping domain decomposition techniques have been proposed for dynamic fracture. For instance, Svolos *et al.* [121] introduced a decomposition

of the computational domain into localized regions containing shear bands and cracks, while healthy regions remain unaffected. Each subdomain is solved using different preconditioners. In contrast, Hao *et al.* [122] employed the dual-primal finite element tearing and interconnecting (FETI-DP) method, partitioning the mesh into subdomains while maintaining solution continuity through Lagrange multipliers. Regarding mesh adaptivity, meshes are automatically refined in crack regions without prior knowledge of crack paths, thus reducing unnecessary degrees of freedom. Indicators for marking elements for refinement include phase field values [110] [17] or a posteriori error estimators [123]. While the PF-CZM model selected in this work offers advantages over the standard PF-AT2 model—such as length scale insensitivity and the incorporation of material strength—it also faces severe numerical convergence challenges, requiring more iterations to achieve convergence than the AT2 model. Recent strategies, such as those employing the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method [30], have not effectively mitigated the convergence issues for this model.

In this work, we focus on modeling rate dependency and enhancing numerical efficiency using a hyperbolic phase field model. We develop a general thermodynamically consistent framework for gradient models, which systematically incorporates micro-inertia and viscous damping terms—elements that are absent in elliptic models. This approach contrasts with the more intuitive derivations by Kamensky *et al.* [72] using a PF-AT2 model and Hai *et al.* [73] using a PF-CZM model. The key step in our framework is the decomposition of micro and macro stresses into elastic and dissipative components, defined through a pseudo-dissipative potential function. We validate the proposed model against experimental data for PMMA under high-rate loading, an evaluation not previously conducted by [72] [73]. We demonstrate that accurate crack patterns at high rates, where crack initiation can be erroneously activated due to prestrain, require a modification to control crack initiation effectively. Leveraging the hyperbolic form of the phase field equation, we introduce a fully explicit time integration scheme to solve the coupled equations

simultaneously. This approach eliminates the need for advanced preconditioners and nonlinear solvers, thereby overcoming convergence issues commonly encountered in implicit schemes. Additionally, we construct a parallel algorithm for the proposed scheme, achieving superlinear speedup for the linear solve and sublinear speedup for the overall algorithm. In contrast, prior work by [120] achieved linear speedup only for the linear solve by using an advanced preconditioner within a complex nonlinear solver (the primal-dual active set method). Meanwhile, Svolos *et al.* [121] and Hao *et al.* [122] reported rapid performance degradation as the number of cores increased beyond one. Their use of an elliptic phase field model required a staggered scheme for phase field solution, which is slower than the monolithic scheme implemented in our approach.

3.3 Formulations

Consider an arbitrarily solid body $\omega \in R^d$, where d denotes its dimension, within a specified time range T for cracking. The external boundary $\partial\omega$ is composed of Dirichlet boundary $\partial\omega_u$ and Neumann boundary $\partial\omega_t$, such that $\partial\omega = \partial\omega_u \cup \partial\omega_t$ and $\emptyset = \partial\omega_u \cap \partial\omega_t$. The mechanical response of the solid is described by the displacement field at a spatial position $\mathbf{x} \in \omega$ and time instant $t \in T$, $\mathbf{u}(\mathbf{x}, t) : \omega \times T \rightarrow R^d$, which satisfies $\mathbf{u} = \tilde{\mathbf{u}}$ on $\partial\omega_u$ and the Neumann boundary condition on $\partial\omega_t$. Assuming small deformations, the infinitesimal strain measure is defined as, $\epsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$, with $i, j \in \{1, \dots, d\}$, where it is associated with a dual stress σ_{ij} .

The topology of a sharp crack within the solid is characterized by $\Gamma(t)$, which evolves over time $t \in T \subset R$. The sharp crack is regularized by a continuous damage variable $d(\mathbf{x}, t)$, referred to as the phase field. An intact material state at a point $\mathbf{x} \in \omega$ is represented by $d = 0$, whereas a fully broken state corresponds to $d = 1$. The evolution of the phase field d and its gradient ∇d describe crack propagation in solids, aligned with the micro-force σ^d and micro-stress $\boldsymbol{\sigma}^{\nabla d}$, analogous to the solid behavior.

3.3.1 Thermodynamically consistent framework

The deterioration of materials from micro-scale defects—such as micro-cracks, voids, or pores—culminates in macro-scale crack formation. Therefore, it is necessary to integrate micro-quantities into the energy balance. Building on the gradient model framework proposed by Stumpf *et al.* [64] and Nguyen [124], we develop a thermodynamically consistent framework for the hyperbolic phase field model, facilitating a systematic and modular identification of micro-quantities. The first law of thermodynamics can be expressed as,

$$\frac{d}{dt} \int_{\omega} (\rho_u e + k) dv = \int_{\omega} (\mathbf{b}^u \cdot \dot{\mathbf{u}} + b^d \dot{d} + \rho_u r) dv + \int_{\partial\omega} (\boldsymbol{\sigma} \mathbf{n} \cdot \dot{\mathbf{u}} + \boldsymbol{\sigma}^{\nabla d} \cdot \mathbf{n} \dot{d} - \mathbf{q} \cdot \mathbf{n}) ds, \quad (3.1)$$

where e is the internal energy density and k represents kinetic energy density. $\mathbf{b}^u$ denotes the macro-level body force, while b^d is the extrinsic force contributing to the breaking of material linkages. ρ_u and r are the solid mass density and heat source respectively, while $\mathbf{q}$ is the heat flux, and $\mathbf{n}$ is the outward normal vector at the boundary $\partial\omega$. In the phase field framework, $\mathbf{b}^u$ and b^d are often neglected and will be disregarded here. The kinetic energy density is defined by,

$$k = \frac{1}{2} \rho_u \dot{\mathbf{u}} \cdot \dot{\mathbf{u}} + \frac{1}{2} \rho_d \dot{d} \dot{d} + \frac{1}{2} \rho^{\nabla d} \nabla_{\mathbf{x}} \dot{d} \cdot \nabla_{\mathbf{x}} \dot{d}, \quad (3.2)$$

where ρ_d and $\rho^{\nabla d}$ denote phase field micro-mass density, which becomes significant in acceleration-dominated defect scenarios, such as micro-crack propagation driven by inertia, even in the absence of external forces. See [63] and [125] for the existence of micro inertia effects from homogenization approaches. Here, we assume that the contribution of the higher order term $\frac{1}{2} \rho^{\nabla d} \nabla_{\mathbf{x}} \dot{d} \cdot \nabla_{\mathbf{x}} \dot{d}$ in Eq. 3.2 can be neglected.

The second law of thermodynamics demands the non-negativity of entropy generation,

$$\mathcal{G} = \int_{\omega} \rho_u \zeta dv = \frac{d}{dt} \int_{\omega} \rho_u \vartheta dv - \int_{\omega} \frac{\rho_u r}{\theta} dv + \int_{\partial\omega} \frac{\mathbf{q} \cdot \mathbf{n}}{\theta} ds \geq 0, \quad (3.3)$$

where ζ is specific entropy production, and ϑ is the specific entropy. By applying the divergence theorem to the last term of Eq. 3.3, the entropy production becomes,

$$\mathcal{G} = \int_{\omega} \rho_u \dot{\vartheta} dv - \int_{\omega} \frac{\rho_u r}{\theta} dv + \int_{\omega} \frac{\nabla_{\mathbf{x}} \cdot \mathbf{q}}{\theta} dv - \int_{\omega} \frac{\mathbf{q} \cdot \nabla_{\mathbf{x}} \theta}{\theta^2} dv \geq 0. \quad (3.4)$$

The dissipated energy density of the system is related to the specific entropy production by temperature such that,

$$\phi_d = \theta \rho_u \zeta = \rho_u \theta \dot{\vartheta} - \rho_u r dv + \nabla_{\mathbf{x}} \cdot \mathbf{q} - \frac{\mathbf{q} \cdot \nabla_{\mathbf{x}} \theta}{\theta} \geq 0. \quad (3.5)$$

The last term in Eq. 3.5 is always non-negative. Thus, the satisfaction of the reduced form of the dissipated energy density,

$$\phi_d^{\text{red}} = \rho_u \theta \dot{\vartheta} - \rho_u r + \nabla_{\mathbf{x}} \cdot \mathbf{q} \geq 0. \quad (3.6)$$

is a sufficient but not necessary condition for the satisfaction of Eq. 3.5.

To eliminate the derivative of specific entropy ϑ in Eq. 3.6, we use the relation between the specific free energy function ψ , the internal energy density e , and the specific entropy ϑ ,

$$e = \psi + \theta \vartheta. \quad (3.7)$$

Setting $\phi = \rho_u \psi$, Eq. 3.7 can be modified as,

$$\rho_u \dot{e} = \dot{\phi} + \rho_u \dot{\theta} \vartheta + \rho_u \theta \dot{\vartheta}. \quad (3.8)$$

Substituting Eq. 3.8 into Eq. 3.6 results in,

$$\phi_d^{\text{red}} = \rho_u \dot{e} - \dot{\phi} - \rho_u \dot{\theta} \vartheta - \rho_u r + \nabla_{\mathbf{x}} \cdot \mathbf{q} \geq 0. \quad (3.9)$$

Next, we define the Newtonian balance laws by incorporating both classical elastodynamics in the physical space and micro-quantities in the material space,

$$\frac{d}{dt} \int_{\omega} \rho_u \dot{\mathbf{u}} = \int_{\partial\omega} \boldsymbol{\sigma} \cdot \mathbf{n} ds, \quad (3.10a)$$

$$\frac{d}{dt} \int_{\omega} \rho_d \dot{d} = \int_{\omega} (-\sigma^d) dv + \int_{\partial\omega} \boldsymbol{\sigma}^{\nabla d} \cdot \mathbf{n} ds. \quad (3.10b)$$

Applying the divergence theorem to Eq. 3.10, and assuming the regularity condition holds, we derive the governing equations for deformation and damage, respectively,

$$\rho_u \ddot{\mathbf{u}} = \nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma}, \quad (3.11a)$$

$$\rho_d \ddot{d} = \nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma}^{\nabla d} - \sigma^d. \quad (3.11b)$$

Eqs. (3.11a) and (3.11b) are supplemented by the initial conditions, $\mathbf{u}(\mathbf{x}, t = 0) = \tilde{\mathbf{u}}_0$, $\dot{\mathbf{u}}(\mathbf{x}, t = 0) = \dot{\tilde{\mathbf{u}}}_0$, $d(\mathbf{x}, t = 0) = \tilde{d}_0$, and $\dot{d}(\mathbf{x}, t = 0) = \dot{\tilde{d}}_0$. In Eq. 3.11a and Eq. 3.11b.

Substituting Eqs. 3.11a and 3.11b into Eq. 3.1 and applying the divergence theorem, we obtain the rate of internal energy as,

$$\rho_u \dot{e} = \boldsymbol{\sigma} : \nabla_{\mathbf{x}} \dot{\mathbf{u}} + \sigma^d \dot{d} + \boldsymbol{\sigma}^{\nabla d} \cdot \nabla_{\mathbf{x}} \dot{d} + \rho_u r - \nabla_{\mathbf{x}} \cdot \mathbf{q}. \quad (3.12)$$

Assuming the free energy density ϕ is a function of $\boldsymbol{\epsilon}$, d , $\nabla_{\mathbf{x}} d$, and temperature θ , its rate can be expressed as,

$$\dot{\phi}(\boldsymbol{\epsilon}, d, \nabla_{\mathbf{x}} d, \theta) = \frac{\partial \phi}{\partial \boldsymbol{\epsilon}} \dot{\boldsymbol{\epsilon}} + \frac{\partial \phi}{\partial d} \dot{d} + \frac{\partial \phi}{\partial \nabla_{\mathbf{x}} d} \nabla_{\mathbf{x}} \dot{d} + \frac{\partial \phi}{\partial \theta} \dot{\theta}. \quad (3.13)$$

Combining Eqs. 3.13 and 3.12 in Eq. 3.6 results in a thermodynamic requirement for the coupled problem of evolving damage,

$$\phi_d^{\text{red}} = (\boldsymbol{\sigma} - \frac{\partial \phi}{\partial \boldsymbol{\epsilon}}) : \dot{\boldsymbol{\epsilon}} + (\sigma^d - \frac{\partial \phi}{\partial d})\dot{d} + (\boldsymbol{\sigma}^{\nabla d} - \frac{\partial \phi}{\partial \nabla_{\mathbf{x}} d}) \cdot \nabla_{\mathbf{x}} \dot{d} - (\rho_u \vartheta + \frac{\partial \phi}{\partial \theta})\dot{\theta} \geq 0. \quad (3.14)$$

The last term in Eq. 3.14 leads to a new relation, $\rho_u \vartheta = -\frac{\partial \phi}{\partial \theta}$. Its time derivative is,

$$\rho_u \dot{\vartheta} = -\frac{\partial^2 \phi}{\partial \theta \partial \boldsymbol{\epsilon}} \dot{\boldsymbol{\epsilon}} - \frac{\partial^2 \phi}{\partial \theta \partial d} \dot{d} - \frac{\partial^2 \phi}{\partial \theta \partial \nabla_{\mathbf{x}} d} \nabla_{\mathbf{x}} \dot{d} - \frac{\partial^2 \phi}{\partial \theta \partial \theta} \dot{\theta}. \quad (3.15)$$

Premultiplying Eq. 3.15 by θ and substituting it back into Eq. 3.6 result in the governing equation for heat conduction,

$$\rho_u c \dot{\theta} = -\nabla_{\mathbf{x}} \cdot \mathbf{q} + \rho_u r + \phi_d^{\text{red}} + L, \quad (3.16)$$

where the latent heat is defined as, $L = \theta \frac{\partial^2 \phi}{\partial \theta \partial \boldsymbol{\epsilon}} \dot{\boldsymbol{\epsilon}} + \theta \frac{\partial^2 \phi}{\partial \theta \partial d} \dot{d} + \theta \frac{\partial^2 \phi}{\partial \theta \partial \nabla_{\mathbf{x}} d} \nabla_{\mathbf{x}} \dot{d}$, and the heat capacity is given by, $c = -\theta \frac{\partial^2 \phi}{\partial \theta \partial \theta}$.

To complete the governing equations 3.11a and 3.11b, we determine closed forms for the micro-damage density ρ_d , micro-force σ^d , and micro-stress $\boldsymbol{\sigma}^{\nabla d}$. According to the theory of generalized standard materials [124], the classical Cauchy stress $\boldsymbol{\sigma}$, micro-force σ^d , and micro-stress $\boldsymbol{\sigma}^{\nabla d}$ can be decomposed into nondissipative parts $(\cdot)_{\text{elas}}$ and dissipative parts $(\cdot)_{\text{diss}}$,

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_{\text{elas}} + \boldsymbol{\sigma}_{\text{diss}}, \quad \sigma^d = \sigma_{\text{elas}}^d + \sigma_{\text{diss}}^d, \quad \boldsymbol{\sigma}^{\nabla d} = \boldsymbol{\sigma}_{\text{elas}}^{\nabla d} + \boldsymbol{\sigma}_{\text{diss}}^{\nabla d}, \quad (3.17)$$

where

$$\boldsymbol{\sigma}_{\text{elas}} = \frac{\partial \phi}{\partial \boldsymbol{\epsilon}}, \quad \sigma_{\text{elas}}^d = \frac{\partial \phi}{\partial d}, \quad \boldsymbol{\sigma}_{\text{elas}}^{\nabla d} = \frac{\partial \phi}{\partial \nabla_{\mathbf{x}} d}, \quad (3.18a)$$

$$\boldsymbol{\sigma}_{\text{diss}} = \frac{\partial \dot{\phi}_{\text{diss}}}{\partial \dot{\boldsymbol{\epsilon}}}, \quad \sigma_{\text{diss}}^d = \frac{\partial \dot{\phi}_{\text{diss}}}{\partial \dot{d}}, \quad \boldsymbol{\sigma}_{\text{diss}}^{\nabla d} = \frac{\partial \dot{\phi}_{\text{diss}}}{\partial \nabla_{\mathbf{x}} \dot{d}}. \quad (3.18b)$$

The dissipative parts $(\cdot)_{\text{diss}}$ in Eq. 3.18b are derived from a pseudo-dissipative potential function $\dot{\phi}_{\text{diss}}(\dot{\epsilon}, \dot{d}, \nabla_{\mathbf{x}} \dot{d})$, provided this function exists. This potential function will be introduced in the next section, enabling a systematic and modular approach to determine the micro-terms in Eq. 3.11b. Accordingly, Eqs. 3.11a and 3.11b, along with the constitutive relations in Eqs. 3.18, expressed through the general functions $\phi(\epsilon, d, \nabla_{\mathbf{x}} d)$ and $\dot{\phi}_{\text{diss}}(\dot{\epsilon}, \dot{d}, \nabla_{\mathbf{x}} \dot{d})$, establish the primary components for the coupled problem.

Using Eq. 3.18, Eq. 3.9 can be reduced as,

$$\phi_d^{\text{red}} = \sigma_{\text{diss}} : \dot{\epsilon} + \sigma_{\text{diss}}^d \dot{d} + \sigma_{\text{diss}}^{\nabla d} \cdot \nabla_{\mathbf{x}} \dot{d} \geq 0. \quad (3.19)$$

To ensure the non-negativity of dissipation, Eq. 3.9 is locally satisfied by imposing the following conditions,

$$\sigma_{\text{diss}}^d \geq 0, \quad \dot{d} \geq 0. \quad (3.20)$$

3.3.2 Energy functionals and constitutive equations

3.3.2.1 Stored energy

For the scope of the numerical results in this work, an isothermal condition is assumed. The stored energy is defined as,

$$\phi(\epsilon, d) = \omega(d) \phi_e(\epsilon), \quad (3.21)$$

with $\phi_e(\epsilon)$ is a reference elastic energy stored in the bulk of a solid, degraded by the function $\omega(d)$ during the damage process. For isotropic linear elastic materials, assumed in this work, ϕ_e is given by,

$$\phi_e = \frac{1}{2} \lambda \text{tr}[\epsilon] + \mu \text{tr}[\epsilon^2], \quad (3.22)$$

where λ and μ are the Lamé constants.

3.3.2.2 Fracture energy density and pseudo dissipative potential function

According to Griffith's theory in fracture mechanics, the energy required to create a new crack surface is represented by the critical energy release rate G integrated over the newly formed crack surface, $\int_{\omega} \phi_f dv = \int_{ds} G ds$. For finite element implementation, this surface integral is approximated by a volume integral, as proposed by Bourdin *et al.* [66],

$$\int_{\omega} \phi_f dv \approx G \int_{\omega} \gamma dv, \quad (3.23)$$

where γ is the crack surface density function, defined generally as,

$$\gamma = \frac{1}{bc_{\alpha}} (\alpha(d) + b^2 |\nabla_{\mathbf{x}} d|^2). \quad (3.24)$$

In Eq. (3.24), $\alpha(d)$ represents the local effect of damage processes, b is the length scale controlling the width of damage zone, and c_{α} is a coefficient that depends on the choice of the function $\alpha(d)$, as described by Braides [126].

