1 ABSTRACT

Through this STIR proposal we propose to initiate research in a challenging new direction of theoretical solid mechanics. Variational, regularized fracture (VRF) theory shows tremendous potential for revitalizing fracture mechanics by opening up new paradigms for understanding and modeling fracture phenomena. The VRF theory-based numerical methods are ideally positioned to galvanize revolutionary developments in the computational design of high-toughness materials. However, currently, VRF theory is insufficiently developed from a solid mechanics perspective. Several fundamental mechanics issues must be resolved before VRF theory can be considered a valid theory of fracture. Resolution of these fundamental issues is expected to be quite challenging and hence requires a long-term, concerted effort involving techniques from many sub-fields of mechanics and applied mathematics. However, even a partial resolution of the identified issues could lead to revolutionary developments in theoretical and computational solid mechanics. Therefore, in order to gauge the magnitude of the challenge and the potential effectiveness of future research, we propose a pilot research program to address a key mechanics issue in the VRF theory termed the "non-localization problem". This issue is foremost among those that need to be resolved before VRF can be considered a valid theory of fracture. Furthermore, the scope of this problem is ideally suited for the time frame of the STIR project.

In classical theories, fracture is modeled as displacement discontinuities across curves and surfaces. In VRF theories fracture is represented using a scalar field. When the scalar variable, ϕ, is zero at a certain point in the domain, the material there is taken to be completely intact, whereas when ϕ is unity the material is taken to be completely disintegrated. The solid's elastic strain energy density is reduced to zero as ϕ increases to unity. The specific form of this strain energy reduction is given by the degradation function $g(\phi)$.

For the $\phi = 1$ level set to be considered a reasonable approximation of the crack path it is necessary that the thickness of the region over which ϕ is not close to zero be small compared to the other length scales in the problem. In this case, we refer to the damage field as "localized". It is generally believed that when the length scale parameter in the VRF theory, ℓ_0, is small compared to the other length scales in the problem, then the damage field will be localized. However, through our preliminary research we found that this is not always the case. We found that even when $\ell_0 \to 0$ there exists a mode of damage that is "non-localized". Specifically, through our preliminary research we have found that in certain cases the VRF theory predicts a failure mode that is spatially spread out and produces a stress-strain response closer to plastic yielding than to fracture. We plan on resolving this issue by deriving a list of constraints that $g(\phi)$ must satisfy. These constraints will ensure that the failure mode in the VRF theory is always localized. We will begin by treating the governing equations of the VRF theory analytically and capturing the asymptotic behavior of the stress, strain, and ϕ close to the tip of a propagating crack. Motivated by linear elastic fracture mechanics (LEFM), we expect the asymptotic behavior to have certain universal forms for a given $g(\phi)$. The constraints on $g(\phi)$ will be derived by requiring that ϕ ahead of the crack tip always remains localized irrespective of the nature of the far-field loading.

By resolving the issue of localization, the proposed research will inaugurate an important line of investigation that will ultimately culminate with the realization of the VRF theory's tremendous potential.

Introduction-vision

2 VARIATIONAL, NON-SINGULAR THEORY OF FRACTURE FOR THE COMPUTATIONAL DESIGN OF HIGH-TOUGHNESS COMPOSITES

2.1 INTRODUCTION

Understanding the mechanics and physics of fracture is of great scientific and engineering importance. In classical fracture theories, such as LEFM and Dugdale-Barenblatt, fracture is modeled as displacement discontinuities across curves and surfaces. The classical theories are numerically solved using techniques such as cohesive zone methods (CZM) [1, 2], and extended finite element method (XFEM) [3], which have proven extremely useful over the years. However, those numerical methods run into difficulties when solving for the evolution of complicated systems of cracks (see Fig. 1), especially in 3D and/or heterogeneous materials. Handling the evolution of crack networks that consist of intersecting and branching cracks is even more difficult. Variational, regularized fracture (VRF) theory is a technique that circumvents these difficulties.

The VRF theory is an approximate model for fracture in which complex crack patterns are represented by the level set of a scalar-valued field, ϕ, termed the damage field. The VRF theory is briefly reviewed in §2.4.1. Numerical methods based on the VRF theory have emerged as highly attractive and powerful computational tools that can simulate the evolution of complex crack patterns. The VRF methods are usually implemented using finite element (FE) methods. In standard FE-based computational fracture mechanics frameworks, such as singularity element based methods [4], as the crack pattern evolves the domain of the problem continually changes. The traction free boundaries of the problem change in a similar fashion. Therefore, a new computational mesh must be generated after each crack growth increment. Preparing meshes of sufficient quality to ensure convergence of the numerical solution procedures in fracture problems is a very challenging task, especially when dealing with branched or intersecting cracks [5]. In VRF methods there is no need to re-mesh the solid after each crack growth increment. This is because the crack is represented by a scalar field, and therefore from a mathematical perspective there is no change in either the domain or the boundary of the problem. In this sense, solving for the evolving damage field in VRF methods is akin to solving for an evolving temperature field in a coupled thermoelastic problem. This leads to a substantial simplification in setting up and running the simulations, especially when dealing with complicated crack patterns or 3D problems.

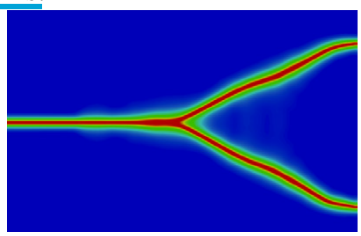

Figure 1: The phenomenon of crack branching is observed in glass under dynamic loads and is captured using VRF methods (see [5] for more details).

