Doctoral Program in Mechanical Engineering
Montana State University

PhD Research Proposal

A Selectively Activated Cohesive Zone Model with Arbitrary Interelement Crack Growth for the Finite Element Method

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Executive Summary

A novel formulation of the cohesive zone model for progressive fracture analysis is proposed. Motivated by both practical and physical considerations, the anticipated merits of this work are (1) to allow fracture to occur at any interelement boundary of a finite element mesh without adaptive remeshing procedures; (2) to reduce the computational expense and eliminate the effect of artificial compliance associated with traditional cohesive zone models; and (3) to couple the damage initiation criteria and cohesive constitutive laws to the state of the adjacent continuum elements in a physically realistic manner. The proposed model is well-suited for a variety of material systems, including composite materials and adhesive joints. The implementation will consist of two main parts: a finite element mesh preprocessing package, and an analysis package. This software will be integrated with a widely-used commercial finite element code to provide a computational framework that is useful and accessible to a large user-base.

Introduction

Background

Durability and damage tolerance are essential elements of engineering design. To reduce the risk of structural failures, engineers seek to discover and quantify the relationships between critical events leading to damage and the characteristic properties of a material – including stiffness, strength, fracture toughness, and environmental resistance. Geometric factors also play a role in the initiation and evolution of damage. Indeed, forensic investigations and experimental tests reveal that discontinuities such as cracks, voids, holes, and bonded or fastened joints are often directly linked to the emergence and propagation of damage.

The effect of physical flaws and manufacturing defects on durability and damage tolerance are the subject of ongoing research, particularly in the composites community. Composite material technology is based on the observation that the physical, mechanical, and even aesthetic properties of heterogeneous materials can be customized by selecting constituent materials with the desired characteristics. For example, fiber-reinforced polymer (FRP) composites provide a combination of high strength, stiffness, fatigue resistance, and low weight.

However, composite materials also introduce a unique set of challenges for engineering design and analysis. The challenges exist, in part, because the effective behavior and strength of a composite material is a function of interrelated factors that occur over multiple scales. For instance, the propagation of damage in FRP composite laminates is influenced by:

- Macroscopic features, such as the part geometry, structural loads, and boundary conditions;
- Mesoscale features, such as the laminate stacking sequence, ply orientations, and structural joints;

- Microstructural details, such as the individual material properties, physical form, volume fraction, and geometric arrangement of the constituent phases.

When damage does occur, the loads carried by a structure are redistributed among damaged and undamaged regions. In some cases, the interaction between constituent phases in a composite material is beneficial, and damage propagation is prevented or delayed. In other cases, the composite offers relatively little resistance. For example, FRP composites are strong and stiff in the fiber directions, but relatively weak in the matrix-dominated transverse and shear directions. The effect of the microstructure on the laminate strength can be appreciated by examining the micrograph in Figure 1, which shows the cross-section of a typical glass-fiber/epoxy-resin laminate, including individual fibers, fiber tows, resin-rich pockets, and porosity.

To understand this complexity, engineers and scientists have developed a variety of experimental techniques and computational models. Despite many advances, progressive damage and fracture models often suffer from one or more shortcomings, including poor accuracy or limited generality, high computational expense, and a reliance on purely numerical (non-physical) parameters. Thus, there is a need for practical, efficient, physics-based techniques to model the initiation and propagation of damage.

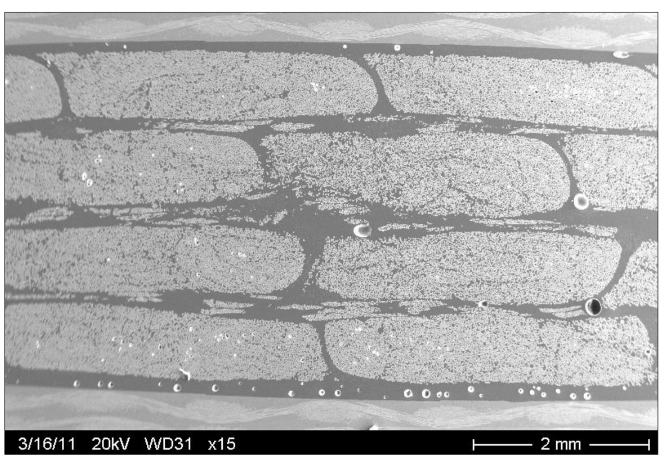

Figure 1. Scanning Electron Micrograph (SEM) of a glass fiber/epoxy resin laminate at x15 magnification (source: [1]).

Needs Assessment

The Blade Reliability Collaborative

The proposed research will contribute to Montana State University's support of the Blade Reliability Collaborative (BRC). The BRC is an ongoing program led by Sandia National Laboratories to improve the quality and reliability of wind turbine blades, with important contributions from academic, national labs, and industrial partners [2].

Modern industrial wind turbine blades must endure static and fatigue loads under a wide range of demanding environmental conditions over an expected service life of 20 years. However, blade failures are emerging as one of the most costly elements of wind plant installation and operation today, with a mean time-between-failure of only 12-14 years [2]. Therefore, the BRC aims to promote the improvement of quality metrics and inspection capabilities, and to develop advanced analysis techniques to evaluate the effects of defects found in wind blades.

Aerospace Structures and Components

The damage model proposed in this work is also designed to fulfill a major objective of a project sponsored by the Boeing Company at the Montana State University Composites Research Group. Due to the increasing use of composite materials in primary aircraft structures, there is a need for fast and accurate progressive crack growth models in the aerospace industry. The primary analysis capabilities desired by this project include accurate criteria for crack initiation and crack propagation, especially with respect to delamination and crack migration between plies.

Summary of Needs and Research Statement

As larger wind turbines blades are developed, rigorous testing and quality metrics, refined manufacturing techniques, and predictive numerical models become ever more important. In addition, the aircraft manufacturers are increasingly interested in expanding the use of FRP composite materials. Consequently, there is a growing awareness that the needs and best practices from the wind industry and those from the aerospace industry are increasingly similar and sophisticated. For example, a recent symposium hosted by Montana State University attracted an international group of experts from aerospace corporations, national research labs, and university research labs to discuss the current state-of-the-art and shared future opportunities [3].

There is a need for practical, efficient, physics-based techniques to model the initiation and propagation of damage. I propose to develop a novel formulation of the cohesive zone model (CZM) for progressive fracture analysis using the finite element method (FEM). Motivated by both practical and physical considerations, the anticipated merits of the proposed work include:

- Fracture is permitted to occur at any interelement boundary of an arbitrary finite element mesh as a natural outcome of an analysis, without adaptive remeshing procedures.
- Damage initiation criteria and cohesive constitutive laws are coupled to the state of the adjacent continuum elements in a physically meaningful manner, in contrast to traditional cohesive zone models.
- Elimination of artificial compliance associated with traditional cohesive zone models.
- Reduced computational expense compared with traditional cohesive zone models.

The work proposed here can be used to create models that account for the combined effects of stress in the material, microstructural details, and material defects. The goals of the research are structured to ensure that the proposed model is *flexible*, *accurate*, *efficient,* and *accessible*. Flexibility is used here to describe the generality of a theoretical framework for various types of analyses (e.g. static or dynamic problems), as well as the ability to represent different types of damage and failure (e.g. ductile or brittle fracture). Efficiency and accuracy are generally desirable in any computational method, though much room for improvement exists in many progressive damage models. Finally, accessibility is used here to describe a conscious effort taken to facilitate users, analysts, and future researchers.

Theoretical Background

The proposed work fits within a theoretical framework known as the cohesive zone model (CZM). A sizable body of work on the use and development of the CZM has been produced over the last two decades. During this time, the CZM has been implemented in many commercial and non-commercial finite element analysis (FEA) programs, such as Abaqus, ANSYS, and WARP3D [4-6]. Therefore, to clarify the purpose of the proposed work, the following sections describe the current state-of-the-art methods, as well as their pros and cons.

The Cohesive Zone Model

The CZM is a versatile progressive fracture model that describes both the initiation and growth of damage as a gradual phenomenon over an extended crack-like process zone within a solid body. Within the cohesive process zone, the CZM posits the existence of cohesive tractions, $\boldsymbol{t}$, which act to prevent material separation across the damage surfaces. As damage accumulates, the cohesive forces weaken until they can no longer resist further separation of the material and the crack tip embedded within the cohesive zone is assumed to have moved on.