The pseudo-dissipative potential, $\dot{\phi}_{\text{diss}}$, quantifies the rate of energy loss in the system over time. To model this, we introduce a closed form for $\dot{\phi}_{\text{diss}}$ that includes both the rate of fracture energy and viscous damping terms. This formulation differs from [124], which only considers the viscous damping terms as the source of dissipative processes. Our modified expression for $\dot{\phi}_{\text{diss}}$ is defined as follows,

$$\dot{\phi}_{\text{diss}} = \dot{\phi}_f(d, \nabla_{\mathbf{x}} d) + \frac{1}{2} \eta^d \dot{d}^2 + \frac{1}{2} \eta^{\nabla d} (\nabla_{\mathbf{x}} \dot{d})^2. \quad (3.25)$$

Here, η^d and $\eta^{\nabla d}$ are viscosity coefficients for the phase field d and its gradient respectively, which add more dissipative mechanisms to the system. These viscous terms can be experimentally determined at various applied velocities, as demonstrated by [65]. In this work, the contribution of the higher-order viscous term is assumed to be negligible and is therefore excluded from the analysis. The simplified form of Eq.

3.25 becomes,

$$\dot{\phi}_{\text{diss}} = \frac{G}{bc_\alpha}(\alpha(d)' \dot{d} + 2b^2 \nabla_{\mathbf{x}} d \cdot \nabla_{\mathbf{x}} \dot{d}) + \frac{1}{2} \eta^d \dot{d}^2. \quad (3.26)$$

3.3.3 Constitutive equations

In the preceding sections, we established a general framework for a dynamic system involving damage evolution. By substituting Eqs. (3.21) and (3.26) into Eq. (3.18), we obtain the following expressions for the constitutive relations,

$$\boldsymbol{\sigma}_{\text{elas}} = \omega(d) \boldsymbol{\sigma}_0, \quad \sigma_{\text{elas}}^d = \omega'(d) \phi_e, \quad \boldsymbol{\sigma}_{\text{elas}}^{\nabla d} = \mathbf{0}, \quad (3.27a)$$

$$\boldsymbol{\sigma}_{\text{diss}} = \mathbf{0}, \quad \sigma_{\text{diss}}^d = \frac{G}{bc_\alpha} \alpha'(d) + \eta^d \dot{d}, \quad \boldsymbol{\sigma}_{\text{diss}}^{\nabla d} = \frac{2Gb}{c_\alpha} \nabla_{\mathbf{x}} d. \quad (3.27b)$$

Here, the reference stress is defined as $\boldsymbol{\sigma}_0 = \frac{\partial \phi_e}{\partial \boldsymbol{\epsilon}} = \lambda \text{tr}[\boldsymbol{\epsilon}] \mathbf{I} + 2\mu \boldsymbol{\epsilon}$. The thermodynamic requirements specified Eq. 4.31 are satisfied by ensuring that $\alpha'(d) \geq 0$ and $\dot{d} \geq 0$, which will be addressed in the next section through modeling and numerical treatment.

Combining Eqs. 3.27 and 3.17, the constitutive relations are expressed as,

$$\boldsymbol{\sigma} = \omega(d) \boldsymbol{\sigma}_0, \quad \sigma^d = \omega'(d) \phi_e + \frac{G}{bc_\alpha} \alpha'(d) + \eta^d \dot{d}, \quad \boldsymbol{\sigma}^{\nabla d} = \frac{2Gb}{c_\alpha} \nabla_{\mathbf{x}} d. \quad (3.28a)$$

At this stage, the only undetermined term in the balance equations (3.11a) and (3.11b) is the micro-damage mass density, ρ_d , which has not been experimentally measured in the literature. It was introduced intuitively by Kamensky *et al.* [72] and Hai *et al.* [73]. Here, to estimate this quantity, we assume that the damage speed c_d is related to the longitudinal wave speed of the material, c_u , which represents the fastest wave speed in the material. This relation is given by $c_d = \kappa c_u$, where κ as a ratio between the two velocities. For an isotropic material $c_u = \sqrt{(\lambda + 2\nu)/\rho_u}$. In the 1D setting, $c_u = \sqrt{E/\rho_u}$, where E is the Young's modulus. Eq. 3.11b, is an hyperbolic PDE with the wave speed c_d as $c_d = \kappa c_u = \sqrt{E_d/\rho_d}$; $E_d = 2Gb/c_\alpha$, obtained from

Eq. 3.28, plays the role of micro-stiffness of the phase field equation for wave speed calculation. Therefore, the micro-damage mass density is defined as,

$$\rho_d = \frac{E_d}{\kappa^2 c_u^2}. \quad (3.29)$$

3.3.4 Governing equations

Substituting Eq. 3.28 into Eqs. 3.11a and 3.11b, and scaling the evolution equation by $\tilde{s} := 2G/bc_\alpha$, with some simplifications, yields,

$$\rho_u \ddot{\mathbf{u}} = \nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma} \quad \text{in } \omega \times [0, T], \quad (3.30a)$$

$$\tau_d^2 \ddot{d} + d_f \tau_d \dot{d} - b^2 \nabla_{\mathbf{x}}^2 d = -\frac{\omega'(d)}{\tilde{s}} \phi_e - \frac{1}{2} \alpha'(d) \quad \text{in } \omega \times [0, T]. \quad (3.30b)$$

Here, a time scale $\tau_d^2 = \rho_d / \tilde{s} = b^2 / c_u^2$ is introduced in Eq. 3.30. The nondimensional damping factor d_f is defined from the relation $\eta^d / \tilde{s} = d_f \tau_d$. τ_d^2 and $d_f \tau_d$ represent micro-inertia and micro-viscosity terms for the phase field equation in its nondimensional form. The form of the viscous term in Eq. 3.30 differs from that in Kamensky *et al.* [72], which is based on a single-degree-of-freedom system analysis.

The elastic energy term ϕ_e in Eq. 3.30b serves as a driving force for crack evolution. To ensure cracks form only in tension and not in compression, ϕ_e is replaced by its positive part, defined using the Rankine criterion [28],

$$\phi_e^+ = \frac{\langle \sigma_1 \rangle_+^2}{2E}, \quad (3.31)$$

where σ_1 is the first principle component of the reference stress tensor $\boldsymbol{\sigma}_0 = \lambda \text{tr}[\boldsymbol{\epsilon}] \mathbf{I} + 2\mu \boldsymbol{\epsilon}$. As a result, Eq. 3.30 is modified to,

$$\rho_u \ddot{\mathbf{u}} = \nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma} \quad \text{in } \omega \times [0, T], \quad (3.32a)$$

$$\tau_d^2 \ddot{d} + d_f \tau_d \dot{d} - b^2 \nabla_{\mathbf{x}}^2 d = -\frac{\omega'(d)}{\tilde{s}} \phi_e^+ - \frac{1}{2} \alpha'(d) \quad \text{in } \omega \times [0, T]. \quad (3.32b)$$

Eqs. 3.32 are subject to the following *Boundary Conditions* (BCs),

$$\left\{ \begin{array}{ll} \mathbf{u}(\mathbf{x}, t) = \tilde{\mathbf{u}} & \text{on } \partial\omega_u \times [0, T] \\ \boldsymbol{\sigma} \cdot \mathbf{n} = \tilde{\mathbf{t}} & \text{on } \partial\omega_t \times [0, T] \\ \nabla_{\mathbf{x}} d \cdot \mathbf{n} = 0 & \text{on } \partial\omega \times [0, T]. \end{array} \right. \quad (3.33)$$

where $\partial\omega_u$ and $\partial\omega_t$ are the Dirichlet and Neumann boundaries for the elastodynamic problem, satisfying $\partial\omega_u \cup \partial\omega_t = \partial\omega$ and $\partial\omega_u \cap \partial\omega_t = \emptyset$. The initial conditions are defined as,

$$\left\{ \begin{array}{ll} \mathbf{u}(\mathbf{x}, 0) = \tilde{\mathbf{u}}_0(\mathbf{x}) \\ \dot{\mathbf{u}}(\mathbf{x}, 0) = \dot{\tilde{\mathbf{u}}}_0(\mathbf{x}) \\ d(\mathbf{x}, 0) = \tilde{d}_0(\mathbf{x}) \\ \dot{d}(\mathbf{x}, 0) = \dot{\tilde{d}}_0(\mathbf{x}). \end{array} \right. \quad (3.34)$$

for $\mathbf{x} \in \omega$. These equations collectively describe the deformation and crack evolution in solids.

3.3.5 Degradation functions

The degradation function $\omega(d)$, which reduces material strength during damage processes, must satisfy the following conditions,

$$\omega(0) = 1, \quad \omega(1) = 0, \text{ and } \omega'(d) \leq 0. \quad (3.35)$$

Several candidates have been proposed in literature. In this work, we adopt the PF-CZM model developed by Wu [28] whose degradation function has a rational form,

$$\omega(d) = \frac{(1-d)^2}{(1-d)^2 + Q(d)}, \quad (3.36)$$

where the polynomial function $Q(d) = a_1d(1 + a_2d(1 + a_3d))$, with a_1 , a_2 , and a_3 being constant coefficients defining the softening curve of the model as summarized in Table 3.1.

The introduction of the material strength $\tilde{\sigma}_c$ in Table. 3.1 represents a significant improvement over classical phase field models [24], [16]. For the importance of material strength in crack initiation, see [127].

3.3.6 Local crack geometric function

The crack geometric function $\alpha(d)$, associated with the critical energy release rate G , contributes locally to the energy needed to create new crack surfaces. It must satisfy the following conditions,

$$\alpha(0) = 0, \quad \alpha(d \geq 0) > 0, \quad \text{and} \quad \alpha'(d) > 0. \quad (3.37)$$

Eq. 3.37³ ensures that $\alpha(d)$ is a monotonically increasing function during dissipative processes, fulfilling the thermodynamic requirement in Eq. 4.31². In Wu's model [28], $\alpha(d)$ is defined as,

$$\alpha(d) = 2d - d^2. \quad (3.38)$$

Based on the definition of $\alpha(d)$, the coefficient c_α in Eq. 3.24 can be determined as,

$$c_\alpha = 4 \int_0^1 \sqrt{\alpha(\beta)} \, d\beta = \pi. \quad (3.39)$$

3.3.7 Irreversibility constraint

The irreversibility condition in Eq.4.31² enforces the non-reversibility of damage. Given the functional form of $\alpha(d)$ in Eq. 3.38, the RHS of Eq. 3.30b is initially negative. To address this issue and ensure damage irreversibility, we use a history variable that records the maximum value of the positive part of the elastic energy ϕ_e^+ ,

as introduced by Miehe *et al.* [16]. Additionally, we introduce a fracture initiation energy ϕ_{0e} to prevent negative damage. Assuming no damage occurs until the reference elastic energy ϕ_e^+ exceeds ϕ_{0e} , we have,

$$\phi_{0e} = \lim_{d \rightarrow 0^+} -\frac{\tilde{s}\alpha'(d)}{\omega'(d)} = \chi \frac{\tilde{\sigma}_c^2}{2E}. \quad (3.40)$$

In Eq. 3.40, the scaling factor $\chi \geq 1$ is introduced to control crack initiation under high loading rates. The effect of this parameter is further investigated in Section 3.5. The history variable then becomes a comparison between the accumulated elastic energy ϕ_e^+ during loading and the initial energy ϕ_{0e} , such that, *

$$\mathcal{H} = \max_{s \in [0, t]} \{\phi_e^+(\boldsymbol{\epsilon}(\mathbf{u}), s), \phi_{0e}\}. \quad (3.41)$$

Interestingly, the energy threshold in Eq. 3.40 is independent of the choice of length scale and can be considered a material property.

3.4 Numerical schemes and discretization

3.4.1 Weak form

The trial solution spaces for displacement and phase field are defined as follows,

$$\mathcal{V}_u = \{\mathbf{u}(\mathbf{x}, t) \in H^1(\omega) \mid \mathbf{u} = \tilde{\mathbf{u}} \text{ on } \partial\omega_u\}, \quad (3.42a)$$

$$\mathcal{V}_d = \{d(\mathbf{x}, t) \in H^1(\omega)\}. \quad (3.42b)$$

*To enhance convergence in the discrete setting for solving the system of coupled equations at time step $n + 1$, we take the the maximum of $\phi_e^+(\boldsymbol{\epsilon}(\mathbf{u}))$ across time step from 0 to n , excluding the iterative updates within the nonlinear solver. This contrasts with the approach presented by Wu *et al.* [30], where the maximum of $\phi_e^+(\boldsymbol{\epsilon}(\mathbf{u}))$ is tracked at every iterative step in implicit solvers. Our numerical experiments indicate that the latter approach significantly impairs the convergence behavior of implicit schemes.

The corresponding weighted spaces are given by,

$$\mathcal{W}_u = \{\hat{\mathbf{u}}(\mathbf{x}, t) \in H^1(\omega) \mid \hat{\mathbf{u}} = \mathbf{0} \text{ on } \partial\omega_u\}, \quad (3.43a)$$

$$\mathcal{W}_d = \{\hat{d}(\mathbf{x}, t) \in H^1(\omega)\}. \quad (3.43b)$$

In Eq. 3.43, the weight functions can be chosen as the velocities of the displacement and phase field variables. This choice enables the recovery of the energy balance law described in Eq. 3.10 for the domain ω .

The *Weighted Residual Statement* (WRS) of the coupled equations is derived by multiplying Eqs. 3.32a and 3.32b with the weight functions $\hat{\mathbf{u}} \in \mathcal{W}_u$ and $\hat{d} \in \mathcal{W}_d$ and integrating over the domain ω . The *weak statement* is then obtained by forming complete spatial divergence terms, applying the divergence theorem, and simplifying the resulting equation by employing the BCs from Eq. 4.34: Given the BCs and ICs, Eqs. 4.34 and 4.35, find $\mathbf{u} \in \mathcal{V}_u$ and $d \in \mathcal{V}_d$ such that for all $\hat{\mathbf{u}} \in \mathcal{W}_u$, and $\hat{d} \in \mathcal{W}_d$, the following holds,

$$(\hat{\mathbf{u}}, \rho_u \ddot{\mathbf{u}})_\omega + (\nabla_{\mathbf{x}} \hat{\mathbf{u}}, \boldsymbol{\sigma})_\omega = (\hat{\mathbf{u}}, \tilde{\mathbf{t}})_{\partial\omega_t}, \quad (3.44a)$$

$$\left(\hat{d}, \tau_d^2 \ddot{d}\right)_\omega + \left(\hat{d}, d_f \tau_d \dot{d}\right)_\omega + \left(\nabla_{\mathbf{x}} \hat{d}, b^2 \nabla_{\mathbf{x}} d\right)_\omega = - \left(\hat{d}, \frac{\omega'(d) \mathcal{H}}{\tilde{s}}\right)_\omega - \left(\hat{d}, \frac{1}{2} \alpha'(d)\right)_\omega, \quad (3.44b)$$

where $(f, g)_\mathcal{S}$ refers to the integral of fg over the domain $\mathcal{S}$. In Eq. 3.44 f refers to a weight function and g refers to a solution of boundary condition field.

3.4.2 Discretization

We first discretize Eq. 3.44 in space. Let $\omega^h = \mathcal{T}(\omega)$ be a partition of the domain into n_e open subdomains $\{e_\alpha\}$ with regular boundaries. The set $\{e_\alpha\}$ corresponds to finite elements for the solution of solid and phase field problems. The discrete

solution spaces are defined as,

$$\mathcal{V}_u^h = \{\mathbf{u}(\mathbf{x}, t) \in H^1(\omega^h) \mid \mathbf{u} = \tilde{\mathbf{u}} \text{ on } \partial\omega_u^h\}, \quad (3.45a)$$

$$\mathcal{V}_d^h = \{d(\mathbf{x}, t) \in H^1(\omega^h)\}, \quad (3.45b)$$

where the superscript h denotes sets and fields in the discrete solution space. Similarly, the discrete weight spaces are defined as,

$$\mathcal{W}_u^h = \{\hat{\mathbf{u}}(\mathbf{x}, t) \in H^1(\omega^h) \mid \hat{\mathbf{u}} = \mathbf{0} \text{ on } \partial\omega_u^h\}, \quad (3.46a)$$

$$\mathcal{W}_d^h = \{\hat{d}(\mathbf{x}, t) \in H^1(\omega^h)\}. \quad (3.46b)$$

The displacement and phase field are interpolated using standard linear finite element shape functions, with nodal unknowns treated as functions of time. Thus, the expressions of displacement and phase field and their corresponding velocity and acceleration quantities are,

$$u_i = N_I(\mathbf{x})c_{Ii}^u(t), \quad \dot{u}_i = N_I(\mathbf{x})\dot{c}_{Ii}^u(t), \quad \ddot{u}_i = N_I(\mathbf{x})\ddot{c}_{Ii}^u(t), \quad (3.47a)$$

$$d = N_I(\mathbf{x})c_I^d(t), \quad \dot{d} = N_I(\mathbf{x})\dot{c}_I^d(t), \quad \ddot{d} = N_I(\mathbf{x})\ddot{c}_I^d(t), \quad (3.47b)$$

where $c_{Ii}^u(t)$ and $c_I^d(t)$ represent the nodal solution variables for displacement and phase field variables, respectively. I is the nodal index, while $i \in \{1, \dots, d\}$ indicates the spatial component.