While methods like CZM and XFEM also do not require remeshing, the VRF methods still have certain important advantages. The evolution of ϕ in the VRF theory is coupled to the macroscopic, mechanical constitutive law of the solid through the length scale parameter ℓ_0, which is termed the regularization parameter. The parameter ℓ_0 is crudely analogous to the size of the cohesive zone in the Dugdale-Barenblatt theory. The introduction of ℓ_0 makes the results of the VRF methods insensitive to the FE mesh. In contrast, the results of CZM and XFEM are strongly affected by the FE mesh. Furthermore, in CZM and XFEM, *a priori* knowledge of topology changes in the evolving crack pattern, such as crack branching, is needed in order to capture those scenarios correctly. In VRF methods, however, this *a priori* knowledge is not needed. Crack branching, merging, and nucleation are all handled automatically in VRF methods (see Fig. 1). A drawback

specific to XFEM is that during the simulation the crack growth can cut elements into arbitrarily small pieces, which leads to ill-conditioned matrices. This ill-conditioning leads to serious convergence problems [6, 7].

Research Question

PROBLEM STATEMENT. Owing to the VRF methods' attractive computational features, they can be used to perform robust, virtual experiments for a variety of complex fracture problems, such as hydraulic fracturing and dynamic crack branching. Despite their tremendous potential, the VRF methods have not been well-accepted by the solid mechanics community. The primary reason behind this is the concern that the VRF theory may not be valid as a reasonable and predictive fracture mechanics theory. The VRF theory has been well-analyzed from a mathematical perspective. However, it was formulated with minimal inclusion of mechanics principles, such as the irreversible nature of fracture, material frame indifference, and crack tip physics, such as material deformation behavior, dissipative mechanisms, and cohesive forces. For this reason it is natural to question – are the predictions of the VRF theory always meaningful? More specifically, one would like to know: Q.I Does the damage field in the VRF theory share the essential physical characteristics of fracture? If not, how can that be rectified? Q.II ~~Will a VRF model's predictions always match those of some particular classical fracture mechanics model?~~ Q.III What is the specific form of a VRF model that corresponds to a particular classical nonlinear fracture model, e.g., the Dugdale-Barenblatt model? ~~Q.IV How should one revise the VRF theory so that the irreversibility of the fracture process is built into the variational formalism?~~

2.2 RESEARCH OBJECTIVE AND JUSTIFICATION

OVERARCHING OBJECTIVE AND CONTRIBUTION TO FUNDAMENTAL SCIENCE. The overarching objective of the proposed research is to answer questions Q.I–IV. Investigating these questions and revising the VRF theory will build a strong solid mechanics foundation for the VRF theory and its related methods. It will shine light on the issues of validity, predictive potential and on the limitations of the VRF theory. This knowledge is critical if the VRF theory and its related methods are to be adopted by the solid mechanics and the engineering science communities.

Intellectual merit

We believe that once provided with a strong solid mechanics foundation, the VRF methods will emerge as revolutionary computational tools that will re-energize the important field of fracture mechanics. These tools will provide invaluable support and guidance in answering some long-standing questions in fracture mechanics that are of fundamental scientific importance, such as the effect of disorder in fragmentation [8]. We also believe that by providing a new paradigm for understanding fracture, the VRF theory will open up new questions, challenges, and applications in the fundamental science of fracture.

SPECIFIC RESEARCH OBJECTIVE (*SRO*): *To resolve the problem of "non-localization" in the VRF theory presented in [5].* Different versions of the VRF theory can be found in the literature [5, 9, 10]. We will focus on the VRF theory presented in [5]. Through our literature survey we found that this version of the theory has a stronger mathematical foundation, and is more suitable for handling engineering problems. We refer to the VRF theory presented in [5] simply as the VRF theory in the remainder of this document. The VRF theory predicts two different failure modes. One mode is spatially localized and corresponds to fracture type failure. Another mode exists, however, that is spatially spread out ("non-local"). This non-local failure mode is an artifact of the VRF theory. This spurious, non-local failure mode appears in other versions of the VRF theory as well, such as the one presented in [9]. We describe the non-local failure mode further in §2.4.3

JUSTIFICATION OF THE *SRO*. Over the course of this STIR project we will reformulate the

VRF theory to remove the spurious, non-local failure mode. The tasks we plan to undertake to achieve the *SRO* are described in §2.5. The issue of non-localization is foremost among the issues that need to be resolved before the VRF theory can be considered a valid theory of fracture. Therefore, achieving the *SRO* will help to answer the fundamental question Q.I and will place the VRF theory on a stronger solid mechanics foundation.

Research Question

The overall research objective (answering questions Q.I–IV) is quite challenging and high risk. The research conducted to achieve the *SRO* will allow us to better gauge the magnitude of the challenges posed by Q.I–IV. It will provide the information needed to launch a large-scale, concerted effort to answer Q.I–IV, and it will also help to ascertain the effectiveness and appropriateness of the research strategy the PI plans to adopt to answer Q.I–IV.

2.3 Relevance of the Proposed Research to the Army's Mission

The proposed research is highly relevant to the Army's mission and vision. It specifically contributes to the following solid mechanics goals of the Army Research Office: (a) *Deterministic scaling methodology for toughness that accounts for heterogeneities*, (b) *Techniques to eliminate trade-off of strength and toughness*. The VRF numerical methods are ideally suited for the computational design of the next generation of high-toughness, composite materials that are based on μ-structural design motifs. We found using VRF methods, that the "Wavy-Interface" (WI) design motif has especially strong potential for serving the Army's need for high-toughness materials (see §2.4.2 and Fig. 4). Protective materials such as body armor, and vehicle cladding must have high-toughness and damage tolerance in order to be able to endure intense mechanical loads without failing catastrophically. As we describe below, the WI motif has been inspired by structural biomaterials (SBs) that show an exceptional capability for containing damage and absorbing energy during impact or shock loading.