As in continuum damage mechanics (CDM), the onset of damage within the cohesive zone is characterized by a critical threshold strength, t_c. However, the evolution of damage and the essential criterion for crack growth is directly related to a critical fracture energy, $\mathcal{G}_c$, as in fracture mechanics. This two-parameter approach provides considerable flexibility in how the cohesive tractions evolve within the cohesive zone. As a result, the CZM can be formulated to capture a broad range of damage processes, including brittle, quasi-brittle, and ductile fracture.

In general, cohesive tractions are defined as a function of the relative displacement gap across the cohesive zone, Δ, in a relation known as the traction-separation law (TSL). For example, the evolution of cohesive tractions for both damaged and undamaged regions within a cohesive zone is illustrated in Figure 2. As shown, a simple bilinear TSL governs the cohesive behavior. This TSL can be expressed within a thermodynamically consistent framework using the general expression:

$$\boldsymbol{t} = \boldsymbol{t}(\Delta) = (1 - \Phi)\mathbf{K} \cdot \Delta \tag{1}$$

In Eqn. (1), Φ is a damage parameter defined in the range $0 \leq \Phi \leq 1$, and can be interpreted as the ratio between the damaged area and the original cross-sectional area of the undamaged interface. An initial elastic penalty stiffness prior to the onset of damage is represented by $\mathbf{K}$. The fracture energy is defined as a function of the cohesive tractions and the separation gap:

$$\mathcal{G} = \int \boldsymbol{t}\, \mathrm{d}\Delta \tag{2}$$

Fracture occurs when $\mathcal{G} = \mathcal{G}_c$, which is also equal to the total area under the TSL.

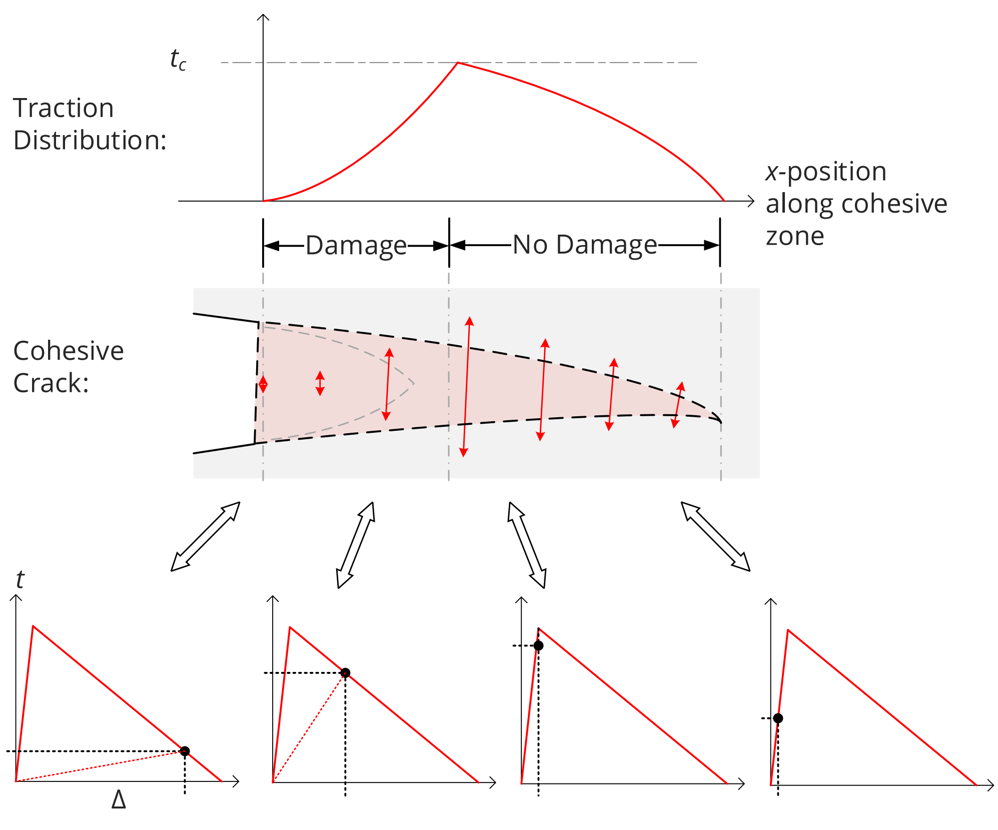

Figure 2. Example distribution of tractions within a cohesive zone. The corresponding (t, Δ) value for a bilinear TSL is shown for selected points along the cohesive zone.

In a finite element implementation, the cohesive zone is represented by special interface elements placed at the boundary between two "bulk material" solid elements, as shown in Figure 3.

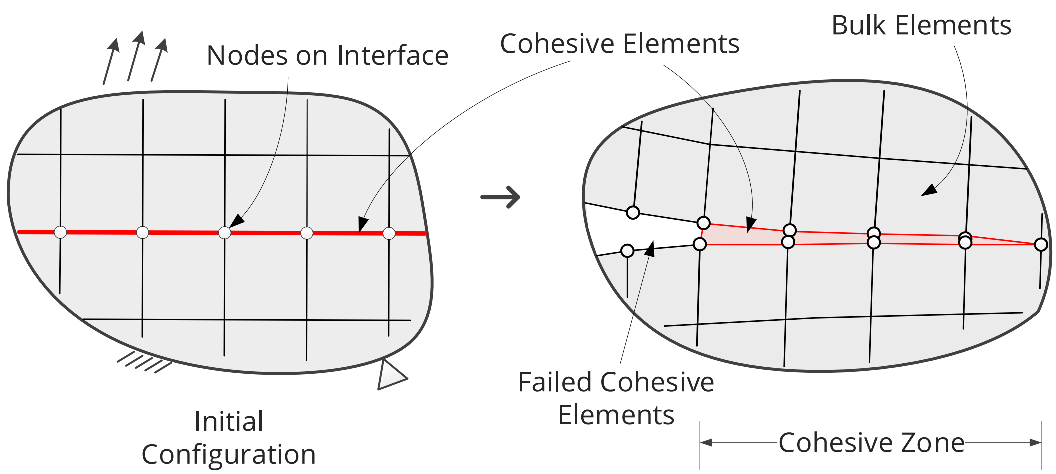

Figure 3. Cohesive elements placed at element boundaries along a plane.

As shown in Figure 4 below, cohesive elements are defined by the nodes at the interface of two adjacent continuum elements, forming a "top" ("+") surface and a "bottom" ("-") surface. The cohesive elements in the initial undamaged configuration have a geometric thickness of zero, so that corresponding nodes on either side of the interface initially share the same position but retain independent degrees of freedom (DOF). As loading is applied to the model, each cohesive element works to control the separation gap according to the specified traction-separation law. Damage initiation and progressive crack growth proceeds as the surfaces separate under continued loading. The relative motion between the top and bottom surfaces is assumed to directly represent the kinematics of crack opening and shearing modes. Each mode may then be related to an experimentally determined fracture energy, for example, $\mathcal{G}_{Ic}$ and $\mathcal{G}_{IIc}$ for Mode I and Mode II type fractures, respectively.

Note that the explicit use of the displacement gap injects a beneficial scale-dependency into the finite element model [7], so that the numerical solution is expected to converge upon mesh refinement. This represents a significant advantage when compared to unregularized continuum damage mechanics techniques.

By restricting crack growth to interelement boundaries, we acknowledge that the CZM may only approximate the “true” crack path. Fortunately, it has been shown that mesh bias can be alleviated with a suitably randomized mesh, such as produced with the so-called K-means or conjugate-gradients mesh generation methods [8, 9].

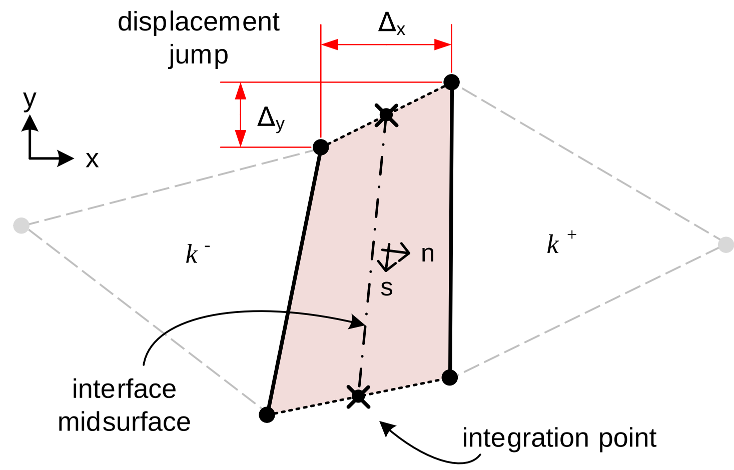

Figure 4. Illustration of a 2D cohesive interface element opening in mixed normal and shear modes. The two adjacent continuum elements, $k^{\pm}$, are shown with dashed gray lines.