Substituting Eq. 3.47 into Eq. 3.44 yields the semi-discrete system of *Ordinary Differential Equations* (ODEs),

$$\mathbf{M}^{(\cdot)}\ddot{\mathbf{c}} + \mathbf{D}^{(\cdot)}\dot{\mathbf{c}} = \mathbf{F}^{(\cdot)}, \quad (3.48a)$$

$$\mathbf{F}^{(\cdot)} := \mathbf{F}^{(\cdot),\text{ext}} - \mathbf{F}^{(\cdot),\text{int}}. \quad (3.48b)$$

In this formulation, $\mathbf{M}^{(\cdot)}$, $\mathbf{D}^{(\cdot)}$, $\mathbf{F}^{(\cdot),\text{int}}$, and $\mathbf{F}^{(\cdot),\text{ext}}$ represent the mass, damping, internal force vector, and the external force vector, respectively, applicable to both the solid and phase field parts. For the solid problem, these are,

$$M_{ab}^u = (N_I, \delta_{ij} \rho_u N_J)_\omega, \quad (3.49a)$$

$$D_{ab}^u = 0, \quad (3.49b)$$

$$F_a^{u,\text{int}} = (B_{I(ijk)}, \sigma_{jk})_\omega, \quad (3.49c)$$

$$F_a^{u,\text{ext}} = (N_I, \tilde{t}_i)_{\partial\omega_t}, \quad (3.49d)$$

where $a = Id + i$ and $b = Jd + i$ denote the degrees of freedom indices. The linear operator $B_{I(ijk)}$ is defined as $B_{I(ijk)} = 1/2 (\delta_{ik} \partial N_I / \partial x_j + \delta_{ij} \partial N_I / \partial x_k)$. For the phase field part, the corresponding components are,

$$M_{IJ}^d = (N_I, \tau_d^2 N_J)_\omega, \quad (3.50a)$$

$$D_{IJ}^d = (N_I, d_f \tau_d N_J)_\omega, \quad (3.50b)$$

$$F_I^{d,\text{int}} = (N_{I,i}, b^2 d_{,i})_\omega, \quad (3.50c)$$

$$F_I^{d,\text{ext}} = - \left(N_I, \frac{\omega'(d) \mathcal{H}}{\tilde{s}} \right)_\omega - \left(N_I, \frac{1}{2} \alpha'(d) \right)_\omega. \quad (3.50d)$$

The fully discrete form of the coupled equations is derived by applying time discretization to Eq. 3.48. To ensure second-order accuracy in time, the Newmark update formulation is employed to solve Eq. 3.48. In this method, the discrete values of a field, $\mathbf{c}^n$, along with its first and second time derivatives, $\dot{\mathbf{c}}^n$ and $\ddot{\mathbf{c}}^n$, are updated from time step n to $n + 1$,

$$\mathbf{c}^{n+1} = \mathbf{c}^n + \Delta t \dot{\mathbf{c}}^n + \frac{(\Delta t)^2}{2} ((1 - 2\beta) \ddot{\mathbf{c}}^n + 2\beta \ddot{\mathbf{c}}^{n+1}), \quad (3.51a)$$

$$\dot{\mathbf{c}}^{n+1} = \dot{\mathbf{c}}^n + \Delta t ((1 - \gamma) \ddot{\mathbf{c}}^n + \gamma \ddot{\mathbf{c}}^{n+1}), \quad (3.51b)$$

$$\ddot{\mathbf{c}}^{n+1} = \frac{1}{\beta(\Delta t)^2} (\mathbf{c}^{n+1} - \mathbf{c}^n) - \frac{1}{\beta \Delta t} \dot{\mathbf{c}}^n - \left(\frac{1}{2\beta} - 1 \right) \ddot{\mathbf{c}}^n. \quad (3.51c)$$

The parameters γ and β in Eqs. 3.51 define the characteristics of the scheme [107]. For achieving second-order accuracy, $\gamma = 1/2$ is selected. Setting $\beta = 0$ results in an explicit scheme, while $\beta = 1$ produces an implicit scheme.

3.4.2.1 Explicit scheme

A monolithic explicit scheme is proposed to solve for the acceleration of both the solid and phase field components. Unlike the approaches of Borden *et al.* [17], and Kamensky *et al.* [72], where the phase field equation is solved implicitly, and the elastodynamic is solved either implicitly or explicitly without mass lumping, our method achieves the solution in a single step without requiring a matrix solve. To achieve this, we restate Eq. 3.48 as,

$$\mathbf{M}\ddot{\mathbf{c}}^{n+1} + \mathbf{D}\dot{\mathbf{c}}^{n+1} = \mathbf{F}^n. \quad (3.52)$$

By substituting Eq. 3.51b into Eq. 3.52, we obtain,

$$(\mathbf{M} + \frac{1}{2}\Delta t \mathbf{D})\ddot{\mathbf{c}}^{n+1} = \mathbf{F}^n - (\dot{\mathbf{c}}^n + \frac{1}{2}\Delta t \ddot{\mathbf{c}}^n)\mathbf{D}. \quad (3.53)$$

While Eq. 3.53 facilitates the explicit computation of the coupled solution $\ddot{\mathbf{c}}^{n+1}$, it still requires a linear solver. To eliminate the need for a matrix solve, we employ the mass-lumping technique [107] on both the mass and damping matrices, storing non-zero entries on their diagonal components only. In a representative example in 3.5.1, we will illustrate that using lumped matrices can lead to superlinear parallel speedup in solving the linear system.

After determining the acceleration of the primary fields in 3.53, the velocity is updated using 3.51b. Solutions at the current step $n + 1$ are then assigned to the previous step n . In the subsequent time step, Eq. 3.51a is used to update $\mathbf{c}^{n+1}$ before solving 3.53 again.

3.4.2.2 Implicit scheme

To analyze the performance of the explicit scheme, a monolithic implicit scheme is introduced for both the hyperbolic and elliptic phase field models. This scheme simultaneously solves for displacement and phase field using a unified approach. This is in contrast to previous hyperbolic models [72, 73] which solve the acceleration of the primary fields (displacement and phase field) in an alternating manner [73].

Eq. 3.48 is reformulated as,

$$\mathbf{M}\ddot{\mathbf{c}}^{n+1} + \mathbf{D}\dot{\mathbf{c}}^{n+1} = \mathbf{F}^{\text{ext},n+1} - \mathbf{F}^{\text{int},n+1}. \quad (3.54)$$

This equation can be iteratively solved using the standard Newton-Raphson method,

$$\Delta \mathbf{c} = -(\mathbf{M}^*)^{-1} \mathbf{R}^{n+1}, \quad (3.55)$$

where the residual vector is defined as $\mathbf{R}^{n+1} = \mathbf{F}^{\text{ext},n+1} - \mathbf{F}^{\text{int},n+1} - \mathbf{M}\ddot{\mathbf{c}}^{n+1} - \mathbf{D}\dot{\mathbf{c}}^{n+1}$.

The matrix $\mathbf{M}^*$ is constructed by incorporating Eqs. 3.51b and 3.51c,

$$\mathbf{M}^* = \frac{1}{\beta(\Delta t)^2} \mathbf{M} + \frac{1}{\beta \Delta t} \mathbf{D} + \mathbf{K}, \quad (3.56)$$

where $\mathbf{K} = -\partial \mathbf{F} / \partial \mathbf{c}$ is the stiffness matrix. In the case of elliptic phase field models, the phase field component does not contribute to the mass and damping matrices in Eq. 3.56.

Once the solution increment $\Delta \mathbf{c}$ is obtained from Eq. 3.55, the solution at the current time $n + 1$ is updated by $\mathbf{c}^{n+1} = \mathbf{c}^n + \Delta \mathbf{c}$. Subsequently, the velocities and accelerations of the primary fields are updated using Eqs. 3.51b and 3.51c, respectively, completing the time step update for the implicit scheme.

3.4.3 Adaptive mesh refinement scheme

To accurately resolve crack paths, fine meshes are required in regions where cracks are likely to form. A common approach is to apply a priori mesh refinement in critical areas, which requires prior knowledge of crack paths. This strategy is impractical for realistic problems, where crack paths are typically unknown. Moreover, a priori refinement often results in redundant fine elements around the actual cracks, unnecessarily increasing the computational cost. Previous studies, such as those by [17] [110], have successfully applied mesh adaptive schemes for the AT2 phase field model. These schemes determine a total refinement level, tr , in advance to ensure that the smallest element size satisfies $h_{min} \leq \frac{b}{2}$. However, this condition holds only after the refinement process begins, as elements are flagged for refinement when the phase field nodal values within an element exceed a specified threshold.

Our numerical experience indicates that this approach can lead to convergence issues for the PF-CZM model when cracks start to propagate, or it may prevent crack initiation during loading. To address these limitations, we apply localized pre-refinement around critical areas, such as initial crack tips and domain corners, to a specified level, $gr + pr$. This strategy improves the accuracy of initial stress distribution, which is often highly concentrated in these regions, thereby ensuring precise spatial and temporal crack initiation. Additionally, the resulting mesh size from this local refinement is kept no larger than the phase field length scale b , maintaining a consistent length scale throughout the computation. In contrast, Heister *et al.* [110] adjusted the length scale b based on changing mesh sizes. Our modified adaptive scheme for the PF-CZM model is detailed in Algorithm 1.

3.5 Numerical results

In this section, we evaluate the efficiency and robustness of the proposed explicit time integration scheme for the HPF model, comparing it against its implicit counterpart

Algorithm 1 Adaptive mesh refinement scheme

(0.0) Determine local refinement level lr , global refinement level gr , and locally pre-refined level pr satisfying,

$$h_{\min} = \frac{h_{\max}}{2^{gr+pr+lr}} \leq \frac{b}{2}$$

(0.1) Locally refine the mesh in critical regions for $gr + pr$ level with,

$$\frac{h_{\max}}{2^{gr+pr}} \leq b$$

(1) Solve the coupled problem at time step t_{n+1} .

(2) Flag element e for refinement that has a maximum damage value $d_I^{(e),n+1} \geq 0.25$.

(3) Refine the flagged elements.

(4) Transfer solutions and history field at time t_n from the old mesh to the new mesh.

(5) Rerun the simulation with the new mesh.

(6) Repeat steps (2)-(5) until the mesh does not change for the solution of time t_{n+1} , then go to the next time step.

for both HPF and EPF models, with and without adaptive mesh refinement. We demonstrate superlinear speedup in the linear solve and sublinear speedup for the overall algorithm, achieved through a parallelized explicit scheme. One benchmark problem in dynamic fracture is considered in the first part. Subsequently, we utilize the explicit solver to examine the effects of the micro-inertia term on crack velocities and crack patterns in a PMMA experiment. We provide both quantitative and qualitative comparisons between the results of the EPF and HPF models under high-rate loading conditions. In all subsequent examples, the default speed ratio, $\kappa = 1$, is applied, except in the high-rate loading case of the PMMA experiment, where it is adjusted to match experimental observations.

The code implemented in this work is built on the deal.II framework [105] and is fully parallelized using the Message Passing Interface (MPI). Adaptive mesh refinement, as described in Section 3.4.3, is managed by p4est [128], while linear algebra computations are performed using Trilinos [129]. The simulations conducted in this study were executed on the ISAAC-ORI HPC cluster at the University of Tennessee, Knoxville. The cluster utilizes Intel Xeon Gold 6148 Processors with 27.5MB cache, a base clock speed of 2.40 GHz, and support for 40 threads per processor.

3.5.1 Dynamic shear loading

We begin with a dynamic shear loading example based on Kalthoff’s experiment [130], where a projectile impacts a prenotched plate at low and high impact velocities ($\bar{v} = 33 \text{ m/s}$ and $\bar{v} = 70 \text{ m/s}$ respectively). As the high velocity case leads to the existence of plastic zones around the notch tip, it is out of the scope of this work that only concentrates on brittle fracture. Following the work by Borden *et al.* [17], we model only half of the target plate to reduce computational cost, with an external velocity applied to the lower part of the left edge to simulate impact, as shown in Fig. 3.2a. Material properties are set as $\rho_u = 8000 \text{ kg/m}^3$, $E = 190 \text{ GPa}$, $\nu = 0.3$, $G = 2.213 \cdot 10^4 \text{ N/m}$, and $\tilde{\sigma}_c = 2.812 \text{ GPa}$, with a fracture length scale of $b = 0.25 \cdot 10^{-3} \text{ m}$.

A mesh convergence study is conducted using five different configurations (Table. 3.2). For adaptive meshes ($lr \geq 1$), a priori mesh refinement is applied around the initial crack tip, while meshes 4 and 5 were uniformly refined across the entire plate. Simulations for meshes 4 and 5 were executed using 32 cores to ensure reasonable computation times, while the remaining configurations were run on a single core. The time step was calculated based on the mesh size, $\Delta t = \text{CFL} \frac{h}{c_u}$. As shown in 3.1, crack evolution for mesh 2 begins at the notch tip and propagates at a 70° towards the top right corner, consistent with results from [130] [17] [131]. The crack patterns for the other configurations are similar and therefore not repeated here.

Fig. 3.3b and Fig. 3.3a display the plots of elastic energy and crack velocity over time, respectively. The coarser meshes (meshes 1 and 4) dissipate more energy than the finer meshes and tend to underestimate crack velocity. In contrast, the results for meshes 2, 3, and 5 are nearly identical, indicating convergence.

Next, we compare the performance of the implicit schemes for the EPF and HPF models with the explicit scheme for the HPF model, using mesh 2 from Table 3.2. For the explicit scheme, a CFL number of 0.5 is used. In comparison, the CFL number for the implicit scheme is varied among $\{0.5, 1, 2\}$. Table. 3.3 presents the CPU time for each time integration scheme. The explicit scheme is approximately 5 times

faster than the implicit scheme at a CFL number of 0.5. When the CFL number is increased to 2, for the implicit scheme, the CPU time is reduced by a factor of 2 to 3 but remains about 1.4 times slower than the explicit scheme. Additionally, using a larger time step tends to delay crack propagation, as illustrated in Figure 3.4.

To further evaluate the efficiency of the explicit scheme, we conducted a strong scaling analysis to measure its parallel performance. Figure 3.6 presents the scaling results in a log – logplot, illustrating three key components of the explicit solver: the solution phase, system assembly, and the overall time-stepping loop of the algorithm. Notably, the solution phase, which benefits from the mass-lumping technique for directly solving the linear system of equations, demonstrates superlinear scaling. In contrast, the system assembly exhibits sublinear scaling, although its performance closely approaches the ideal scaling curve (black line). As a result, the overall algorithm achieves sublinear scaling.

3.5.2 Dynamic PMMA plate

This example aims to demonstrate the quantitative and qualitative differences between the HPF and EPF models in simulating dynamic fracture. A PMMA plate of $32 \times 16 \text{ mm}^2$ with a preexisting crack of 4 mm is considered, based on an experiment conducted by Zhou *et al.* [23]. The plate is first loaded statically in tension until the prescribed displacement, $\Delta\tilde{u}$, is reached and then held constant. This initial step allows stress to become highly localized around the preexisting crack tip. Subsequently, a razor is used to quickly cut the plate, initiating rapid crack propagation. The geometry and boundary conditions are illustrated in Figure 3.7a.

The material parameters used in this study are: $E = 3090 \text{ MPa}$, $\nu = 0.35$, $\rho_u = 1180 \text{ kg/m}^3$, $G = 580 \text{ N/m}$, and $\tilde{\sigma}_c = 72 \text{ MPa}$. The phase field length scale is set to $b = 0.1 \text{ mm}$. In this work, we consider only the prescribed displacements $\Delta\tilde{u} = \{0.1, 0.14\} \text{ mm}$, corresponding to the steady crack speeds observed in Zhou’s experiment: $\{578, 660\} \text{ m/s}$.

3.5.2.1 Load case $\Delta\tilde{u} = 0.1$

Figures 3.8a and 3.8b show the final crack patterns for the EPF and HPF models, respectively. Both models exhibit similar crack trajectories with two main sub-branches; however, the HPF model displays more micro-branches along each sub-branch. This difference can be attributed to the higher average crack velocity of 683m/s in the HPF model compared to 653m/s in the EPF model, as illustrated in Figure 3.8c. Notably, both models significantly overestimate the experimental crack velocity of 578m/s.

The crack velocity in the HPF model can be adjusted by modifying the speed ratio, κ . Figure 3.9a demonstrates a straight crack path at $\kappa = 0.2$, contrasting with the two main sub-branches observed at $\kappa = 1$ with two main sub-branches in Figure 3.8b. As κ is reduced, the two sub-cracks seen in Figure 3.8b merge into a single main crack shown in Figure 3.9a with a thicker damage zone that encompasses micro-cracks. The predicted crack velocity at $\kappa = 0.2$ is 608m/s, which is 5.2% of the experimental result of 578m/s.

To accurately capture micro-cracks observed in experiments, a reduced length scale of $b = 0.025$ was used in Figure 3.9b. This adjustment narrows the damage zone, revealing multiple micro-cracks emanating from the main crack, which aligns well with experimental observations. The crack velocity at $b = 0.025$ is 592m/s, slightly lower than at $b = 0.1$. This is the first numerical prediction to capture micro-cracks both qualitatively and quantitatively for this loading case.

In comparison with prior literature, the sub-cracks predicted by Zhou *et al.* [23] in Figure 3.10a are longer than those observed experimentally in Figure 3.10d by Zhou *et al.* [23]. Meanwhile, the micro-cracks predicted in Figures 3.10b and 3.10c are merged into the main damage zone and are not clearly visible.

3.5.2.2 Load case $\Delta\tilde{u} = 0.14$

Figures 3.11a and 3.11d illustrate the crack patterns obtained using the EPF and HPF models, respectively. Both models produce nearly identical crack patterns, with crack velocities around 700m/s, closely matching the experimental velocity of 660m/s reported by Zhou *et al.* [23]. However, non-physical mushy zones are observed ahead of the main crack branching location and around sub-cracks, consistent with previous findings by Wolff *et al.* [22] and Wang *et al.* [132].

To address these undesired zones, we introduce a correction factor, χ , which adjusts the initial damage threshold defined in Eq. 3.40. Increasing χ will remove the mushy zones as shown in Figures 3.11c and 3.11d, where $\chi = 2$ is used for both the EPF and HPF models. Notably, with $\chi = 3$, shown in Figures 3.11e and 3.11f, the models produce asymmetric crack patterns similar to the experimental results in Figure 3.13e. Despite this improvement, the resulting crack velocities from both models still slightly exceed the experimental value, as depicted in Figures 3.11g and 3.11h.

As in the load case with $\tilde{u} = 0.1$, reducing the speed ratio κ in the HPF model decreases crack velocities, as shown in Figures 3.12a and 3.12b, with values of 644m/s and 687m/s, respectively. These velocities are slightly below and above the experimental result of 660m/s. In terms of crack patterns, good agreement with experimental observations is achieved at $\kappa = 0.4$ as shown in Figure 3.12b. In contrast, for $\kappa = 0.2$, a straight crack trajectory with short surrounding cracks is observed, as depicted in Figure 3.12a.

Compared to previous results in the literature, the crack pattern shown in Figure 3.12b provides the best qualitative and quantitative fit with the experimental data. Although Zhou *et al.* [23] predicted asymmetric crack patterns (Figure 3.13a), they did not capture the short cracks around the lower crack branch observed in the experiment. Similarly, the patterns predicted by Wang *et al.* [132] (Figure 3.13b),

and by Wolf *et al.* [22] (Figures 3.13c and 3.13d) show significant discrepancies from the experimental observations.

3.6 Conclusions

In this study, we demonstrate the numerical efficiency and modeling capabilities of the hyperbolic phase field cohesive zone model for fast crack propagation. We begin by deriving a general framework for the hyperbolic phase field model, enabling systematic and modular identification of micro-mass density and micro-viscosity, which were introduced intuitively in previous research.

Leveraging the advantages of hyperbolic partial differential equations (PDEs), we propose a fully explicit time integration scheme to solve the coupled equations without requiring iterative steps. Our results show that the explicit scheme is more efficient in terms of computational resources and CPU time than the implicit approach, which incorporates a coupled solution for both hyperbolic and elliptic models within the same implementation. Although the implicit scheme permits a larger time step, we found that excessive time stepping can delay crack propagation and overestimate crack velocities and elastic energy. Furthermore, using the explicit scheme, we implemented a parallel solver that achieved sublinear strong scaling for the entire algorithm and superlinear scaling for the solution phase, thanks to the mass-lumping technique. This approach stores all non-zero components on the diagonal of the resulting mass matrices, enabling direct solutions through the inverse of the diagonal components and eliminating the need for a linear solver. Computational cost is further reduced by employing an adaptive mesh refinement strategy based on phase field values as indicators.