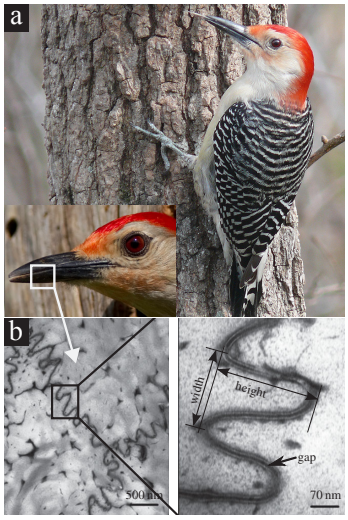

Figure 2: (a) Shows a red-bellied woodpecker (*Melanerpes carolinus*) [11]; the inset provides a closer view of its beak [12]. (b) The μ-structure of the beak consists of wavy interfaces between keratin scales on the outermost layer [13].

Structural biomaterials such as shells, and antlers have evolved to withstand impacts without failing [14, 15]. These materials are composites that consist of a stiff, often ceramic, phase and a compliant, organic phase arranged in intricate patterns at the μ-meter scale. While the stiff phase, which constitutes 95% of the material by volume, is often quite brittle and weak, the bulk toughness of SBs can be hundreds to thousands of times larger than what is predicted by the rule of mixtures [14]. It has been shown that the SBs' μ-structure – i.e., the arrangement of the individual phases – is the key to this remarkable toughness [16]. One μ-structural motif that appears in many tough SBs is the wavy interface. This is an undulating junction that joins two pieces of the stiff phase, often using a thin layer of the organic phase. Wavy interfaces can be found in the outermost layer of woodpecker beaks [13] (see Fig. 2) and between the cranial bones of rams [17]. Interestingly, these SBs experience impact or cyclic dynamic loads and must remain intact in order to perform their mechanical functions. This suggests that WIs are a key ingredient for enhancing toughness in these SBs.

Many researchers have produced model structures that contain synthetic analogues of the WIs observed in SBs and have shown experimentally that the wavy nature of the interfaces does indeed

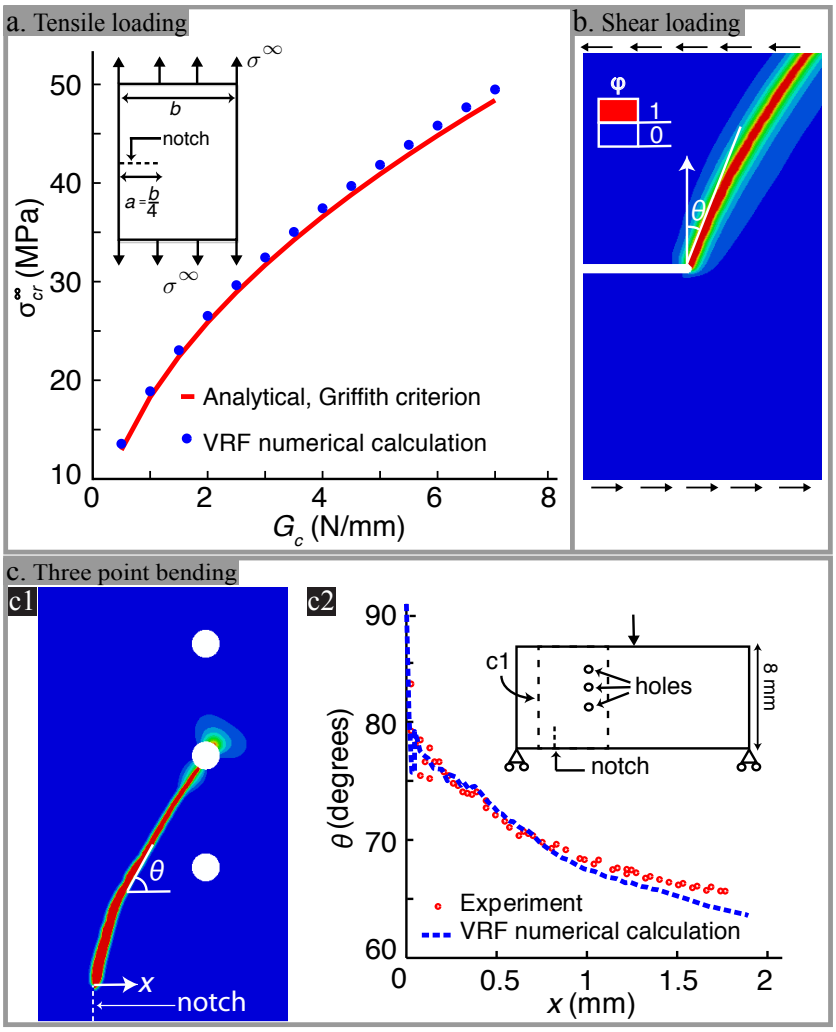

Figure 3: (a) Edge-notched geometry subjected to a far-field stress σ^∞. The stress σ^∞_{cr}, which is the far-field stress at which crack growth initiates, is plotted as a function of fracture toughness, G_c. The red curve is the analytical prediction from the Griffith criteria, the blue points are results from VRF simulations. (b) shows the damage field ϕ ($\phi = 1$ being the crack path) for a notched plate subjected to pure shear (Mode II) loading on the horizontal boundaries. The VRF simulations show a kinked crack propagating at an angle of $\theta = 21.4°$ from the notch tip. This value is close to the kink angle of 19.5° that is predicted by the principle of local symmetry. (c1) shows the crack path for an edge-notched geometry with 3 holes subjected to 3-point bending (see inset in (c2)) predicted by the VRF simulation. (c2) The crack path from the VRF simulations (shown in (c1)) compares very well with the experimentally observed crack path (see [20] for experiment details).

enhance the work of fracture [18]. Even before WIs in nature drew the attention of engineers, it was shown using fracture mechanics calculations [19] that making an interface wavy can indeed increase a material's effective toughness. The examples from biology as well as the theoretical and experimental studies strongly suggest that the WI μ-structural motif can indeed enhance toughness and damage tolerance in composite materials without causing an appreciable loss of strength. However, despite the toughness enhancing potential of WIs and the critical need for high-toughness materials, WIs are seldom seen leveraged in engineering materials. In addition to manufacturing difficulties, we believe that the absence of WIs is primarily due to the lack of robust computational fracture mechanics tools that can resolve the highly nonlinear, toughening mechanisms occurring in WIs. We found examples of such mechanisms during our preliminary research using a VRF model (see §2.4.2 and Fig. 4). Such computational tools are needed for the design and optimization of WIs, and other similar μ-structural motifs. We believe that the proposed research will ultimately lead to the development of such computational tools.