The Intrinsic CZM

Current implementations of the CZM can be categorized into two basic approaches. The first and most common approach (by far) is referred to as the **intrinsic CZM**, or simply the CZM. In this method, cohesive elements are placed within the mesh *ab initio*, prior to running an analysis, and are an inherent feature of the model. In practice, the cohesive elements are typically inserted along an expected fracture path, such as in Figure 3 above. This approach has been used successfully to model the delamination of FRP composites, or other cases where the fracture path is already known. However, it also effectively imposes restrictions upon where fracture may occur and can severely limit the predictive capability of the model for new load conditions or part geometries, where a different crack path may be more appropriate.

Nevertheless, the CZM is capable of modeling non-self-similar crack growth, multiple cracks, and even fragmentation without predefining the crack path if cohesive elements are placed at every interelement boundary. As shown in Figure 5, this alternative cohesive modeling approach provides a network of potential fracture paths and orientations. Note that the mesh shown in the figure was created with a model preprocessor already developed during preliminary research conducted for this proposal. Also note that in this figure, the continuum elements have been visually reduced by a shrink-factor of 5% so that the position of the embedded zero-thickness cohesive elements can be seen. In the actual mesh, the element edges and corresponding nodes at each interface are coincident, and no gap exists.

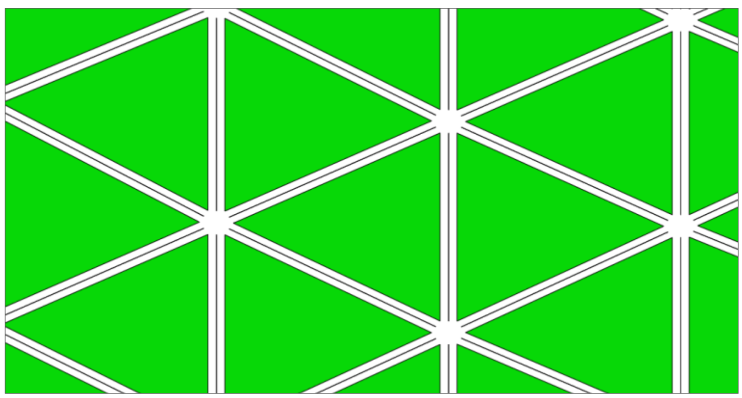

Figure 5. Detail of an example 2D intrinsic CZM mesh with zero-thickness cohesive elements at all element boundaries.

Despite the potential advantages, models with intrinsic cohesive elements at every interelement boundary are not common in the literature [10, 11]. Furthermore, no specific name has yet been assigned to distinguish this cohesive modeling approach, which is clearly distinct from the practice of inserting cohesive elements along a fracture path that is known *a priori*. Therefore, for clarity we will refer to a mesh with an assumed, predefined fracture path(s) as a **first-generation CZM mesh**, or more simply as a Gen-1 cohesive mesh. A mesh with cohesive interface elements at *all* interelement boundaries within a region of interest will be referred to as a **second-generation CZM mesh**, or a Gen-2 cohesive mesh.

However, with research and practical experience it becomes clear that placing many cohesive elements throughout the mesh to allow arbitrary interelement crack propagation (i.e. the creation of a Gen-2 mesh) is relatively rare due to challenges in at least three areas:

- **Mesh generation and cohesive element insertion.** Developing procedures to reliably generate a mesh for arbitrary 2D/3D models with cohesive elements at all interelement boundaries is a prerequisite for the technique. However, at the time of this report there does not appear to be a suitable open-source or commercial off-the-shelf (COTS) program available that offers this capability.
- **Computational expense.** The computational expense of an analysis is significantly increased due to the large number of additional degrees of freedom (DOF) associated with the extra nodes needed to split the mesh and insert cohesive elements. In addition, cohesive elements may be numerically sensitive to relatively small changes in the applied loading, especially when they begin to soften and fail. Many small load steps may be needed to achieve numerical convergence.
- **Artificial compliance.** Each additional intrinsic cohesive element deforms under load, even in the undamaged state. The total effect may be dependent on the specific mesh, load conditions, material properties, and structural geometry. If not suitably controlled, artificial compliance alters the response of the structure being analyzed.

As noted in the first bullet, mesh generation and cohesive element insertion presents a non-trivial technical challenge, yet it is required for any technique proposing to use cohesive elements for arbitrary crack propagation. Generating a suitable mesh can be solved in a variety of ways. For the proposed research, I have already developed a fast, robust, and versatile solution which integrates directly with the commercial finite element analysis (FEA) package, Abaqus. To the best of my knowledge, no other software currently available offers similar capabilities.

As noted in the second bullet point, the computational requirements of the intrinsic CZM may quickly become prohibitively expensive, particularly for realistic fracture models and applications where multiple analyses are needed. Fortunately, the intrinsic CZM may be used with parallel (multi-core and distributed) computational techniques, and much of this problem can be reduced with a suitable hardware and software setup.

As introduced in the third bullet, **artificial compliance is perhaps the most problematic issue related to the intrinsic CZM**. Ideally, the presence of undamaged cohesive elements would not unduly affect the overall response of a structure. However, a consequence of the intrinsic approach is that a small but unavoidable elastic response occurs in each cohesive element, even before the onset of damage. Therefore, a structure with cohesive elements will deform further under an applied load than it normally would if cohesive elements were not present. This effect can be observed even when the penalty stiffness, $\mathbf{K}$, becomes very large. Likewise, under a prescribed displacement boundary condition, the stresses computed within the continuum elements is underestimated since part of the deformation is absorbed by the embedded cohesive elements. In either case, the displacement, stress, and strain computed for the model may be unreliable or inaccurate. When many cohesive elements are used, the additional compliance is cumulative, mesh-dependent, and can be difficult to predict or counteract.

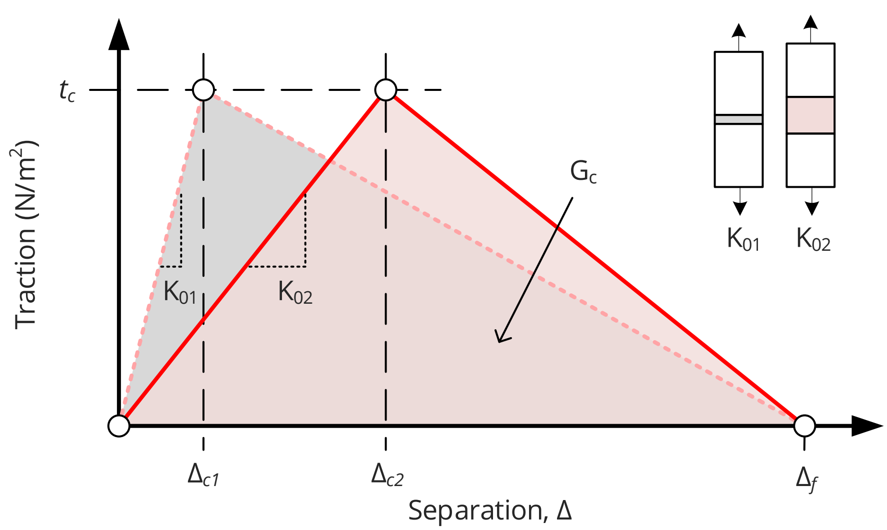

Figure 6. Example bilinear intrinsic traction-separation law.

The source of artificial compliance in the intrinsic CZM can be better understood by referring to the TSL that governs the interface behavior. Consider the bilinear TSL shown in Figure 6, which is fully defined by three parameters: the critical traction at the onset of damage, t_c, the critical fracture energy, $\mathcal{G}_c$, and either the initial penalty stiffness, K_0, or the interface displacement gap at failure, Δ_f. Note that when either K_0 or Δ_f are chosen, the other is known due to the triangular shape of the TSL.