From a modeling perspective, the hyperbolic phase field model allows for the adjustment of crack velocities through the speed ratio between elastic and damage wave speeds. To accurately replicate crack velocities and patterns observed in PMMA experiments, it is essential to introduce uncertainty in material properties and a

correction factor for crack initiation. This factor is crucial for eliminating non-physical damage zones that can arise under high-rate loading. The results obtained align closely with experimental observations, surpassing previous outcomes reported in the literature.

For future work, we plan to explore the correction factor based on strain-rate-dependent variables, such as strain rate and damage, to avoid extensive parametric studies currently required to determine the optimal correction factor for crack initiation.

Appendix

Tables

Table 3.1: Constant parameters for the polynomial function $Q(d)$.

PF model	Softening curve	p	a_1	a_2	a_3
PF-CZM [28]	Linear	2		-0.5	0
	Exponential	$\frac{5}{2}$	$\frac{4EG}{c_\alpha \bar{\sigma}_c^2 b}$	$2^{5/3} - 3$	0
	Cornelissen	2		1.3868	0.6567

Table 3.2: Dynamic shear loading example. Mesh configurations for a convergence study.

	$gl + pr + lr$	Number of elements	
		Initial mesh	Final mesh
Mesh 1	$0 + 4 + 1$	2653	13500
Mesh 2	$1 + 4 + 1$	9307	34100
Mesh 3	$1 + 4 + 2$	9307	71500
Mesh 4	$4 + 0 + 0$	102400	102400
Mesh 5	$5 + 0 + 0$	409600	409600

Table 3.3: Dynamic shear loading example. Measure of CPU time in second.

	Implicit						Explicit
CFL	0.5		1.0		2.0		0.5
Model	HPF	EPF	HPF	EPF	HPF	EPF	HPF
CPU time	105740.0	95903.2	78018.4	54874.6	39475.0	31873.7	24857.3

Figures

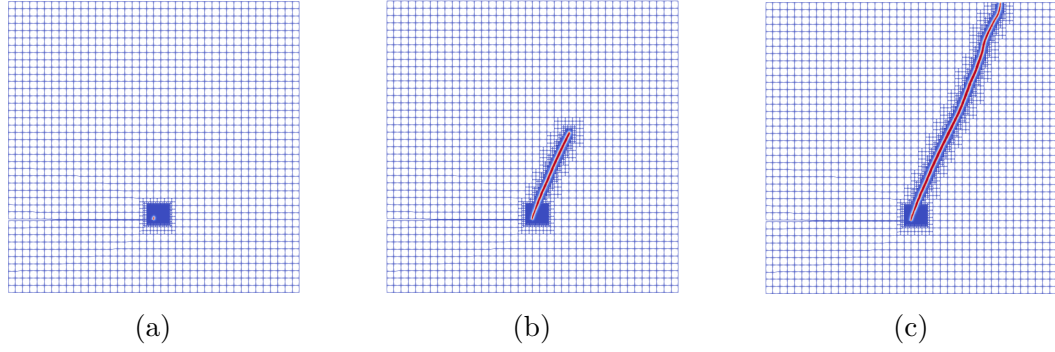


Figure 3.1: Dynamic shear loading example. Crack path at different instants

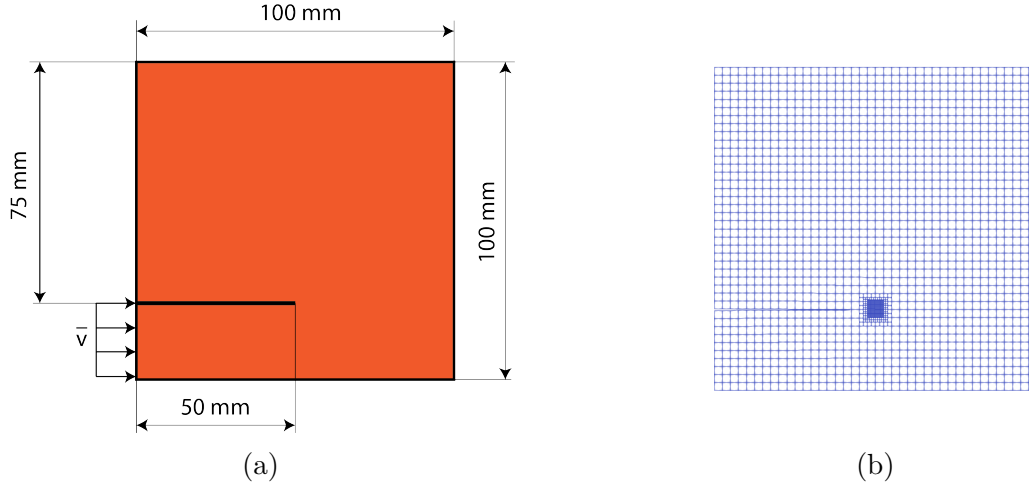


Figure 3.2: Dynamic shear loading example. a) Problem setup and boundary condition b) An original mesh with a priori refinement at the tip.

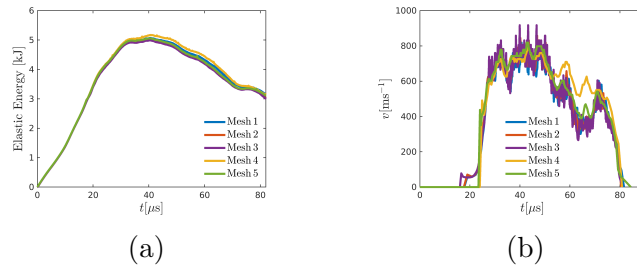


Figure 3.3: Dynamic shear loading. a) Elastic energy b) crack velocity

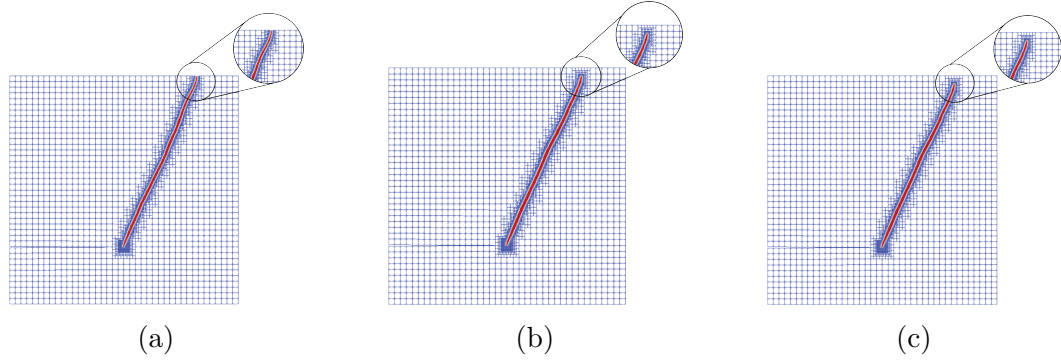


Figure 3.4: Dynamic shear loading example. Crack patterns at $T = 7.8e - 2(ms)$ using HPF with a) $CFL = 0.5$, b) $CFL = 1$, and c) $CFL = 2$.

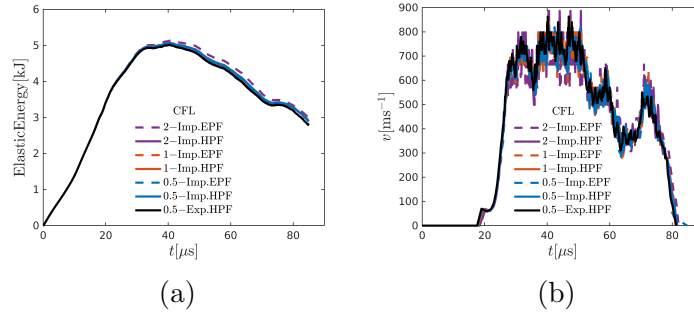


Figure 3.5: Dynamic shear loading example. Quantitative comparisons for hyperbolic and elliptic models using implicit and explicit schemes for a) elastic energy b) crack speed.

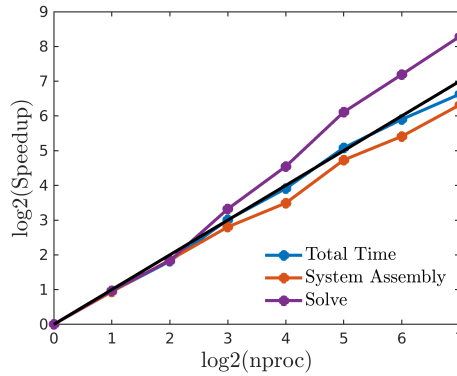


Figure 3.6: Dynamic shear loading example. Strong scaling analysis.

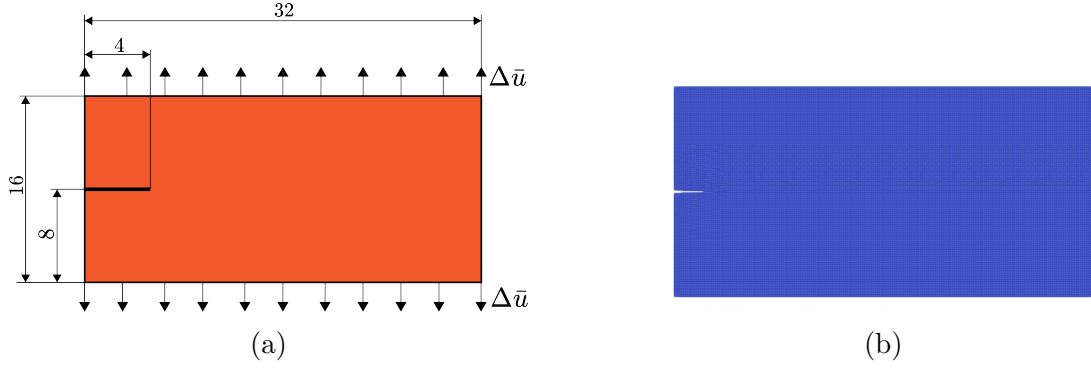


Figure 3.7: Dynamic PMMA plate example. a) Problem setup and boundary condition b) a discretized mesh with 128000 elements.

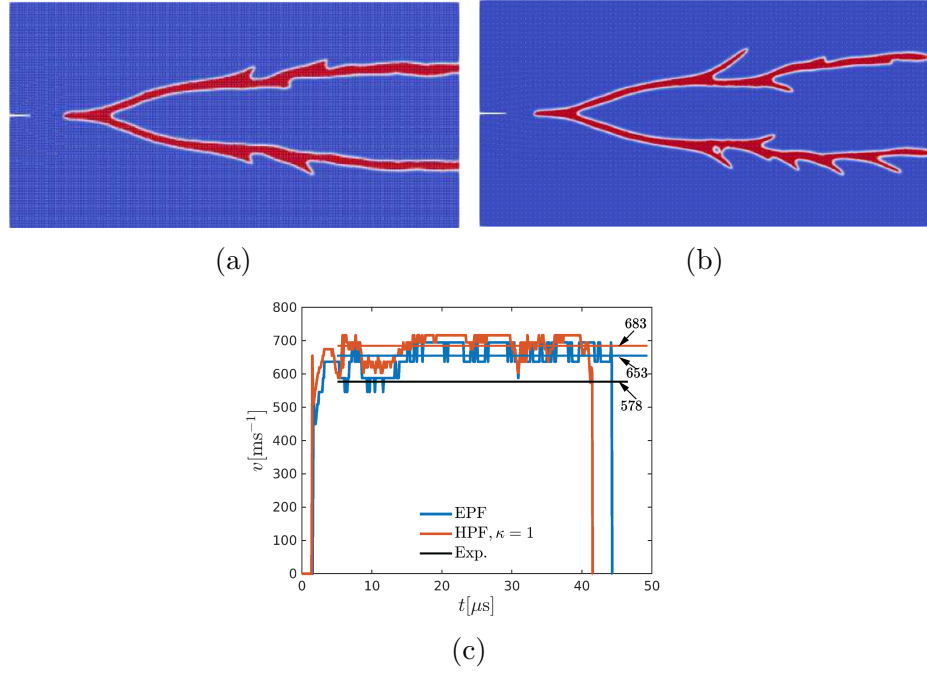


Figure 3.8: Dynamic PMMA plate example. Final crack patterns with $b = 0.1$ for a) EPF, b) HPF, and c) crack velocity

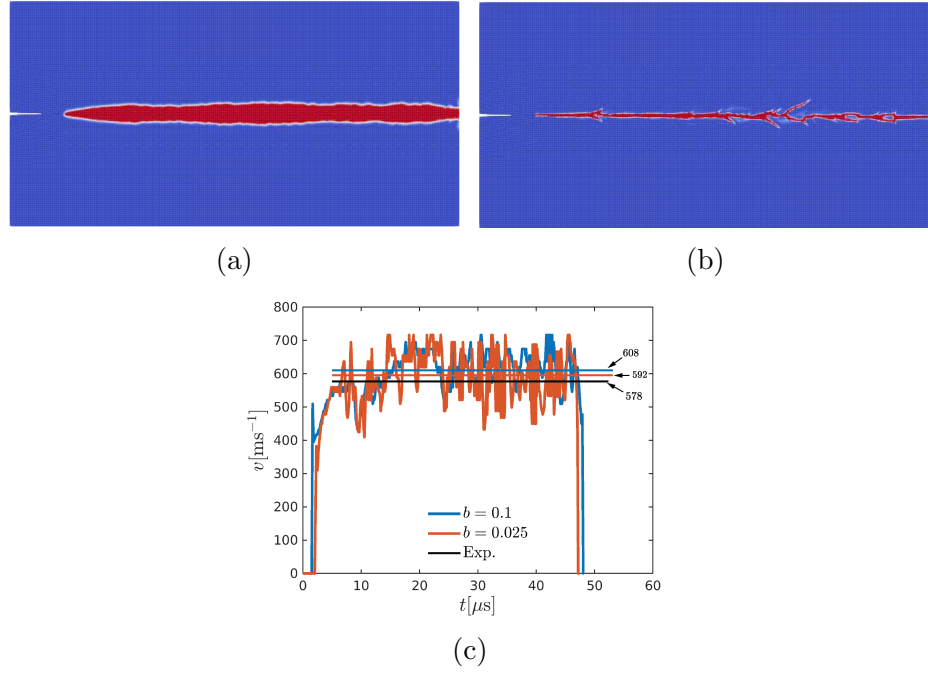


Figure 3.9: Dynamic PMMA plate example. Final crack patterns using the HPF model and the speed ratio $\kappa = 0.2$ with a) $b = 0.1$, b) $b = 0.025$ and c) crack velocity

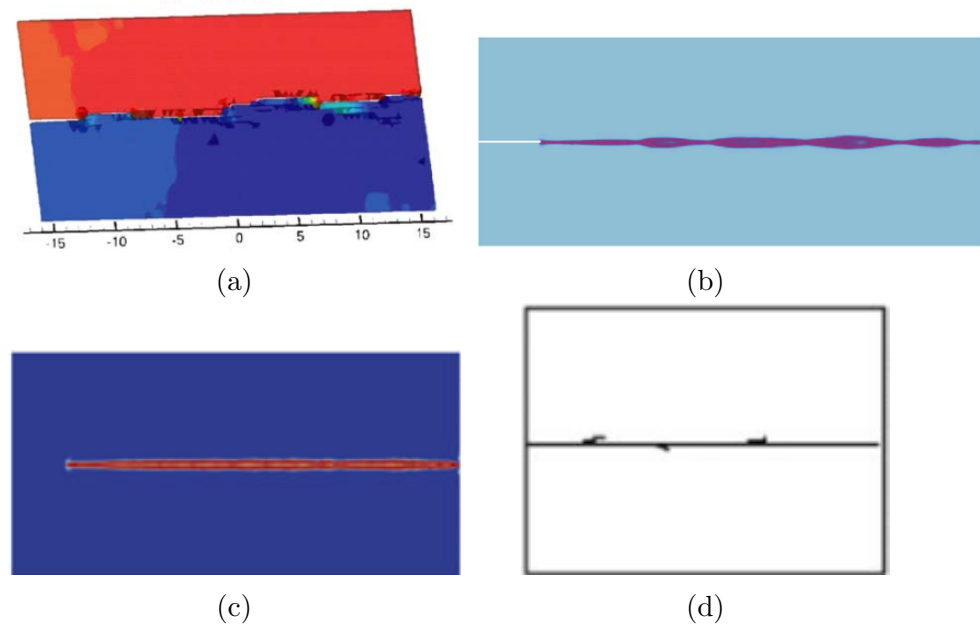


Figure 3.10: Dynamic PMMA plate example. Numerical results by a) [23] b) [132] c) [22] and experimental observation by d) [23]

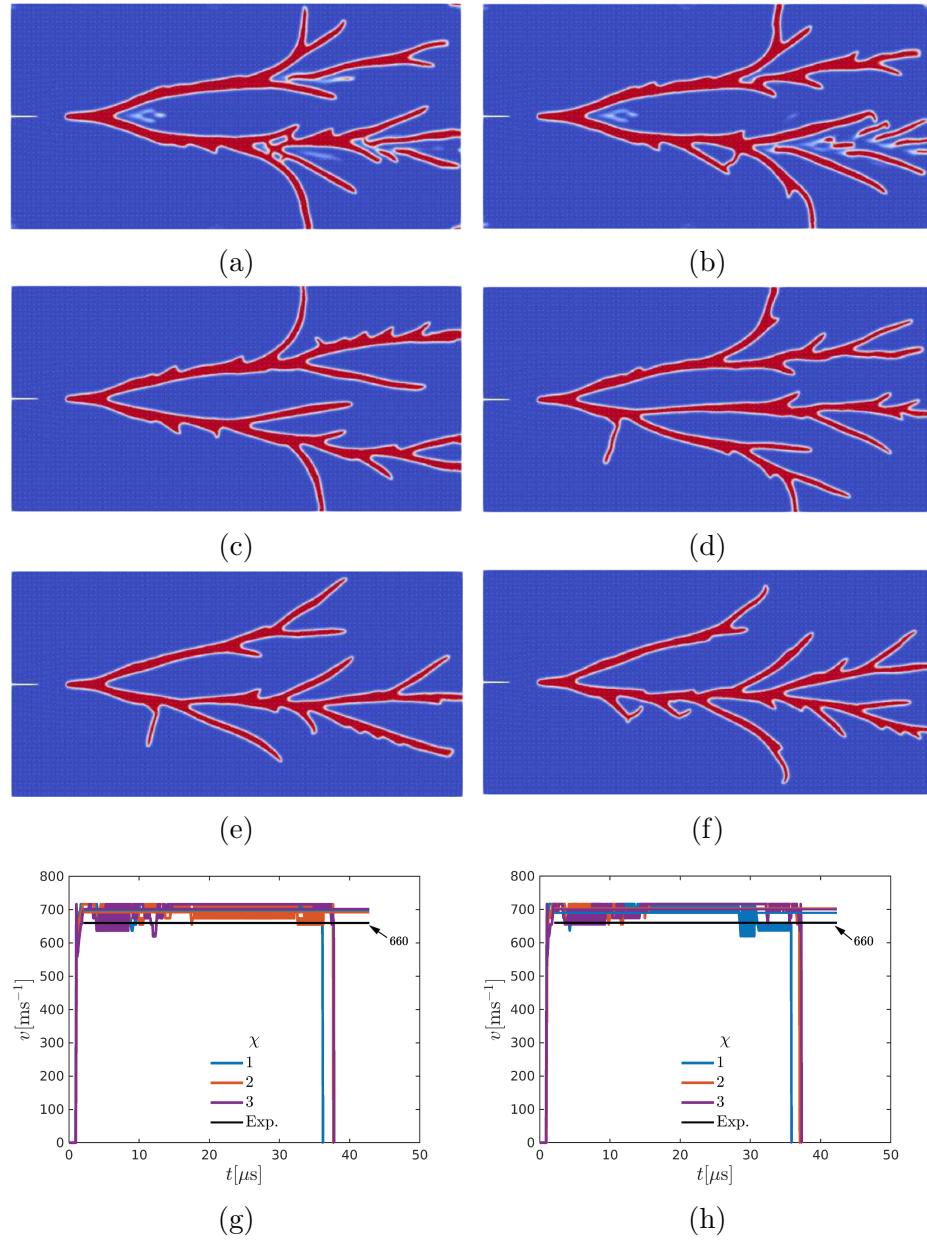


Figure 3.11: Dynamic PMMA plate example. Crack patterns using the EPF models a), c) and e), and using hyperbolic models b), d) and f). Results are obtained using the correction factor $\chi = 1$ for (a) and (b), $\chi = 2$ for (c) and (d), and $\chi = 3$ for (e) and (f). Crack velocity is obtained for the EPF model in (g) and for the HPF model in (h).