Phase field theory

In order to grasp the fundamental theory of phase field, I need to carefully read the following papers [1–8].

Griffith's contribution: the criterion for crack propagation. Drawbacks: cannot predict the crack initiation, kinking, branching, and curvilinear crack paths. Such shortcomings of Griffith-type brittle fracture theory can be overcome by the variational method based on energy minimization principle, as first proposed by Francfort and Marigo [1].

The total energy of the body containing cracks includes bulk elastic energy and surface energy. It is a postulation, instead of derived from any known thermodynamical argument, that the evolution of crack surface should always minimize the total energy. The evolution of the crack obeys the following law: (a) Irreversibility condition requires the crack grows with time or external loading; (b) The total energy of the actual crack is minimal among all the possible compatible cracks at a given time; and (c) The total energy of the actual crack at the current time should be lower than that of all prior cracks for a fixed loading [1].

The strong formulation of the problem lies in a domain containing a sharp crack surface topology with displacement discontinuity, which is very difficult to solve mathematically. The regularization of the strong formulation of variational brittle fracture problem is inspired by the work of Ambrosio and Tororelli [9], which proposed a regularized formulation to approximate the Mumford-Shah [10] image segmentation functional depending on jumps. The functional form of weak formulation is borrowed from [9] (very similar form). An auxiliary variable, called as phase field parameter, is introduced to represent the jump set. The two-field functional approximation has been proved to be Γ-convergent to the one-field one for free discontinuity problems. See the details of Γ-convergence proof in [9]. A numerical implementation of the regularized formulation is first presented by Bourdin et. al [2].

Miehe et. al [5, 6] present a thermodynamically consistent phase field model in which the sharp crack discontinuity is overcome by a diffusive crack. The regularized diffusive crack surface functional Γ-converges to a sharp crack topology functional for vanishing length-scale parameter [11]. The two-field setting of the variational frame work is close to that of Bourdin et. al [2, 3]. One of the major contributions is the proposed energy decomposition based on operator splits, which suppresses the crack growth under compression stress state.

Borden et. al [7] extend the Miehe's model of quasi-static brittle fracture to the dynamic case. The essence of the model is the same except including the kinetic energy.

The framework of phase field fracture by Hakim and Karma [4] is different in spirit from Bourdin et. al [3] and Miehe et. al [5]. It is based on the classical Ginzburg-Landau type evolution equation. The evolution of the phase field parameter is governed by the dissipative dynamics. The model based on Ginzburg-Landau phase transition is particular to dynamic fracture problems.

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2.4 Scientific Approaches

2.4.1 VRF Theory: Some Technical Details

For a detailed discussion of the VRF theory see [9, 10]. The VRF formalism is a generalization of the configurational force balance ideas put forward by Griffith. The fundamental postulate underlying the theory is that the crack pattern and the associated displacement field simultaneously evolve in the "direction" that reduces the total energy of the system by the maximum possible amount[1]. Here, the term "direction" is used in a functional analysis sense. Traditionally, the total energy is written as the sum of two terms that are written as $\int_\Omega \psi_e(\nabla u, x)\, d\Omega$ and $\int_\Gamma G_c\, d\Gamma$, where $\psi_e(\nabla u, x)$ is the solid's strain energy density, G_c is the fracture toughness, and Γ is the crack curve/surface in the reference configuration. The first term is an area/volume integral, whereas the second term is a line/surface integral. This makes it very difficult to calculate the direction, and consequently the crack path. In order to circumvent this problem the damage field ϕ is introduced to convert the surface energy term to an area/volume integral. Thus, in the VRF theory the surface energy term becomes $\int_\Omega G_c/2 \left(\ell_0 \|\nabla\phi\|^2 + \phi^2/\ell_0\right) d\Omega$, where $\|\cdot\|$ is the Euclidean 2-norm. Additionally, as ϕ increases to unity at a point, the elastic strain energy density there is reduced to zero. The specific form of the reduction is given by the degradation function $g(\phi) = (1-\phi)^2$. Thus, in the VRF theory the elastic strain energy is $\int_\Omega g(\phi)\psi_e(\nabla u, x)\, d\Omega$.

Having the energy functional consist of only area/volume integrals, the governing equations can now be derived using standard techniques from the calculus of variations (see [5] for details). Even when modeling a linear elastic solid the governing equations come out to be a coupled system of nonlinear PDEs. The PDEs are solved using FE methods (see [5] for details).

2.4.2 Preliminary results

In classical fracture models there are several criteria that are used to predict the direction of crack growth, such as the principle of local symmetry, and the maximum energy release rate (MERR). In VRF theory, the crack growth and crack pattern evolution laws emerge naturally from the variational formalism. For example, for a single crack it has been shown that the kink angle, θ, is selected by requiring that at the crack tip (i) $G = G_c(\theta)$, and (ii) $\partial G/\partial\theta = \partial G_c(\theta)/\partial\theta$, where G is the local energy release rate at the crack tip, and $G_c(\theta)$ is the anisotropic material toughness [9]. We have performed extensive numerical experiments to compare the results of the VRF theory with analytical solutions and experimental measurements from literature. In all the cases that we studied, the VRF results match the analytical and experimental results to a remarkable degree (see Fig. 3).