The intrinsic TSL exhibits initially elastic behavior before t_c is reached. This initial (undamaged) response is not usually considered a material or fracture property, but rather as an unfortunate side effect required by the standard numerical implementation of cohesive interface elements in the finite element method. Therefore, the penalty stiffness K_0 is typically used as a numerical parameter to reduce the separation gap prior to the actual onset of damage.

However, this introduces ambiguity in the solution and a false dependence on a purely numerical parameter. For example, as shown in Figure 6, the initial penalty stiffness K_{01} is greater than K_{02}. Evidently, holding t_c and $\mathcal{G}_c$ constant while increasing the penalty stiffness reduces the critical separation at damage initiation, Δ_c. Since the initial behavior is linear, the amount of separation that occurs at the onset of damage can easily be expressed using the simple relation:

$$\Delta_c = \frac{t_c}{K_0} \tag{3}$$

Theoretically, as K_0 becomes very large such that $K_0 \to \infty$, the initial displacement $\Delta_c \to 0$, so that the interface becomes nearly rigid and the exact continuum solution may be asymptotically achieved. Unfortunately, in the limit as $K_0 \to \infty$ numerical problems may appear, such as ill-conditioning of the system of equations and other instabilities that lead to very small step sizes and numerical non-convergence. Therefore, an acceptable value is often a compromise between accuracy and stability, which can usually only be found through iteration.

The Extrinsic CZM

Rather than placing cohesive elements within the mesh at the beginning of an analysis as done in the intrinsic CZM, cohesive elements may instead be adaptively inserted as the solution proceeds. This method is known as the **extrinsic CZM**, or sometimes the initially rigid cohesive model, and requires the calculation of an insertion criterion at each interface. Once the insertion criterion is satisfied, the mesh must first be split by duplicating the nodes along the critical interface. The neighboring continuum elements must then be redefined with an updated nodal connectivity, and finally a cohesive element may then be defined with the updated set of nodes from either side of the interface in the new mesh configuration.

As shown in Figure 7, the extrinsic TSL is usually defined as a monotonically decreasing function of the interface displacement gap with a nonzero initial traction, $t_0 = t_c > 0$.

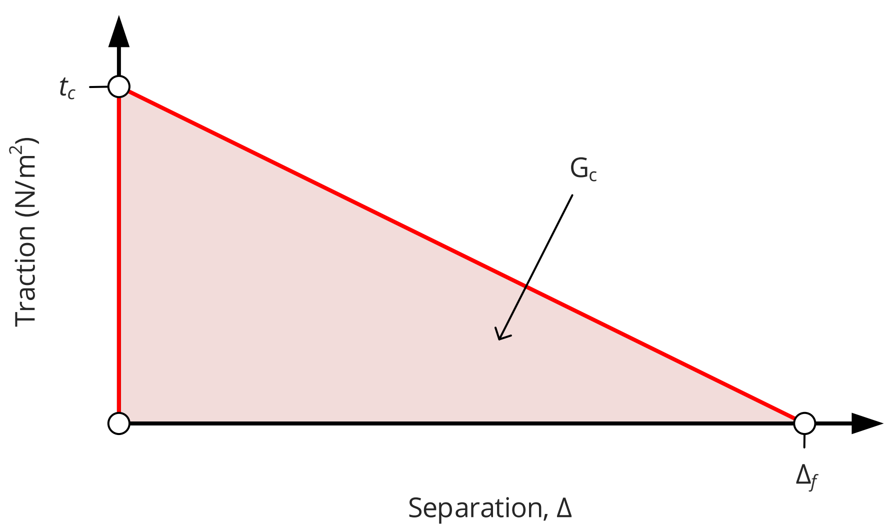

Figure 7. Example linear extrinsic traction-separation law.

Therefore, the adaptive insertion procedure coupled with the extrinsic TSL ensures that the global response of the structure is free from artificial compliance, while the increase in the number of active DOF is minimized.

In summary, the main advantages of the extrinsic CZM compared to the intrinsic CZM are:

- **Additional DOF are minimized.** Cohesive elements are adaptively inserted as the solution progresses only where a criterion has been satisfied.
- **Artificial compliance is eliminated.** Because the cohesive elements are adaptively inserted without an initial undamaged elastic response, artificial compliance is no longer an issue.

Although the extrinsic CZM is an effective technique to remove the problem of artificial compliance, it introduces a new complication:

- **Complex implementation and potential inefficiencies.** Remeshing operations usually come with significant overhead and are dependent on the use of sophisticated data storage and solution transfer routines. Additional complications arise due to requirements imposed by parallel computing environments.

The extrinsic technique must be closely integrated with the specific analysis software to adaptively insert cohesive elements in an efficient manner. Otherwise, if implemented with a COTS finite element package such as Abaqus, the adaptive insertion routines may need to be handled by stopping the analysis, modifying the mesh, and then beginning a completely new analysis with the additional cohesive element. Unfortunately, repeating this procedure many times would become a severe bottleneck.

As noted above, the total number of additional DOF introduced by adaptively inserting cohesive elements will generally be much lower with the extrinsic approach than for a Gen-2 intrinsic CZM mesh. Note that some researchers have developed other methods which appear to overcome the complexity and potential inefficiency of the adaptive/extrinsic CZM technique [11-15]. However, so far these improvements have only been achieved with in-house research codes or where the source code of the FEA package was otherwise available. In contrast, the approach proposed here may be employed with any FEA program with a minimal impact on the overall computational expense.

Research Objectives

Objective 1: Non-Self-Similar Cohesive Fracture

Objective: Allow cohesive fracture to occur as an outcome of the analysis without specifying the fracture path, by inserting cohesive elements at all interelement boundaries within any region of interest of a finite element mesh.

To satisfy this objective, cohesive elements must be inserted as needed throughout a mesh, including at every interelement boundary in 2D and 3D meshes. A key outcome of this project is the development of a robust preprocessing code that integrates with Abaqus/CAE to operate on an internal model database directly. Examples are shown in Figure 5 above, and in Figure 8 below.

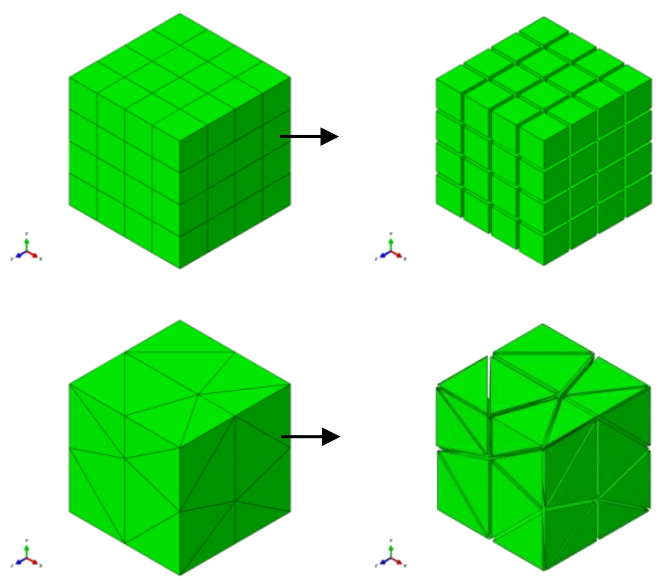

Figure 8. Example meshes before and after splitting and cohesive element insertion. Gaps are shown for illustration purposes only.

Objective 2: Alleviate or Eliminate Artificial Compliance

Objective: Alleviate or eliminate the effects of artificial compliance that are normally associated with the use of cohesive elements.

Note that while Objective 1 is necessary for the practical deployment of the new fracture model, Objective 2 requires improvements to the implementation and/or formulation of the standard cohesive zone model.

Once a finite element mesh has been split and cohesive interface elements have been inserted, the model has been enriched by a set of new nodes and their associated degrees of freedom. These extra nodes are necessary to permit interelement crack growth but result in a significant increase of the total computational expense. More importantly, each cohesive element introduces a small amount of additional compliance to the model.

I propose to demonstrate two distinct approaches that successfully alleviate or eliminate artificial compliance. In the first approach, a strategy using controllable multipoint constraints will be developed. With this technique, artificial compliance is exactly eliminated, and the embedded cohesive elements remain dormant until activation. However, this approach is only possible using the implicit FEM.

In the second approach, an advanced interface formulation based on the Interior Penalty Discontinuous Galerkin Method (IP-DGM) is used. The IP-DGM can be thought of as a stable and consistent penalty method, where continuity of the solution across discontinuous interelement boundaries is weakly enforced in an integral sense. Prior to damage initiation, interface separation remains negligibly small and artificial compliance is effectively eliminated. This technique is suitable for both implicit and explicit FEM.