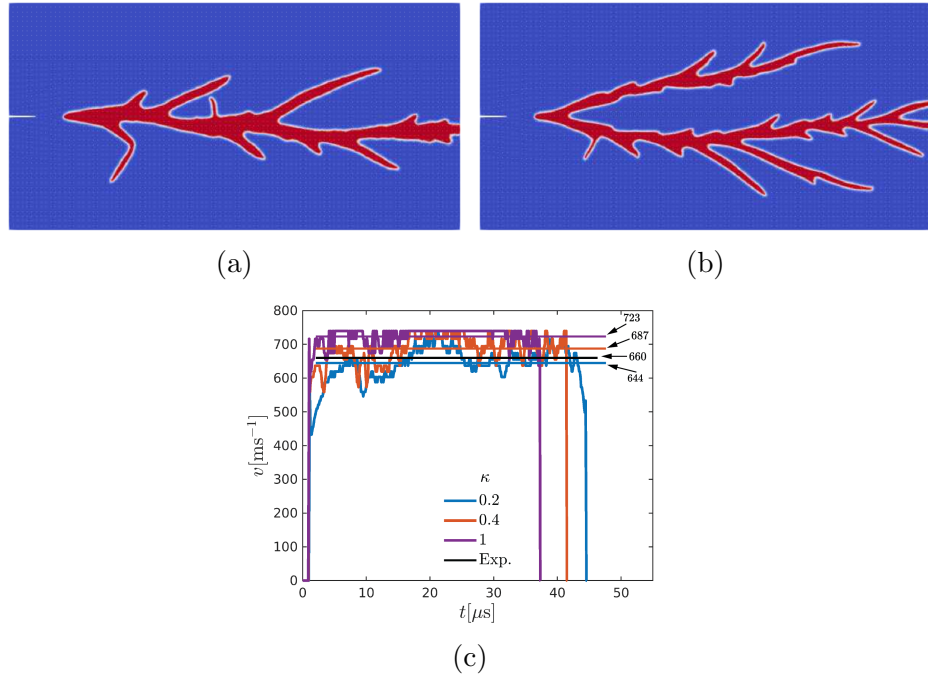


Figure 3.12: Dynamic PMMA plate example. Final crack patterns using the HPF model is obtained with the speed ratio $\kappa = 0.2$ in (a) and $\kappa = 0.4$ in b). Crack velocity are plotted in (c).

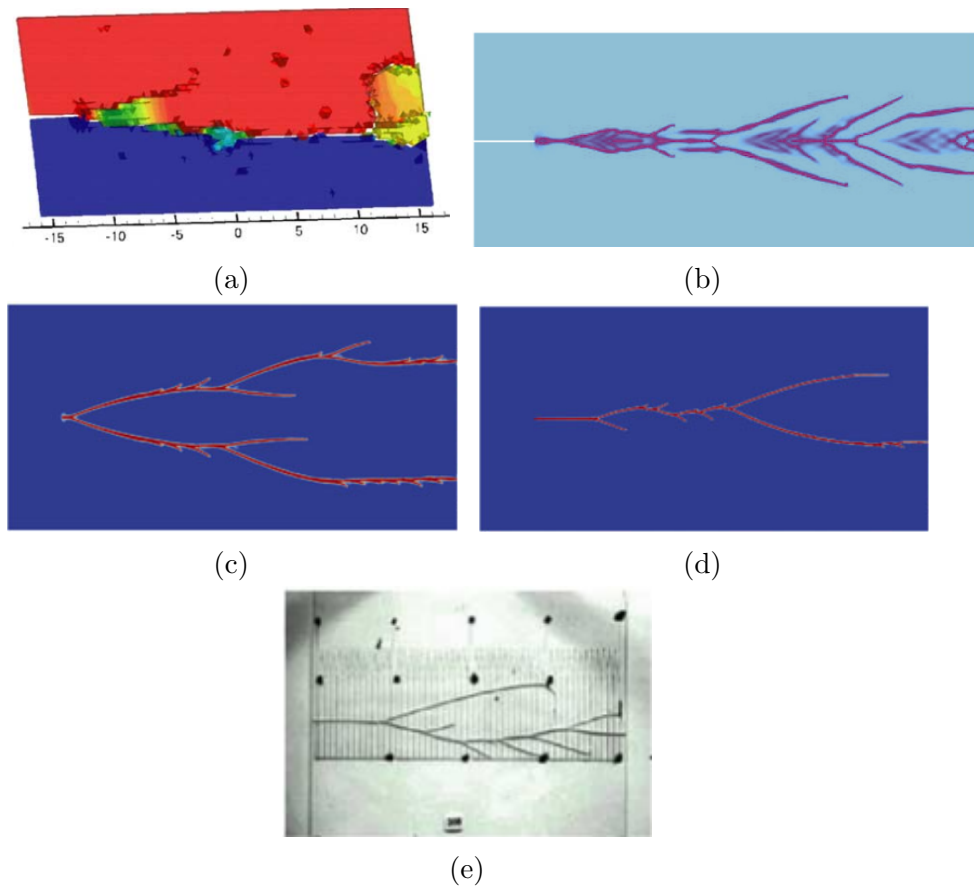


Figure 3.13: Dynamic PMMA plate example. Numerical results by a) [23] b) [132] c) [22] and experimental observation by d) [23]

Chapter 4

A hyperbolic phase field model for ductile fracture at finite strain

4.1 Abstract

The phase field cohesive-zone (PF-CZM) model has been proven to be more accurate and convenient in modeling crack propagation compared to traditional models, primarily due to its insensitivity to length scales and the inclusion of material strength. However, it faces significant convergence challenges, which limit its applicability to highly nonlinear problems. In this study, we extend the PF-CZM model from linear elasticity to ductile fracture at finite strains, addressing both quasi-static and dynamic regimes. For the dynamic case, a hyperbolic form of the evolution equation is utilized, enabling the implementation of a fully explicit time integration scheme. Additionally, to mitigate volumetric locking, a common issue in large strain and deformation problems the Hu-Washizu three-field formulation is employed. By applying a mean dilatation technique, two additional variables are condensed, resulting in a standard displacement-based framework that avoids the complexity of solving a large system of equations. Several numerical examples illustrate the effectiveness of the proposed framework.

4.2 Introduction

Many materials exhibit plastic behavior under high stress levels or extreme loads, resulting in permanent deformation once a new stress-free state is reached. If the applied load exceeds a critical threshold, shear bands and eventually fractures may develop. Consequently, accurately predicting the ductile fracture process is crucial for the effective and optimal design of engineering structures and materials, especially in extreme environments where these phenomena become more complex. While computational tools significantly reduce costs and efforts compared to experimental approaches, challenges remain in both modeling and numerical accuracy to robustly capture the entire failure process.

Phase field modeling has gained considerable attention over the past two decades for its ability to capture complex fracture patterns. Crack paths evolve automatically with the solution of coupled equations, eliminating the need for additional crack-tracking algorithms. Initially formulated for brittle materials by Bourdin et al. [15] using a variational approach suitable for finite element implementation, phase field modeling has since been extended to ductile fracture through various modifications. Duda et al. [133] introduced an elastic-plastic model in which the plastic potential remains unaffected by phase field evolution. Ambati et al. [134] proposed coupling damage and plasticity within a degradation function that controls the contribution of plastic deformation to fracture via an internal plastic variable. In contrast, Miehe et al. [135] linked the phase field to the hardening work, incorporating both local and nonlocal contributions. Borden et al. [119] further integrated the phase field with hardening and plastic dissipative work, resulting in a reduced yield surface. Their modified formulation accurately reflected experimental observations of ductile fracture in aluminum alloys, where plastic strain dominates before failure. For a comprehensive comparison of ductile fracture models, see the overview by Alessi et al. [136].

In this work, we extend the ductile fracture mechanism proposed by [119] using the AT2 classical model to the phase field cohesive-zone (PF-CZM) model developed by Wu [28] in a dynamical setting with a hyperbolic form of the phase field equation. Our contributions are as follows. First, unlike previous studies using classical phase field models, the PF-CZM model demonstrates length-scale insensitivity in mechanical responses. It also incorporates material strength into its formulation, leading to more accurate predictions of crack initiation [137]. However, the PF-CZM model by Wu [28] has encountered significant convergence issues, limiting its applicability to ductile fracture at finite strains. Second, in contrast to prior works that employed an elliptic form of the evolution equation, we adopt a hyperbolic form that enables fully explicit time integration without requiring complex calculations of the elasto-plastic tangent modulus in ductile fracture. Third, to address volumetric locking in finite strain

settings, various strategies have been proposed, such as the enhanced assumed strain [138], the assumed natural strain [134], and the three-field formulation [139]. Here, we use a mean dilatation technique, which is straightforward and requires minimal modifications to the volumetric stress calculation. This technique, derived from the three-field formulation similar to Talamini et al. [139], simplifies to a standard displacement-based formulation, thereby avoiding the complexity of solving a large system of equations due to the inclusion of additional fields.

4.3 Formulations

Consider a solid body occupying the domain $\Omega \in R^d$ in the undeformed configuration and $\omega \in R^d$ in the deformed configuration. The displacement of a material point $\mathbf{X} \in \Omega$ is defined as,

$$\mathbf{u} = \mathbf{x} - \mathbf{X}, \quad (4.1)$$

where $\mathbf{x} = \mathbf{x}(\mathbf{X}, t)$ represents the current position of the material point $\mathbf{X}$ at time t .

4.3.1 Finite deformation theory

The deformation gradient tensor, mapping the undeformed configuration to the current configuration, is expressed as, $\mathbf{F} = \nabla_{\mathbf{X}} \mathbf{x}$. The gradients of velocity with respect to the undeformed (Lagrangian) and deformed (Eulerian) positions are,

$$\mathbf{l} = \nabla_{\mathbf{x}} \dot{\mathbf{u}}, \quad (4.2a)$$

$$\nabla_{\mathbf{X}} \dot{\mathbf{u}} = \mathbf{l} \mathbf{F}. \quad (4.2b)$$

In the material space, damage, plastic deformation, and hardening effects are represented by the variables d , $\mathbf{C}_p$, and β respectively.

The deformation gradient tensor $\mathbf{F}$ is further decomposed into elastic and plastic parts,

$$\mathbf{F} = \mathbf{F}_e \mathbf{F}_p. \quad (4.3)$$

This split accommodates a new potential stress-free state when the solid is unloaded with a permanent deformation represented by $\mathbf{F}_p$.

The mapping between the distances of the material point in the deformed and undeformed configurations is defined using the right and left Cauchy deformation gradients,

$$\mathbf{C} = \mathbf{F}^T \mathbf{F}, \quad \mathbf{b} = \mathbf{F} \mathbf{F}^T. \quad (4.4)$$

Based on the decomposition of the deformation gradient $\mathbf{F}$, the right and left Cauchy-Green deformation gradients $\mathbf{C}$ and $\mathbf{b}$ can be further split into elastic and plastic components. The relationship between them is,

$$\mathbf{b}_e = \mathbf{F} \mathbf{C}_p^{-1} \mathbf{F}^T. \quad (4.5)$$

The rate of $\mathbf{b}_e$ is expressed as,

$$\dot{\mathbf{b}}_e = \left. \frac{d\mathbf{b}_e}{dt} \right|_{\mathbf{C}_p=\text{const.}} + \left. \frac{d\mathbf{b}_e}{dt} \right|_{\mathbf{F}=\text{const.}}. \quad (4.6)$$

Eq. 4.6 implies two steps in the so-called return mapping algorithm [140]; the first term represents the trial stage with frozen plastic deformation, while the second term corresponds to the correction phase, accounting for plastic flow to satisfy the updated yield surface.

In this study, the von Mises yield criterion is adopted. It depends on the deviatoric part of the Kirchhoff stress $\boldsymbol{\tau}$ and the hardening variable β . It is defined as,

$$f(\boldsymbol{\tau}, \beta) = \|\boldsymbol{\tau}_{\text{dev}}\| - \omega(d) \sqrt{\frac{2}{3}} K(\beta) \leq 0, \quad (4.7)$$

where $K(\beta)$ is the kinematic hardening function. Following [119], the degradation function $\omega(d)$ in Eq. 4.7 is used to reduce the yield surface due to plastic deformation. The inequality in Eq. 4.7 can be restated using the Kuhn-Tucker conditions,

$$\dot{\gamma} \geq 0, \quad f \leq 0, \quad \dot{\gamma}f = 0, \quad (4.8)$$

where $\dot{\gamma}$ is introduced as the Lagrange multiplier. These conditions determine whether the current stress state remains elastic or needs to be projected back to the updated yield surface due to plastic deformation.

In the following sections, three stress tensors are encountered,

$$\mathbf{P} \quad \text{First Piola-Kirchoff stress,} \quad (4.9a)$$

$$\boldsymbol{\sigma} = J^{-1}\mathbf{P}\mathbf{F}^T \quad \text{Cauchy stress,} \quad (4.9b)$$

$$\boldsymbol{\tau} = J\boldsymbol{\sigma} \quad \text{Kirchoff stress.} \quad (4.9c)$$

The first Piola-Kirchoff stress tensor $\mathbf{P}$ is obtained directly from the energy potential; however, it is not symmetric. In addition, the Cauchy stress is the physically meaningful stress tensor in the actual deformed configuration. Therefore, in finite element implementations, symmetric stress tensors, including the Cauchy stress $\boldsymbol{\sigma}$ and Kirchoff stress $\boldsymbol{\tau}$, are interchangeably used for various stress tensor operations.

4.3.2 Internal potential energy functional

The internal potential density is assumed to be the sum of the stored and dissipated components,

$$\phi_{\text{int}} = \phi_{\text{stor}} + \phi_{\text{diss}}, \quad (4.10)$$

where ϕ_{stor} includes elastic and plastic contributions, whereas ϕ_{diss} includes damage ϕ_f and viscous ϕ_{vis} contributions,

$$\phi_{\text{stor}} = \omega(d)\phi_e(\mathbf{F}, \mathbf{F}_p, d, \nabla_{\mathbf{X}}d) + \omega(d)\phi_p(\beta), \quad (4.11a)$$

$$\phi_{\text{diss}} = \phi_f(d, \nabla_{\mathbf{X}}d) + \phi_{\text{vis}}(\dot{d}). \quad (4.11b)$$

The degradation function reduces both the elastic free energy ϕ_e and the plastic energy ϕ_p functions in Eq. 4.11a. ϕ_e is further decomposed into deviatoric and volumetric parts,

$$\phi_e = \phi_{\text{dev}}(\mathbf{F}, \mathbf{F}_p) + \phi_{\text{vol}}(J_e), \quad (4.12)$$

where,

$$\phi_{\text{dev}} = \frac{G}{2} (\text{tr}[\bar{\mathbf{b}}_e] - 3), \quad \phi_{\text{iso}} = \frac{K_d}{2} \left(\frac{J_e^2 - 1}{2} - \ln J_e \right), \quad (4.13)$$

with $\bar{\mathbf{b}}_e = J_e^{-2/3} \mathbf{b}_e$ and $J_e = \det[\mathbf{F}_e]$. G and $K_d = \lambda + 2\mu/d$ are the shear and bulk moduli, respectively.

The fracture energy density ϕ_f in Eq. 4.11b, defined in the reference configuration, is,

$$\phi_f = \frac{G}{bc_\alpha} (\alpha(d) + b^2 |\nabla_{\mathbf{X}}d|^2), \quad (4.14)$$

while the potential related to viscosity, $\phi_{\text{vis}}(\dot{d})$, can be defined in its rate form,

$$\dot{\phi}_{\text{vis}}(\dot{d}) = \frac{1}{2} \eta^d \dot{d}^2. \quad (4.15)$$

where the *micro-viscosity* term η^d , incorporate fracture viscous effects [48]. As a consequence, the rate expressions for the stored potential and the dissipated potential are,

$$\dot{\phi}_{\text{stor}}(\mathbf{F}, \mathbf{F}_p, d, \nabla d, \beta) = \frac{\partial \phi_{\text{stor}}}{\partial \mathbf{F}} \dot{\mathbf{F}} + \frac{\partial \phi_{\text{stor}}}{\partial \mathbf{F}_p} \dot{\mathbf{F}}_p + \frac{\partial \phi_{\text{stor}}}{\partial d} \dot{d} + \frac{\partial \phi_{\text{stor}}}{\partial \nabla_{\mathbf{X}}d} \nabla_{\mathbf{X}} \dot{d} + \frac{\partial \phi_{\text{stor}}}{\partial \beta} \dot{\beta}, \quad (4.16)$$

$$\dot{\phi}_{\text{diss}} = \dot{\phi}_f(d, \nabla d) + \dot{\phi}_{\text{vis}}(\dot{d}) = \frac{G}{bc_\alpha} \left(\alpha'(d) \dot{d} + 2b^2 \nabla_{\mathbf{X}}d \cdot \nabla_{\mathbf{X}} \dot{d} \right) + \frac{1}{2} \eta^d \dot{d}^2. \quad (4.17)$$

4.3.3 Evolution equations for internal variables

With the forms of the yield function 4.7 and the stored energy 4.12, the flow rule can be obtained from Lie derivative and the principle of maximum dissipation [141, 140] as,

$$\mathbf{L}[\mathbf{b}_e] = \mathbf{F} \dot{\mathbf{C}}_p^{-1} \mathbf{F}^T = -\frac{2}{3} \dot{\gamma} \text{tr}[\mathbf{b}_e] \mathbf{n}, \quad (4.18a)$$

$$\dot{\beta} = \sqrt{\frac{2}{3}} \dot{\gamma}, \quad (4.18b)$$

where $\mathbf{n} = \boldsymbol{\tau}_{\text{dev}} / \|\boldsymbol{\tau}_{\text{dev}}\|$. The solutions for $\mathbf{C}_p$ at the current time step $n + 1$ can be incrementally updated from the previous time step n using the backward Euler method,

$$\mathbf{C}_{p,n+1}^{-1} = \mathbf{C}_{p,n}^{-1} - \frac{2}{3} \Delta\gamma \text{tr}[\mathbf{b}_{e,n+1}] \mathbf{F}_{n+1}^{-1} \mathbf{n} \mathbf{F}_{n+1}^{-T}, \quad (4.19a)$$

$$\beta_{n+1} = \beta_n + \sqrt{\frac{2}{3}} \Delta\gamma. \quad (4.19b)$$

4.3.4 Thermodynamically consistent framework for finite strain setting

The Newtonian balance laws, applied to both the physical and material spaces in the reference configuration, are expressed as,

$$\frac{d}{dt} \int_{\Omega} \rho_u \dot{\mathbf{u}} \, dV = \int_{\partial\Omega} \mathbf{P} \mathbf{N} \, dS, \quad (4.20a)$$

$$\frac{d}{dt} \int_{\Omega} \rho_d \dot{d} \, dV = - \int_{\Omega} \sigma^d \, dV + \int_{\partial\Omega} \boldsymbol{\sigma}^{\nabla d} \cdot \mathbf{N} \, dS, \quad (4.20b)$$

where ρ_u and ρ_d are the solid and micro-damage densities in the reference configuration, respectively; $\mathbf{P}$ is the first Piola-Kirchhoff stress tensor, $\mathbf{N}$ is the normal vector, σ^d is the micro-force value, and $\boldsymbol{\sigma}^{\nabla d}$ is the micro-stress vector, respectively.