We were also able to simulate crack propagation in materials with WIs, which is important to the Army's mission (§2.3). We did so by allowing G_c to vary spatially, so that in most of the solid it had a high value, G_∞, and at a predefined wavy interface of finite thickness, it had a low value, G_I. In our preliminary simulations depending on the parameter regime of A/λ and G_I/G_∞ the failure of the interface displayed very rich mechanics. Here, A and λ are the amplitude and the wavelength of the WI, respectively. For example, we found that at small A/λ the crack always propagated along the interface, see Fig. 4 (a). However, at larger A/λ the crack repeatedly ventured out of the interface into the bulk and then back into the interface through a series of energy dissipating

[1] We do not adopt the perspective that the crack pattern is a global minimizer of the energy functional, as done, e.g., in [10].

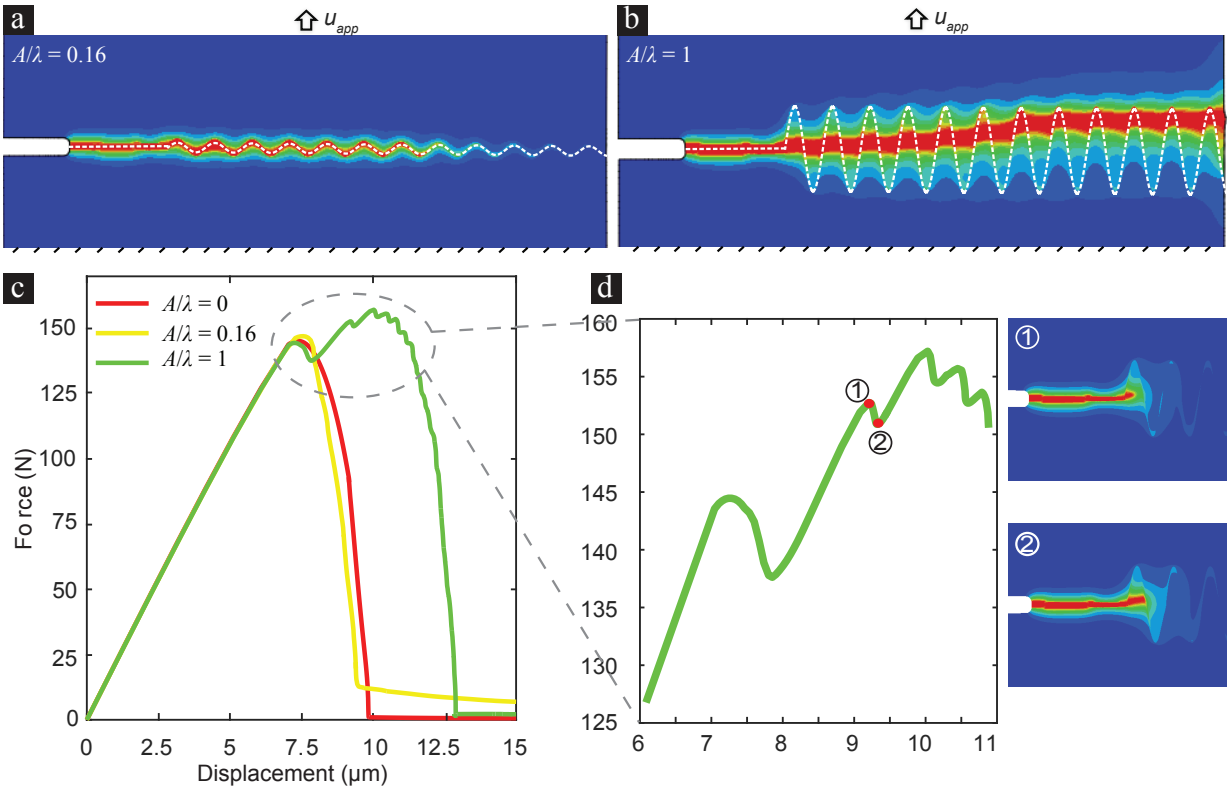

Figure 4: Simulation of fracture of WIs. The specimens are 1 mm squares. The interface is shown as a dashed line in (a) and (b). The material shear and bulk moduli are 8 and 17 GPa, respectively, and G_∞ =0.5 N/mm. At the interface, $G_I = G_\infty/10$. The interface wavelength λ is 0.0625 mm, and the regularization parameter ℓ_0 =0.009 mm is used in the simulation. (a) Crack propagation along the interface for small amplitude, $A = 0.01$ mm. (b) Crack jumping out of the interface and through the bulk material for large amplitude, $A = 0.0625$ mm. (c) Load-displacement curves. (d) Close-up view of the load-displacement curve indicated by the dashed ellipse in (c) showing the instabilities during the crack propagation. The transition from configuration 1 to 2 corresponds to the sudden movement of the crack from the interface into the bulk.

instabilities (see Fig. 4 (b)–(d)). This lead to substantial toughening in the load-displacement response (see Fig. 4 (c)–(d)).

2.4.3 Spurious, Non-local Failure Mode in the VRF Theory

The issue of non-localization can be best described in the 1D case. While a crack path only makes sense in 2 or 3D, in 1D one can still study the occurrence of a rupture event, which is analogous to unstable crack initiation in higher dimensions.