In addition, I propose to demonstrate, for the first time, a combination of the MPC and the IP-DGM approaches specifically designed to address challenges in modeling cohesive fracture with composite materials, while simultaneously reducing the total computational expense of an analysis.

Objective 3: 2D and 3D Fracture Analysis Capability

Objective: Implement fracture analysis capabilities for 2D and 3D analysis.

One of the tasks of this project is to provide the capability to investigate crack growth for complex loads, materials, and structural geometries where 2D assumptions may not apply. The computational savings offered by the proposed model should be very substantial, especially for the 3D modeling space.

Objective 4: Abaqus-based Implementation

Objective: Each previous objective must be implemented for use with the commercial finite element code, Abaqus.

An important goal of the project is to provide a useful and approachable technique that can be executed with commercial FEA platforms, such as Abaqus. This decision offers many advantages, such as access to high-quality and extensively tested functionality, expansive documentation, and technical support options. On the other hand, the use of a closed-source program places certain restrictions on the access granted to any user-developed code. Fortunately, Abaqus provides a rich set of APIs and other utilities that, with some ingenuity, can be harnessed to suit many needs.

The Abaqus FEA package encompasses several products. The code implemented in this proposal is integrated with three core components:

- Abaqus/Standard: An implicit FEM solver and related utilities. Ideally suited for static and quasi-static scenarios.
- Abaqus/Explicit: An explicit FEM solver and related utilities. Best for dynamic or highly nonlinear processes, such as impact fracture and fragmentation.
- Abaqus/CAE: The “Complete Abaqus Environment” provides a convenient Graphical User Interface (GUI) to build models, run analyses, and view results.

In the proposed work, the chosen modeling strategy depends on whether the analysis is submitted to Abaqus/Standard or Abaqus/Explicit. This is primarily due to differences in the specific computational procedures used by each solver.

The implementation of the proposed work consists of a set of scripts, subroutines, and data structures designed to integrate with the capabilities offered by Abaqus. However, a similar approach should be possible with other FEA packages which allow user-defined analysis subroutines, such as ANSYS and LS-DYNA.

In the current work, we shall take advantage of several user-defined analysis subroutines for Abaqus/Standard and Abaqus/Explicit. In addition, we use the Python API provided by Abaqus/CAE to generate a suitable FE model that makes the proposed selectively activated CZM possible.

Proposed Research and Modeling Techniques

As described above, current CZM techniques must either insert cohesive elements prior to running an analysis (the intrinsic CZM) or dynamically update the FE model and mesh connectivity during the solution (the extrinsic CZM). In the proposed model, cohesive elements are embedded within a mesh prior to an analysis, so that cracks may form along interelement boundaries as a natural outcome of the solution. This is like the approach used in the intrinsic CZM. However, in the proposed model, interface separation within an undamaged material is prevented and artificial compliance is eliminated. The proposed model uses two special techniques to accomplish this:

- **Controllable Multipoint Constraints (MPCs).** The MPC approach is an efficient strategy available for the implicit solver only. Constrained nodal DOF are eliminated from the system of equations submitted to the solver.
- **The Interior Penalty Discontinuous Galerkin Method (IP-DGM).** The IP-DGM is an advanced interface element formulation that may be used for either implicit or explicit solvers.

Thus, undamaged cohesive elements embedded within the mesh lie dormant and have no effect on the analysis. In the proposed model, the stresses in the bulk material adjacent to each cohesive interface are then monitored and used to compute a cohesive activation criterion. Once the activation criterion is satisfied at any point in the proposed model, the constraints at the critical interface can be selectively released and the cohesive element automatically becomes an active participant in the solution. Subsequent interfacial behavior is governed by an appropriate cohesive TSL. Therefore, the proposed technique may be referred to as a **Selectively Activated Cohesive Zone Model**.

Mesh Splitting and Cohesive Element Insertion

One objective of this research is to provide a framework that allows cohesive fracture to occur at any interelement boundary in a finite element mesh. To make this possible, a procedure is proposed wherein an existing (continuous) mesh is first generated and then modified by splitting and inserting cohesive interface elements. Because the split-insert procedure is completed as a preprocessing step prior to running the analysis, it may also be used to create a Gen-2 intrinsic cohesive mesh. The proposed split-insert concept is illustrated in Figure 9 using a simple 3D "parent" mesh.

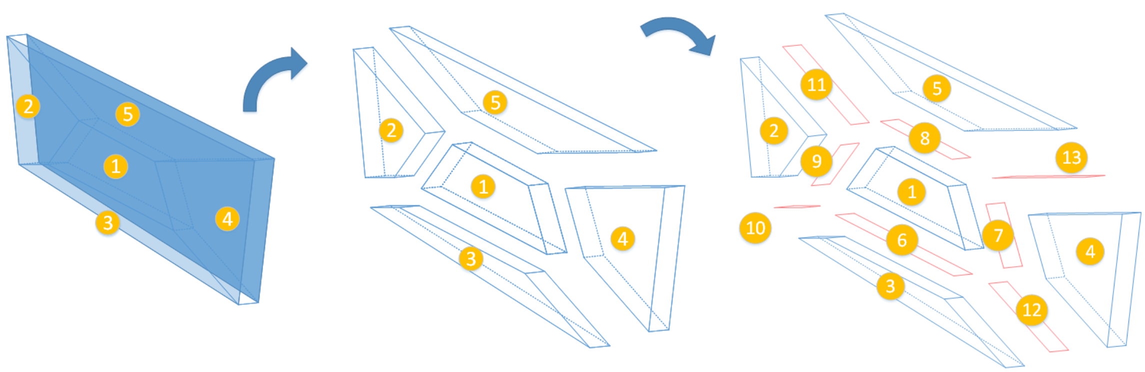

Figure 9. Exploded view of mesh splitting and element insertion process.

Referring to Figure 9, we can describe the proposed split-insert procedure with the following observations:

- Note that the mesh in the figure is shown in an exploded configuration for clarity only, and corresponding nodes across each interface are coincident.
- The parent mesh, shown on the left, originally consists of 5 linear hexahedral elements, and a total of 16 nodes.

- In the center of the figure, the mesh has been split at all element boundaries (gaps are shown for illustration only). This requires duplicating any node shared by two or more elements at each interface.
- Each child node is defined at the same coordinates of the parent node.
- Each element is then redefined with a proper sequence of 8 unique nodes, not shared by any other element. The outcome is a new discontinuous mesh where each element is independent from its neighbors.
- In the final step, shown in the right, 8 additional zero-thickness cohesive interface elements have been inserted at the internal boundaries between the discontinuous elements, using corresponding nodes on the adjacent surfaces to define their nodal connectivity.
- The final mesh consists of 13 elements and 40 nodes in total.

Using a remeshing tool developed as part of this proposal, any arbitrary 2D or 3D parent mesh may be split in a variety of ways. For example, an entire model can be modified so that cohesive elements are inserted at every interelement boundary in the mesh, or within certain regions only, or even along a specified interface only.

Multipoint Constraints

In the proposed model, interface separation prior to the onset of damage may be prevented by constraining the nodes on either side of every cohesive element with controllable **multipoint constraints** (MPCs). In the proposed work, a master-slave DOF elimination method is used. This method ensures that the displacements of two nodes are exactly equal. The MPC relation can be interpreted as a perfectly rigid link between the master and slave nodes, as illustrated in Figure 10.

One of the nodes is chosen as the “master” and the other as a “slave”. Then each DOF of the slave node in an active MPC is constrained to the corresponding DOF of the master node using a linear homogeneous equation of the form:

$$u_i^s = u_i^m \quad \text{for} \quad i = 1, 2, \ldots, ndof \tag{4}$$

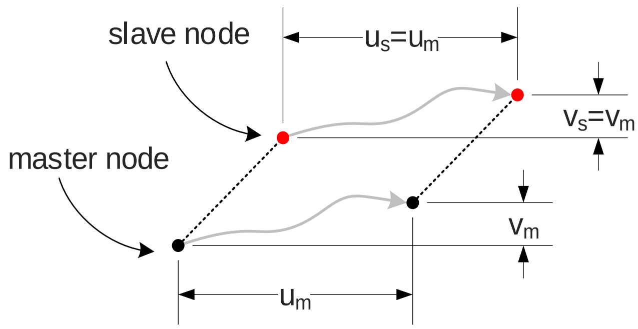

Figure 10. Displacement of a slave node (red) is exactly equal to the displacement of the master node (black) at all times, as if they were connected by a rigid link. Note: the nodes are coincident while the MPC is active, and the gap is shown here for illustration purposes only.