Applying the divergence theorem to Eq. 4.20 yields,

$$\rho_u \ddot{\mathbf{u}} = \nabla_{\mathbf{X}} \cdot \mathbf{P}, \quad (4.21a)$$

$$\rho_d \ddot{d} = \nabla_{\mathbf{X}} \cdot \boldsymbol{\sigma}^{\nabla d} - \sigma^d. \quad (4.21b)$$

The balance of the energy, complying with the first law of thermodynamics, is expressed as,

$$\frac{d}{dt} \int_{\Omega} (\rho_u e + k) \, dV = \int_{\partial\Omega} \left(\dot{\mathbf{u}} \cdot \mathbf{P} \mathbf{N} + \dot{d} \boldsymbol{\sigma}^{\nabla d} \cdot \mathbf{N} \right) \, dS. \quad (4.22)$$

where e is the internal energy density and k represents kinetic energy density, which is defined by,

$$k = \frac{1}{2} \rho_u \dot{\mathbf{u}} \cdot \dot{\mathbf{u}} + \frac{1}{2} \rho_d \dot{d} \dot{d}, \quad (4.23)$$

Applying the divergence theorem to Eq. 4.22, along with the balance laws Eq. 4.21, leads to,

$$\rho_u \dot{e} = \mathbf{P} : \dot{\mathbf{F}} + \sigma^d \dot{d} + \boldsymbol{\sigma}^{\nabla d} \cdot \nabla_{\mathbf{X}} \dot{d}. \quad (4.24)$$

The second law of thermodynamics demands the nonnegativity of dissipated energy,

$$\phi_d^{\text{red}} = \rho_u \dot{e} - \dot{\phi}_{\text{stor}} \geq 0. \quad (4.25)$$

Substituting Eqs. 4.16 and 4.22 into Eq. 4.25 yields,

$$\phi_d^{\text{red}} = \left(\mathbf{P} - \frac{\partial \phi_{\text{stor}}}{\partial \mathbf{F}} \right) : \dot{\mathbf{F}} + \left(\sigma^d - \frac{\partial \phi_{\text{stor}}}{\partial d} \right) \dot{d} + \left(\boldsymbol{\sigma}^{\nabla d} - \frac{\partial \phi_{\text{stor}}}{\partial \nabla_{\mathbf{X}} d} \right) \cdot \nabla_{\mathbf{X}} \dot{d} - \frac{\partial \phi_{\text{stor}}}{\partial \mathbf{F}_p} \dot{\mathbf{F}}_p - \frac{\partial \phi_{\text{stor}}}{\partial \beta} \dot{\beta} \geq 0. \quad (4.26)$$

Using the theory of generalized standard material [124], macro- and micro-stresses are decomposed into the elastic and plastic parts,

$$\mathbf{P} = \mathbf{P}_{\text{elas}} + \mathbf{P}_{\text{diss}}, \quad \sigma^d = \sigma_{\text{elas}}^d + \sigma_{\text{diss}}^d, \quad \boldsymbol{\sigma}^{\nabla d} = \boldsymbol{\sigma}_{\text{elas}}^{\nabla d} + \boldsymbol{\sigma}_{\text{diss}}^{\nabla d}, \quad (4.27)$$

where the elastic parts are,

$$\mathbf{P}_{\text{elas}} = \frac{\partial \phi_{\text{stor}}}{\partial \mathbf{F}} = \omega(d) (\boldsymbol{\tau}_{0,\text{dev}} + \boldsymbol{\tau}_{0,\text{vol}}) \mathbf{F}^{-T}, \quad (4.28a)$$

$$\sigma_{\text{elas}}^d = \frac{\partial \phi_{\text{stor}}}{\partial d} = \omega'(d) \phi_e, \quad (4.28b)$$

$$\boldsymbol{\sigma}_{\text{elas}}^{\nabla d} = \frac{\partial \phi_{\text{stor}}}{\partial \nabla_{\mathbf{X}} d} = \mathbf{0}, \quad (4.28c)$$

with $\boldsymbol{\tau}_{0,\text{dev}} = \mu[\text{dev} \bar{\mathbf{b}}_e]$ and $\boldsymbol{\tau}_{0,\text{vol}} = \frac{K_n}{2}(J^2 - 1)\mathbf{I}$. The dissipative parts are defined as,

$$\mathbf{P}_{\text{diss}} = \frac{\partial \dot{\phi}_{\text{diss}}}{\partial \dot{\mathbf{F}}} = \mathbf{0}, \quad (4.29a)$$

$$\sigma_{\text{diss}}^d = \frac{\partial \dot{\phi}_{\text{diss}}}{\partial \dot{d}} = \frac{G}{bc_\alpha} \alpha'(d) + \eta^d \dot{d}, \quad (4.29b)$$

$$\boldsymbol{\sigma}_{\text{diss}}^{\nabla d} = \frac{\partial \dot{\phi}_{\text{diss}}}{\partial \nabla_{\mathbf{X}} \dot{d}} = \frac{2Gb}{c_\alpha} \nabla_{\mathbf{X}} \dot{d}. \quad (4.29c)$$

Substituting these decompositions into Eq. 4.26 leads to,

$$\phi_d^{\text{red}} = \mathbf{P}_{\text{diss}} : \dot{\mathbf{F}} + \sigma_{\text{diss}}^d \dot{d} + \boldsymbol{\sigma}_{\text{diss}}^{\nabla d} \cdot \nabla_{\mathbf{X}} \dot{d} - \frac{\partial \phi_{\text{stor}}}{\partial \mathbf{F}_p} \dot{\mathbf{F}}_p - \frac{\partial \phi_{\text{stor}}}{\partial \beta} \dot{\beta} \geq 0, \quad (4.30)$$

To ensure the non-negativity of dissipation, Eq. 4.30 is locally satisfied by imposing the following conditions,

$$\sigma_{\text{diss}}^d \geq 0, \quad \dot{d} \geq 0. \quad (4.31)$$

4.3.5 Governing equations

Substitution of the constitutive relations in Eqs. 4.28 and 4.29 into the balance laws in Eq. 4.21 leads to the governing equations,

$$\rho_u \ddot{\mathbf{u}} - \nabla_{\mathbf{X}} \cdot \mathbf{P} = \mathbf{0} \quad (4.32a)$$

$$\rho_d \ddot{d} + \eta^d \dot{d} + \nabla_{\mathbf{X}} \cdot \left(\frac{2bG}{c_\alpha} \nabla_{\mathbf{X}} d \right) = -\omega'(d) (\phi_e + \beta_p \phi_p) - \frac{G}{bc_\alpha} \alpha'(d), \quad (4.32b)$$

Dividing Eq. 4.32b by the scaling factor $\tilde{s} := 2G/bc_\alpha$ results in a PDE for the phase field that is non-dimensional and more suitable in discerning its relevant time scales. Moreover, the first term on the right-hand side of this equation represents the energetic driving force for crack evolution. To prevent crack healing, this term is reformulated as shown below,

$$\tau_d^2 \ddot{d} + d_f \tau_d \dot{d} - b^2 \Delta_{\mathbf{X}} d = -\omega'(d) \frac{\mathcal{H} + \beta_p \langle \phi_p - \phi_0 \rangle_+}{\tilde{s}} - \frac{1}{2} \alpha'(d), \quad (4.33)$$

where $\Delta_{\mathbf{X}} := \nabla_{\mathbf{X}} \cdot \nabla_{\mathbf{X}}$ is the referential Laplacian operator. It is assumed that $\tilde{s}$ is spatially uniform (in each phase of the material). The time scale $\tau_d^2 = \rho_d / \tilde{s} = b^2 / c_u^2$ is introduced in Eq. 4.33. The nondimensional damping factor d_f is defined from the relation $\eta^d / \tilde{s} = d_f \tau_d$. Basically, τ_d^2 and $d_f \tau_d$ represent micro-inertia and micro-viscosity terms for the phase field equation in its nondimensional form.

The history parameter $^* \mathcal{H} = \max_{s \in [0, t]} \{\phi_e^+(\mathbf{F}_n, \mathbf{F}_{p,n}, J_{e,n}), s\}, \phi_{0e}\}$ takes the maximum value of prior time ϕ_e^+ values and the initiation fracture energy ϕ_{0e} . To ensure cracks form only in tension and not in compression, ϕ_e is replaced by its positive part, defined using the Rankine criterion [28], in the history operator. $\phi_{0e} := -\lim_{d \rightarrow 0^+} \tilde{s} \alpha'(d) / \omega'(d) = \tilde{\sigma}_c^2 / 2E$ corresponds to the elastic energy level required to initiate damage accumulation and its inclusion prevents negative damage evolution when $\phi_e^+ < \phi_{0e}$.

The reference plastic energy ϕ_0 is introduced to regulate the degree of plastic contribution to the fracture process. The positive operator is defined as $\langle x \rangle_+ = x$ for $x \geq 0$ and zero otherwise. The coefficient β_p determines whether plastic deformation contributes to crack evolution, with $\beta_p = 0$ representing the elastic-plastic case and $\beta_p = 1$ representing the elasto-plastic case.

*The history parameter was introduced by [67] to guarantee damage irreversibility for an AT2 elliptic phase field formulation. The irreversibility is not guaranteed for non-AT2 degradation functions or non-elliptic phase field formulations. Accordingly, in addition to the history parameter we directly enforce damage irreversibility in numerical setting.

Eqs. 4.32a and 4.33 are subject to the following *Boundary Conditions* (BCs),

$$\begin{cases} \mathbf{u}(\mathbf{X}, t) = \tilde{\mathbf{u}} & \text{on } \partial\Omega_u \times [0, T] \\ \mathbf{P} \cdot \mathbf{N} = \tilde{\mathbf{T}} & \text{on } \partial\Omega_t \times [0, T] \\ \nabla_{\mathbf{X}} d \cdot \mathbf{N} = 0 & \text{on } \partial\Omega \times [0, T]. \end{cases} \quad (4.34)$$

where $\partial\Omega_u$ and $\partial\Omega_t$ are the Dirichlet and Neumann boundaries for the elastodynamic problem, satisfying $\partial\Omega_u \cup \partial\Omega_t = \partial\Omega$ and $\partial\Omega_u \cap \partial\Omega_t = \emptyset$. The initial conditions are defined as,

$$\begin{cases} \mathbf{u}(\mathbf{X}, 0) = \tilde{\mathbf{u}}_0(\mathbf{X}) \\ \dot{\mathbf{u}}(\mathbf{X}, 0) = \dot{\tilde{\mathbf{u}}}_0(\mathbf{X}) \\ d(\mathbf{X}, 0) = \tilde{d}_0(\mathbf{X}) \\ \dot{d}(\mathbf{X}, 0) = \dot{\tilde{d}}_0(\mathbf{X}). \end{cases} \quad (4.35)$$

for $\mathbf{X} \in \Omega$.

These conditions describe the deformation and crack evolution in solids. Additionally, due to the presence of plastic internal variables, a local problem must be solved to determine the constitutive response of the solid. The corresponding equations are,

$$\text{Isochoric assumption: } J_e = J = \det[\mathbf{F}]; \quad (4.36a)$$

$$\text{Stress: } \mathbf{P} = \frac{\partial \phi_{\text{stor}}}{\partial \mathbf{F}}, \quad \boldsymbol{\sigma} = J^{-1} \mathbf{P} \mathbf{F}^T, \quad \boldsymbol{\tau} = J \boldsymbol{\sigma}; \quad (4.36b)$$

$$\text{Yield function: } f = \|\mathbf{s}\| - \omega(d) \sqrt{\frac{2}{3}} K(\beta); \quad (4.36c)$$

$$\text{Flow rule: } L[\mathbf{b}^e] = -\frac{2}{3} \dot{\gamma} \text{tr}[\mathbf{b}^e] \mathbf{n}, \quad \mathbf{n} = \frac{\mathbf{s}}{\|\mathbf{s}\|}; \quad (4.36d)$$

$$\text{Hardening rule: } \dot{\beta} = \sqrt{\frac{2}{3}} \dot{\gamma}; \quad (4.36e)$$

$$\text{Karush-Kuhn-Tucker condition: } \dot{\gamma} f = 0, \quad \dot{\gamma} \geq 0, \quad f \leq 0. \quad (4.36f)$$

4.3.6 Weak form

The *Weighted Residual Statement* (WRS) is obtained by multiplying Eq. 4.32a and Eq. 4.33 by displacement $\hat{\mathbf{u}}$ and phase field $\hat{d}$ weight functions, respectively, and integrating over Ω . The *Weak Statement* is obtained by forming full divergence terms and the application of divergence theorem on the spatial gradient terms. By employing Eq. (4.34), the weak statement is expressed as,

$$(\hat{\mathbf{u}}, \rho_u \ddot{\mathbf{u}})_\Omega + (\hat{\mathbf{l}}, \boldsymbol{\tau})_\Omega = (\hat{\mathbf{u}}, \tilde{\mathbf{T}})_{\partial\Omega_t}, \quad (4.37a)$$

$$\left(\hat{d}, \tau_d^2 \ddot{d} + d_f \tau_d \dot{d} \right)_\Omega + \left(\nabla_{\mathbf{X}} \hat{d}, b^2 \nabla_{\mathbf{X}} d \right)_\Omega = - \left(\hat{d}, \omega'(d) \frac{\mathcal{H} + \beta_p \langle \phi_p - \phi_0 \rangle_+}{\tilde{s}} + \frac{1}{2} \alpha'(d) \right)_\Omega, \quad (4.37b)$$

where $(f, g)_\mathcal{S}$ refers to the integral of fg over the domain $\mathcal{S}$. In Eq. 4.37, g refers to a weight function and g refers to a solution of boundary condition field. In the original form of the weak statement, we encounter the term $(\nabla_{\mathbf{X}} \hat{\mathbf{u}}, \mathbf{P})_\Omega$, which is equivalent to $(\hat{\mathbf{l}}, \boldsymbol{\tau})_\Omega$ in Eq. 4.37a. The latter form is preferred because the stress tensor $\boldsymbol{\tau}$ is symmetric, which is advantageous for the finite element implementation and aligns with the definition of the yield surface in Eq. 4.7.

4.3.7 Treatment of volumetric locking for finite deformation

Volumetric locking commonly occurs in large strain scenarios and under isochoric assumptions in plasticity problems. We adopt the three-field formulation developed by Hu and Washizu [142]. For clarity, the formulation is briefly outlined here for the free energy without internal variables. The total potential in the original three-field formulation, with the inclusion of the phase field variable for fracture modeling as considered in this work, is expressed as follows,

$$\hat{\phi}_{\text{stor}}(\mathbf{C}, d, p, \tilde{J}) = \int_{\Omega} \omega(d) [\phi_{\text{dev}}(\mathbf{C}) + \phi_{\text{vol}}(\tilde{J})] \, dV + \int_{\Omega} p(J - \tilde{J}) \, dV, \quad (4.38)$$

where $\tilde{J}$ represents the constrained value for the volume change J (Jacobian), and p acts as the Lagrange multiplier to enforce this constraint on the total potential. The directional derivative of $\hat{\phi}_{\text{stor}}$ with respect to $\{\dot{\mathbf{u}}, \dot{d}, \dot{p}, \dot{\tilde{J}}\}$ is expressed as,

$$\text{D}\hat{\phi}_{\text{stor}}(\mathbf{C}, d, p, \tilde{J})[\dot{\mathbf{u}}, \dot{d}, \dot{p}, \dot{\tilde{J}}] = \text{D}\hat{\phi}_{\text{stor}}[\dot{\mathbf{u}}] + \text{D}\hat{\phi}_{\text{stor}}[\dot{d}] + \text{D}\hat{\phi}_{\text{stor}}[\dot{p}] + \text{D}\hat{\phi}_{\text{stor}}[\dot{\tilde{J}}], \quad (4.39)$$

where,

$$\text{D}\hat{\phi}_{\text{stor}}[\dot{\mathbf{u}}] = \int_{\omega} \mathbf{l} : \boldsymbol{\tau}_{\text{dev}} \, dV + \int_{\omega} \mathbf{l} : \boldsymbol{\tau}_{\text{vol}} \, dV, \quad (4.40a)$$

$$\text{D}\hat{\phi}_{\text{stor}}[\dot{d}] = \int_{\omega} \dot{d}\omega'(d)(\phi_{\text{dev}}(\mathbf{C}) + \phi_{\text{vol}}(\tilde{J})) \, dV, \quad (4.40b)$$

$$\text{D}\hat{\phi}_{\text{stor}}[\dot{p}] = \int_{\Omega} \dot{p}(J - \tilde{J}) \, dV, \quad (4.40c)$$

$$\text{D}\hat{\phi}_{\text{stor}}[\dot{\tilde{J}}] = \int_{\Omega} \dot{\tilde{J}} \left(\frac{d\phi_{\text{vol}}(\tilde{J})}{d\tilde{J}} - p \right) \, dV, \quad (4.40d)$$

with $\boldsymbol{\tau}_{\text{vol}} = \omega(d)p\mathbf{I}J$. From Eqs. 4.40c and 4.40d, we obtain the relation $J = \tilde{J}$ and $p = d\phi_{\text{vol}}(\tilde{J})/d\tilde{J}$. Using the same discretization for the three primary variables p , $\tilde{J}$, $\mathbf{u}$ offers no clear advantage. It is more effective to use different discretizations for p and $\tilde{J}$ compared to $\mathbf{u}$. In this context, we adopt the mean dilatation technique [141], where the interpolated functions for p and $\tilde{J}$ are averaged over a given volume,

$$\tilde{J} = \frac{1}{\Omega} \int_{\Omega} J \, dV, \quad (4.41a)$$

$$p = \left. \frac{d\phi_{\text{vol}}}{d\tilde{J}} \right|_{\tilde{J}=\text{const}}. \quad (4.41b)$$

The directional derivative in Eq. 4.39 now operates along the direction of $\{\dot{\mathbf{u}}, \dot{d}\}$,

$$\text{D}\hat{\phi}_{\text{stor}}(\mathbf{C}, d, p, \tilde{J})[\dot{\mathbf{u}}, \dot{d}] = \text{D}\hat{\phi}_{\text{stor}}[\dot{\mathbf{u}}] + \text{D}\hat{\phi}_{\text{stor}}[\dot{d}], \quad (4.42)$$

where,

$$\mathrm{D}\hat{\phi}_{\text{stor}}[\dot{\mathbf{u}}] = \int_{\Omega} \mathbf{l} : \boldsymbol{\tau}_{\text{dev}} \, \mathrm{d}V + \int_{\Omega} \mathbf{l} : \tilde{\boldsymbol{\tau}}_{\text{vol}} \, \mathrm{d}V, \quad (4.43)$$

with $\tilde{\boldsymbol{\tau}}_{\text{vol}} = \omega(d)p(\tilde{J})\mathbf{I}\tilde{J}$. Eq. 4.43 aligns with the form of the second term in Eq. 4.37a by setting $\hat{\mathbf{u}} = \dot{\mathbf{u}}$, with a slight modification to the volumetric component of the Kirchhoff stress, $\tilde{\boldsymbol{\tau}}_{\text{vol}}$. This adjustment simplifies the numerical implementation and reduces the complexity compared to other methods used to address the volumetric locking [138, 139, 134].