Consider a linear elastic bar of length a and Young's modulus E. The bar is clamped at one end and a displacement of u_{app} is applied at the other. For this problem, one of the governing equations of the VRF theory in dimensionless form reads,

$$\hat{\phi}''(\xi) - \alpha^2\hat{\phi}(\xi) + \beta g'(\hat{\phi}(\xi))\left[g(\hat{\phi}(\xi))\right]^{-2} = 0, \quad \forall \xi \in (0,1), \qquad (1)$$
$$\hat{\phi}'(0) = \hat{\phi}'(1) = 0,$$

where $\hat{\phi}(\xi) = \phi(x)$, $x \in (0,a)$, $\xi = x/a$, and $\alpha = a/\ell_0$. The parameter $\beta = \sigma^2 a^2/EG_c\ell_0$ is the dimensionless, homogeneous stress in the bar. Recall that $g(\hat{\phi}) = (1-\hat{\phi})^2$. Through a phase plane analysis of Eqn. (1) we found that there always exist two qualitatively distinct solutions for the

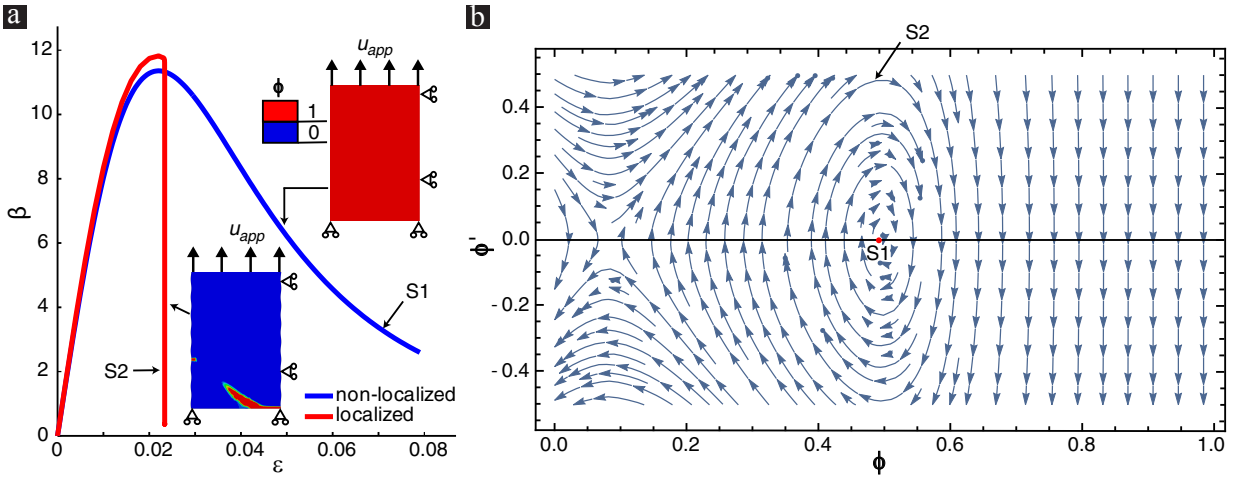

Figure 5: (a) Finite element results from a 2D simulation that approximates the 1D problem discussed in §2.4.3. Dimensionless force β vs. average strain in the bar $\varepsilon = u_{\text{app}}/a$. The red curve corresponds to the localized failure mode, while the blue curve corresponds to the non-local failure mode. Representative damage fields corresponding to these two modes are shown as insets. (b) Phase plane plot of Eqn. (1). The localized failure mode corresponds to the closed orbits. An example orbit is marked as $S2$. The non-local failure mode corresponds to the nonlinear center, marked as $S1$. In (a) $\alpha = 166.67$ and in (b) $\beta = 0.632$ and $\alpha = \sqrt{10}$.

damage field $\hat{\phi}$ (see insets Fig. 5). The first one, which is non-local, corresponds to the nonlinear center marked as $S1$ in the phase plane (Fig. 5 (b)). The localized solution corresponds to one of the closed orbits. A representative closed orbit is marked as $S2$ in Fig. 5 (b).

Even though conceptually simple, we did not have the FE procedures set up to solve Eqn. (1), whereas we readily had FE procedures available to solve the 2D VRF equations. Therefore, we numerically solved a 2D problem that closely approximates the 1D problem represented by Eqn. (1). As the bar, represented by the rectangular geometry in 2D, is elongated, the simulation always selects the non-local failure mode (see Fig. 5 (a) top inset). Alternately, if the rectangular geometry is slightly perturbed, then the localized failure mode is always selected (see Fig. 5 (a) bottom inset). Representative stress-strain curves corresponding to these two cases are shown in Fig. 5 (a). To capture the localized failure mode, we perturbed the rectangular boundary using a sinusoidal waveform whose amplitude is small compared to the dimensions of the rectangle. In the calculations corresponding to the localized failure mode the stress drops abruptly after reaching a critical value. This is consistent with our interpretation of the localized failure mode as a fracture type failure. In the calculations corresponding to the non-local failure mode, the stress-strain curve resembles a strain-softening plastic yielding behavior, rather than a fracture event. In some damage models, the non-local failure mode might have some physical interpretation. But since the VRF theory specifically aims to model fracture, the non-local failure mode is simply an artifact which needs to be eliminated for the results of the VRF theory to be meaningful.

We have found the above conclusions to hold true in a number of 2D FE-based simulations.

COMPETING RESEARCH. The VRF community is aware of the non-local failure mode [5]. It is generally argued that the non-local failure mode will vanish as $\ell_0 \to 0$. Our calculations in 1D, however, show that the non-local failure mode persists even in the limit of $\ell_0 \to 0$.