In this project we are concerned with translational DOF only. This is consistent with a typical continuum solid element formulation, but there is no difficulty in including additional DOF, such as rotation, temperature, etc. For example, in a 2D analysis we assume the nodal DOF are the displacements in the x- and y-directions: $\boldsymbol{u}^T = [u_1, u_2]^T = [\mathrm{u}, \mathrm{v}]^T$.

The constraints defined by (4) are then used to explicitly eliminate the slave DOF to obtain a reduced system of equations. The implementation of this process has been carefully designed so that the reduced system exactly matches the computational structure of the original mesh before cohesive elements were inserted. These concepts are visualized in Figure 11.

When the nodes across an interface are rigidly tied by active MPCs, the embedded cohesive element has no effect on the solution. However, if an MPC is released, the slave DOF are immediately reinjected into the system of equations submitted to the solver in the next increment.

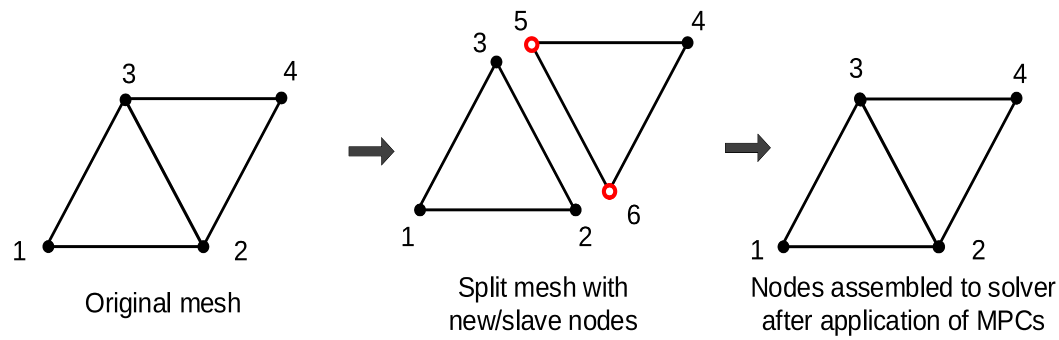

Figure 11. Application of multipoint constraints eliminate all slave node DOF from the system of equations, and exactly prevent interface separation.

Interior Penalty DGM

We propose to develop an advanced interface element formulation based on an **Interior Penalty Discontinuous Galerkin Method** (IP-DGM) to eliminate artificial compliance without requiring the use of multipoint constraints. The IP-DGM (or simply, the IP method) can be thought of as a stable and consistent penalty method, where continuity of the solution across discontinuous interelement boundaries is weakly enforced in an integral sense. We briefly note several reasons why the IP-DGM is suitable for our goals:

- The IP method effectively eliminates artificial compliance prior to the onset of damage, unlike the penalty stiffness-based method used with conventional cohesive elements.
- The IP method can be used in both implicit and explicit FEM techniques. Since user-defined controllable MPC subroutines are not available in Abaqus/Explicit, the IP is used exclusively to implement the selectively activated CZM for the explicit solver in this project.
- The IP method permits nonconforming meshes and hanging nodes, and basis functions are permitted to be discontinuous from element to element. Therefore, the method is naturally suited to facilitate *hp*-adaptivity [16, 17].

In this work, we propose to take advantage of the first two items to ensure an accurate solution free of artificial compliance can be achieved for both Abaqus/Standard and Abaqus/Explicit.

Remark: Unlike the MPC-based strategy, extra nodes resulting from splitting the mesh are not condensed/eliminated with the IP-DGM. Depending on how the mesh is split, this can significantly increase the computational expense of an analysis. However, in our experience the IP-DGM is both more accurate and more efficient than a full intrinsic CZM implementation.

Remark: Unlike the MPC-based strategy, interface constraints are weakly enforced in the IP-DGM. Therefore, a negligibly small (but non-zero) displacement gap may exist across interelement boundaries prior to the onset of damage.

The IP-DGM enforces continuity of the solution across discontinuous elements through additional terms in the finite element weak form. As will be shown in the final thesis, the general formulation is obtained by integrating by parts and summing contributions over each discontinuous element K and at each interior interface Γ in the mesh, to arrive at:

$$\sum_{K} \int_{K} \varepsilon(v) : C : \varepsilon(u) - \sum_{\Gamma \in \Gamma_I} \left(\int_{\Gamma} [\![v]\!] : \{\sigma(u)\} + \int_{\Gamma} [\![u]\!] : \{\sigma(v)\} - \int_{\Gamma} \eta [\![v]\!] : [\![u]\!] \right) = \sum_{K} \int_{K} f \cdot v \qquad (5)$$

where:

$u \equiv vector\ of\ nodal\ displacements$

$v \equiv vector\ test\ function\ (virtual\ displacements)$

$f \equiv vector\ of\ forces$

$C \equiv material\ constitutive\ tensor$

$\eta \equiv penalty\ parameter$

$\varepsilon(v) \equiv \nabla v \equiv tensor\ test\ function\ (virtual\ strains)$

$\varepsilon(u) \equiv \nabla u \equiv strain\ tensor$

$\sigma(v) \equiv \left(C : \varepsilon(v)\right) \equiv Cauchy\ stress\ tensor$

$\sigma(u) \equiv \left(C : \varepsilon(u)\right) \equiv Cauchy\ stress\ tensor$

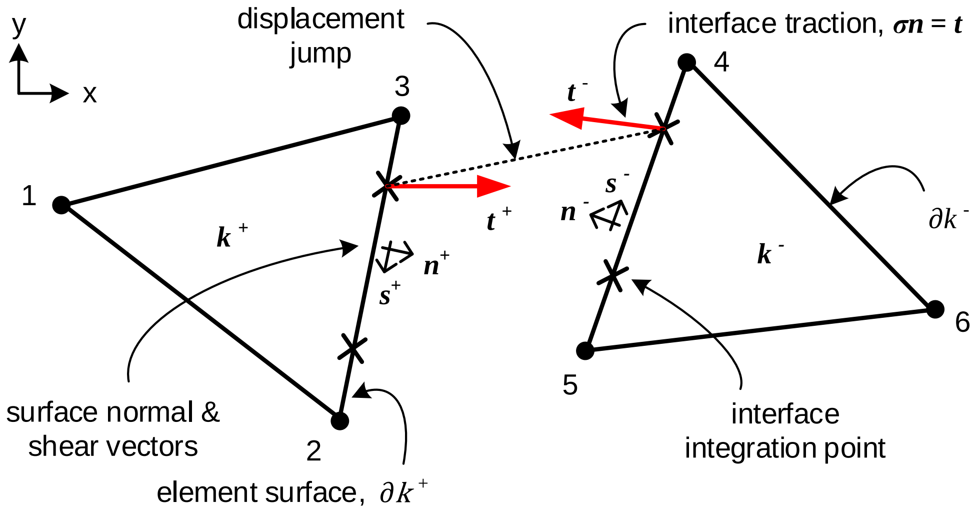

Figure 12. Two adjacent elements in the Interior Penalty method, where the interface is defined as $\Gamma \cup \partial k^{\pm}$ and numerical fluxes are based on the jump and average of element stresses and displacements.

Referring to Figure 12, let the interface between two adjacent, but discontinuous, elements $k^{\pm}$ be represented by Γ, where $\Gamma \cup \partial k$. For convenience, we may denote the "+" or "-" sides of an interface as "1" and "2". We propose to develop a general technique where the order in which the elements are given is not important for the IP-DGM formulation. However, once chosen the sides are fixed.