4.4 Numerical results

In the following examples, we illustrate the effectiveness of the proposed formulations and numerical schemes. The first example involves a simple uniaxial test that evaluates the stress-strain response as model parameters vary. The second example features a notched specimen under tensile loading in a quasi-static regime. Lastly, a dynamic shear loading scenario is used to validate the formulation's applicability to dynamic problems.

4.4.1 Uniaxial test

A unit cube subjected to uniaxial loading is considered. The material properties are selected according to Borden et al. [119], with Young's modulus $E = 68.8 \text{ GPa}$, Poisson's ratio $\nu = 0.33$, yield stress $\sigma_y = 320 \text{ MPa}$, critical energy release rate $G = 138 \cdot 10^6 \text{ J/m}^2$, and length scale $b = 2 \text{ m}$.

We first examine the scenario where the yield function is unaffected by damage evolution, as presented by [134];[135]. Figure 4.1a depicts the stress-strain response for three cases: no fracture, the elastic-plastic model, and the elasto-plastic model. In the absence of fracture, stress increases linearly until it reaches the yield stress, after which the loading path enters the hardening phase. In contrast, the other two cases exhibit a softening phase due to fracture occurrence. Crack initiation is delayed in the

elastic-plastic case, as the sole driver for crack growth is plastic deformation. In the elasto-plastic case, both elastic and plastic deformations contribute to the fracture process, resulting in earlier crack initiation. Figure 4.1b illustrates the energy versus strain behavior for the fracture case, showing that elastic energy dominates over plastic energy in the inelastic phase, which contradicts experimental observations.

Next, we introduce degradation of the yield surface through the degradation function. Figure 4.2a presents stress-strain responses for varying initial plastic energy values $\phi_0 = \{1e7, 5e7, 1e8\}$ which regulate the contribution of plastic deformation to crack propagation. As shown, increasing the initial plastic energy delays the onset of fracture. Notably, the peak stress obtained with the highest value $\phi_0 = 1e8$, matches the tensile strength of the material, contrasting with results from classical phase field models [119] [134], where material strength is not a model parameter. Additionally, Figure 4.1b illustrates the predominance of plastic energy over elastic energy during the softening phase, underscoring the importance of accounting for the degradation function's effect on the yield surface.

4.4.2 I-shaped specimen

To assess the performance of the proposed formulation, an I-shaped specimen is analyzed with its bottom edge fixed and a tensile load applied at the top. The geometry and boundary conditions are illustrated in Figure 4.3. The material properties are defined as follows: Young's modulus $E = 72624$ MPa, Poisson ratio $\nu = 0.33$, yield stress $\sigma_y = 345$ MPa, hardening modulus $H = 250$ MPa, and critical energy release rate $G = 9.31$ MPa mm. A length scale $b = 0.2$ mm is assumed.

Figure 4.4 illustrates the crack patterns observed at various stages of loading. Initially, damage zones form at the center of the specimen, displaying two intersecting inclined trajectories. However, due to perturbations, only one trajectory continues to propagate to the fully damaged state, which aligns with the numerical findings reported by Ambati et al. [134].

The load-deflection curve is shown in Figure 4.5. In the results of Ambati et al. [134], the reaction force increases gradually during the hardening phase, followed by a sharp drop in the softening phase due to crack initiation and propagation. The results presented here exhibit a similar trend; however, the reaction force remains constant during the hardening phase. This behavior occurs because the stress state in this region matches the material’s strength, as demonstrated in the analysis results in Figure 4.2a.

4.4.3 Dynamic shear loading

In the final example, we analyze a benchmark problem in dynamic fracture to demonstrate the importance of using a ductile fracture model under high loading rates. The geometry and boundary conditions are illustrated in Figure 4.6. A projectile impacts a pre-notched plate at high velocity ($\bar{v} = 35 \text{ m/s}$), with the impact modeled as an external velocity applied to the lower part of the left edge. The material properties are chosen as follows: $\rho_u = 8000 \text{ kg/m}^3$, $E = 190 \text{ GPa}$, $\nu = 0.3$, $G = 2.213 \cdot 10^4 \text{ N/m}$, and $\tilde{\sigma}_c = 2.812 \text{ GPa}$. The length scale is set to $b = 0.3 \cdot 10^{-3} \text{ m}$.

Figure 4.7 shows the crack patterns at different time intervals using the brittle fracture model described in §3. Cracks initiate at the notch tip and propagate at an inclined angle before branching into two sub-cracks. This branching is caused by the high-velocity impact on the plate. However, the resulting crack pattern does not align with the experimental observations shown in Figure 4.6b.

In contrast, results from the proposed ductile fracture model are depicted in Figure 4.8. Unlike the brittle model, crack initiation occurs at the notch tip, followed by horizontal propagation toward the right edge, with a slight downward angle toward the bottom right corner. This pattern closely matches the experimental results presented in Figure 4.6b.

4.5 Conclusions

In this study, we developed a hyperbolic phase field cohesive-zone model for simulating ductile fracture at finite strains. The issue of volumetric locking, commonly encountered in finite strain and deformation scenarios, is addressed using a three-field formulation. By applying the mean dilatation technique, this three-field approach is reformulated into a standard displacement-based framework, avoiding the large system of equations inherent in the original method. The performance of the proposed formulation is evaluated through two quasi-static fracture problems. Results indicate that the peak stress predicted by the PF-CZM model does not exceed the material's tensile strength, in contrast to classical phase field models that do not account for material strength.

For dynamic problems, we introduce a fully explicit time integration scheme that enables direct solution computation without iterative steps or the stiffness matrix calculations required by implicit schemes. This approach significantly reduces computational cost and mitigates the convergence issues often observed in implicit methods. Additionally, the importance of considering a ductile fracture model is highlighted by the ability to replicate crack patterns in Kalthoff's experiment under high loading rates. While further calibration of the model is necessary, the numerical results obtained are promising.

Appendix

Figures

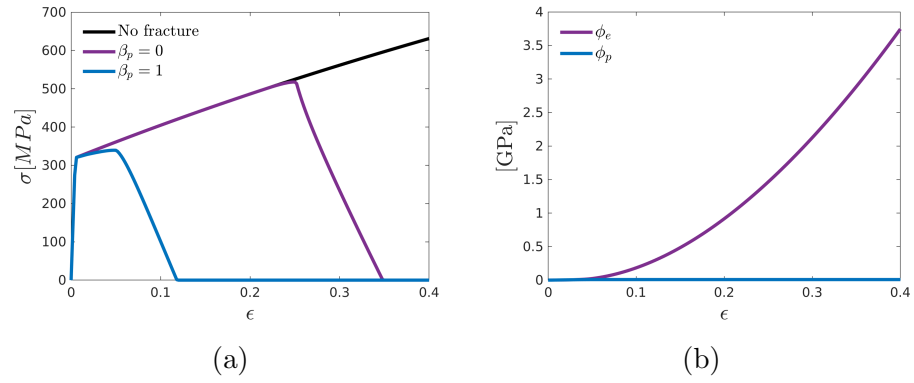


Figure 4.1: Uniaxial test. a) Stress-strain response b) Energy

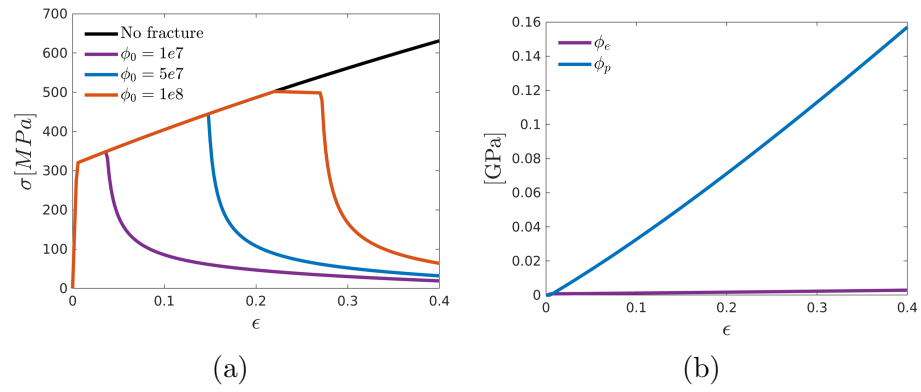


Figure 4.2: Uniaxial test. a) Stress-strain response b) Energy

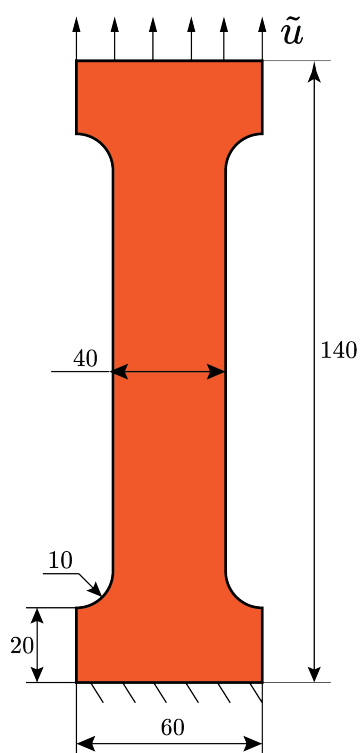


Figure 4.3: I-shaped specimen. Problem setup.

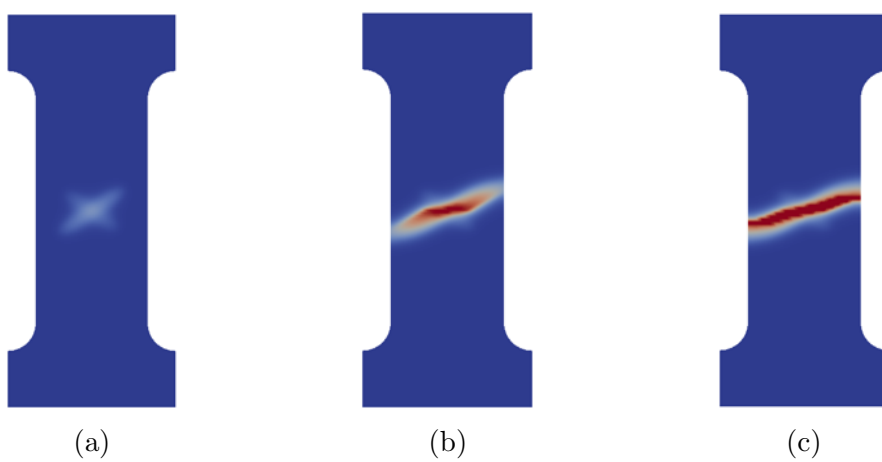


Figure 4.4: Uniaxial test. a) Stress-strain response b) Energy

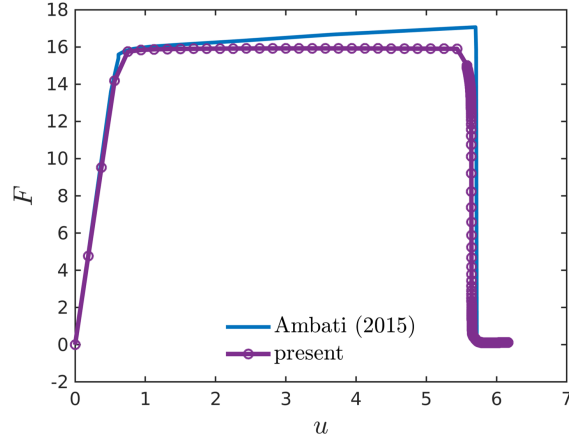


Figure 4.5: I-shaped specimen. Stress-strain response.

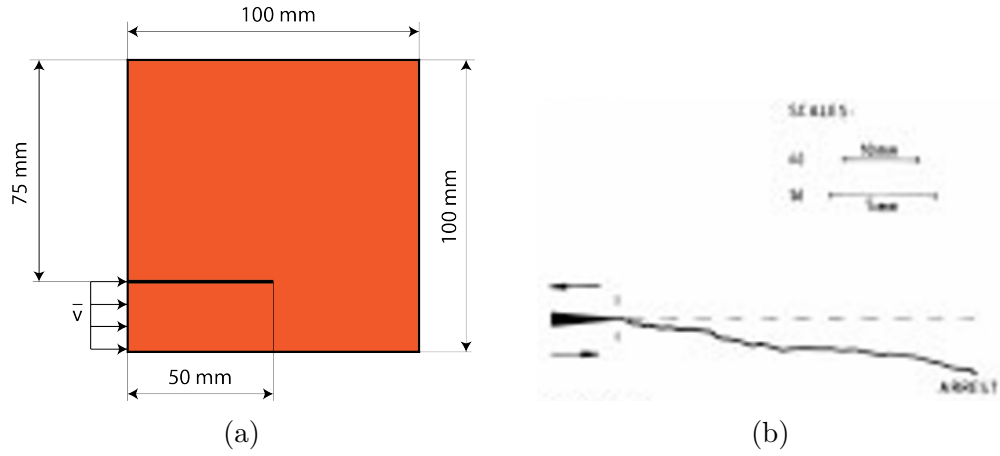


Figure 4.6: Dynamic shear loading example. (a) Problem setup and boundary condition, (b) Experimental observation [130].

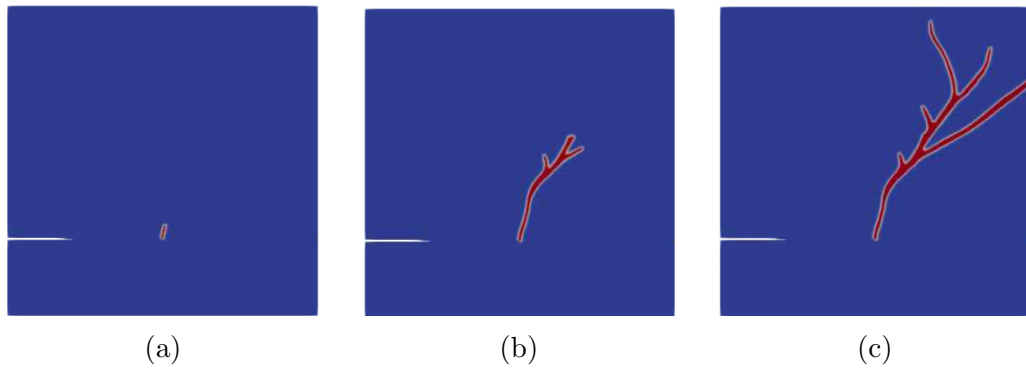


Figure 4.7: Dynamic shear loading example. Crack patterns obtained by the brittle fracture model.

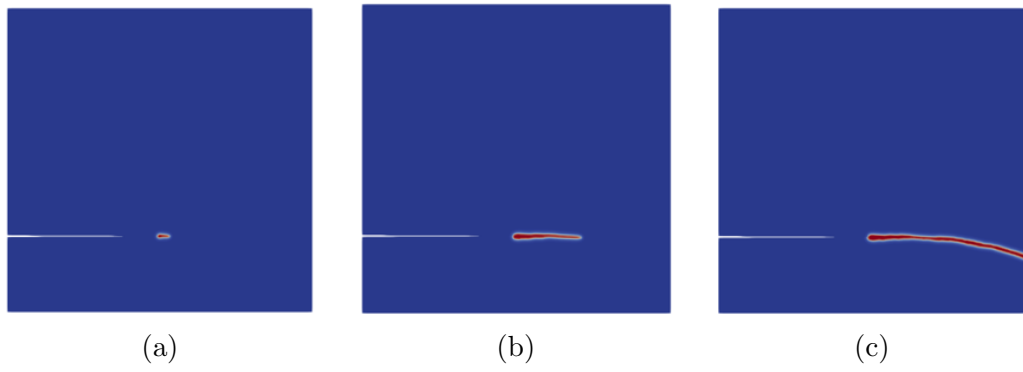


Figure 4.8: Dynamic shear loading example. Crack patterns obtained by the ductile fracture model.

Chapter 5

Conclusions and future work

This dissertation presents hyperbolic phase-field models applicable to both brittle and ductile materials for dynamic fracture. The hyperbolic form of the evolution equations offers notable advantages over other PDE formulations.

From a computational perspective, the hyperbolic model enables the construction of a fully explicit scheme, allowing the solution of primary fields without requiring linear solvers. The proposed algorithm demonstrates efficient parallel performance, achieving superlinear scaling in the linear solve and sublinear scaling for the overall algorithm. The explicit scheme's time step, proportional to the mesh size, is generally larger than that of the parabolic model, which scales with the square of the mesh size. Furthermore, by leveraging the lumped mass matrix and the hyperbolic formulation, the explicit scheme is shown to be approximately five times faster than its implicit counterpart for equivalent time steps in a sample problem.

From a modeling standpoint, the hyperbolic model ensures a finite speed for damage propagation, controllable via the speed ratio between the damage wave speed and the elastic wave speed. This feature contrasts with elliptic models, where the damage propagation speed implied by the differential equation is infinite. We believe this characteristic contributes to some of the unrealistic fracture patterns observed in simulations based on the elliptic phase-field equation. The hyperbolic model,

on the other hand, successfully predicts realistic crack patterns observed in PMMA fracture experiments, provided the parameters of the proposed phase-field equation are appropriately tuned. However, a limitation of this work is the overestimated rate dependency in fragmentation problems at very high rates when compared to Grady’s analytical values.