2.5 Research Strategy and Tasks

Task.1. We will focus on the VRF theory in the context of 1D and 2D problems involving linear elastic solids. In 1D, the non-local failure mode is a consequence of the existence of the nonlinear center $S1$ shown in Fig. 5 (b). The presence or absence of the nonlinear center depends on the function $g(\phi)$. In the current VRF theory, the only constraints on $g(\phi)$ are $(c.1)$ $g(0) = 1$, and $(c.2)$ $g \to 0$ as $\phi \to 1$. The choice of the specific form of $g(\phi) = (1-\phi^2)$ is arbitrary. Therefore, we will achieve the *SRO* by constructing a new $g(\phi)$. Specifically, using nonlinear dynamics techniques, we will first derive the sufficiency conditions on $g(\phi)$ such that there are no nonlinear centers in the region $\phi \in [0,1]$ of the phase plane for all admissible β and α. Then, we will derive additional conditions by requiring that there must exist localized solutions, of the type $S2$ seen in Fig. 5 (b) for all admissible β and α. Essentially, $g(\phi)$ should create a stable limit cycle in the phase plane when $\phi \in (0,1)$. We will construct the simplest $g(\phi)$ that satisfies the newly derived constraints as well as the conditions $c.1$–2. *Task.2.* New FE procedures will be developed and implemented to solve Eqn. (1) for the newly constructed $g(\phi)$. *Task.3.* The FE simulations will be used to check whether the non-local failure mode has indeed been eliminated without also losing the localized one.

Task.4. It is unclear at this stage whether the newly constructed $g(\phi)$ would also eliminate the non-local failure mode in 2D. We plan on performing the following analysis in case the $g(\phi)$ derived from the 1D analysis falls short for the 2D case. We will analyze the governing PDEs of the VRF theory in 2D analytically. The complete solution might not be feasible, however, we have found that after a few transformations the VRF equations share some features with the 2D LEFM equations. Thus, we will use complex variable techniques, often used in LEFM, to solve for the asymptotic behavior of ϕ close to the crack tip. Motivated by LEFM, we expect the asymptotic behavior of ϕ to have certain universal forms for a given $g(\phi)$. Additional constraints on $g(\phi)$ in 2D will be derived by requiring that ϕ ahead of the crack tip always remains localized.

Task.5. The preliminary simulations on WI using VRF methods showed interesting mechanics (Fig. 4). However, we were unable to perform a thorough study of the toughening potential of WIs using VRF due to the problem of non-localization. We will use the VRF theory with our newly constructed $g(\phi)$ to study the toughening potential of the WIs. Specifically, we will investigate the WI's toughening effect as a function of A/λ, G_I/G_∞, and $E\lambda/G_\infty$.

2.6 Project Management

Anticipated difficulties and our plan to handle them. The simulations reported in §2.4.2 were based on FE meshes containing $\sim 500,000$ elements. In order to be prepared for computational difficulties that may arise while testing the new VRF methods we have allocated funds in the budget to procure additional computational resources. The number of Abaqus (finite element software) tokens required is proportional to the number of CPUs used in the parallelized FE calculations. Therefore, funds are requested as part of the budget to purchase additional Abaqus tokens. See §I for details.

Project time line. *Task.1:* Two months. *Task.2:* One month. *Task.3:* One month. *Task.4:* Three months. *Task.5:* Two months.

Research Team. The research team will consist of the PI and a graduate student at Brown. The PI will primarily develop the revised VRF theory, while the graduate student will develop and implement the new numerical methods that are based on the revised VRF theory.

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(a) Professional Preparation

Indian Institute of Technology Guwahati	Mechanical Engineering	B.Tech. 2005
Stanford University	Mechanical Engineering	M.S. 2007
Stanford University	Mechanical Engineering	Ph.D. 2011

(b) Appointments

January 2013-present	Asst. Professor of Engineering, Brown University
May 2011-December 2012	Postdoctoral Research Associate, Brown University

(c) Products

Products Most Closely Related

1. Michael A. Monn, James C. Weaver, Tianyang Zhang, Joanna Aizenberg, and Haneesh Kesari, "New functional insights into the internal architecture of the laminated anchor spicules of *Euplectella aspergillum*," *Proceedings of the National Academy of Sciences,* 112(16) 4976–4981 (2015), DOI: 10.1073/pnas.1415502112

2. David A. Stout, Eyal Bar-Kochba, Jonathan B. Estrada, Jennet Toyjanova, Haneesh Kesari, Jonathan S. Reichner, and Christian Franck, "Mean deformation metrics for quantifying 3D cell–matrix interactions without requiring information about matrix material properties," *Proceedings of the National Academy of Sciences*, published ahead of print (February 29, 2016), DOI:10.1073/pnas.1510935113

3. Haneesh Kesari and Adrian J. Lew, "Adhesive frictionless contact between an elastic isotropic halfspace and a rigid axi-symmetric punch," *Journal of Elasticity*, 106(2) 203–224 (2012), DOI: 10.1007/s10659-011-9323-8

4. Haneesh Kesari and Adrian J. Lew, "Effective macroscopic adhesive contact behavior induced by small surface roughness," *Journal of the Mechanics and Physics of Solids*, 59(12) 2488–2510 (2011), DOI: 10.1016/j.jmps.2011.07.009

5. Haneesh Kesari, Joseph C. Doll, Beth L. Pruitt, Wei Cai, and Adrian J. Lew, "Role of surface roughness in hysteresis during adhesive elastic contact," *Philosophical Magazine Letters*, 90(12) 891–902 (2010), DOI: 10.1080/09500839.2010.521204

Other Significant Products

1. Sohan Dharmaraja, Haneesh Kesari, Eric Darve, and Adrian J. Lew, "Time integrators based on approximate discontinuous hamiltonians," *International Journal for Numerical Methods in Engineering*, 89(1) 71–104 (2012), DOI: 10.1002/nme.3236

2. Lampros C. Kourtis, Haneesh Kesari, Dennis R. Carter, and Gary S. Beaupré, "Transverse and torsional shear stresses in prismatic bodies having inhomogeneous material properties using a new 2D stress function," *Journal of Mechanics of Materials and Structures*, 4(4) 659–674 (2009), DOI: 10.2140/jomms.2009.4.659

3. Lampros C. Kourtis, Dennis R. Carter, Haneesh Kesari, and Gary S. Beaupré, "A new software tool (VA-BATTS) to calculate bending, axial, torsional, and transverse shear stresses within bone cross sections having inhomogeneous material properties," *Computer Methods in Biomechanics and Biomedical Engineering*, 11(5) 463–476 (2008), DOI: 10.1080/10255840801930728

4. Suhas S. Mohite, Haneesh Kesari, Venkata R. Sonti, and Rudra Pratap, "Analytical solutions for the stiffness and damping coefficients of squeeze films in MEMS devices having perforated back plates," *Journal of Micromechanics and Microengineering*, 15(11) 2083–92 (2005), DOI: 10.1088/0960-1317/15/11/013

(d) Academic Honors

1. *Haythornthwaite Foundation Research Initiation Award* (2015). Awarded by the Applied Mechanics Division of the American Society of Mechanical Engineers.