The average operator $\{\,\}$ and the jump operator $[\![\,]\!]$ are used in (5) to describe the limit values of stresses and displacements at each interface, Γ. The average operator simply computes the *average* of the matrix-valued/tensor quantity (σ) at an interface:

$$\{\sigma\} = \frac{1}{2}(\sigma_1 + \sigma_2)$$

The jump operator describes the *difference* in a vector quantity (v) at an interface[1]:

---

[1] **Implementation Note:** Both v and n are column-vectors, so that with the outer product defined as $(\mathrm{v} \otimes n) = (\mathrm{v} \cdot n^T)$ the jump operator results in a matrix-valued output.

$$[\![\mathrm{v}]\!] = \mathrm{v}_1 \otimes n_1 + \mathrm{v}_2 \otimes n_2$$

The first and third terms in (5) are the same as those found in the conventional (continuous Galerkin) FEM weak form to compute the work due to internal element stresses and the work due to external loads, respectively. In addition, the IP-DGM includes three integrals over each interior interface Γ to account for the work done across adjacent element surfaces, with the following important properties (c.f. [16, 18-21]):

- The first interface integral in (5) is called the *consistency* term. This term guarantees that the IP method will find any continuous solution u that can be represented by the finite element shape functions, such that $[\![u]\!] = 0$.
- The second interface integral is called the *symmetry* term. When combined with the consistency term the IP method becomes symmetric in u and v. Accordingly, the resulting interface stiffness matrices are also symmetric.
- The third interface integral is called the *stability* term. This term acts to weakly enforce displacement compatibility and the stability of the IP method. The stability term has a form like that used for the cohesive penalty-based TSL. However, a lower bound for the penalty factor η can be found that stabilizes the method and guarantees that the interface stiffness matrix is positive-definite.

Selective Activation Strategy

In the proposed selectively activated CZM, interface constraints may be enforced by either the MPC or IP methods, or by a combination of the two methods. Thus, in the selectively activated CZM, the mesh contains a set of initially dormant cohesive elements and all interelement separation is exactly prevented. However, once an activation criterion (i.e., the damage initiation criterion) is satisfied at any point in the model, the constraints at the critical interface can be dynamically released and the cohesive element automatically becomes an active participant in the solution. This strategy is called the **selective activation of cohesive interfaces**.

Prior Work

Before closing this section, we note that to the best of our knowledge, MPC-based approaches have been independently developed or suggested by a short list of other researchers. The earliest MPC-based approach to model interelement crack growth that we have found was developed by Gerken [22] for regular 2D quadrilateral meshes. Interestingly, Gerken also implemented the technique with the MPC and UEL user subroutines in Abaqus/Standard but assumed brittle fracture and did not employ a TSL-like interface law to describe damage evolution once the constraints were released. The idea of using controllable node-to-node tie constraints was also suggested by Zavattieri [23] as a potential strategy to obtain initially rigid cohesive elements. However, those ideas were not implemented. Finally, Verhoosel and Gutiérrez [24] state that undamaged cohesive interfaces in an unstructured 2D triangle mesh were initially constrained prior to the onset of damage. These authors did not discuss their approach in any detail, however they noted its ability to limit the total number of active DOF and restrict mesh-dependent artificial compliance.

Therefore, the current proposal introduces a new, more complete framework different than others suggested in the literature.

Current Work and Preliminary Results

To accurately determine the stress state at an interface, we have developed special user-defined macroelements that include the nodal connectivity from the two elements adjacent to an interface, as shown in Figure 13. This has been developed as a User-Element (UEL/VUEL) user subroutine for both Abaqus/Standard and Abaqus/Explicit.

Recall that until released, the corresponding nodes on either side of an interface are coincident, and no gap exists. As shown in the figure, a uniquified interface normal vector n is assumed to point from element 1 to element 2, such that:

$$n = n_1 = -n_2 \tag{6}$$

where n_1 is the outward normal on element 1, and n_2 is the outward normal on element 2.

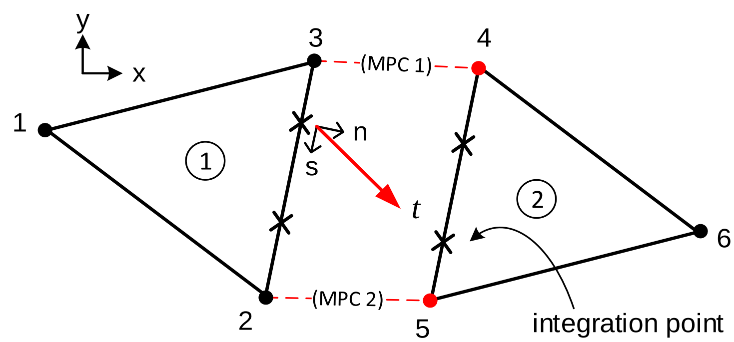

Figure 13. A macroelement used to compute interface values based on solution in adjacent elements.

To evaluate the activation criterion, the stresses are first calculated within each element adjacent to the interface. Because a cohesive element may exist at the boundary between regions with significantly different material properties, a weighted average from corresponding points along the interface is computed:

$$\sigma = \gamma_1 \sigma_1 + \gamma_2 \sigma_2 \quad \text{where} \quad \gamma_1 + \gamma_2 = 1 \tag{7}$$

The interface weight factors, γ_i, are based on element moduli as well as geometric factors such as the characteristic element size. If the material and element size are the same for both element, the weight factors are each given by $y_i = 1/2$, and the weighted average stress is simply the mean value:

$$\sigma = \frac{1}{2}(\sigma_1 + \sigma_2) \tag{8}$$

The average stress is then used to calculate a unique interface traction vector in the global coordinate system, $t_g = \sigma\, n$, which is rotated into a local coordinate system attached to the interface to obtain the local traction vector:

$$t = R\, t_g = R\, \sigma\, n \tag{9}$$

In 2D problems, the local traction components are expressed as a vector with shear and normal components:

$$t = [t_s\, , t_n]^T \tag{10}$$

To determine if an interface should be activated, the traction at each interface integration point is checked against a quadratic traction interaction (QTI) criterion. In 2D, the QTI criterion is written:

$$f = \sqrt{\left(\frac{\langle t_n \rangle}{t_n^c}\right)^2 + \left(\frac{t_s}{t_s^c}\right)^2} \tag{11}$$

The Macaulay brackets ⟨·⟩ are used to indicate that normal tractions only contribute to failure at the interface if $t_n > 0$, such as caused by tensile stresses. The QTI criterion is interpreted as the ratio of the magnitude of the interface traction to the critical traction vector at the onset of damage t^c, where $t^c = [t_s^c\, , t_n^c]^T$, and where t_s^c and t_n^c are the shear and normal components.

In the present work, we release MPCs once a threshold value, f_{rel}, has been satisfied:

$$0 \leq f_{rel} \leq 1 \tag{12}$$

If the QTI criterion exceeds f_{rel} at any integration point on the interface, all nodes on the interface in an active MPC are flagged for release at the beginning of the next increment:

$$\max(f) \geq f_{rel} \Rightarrow interface\ constraint\ is\ released \tag{13}$$

Once an MPC is released, it remains off for the rest of the analysis, and the MPC release criterion at the activated interface will no longer be computed. To honor the MPC release criterion set by the user, an increment is restarted with a smaller time step if $\max(f) > 1.1 f_{rel}$.

The currently developed analysis codes handle all calculations and employ custom data structures to pass non-default data between Abaqus user subroutines, and from increment to increment. An example analysis using the currently developed preprocessor and analysis codes developed for the proposed selectively activated CZM is shown in Figure 14.

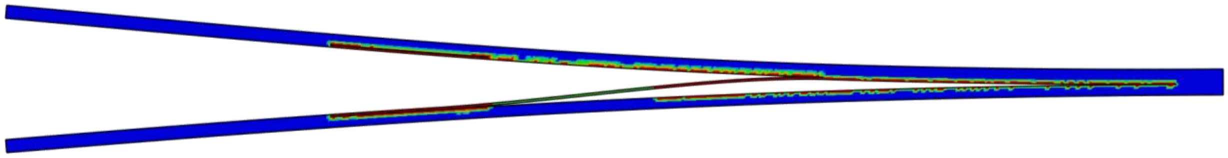

Figure 14. Example Double-Cantilever Beam with crack jumping between plies – red areas indicate where cohesive elements are active

Potential Limitations and Alternatives

Parallel Computing

Computational approaches such as the finite element method benefit from formulations that are well-suited for parallel computing, where calculations are distributed and carried out concurrently by multiple processes to reduce the time needed to reach a solution. Unfortunately, the macroelement-based IP-DGM formulation described above is not well-suited for parallel processing in Abaqus/Standard since read/write access for the elements on either side of an interface may be "owned" by different processes. An alternative approach of the IP-DGM using only the stability term in (5) may be sufficient to prevent artificial compliance. Pilot tests of this concept are promising, resulting in computed solutions which match that of the full IP-DGM formulation. This alternative will be explored in the final report.