The primary contributions of this research are summarized as follows:

I: Mathematical analysis

- Derivation of a thermodynamically consistent framework for hyperbolic models, systematically identifying micro-quantities.
- Development of asymptotic ODEs for phase-field models, enabling the derivation of rate sensitivity for different models and facilitating their comparison with actual phase-field solutions.
- Generalization of closed-form rate dependency from phase-field models to other damage models.

II: Scientific computing

- Implementation of a general phase-field fracture code supporting various models (AT1, AT2, and CZM) with potential extensions to multi-physics problems (*e.g.*, thermo-mechanical models).
- Development of implicit and explicit time integration schemes for hyperbolic, parabolic, and elliptic PDEs.
- Design of a parallel adaptive mesh refinement strategy for dynamic fracture problems.

III: Physical models and findings

- Development of the first hyperbolic ductile fracture model at finite strain.

- Application of fracture models to dynamic fragmentation problems.
- Numerical prediction of realistic crack patterns in PMMA experiments under different loading rates.
- Comparison of the rate dependency of different phase-field equations with analytical and empirical results.

Several avenues for extending the theoretical framework and computational implementations developed in this work are identified.

First, building on the validated 1D fragmentation results in Chapter 2, an extensive parametric study could investigate the effects of key model and loading parameters, including fracture length scale, loading rate, material strength, correlation length, and point-wise variations in random fields for certain material properties. These studies could generate valuable datasets for constructing surrogate machine learning models. Furthermore, extending the 1D study to 2D fragmentation introduces challenges such as fragment counting and high computational costs. Statistical approaches and image recognition techniques, as demonstrated in [143], could address fragment counting, while parallelized and efficient codes from Chapter 3 could mitigate computational expense.

In Chapter 3, although realistic crack patterns in PMMA experiments were successfully reproduced, extensive parametric studies were required to fine-tune key factors such as the speed ratio κ and the correction factor for crack initiation χ . Future work could explore incorporating strain-rate-dependent or phase-field-dependent variations of the speed ratio κ , the correction factor χ , or the critical energy release rate G to enhance the model's generality and predictive accuracy.

The theoretical framework for hyperbolic models developed in Chapter 3 provides a foundation for incorporating additional dissipative processes, such as corrosion or hydrogen embrittlement. These phenomena are particularly relevant in industrial applications, especially in the context of nuclear reactor materials, where such degradation mechanisms significantly affect long-term performance and safety.

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Appendices

Appendix A

Verifications

A.1 Time-marching scheme

For all dynamic simulations, Newmark- β method [107] is utilized. Using the method of manufactured solutions, a bar of unit length is considered, with its response governed by

$$\ddot{u} = (u)'', \quad (\text{A.1})$$

subject to the following initial conditions

$$\begin{cases} u(x, t = 0) &= 0, \\ \dot{u}(x, t = 0) &= -\pi \cos(\pi x), \end{cases} \quad (\text{A.2})$$

and boundary conditions

$$\begin{cases} u(x = 0, t) &= -\sin(\pi t), \\ \dot{u}(x = L, t) &= \sin(\pi t). \end{cases} \quad (\text{A.3})$$

The analytical solution for Eq. A.1 is $u(x, t) = -\sin(\pi t) \cos(\pi x)$. For the explicit scheme, the Courant-Friedrichs-Lewy (CFL) condition must be below 0.6; otherwise, the solution becomes unstable and diverges.

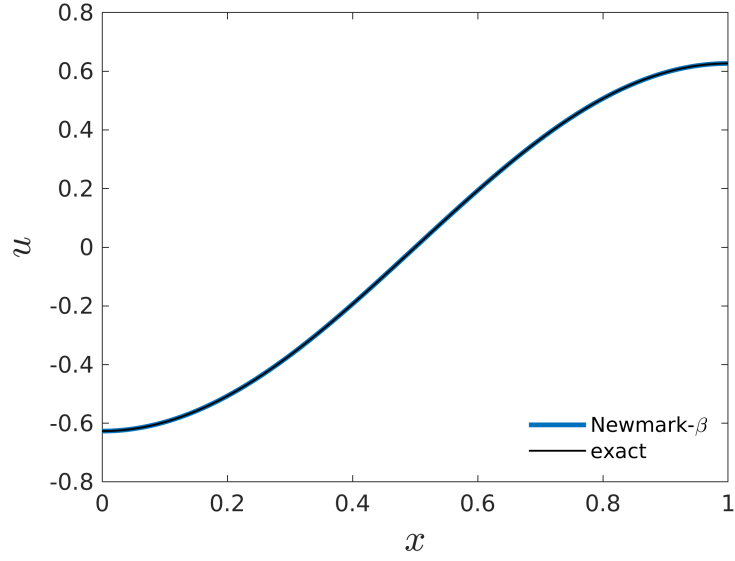


Figure A.1: Harmonic test. $\Delta x = 1/2^{10}$, CFL=0.95

A.2 Quasi-static single phase field element

The problem setup and corresponding analytical solution are described in [144]. A 2D unit square is constrained in both the x and y directions along its bottom edge, while the top edge allows for vertical sliding. The material parameters are set to $E = 210 \text{ kN/mm}^2$, $\nu = 0.3$, $G = 5 \cdot 10^{-3} \text{ kN/mm}$, $b = 0.1 \text{ mm}$. Equal increments of $\Delta u_y = 10^{-4} \text{ mm}$ are applied at the top edge over 1000 steps. Figure A.3 demonstrates a good agreement between the numerical and analytical solutions.

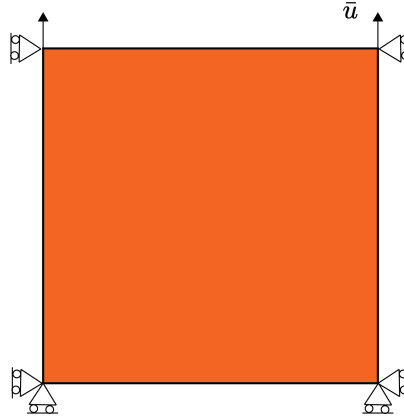


Figure A.2: Single element. Problem setup and boundary conditions.

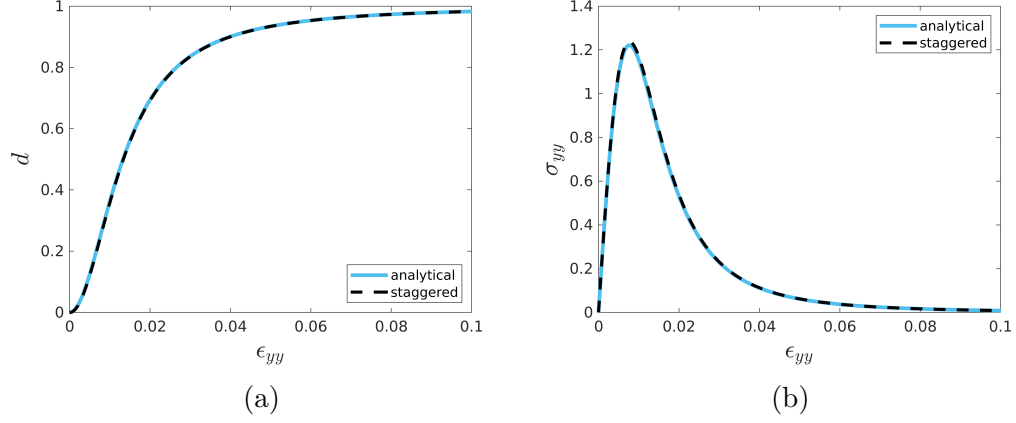


Figure A.3: Single element. a) phase field versus axial strain, b) axial stress versus strain

A.3 Quasi-static bar under tension

A bar of length $L = 200$ mm is subjected to uniaxial loading. The left edge is fixed, while the right end is pulled under an increasing displacement. The material properties are defined as follows: Young's modulus $E = 3.0 \cdot 10^4$ MPa, Poisson's ratio $\nu = 0.2$, failure strength $\tilde{\sigma}_c = 3.0$ MPa and critical energy release rate $G = 0.12 \text{ N} \cdot \text{mm}^{-1}$.

Fig. A.5 illustrates a close agreement between the numerical and analytical solutions.



Figure A.4: Traction bar. Geometry and boundary conditions.

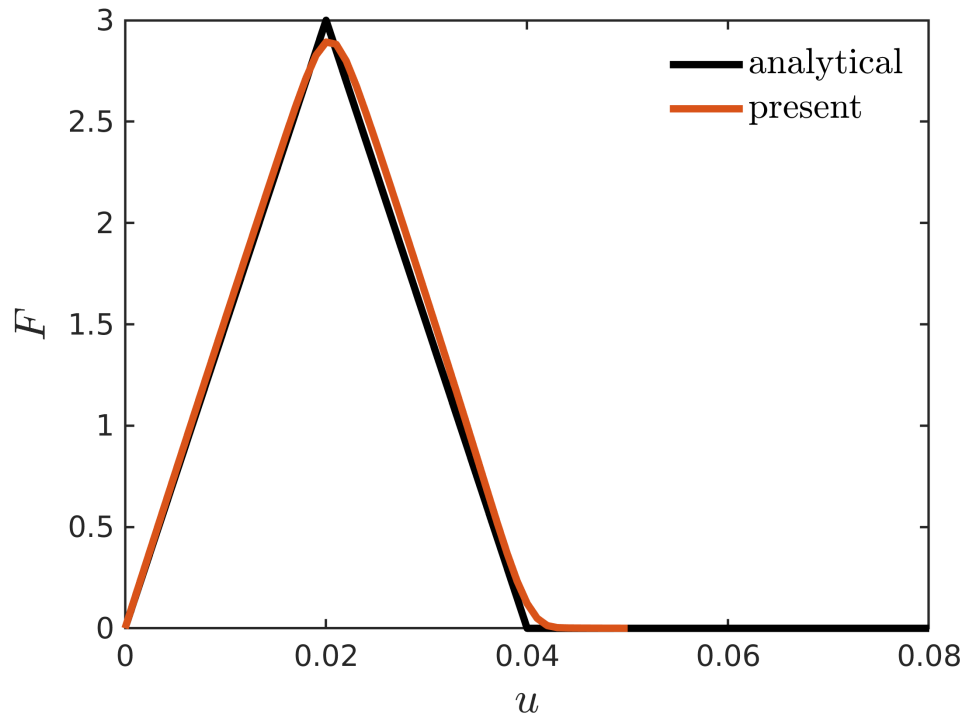


Figure A.5: Traction bar. Load-deflection curve.

Appendix B

Validations

B.1 Single-edge notched shear test

This example is a standard quasi-static benchmark problem in phase field modeling, as proposed by Miehe et al. [16]. A square unit plate $1 \times 1 \text{ mm}^2$ is fully constrained at the bottom edge, while the top edge is subjected to pure shear loading, as shown in Figure B.1a. The material properties are defined as: Young's modulus $E = 210 \cdot 10^3 \text{ N/mm}^2$, failure strength $\tilde{\sigma}_c = 2000 \text{ N/mm}^2$, energy release rate $G = 2.7 \text{ N/mm}$, Poisson ratio $\nu = 0.3$, and length scale $b = 0.005 \text{ mm}$.

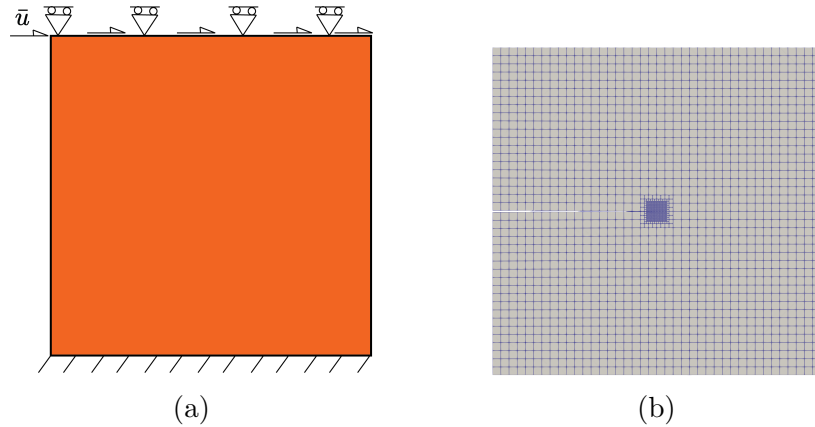


Figure B.1: Single edge notched shear test. a) Problem setup and boundary condition b) An original mesh with a priori refinement at the tip.

A mesh convergence study with respect to the load-deflection curve is conducted. An initial uniform mesh with quadrilateral elements of size $h = 1/2^4$ is generated, followed by local a priori refinement at the crack tip, located at the center of the plate (Figure B.1b), where stress concentration is high and potential crack initiation is expected. Three different mesh refinement strategies are employed during simulation, as listed in Table B.1. A fixed displacement increment of $\Delta\bar{u} = 1e - 5$ mm is applied until the total displacement reaches $\bar{u} = 0.02$ mm.

Figure B.2 shows the crack patterns at different loading stages. Cracks initiate at the pre-defined tip and propagate toward the bottom-right corner. The same crack trajectory is observed across all three meshes, but only the results for Mesh 2 are reported here. The final crack path aligns well with the reference in Miehe et al. [16]. Figure B.3 presents load-deflection curves for each mesh. The coarsest mesh (Mesh 1) shows delayed crack initiation and overestimates the peak load, while the curves for Meshes 2 and 3 are similar and agree well with the reference results in Wu et al. [30], which used a computational domain discretized with 390000 elements.

Further analysis is conducted to study the effect of varying displacement increments, ranging from $\Delta u = 2 \cdot 10^{-4}$ to $\Delta u = 1 \cdot 10^{-5}$, on mechanical responses. The displacement increment remains constant throughout the simulation, and Mesh 2 is utilized. For a fair comparison with Wu et al. [30], the largest increment $\Delta u = 2 \cdot 10^{-4}$ is used. Figure B.4a plots the load-deflection curves, while Figure B.4b shows the iteration count at each loading step. Larger increments prevent crack propagation and overestimate the peak load, a behavior also reported by Singh et al. [145] using a

Table B.1: Single-edge notched shear test. Mesh configurations for a convergence study.

	$gl + pr + lr$	Number of elements	
		Initial mesh	Final mesh
Mesh 1	0 + 3 + 1	796	6484
Mesh 2	1 + 3 + 1	1384	4575
Mesh 3	1 + 4 + 1	2536	19918

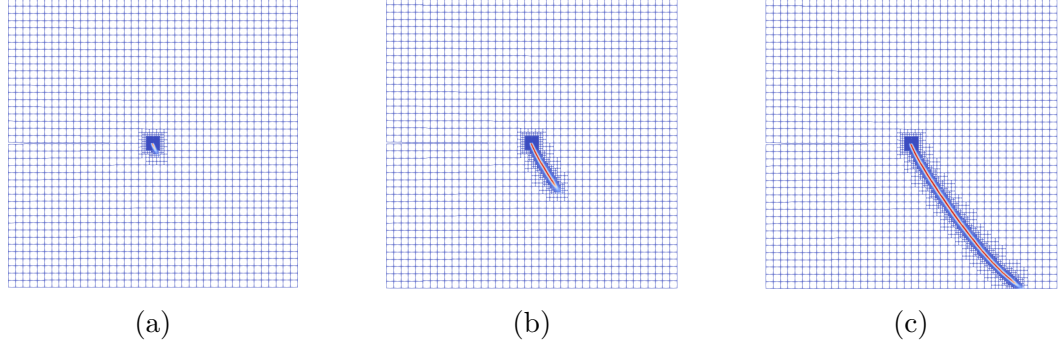


Figure B.2: Single edge notched shear test. Crack path at different instants

standard Newton method. As the increment decreases, the solution converges towards the results obtained by the BFGS solver in Wu et al. [30].

In terms of efficiency, the solution with $\Delta u = 2 \cdot 10^{-4}$ requires only 4 iterations at critical steps out of 125 total loading steps, resulting in 425 total iterations. This compares favorably to the 3,131 iterations required by the BFGS solver in Wu et al. [30], which also used a maximum iteration count of 100. The staggered scheme in Wu et al. [30], claimed to be slower than the monolithic and BFGS solvers, required more than 400 iterations at critical steps and 9,300 total iterations. Table. B.2 lists the total iterations corresponding to other loading increments in this study.

While smaller increments are needed to match the BFGS solutions in Wu et al. [30], the current implementation still performs better than the standard solver and

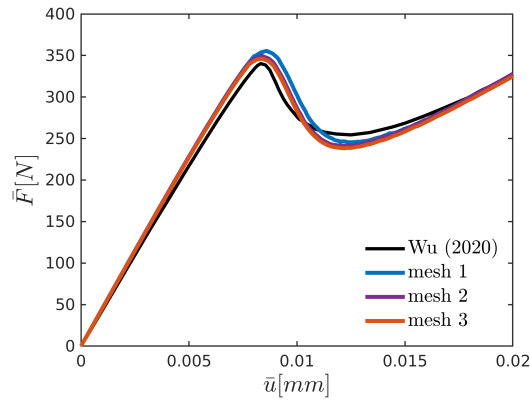


Figure B.3: Single edge notched shear test. a) Load-deflection curve b) iteration number

Table B.2: Single edge notched shear test. The total number of iterations for varying increment.

	Δu				
	$2 \cdot 10^{-4}$	$1 \cdot 10^{-4}$	$5 \cdot 10^{-5}$	$2 \cdot 10^{-5}$	$1 \cdot 10^{-5}$
Total number of iterations	425	324	1089	2669	5334

requires fewer iterations with an intermediate increment ($\Delta u = 2 \cdot 10^{-5}$), which approximates the BFGS solution reasonably well. It is expected that the number of iterations could be further reduced by using adaptive increments, allowing larger increments in the elastic and late post-peak regions. Additionally, the present results are achieved with only 4,575 elements, compared to the 390,000 elements used in Wu et al. [30].

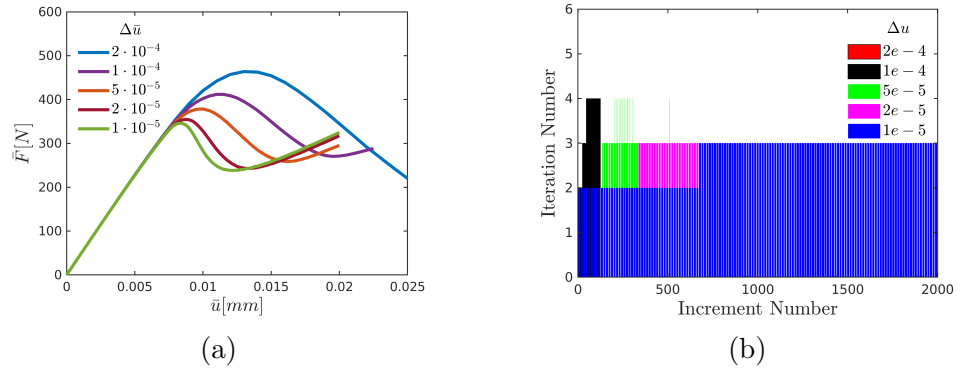


Figure B.4: Single edge notched shear test. Mesh convergence study. a) Load-deflection curve b) iteration number

Vita

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