2. *Juan Simo Memorial Prize* (2011). This is a best thesis award, given by Stanford University to a graduating doctoral candidate on selective years.

3. First authored research article chosen "highly commended" along with two others as part of the *James Clerk Maxwell Young Writers Prize* (2011). Awarded by Philosophical Magazine & Philosophical Magazine Letters.

4. *Herbert Kunzel Stanford Graduate Fellowship* (2007–2010). Awarded by Stanford University considering faculty nominations.

5. Nominated for the *Shankar Dayal Sharma Gold Medal* by the faculty at IIT Guwahati (2005). Medal awarded to the "best student" of the year's graduating undergraduate cohort (129 students from various disciplines).

(e) Collaborators & Other Affiliations

Collaborators and & Co-Editors (over the past 48 months)

Jae-Hyun Kim (KIMM, Korea), Kwan-Seop Kim (KIMM, Korea), Eric Chason (Brown University), Fei Pei (Brown University), Clyde L Briant (Brown University), Allan Bower (Brown University)

Graduate Advisors and Postdoctoral Sponsors (all, Total: 3)

Wei Cai (Ph.D. advisor; Stanford University), Adrian Lew (Ph.D. advisor; Stanford University), and Huajian Gao (Postdoctoral sponsor; Brown University)

Graduate Thesis Advisees (all, Total: 1)

Tianyang Zhang (M.S.; University of California, Los Angeles)

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FACILITIES, EQUIPMENT, AND OTHER RESOURCES

FACILITIES: Identify the facilities to be used at each performance site listed and, as appropriate, briefly indicate their capabilities, pertinent capabilities, relative proximity, and extent of availability to the project. Use "Other" to describe the facilities at any other performance sites listed and at sites for field studies. Use additional pages, if necessary.

Laboratory: The PI directs an over 800 square foot laboratory in the School of Engineering at Brown. The laboratory is equipped with a fume hood, two laboratory benches, a fume extraction arm, an isolation table, and an optical microscope. Other facilities include four student desks, a conference table, and two white boards. This laboratory is located on Brown's campus, and is available to use 24 hours per day by the PI and his students for the proposed project.

Clinical: Not applicable.

Animal: Not applicable.

Computer: There are 3 computer workstations in the PI's laboratory and a 4th in his office. Between these workstations, there are a total of 60 computer cores. At least one of these workstations will be dedicated to the proposed project. Brown provides the license to the research version of Abaqus, which is necessary for implementing the VRF model, for a fee of $1,800 per year. Brown also provides licenses to MATLAB, Mathematica, and Solidworks free of charge.

Office: The PI has an office in close proximity to his laboratory. An 8-core workstation is located in the office, to which the PI has exclusive access.

Other: Brown hosts the Center for Computation & Visualization (CCV). The high performance computing cluster (HPC) at the CCV consists of over 500 terabytes of disk capacity, 570 nodes comprising 7,632 CPU cores (and 334,336 GPU cores) with a peak performance of over 125 TFLOPs (and 540 TFLOPS from GPUs). A large collection of software, including that necessary for the proposed project, is available on CCV systems. The fee to use the CCV is $300 per semester.

MAJOR EQUIPMENT: List the most important items available for this project and, as appropriate, identify the location and pertinent capabilities of each:

8-core (Intel i7 4770 3.4 GHz) custom built workstation with 32 Gb RAM. Located in the laboratory. Pertinent software: Abaqus, MATLAB, Mathematica.

36-core (Intel Xeon E5-2699 2.3 GHz) Dell workstation with 128 Gb RAM, and NVIDIA Quadro K5200 GPU. Located in the laboratory. Pertinent software: Abaqus, MATLAB, Mathematica with GPU acceleration.

ADDITIONAL INFORMATION: Provide any other information describing the other resources available for the project. Identify support services such as consultant, secretarial, machine shop, and electronics shop, and the extent to which they will be available for the project. Include an explanation of any consortium/contractual/subaward arrangements with other organizations.

BUDGET EXPLANATION PAGE

PERSONNEL

Funds totaling roughly $48,000 are requested to support the personnel involved in the proposed research. These funds will be used to fully support one Ph.D. graduate student for the duration of the project ($38,510) and to support the PI at 85% effort for one month in the summer of 2016 ($9,489). Funds to support the graduate student include a stipend, health fees, and tuition to Brown. The details of the personnel expenses can be found in the Budget document. Both the graduate student and the PI will design the computational models used to investigate the toughness enhancements provided by wavy interfaces. The graduate student will develop and implement the numerical VRF methods and also interpret the computational results. The PI will use these results as a guide for developing theoretical models of the toughening mechanisms with assistance from the graduate student.

COMPUTATIONAL RESOURCES

The VRF will be implemented using the research version of Abaqus finite element software. The license fee for a single user is $1,800/per year. Funds totaling $1,350 are requested as part of the Budget to pay the license fee for the duration of the proposed effort. The number of Abaqus tokens required for the numerical simulations is proportional to the number of computer cores used. Funds totaling $651 are requested as part of the Budget to purchase additional Abaqus tokens.