Stochastic Interface Activation Criteria

In the current work, we propose the option to scale the interface release/activation criterion in a non-deterministic fashion based on a 2-parameter Weibull distribution. The Weibull distribution is a statistical model that is widely used to represent the natural variation in the strength and reliability of material, but appears to be rarely applied to cohesive fracture models (for an example, see the work of Zhou and Molinari [8] and the references therein).

Providing this option is primarily motivated to account for uncertainty and/or natural variations present in the measurement of material and fracture properties. Such variation may be due to manufacturing effects, the presence of micro-defects, etc. For example, in Figure 15, the activation traction t^a computed for $N = 200$ cohesive elements are shown, listed by element number. Evidently, the activation tractions are suitably randomized using the Weibull distribution.

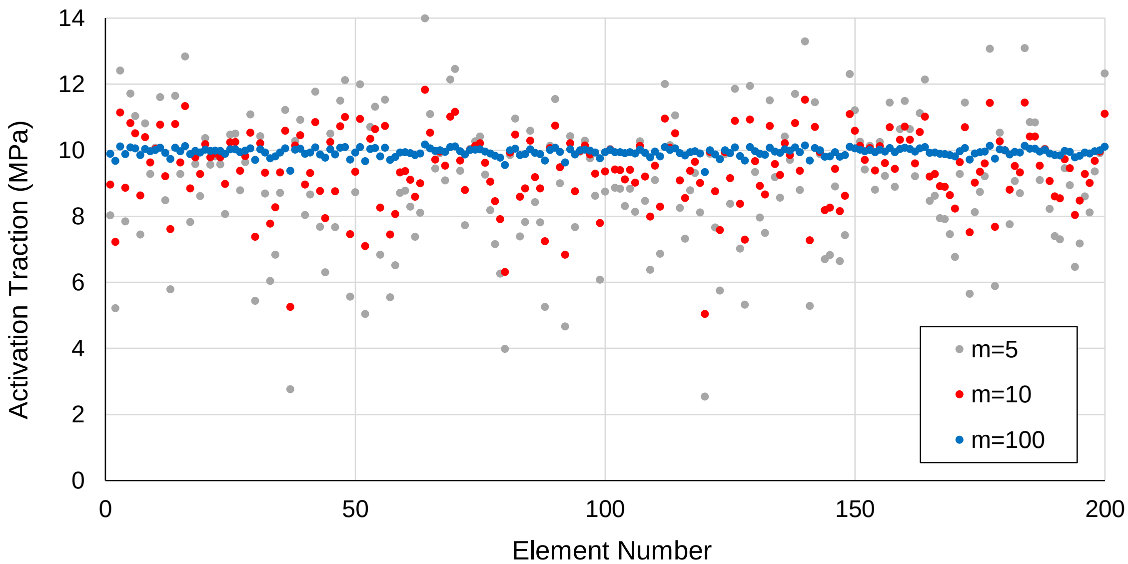

Figure 15. Computed values for activation traction t^a centered about the mean value, $t^c = 10MPa$ for Weibull moduli, $m = 5,10,100$

Significance

Intellectual Merit

Selective activation has advantages like those provided by adaptive insertion techniques but does not require the continuous use of remeshing routines. Cohesive elements actively contribute to the solution only once they have been activated. This effectively solves the problem of artificial compliance inherent to the intrinsic CZM, while avoiding the costly overhead of frequent adaptive remeshing procedures used by the extrinsic CZM.

In addition, the conditions for damage initiation and propagation in the proposed selectively activated CZM are influenced by the physics of the problem, rather than purely numerical parameters such as the cohesive penalty stiffness, $\boldsymbol{K}$. In fact, the solution is influenced only by the load conditions, part geometry, and assumed material properties. As a result, confidence in the outcome of an analysis is increased and verification and validation (V&V) can proceed more quickly.

To the best of our knowledge, the work developed in this project is the most advanced and complete MPC-based selective activation technique to date, and the first selectively activated Discontinuous Galerkin Method.

Due to the overall complexity of the stated goals, a set of integrated software utilities will be developed. This software collection will consist of two main parts: a finite element mesh preprocessing package, and an analysis package. The complete implementation of the proposed selectively activated CZM will be designed to generate a mesh that provides a variety of potential crack paths at interelement boundaries throughout a finite element mesh (i.e., a Gen-2 mesh), and that may be used to predict fracture initiation and non-self-similar crack propagation without *a priori* knowledge of where it may occur. This capability is crucial in the case where damage or manufacturing flaws exist within a material.

The true potential of the MPC-based selectively activated CZM is expected to be realized with 3D analyses, since the method allows arbitrary interelement fracture but offers to dramatically reduce the number of active DOF.

In composite laminates or other nonhomogeneous materials, the combination of the MPC and IP-DGM techniques is a useful and practical technique to prevent fracture in sub-critical interfaces when an MPC is released.

Broader Impacts

The proposed selectively activated CZM is suitable as a general-purpose modeling technique and may be used in any simulation, with or without damage. For any model where damage does not occur, the solution will closely match that of a conventional continuous mesh without cohesive elements. In fact, when the MPC-based strategy is applied, the (undamaged) solution will be *exactly* equal to that obtained from a matching continuous mesh without cohesive elements and the total computational expense is only slightly increased due to extra calls to procedures that enforce the MPC constraints. Each of the MPC procedures are very simple. Thus, the selectively activated CZM offers the capability to run general analysis for a negligible increase in computational expense while including the capability to adaptively introduce cohesive cracks wherever needed as the solution proceeds. This represents a significant improvement over currently available state-of-the-art cohesive zone models.

Note that the implementation of the selectively activated CZM described in this proposal permits the MPC and IP methods to be combined. In this case, if there is no damage the IP method is never utilized. If damage criteria are satisfied, however, then the combination may be advantageous for modeling crack growth in composite materials and adhesive joints – or any model where failure occurs between different constituent materials with different failure properties.

Opportunities for Further Research and Development

In addition, the selectively activated CZM opens opportunities for further research and development and for advanced fracture analyses:

- Multiphysics Analysis: The framework provided by the current implementation also provides a capability to allow coupled thermal and multiphysics-based fracture properties. For example, temperature dependent material properties are accessible via the subroutine implementations currently developed for this work, and the strength of an interface may be influenced accordingly. Another palpable research direction for multiphysics-based fracture analysis is to account for environmental degradation and the effects of water saturation in composite materials for submerged marine hydrokinetics applications.
- Extensible R&D Platform: The framework provided by the current implementation provides useful techniques for communicating data between various subroutines and between different increments of the solution, which is not typically possible with Abaqus subroutines by default. This capability offers opportunities for research

and development – for example, to support requirements for sharing data in non-local mechanics and damage criteria, or for methods which predict the direction of fracture propagation based on non-local averaging.

- The current preliminary implementation is already heavily integrated with Abaqus. However, additional work may be undertaken in the future to provide a convenient graphical user interface (GUI). In fact, a significant amount of work as already been performed to develop a GUI plugin for the Abaqus/CAE.

Finally, we mention that many of the techniques, procedures, logic, and algorithms developed for the Abaqus-based implementation of the selectively activated CZM may be similarly implemented in other finite element codes. For instance, the ANSYS FEA software package offers an ability to access the internal model database (via a convenient Python-based API) and the capability to write user-subroutines such as user-defined elements. Such developments may be very useful for agencies and businesses which are already heavily invested in FEA packages other than Abaqus but would benefit from the capabilities offered by the selectively activated cohesive zone model discussed in this report.

Conclusion

The CZM is a flexible progressive crack growth model that has been successfully applied in many types of analyses, but usually in situations where the crack path is known *a priori* – for example, to model debonding of material interfaces and other cases of self-similar fracture propagation where conventional Linear Elastic Fracture Mechanics (LEFM) may also be successfully applied. However, the reliability of the CZM is limited by artificial compliance, which is mesh-dependent and difficult to predict or counteract. The practical use of the CZM is also restricted by technical challenges related to inserting cohesive elements within an arbitrary finite element mesh. The proposed selectively activated CZM is a natural extension of conventional intrinsic and extrinsic cohesive zone models that addresses their shortcomings by (1) alleviating or eliminating the effect of artificial compliance, (2) minimizing the number of DOF in the system matrix while retaining eliminated DOF for reactivation as needed, and (3) utilizing dormant cohesive elements that are selectively activated at interelement boundaries only as needed by the analysis, without remeshing.

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