Unstructured Methods for Simulating Pervasive Fracture and Fragmentation in Two- and Three-Dimensions

Daniel Spring

Sofie E. Léon, Glaucio H. Paulino

Department of Civil and Environmental Engineering
University of Illinois at Urbana-Champaign
In this presentation, I discuss the use of unstructured methods with interfacial cohesive elements for investigating dynamic fracture problems in quasi-brittle materials.
Outline of Presentation

Dynamic Fracture with Interfacial CZMs

Unstructured Methods for 2D Dynamic Fracture Using Polygonal Finite Elements

Unstructured Methods for 3D Pervasive Fragmentation
Cohesive Zone Models Are Used To Capture the Nonlinear Behavior in the Zone in Front of the Macro Crack-Tip

- A macro-crack forms when the traction in the traction-separation relation goes to zero
- In a numerical setting, we use zero thickness cohesive elements to capture the cohesive zone ahead of the crack-tip

In ductile or quasi-brittle materials, the nonlinear zone ahead of a crack tip is not negligible, and LEFM principles may not be appropriate


In a Finite Element Setting, Zero-Thickness Cohesive Elements are Adaptively Inserted Between Bulk Elements

Cohesive elements consist of two facets that can separate from each other by means of a traction-separation relation.

2D:

Element Opening
($\Delta_n, \Delta_t$)

Separation of Cohesive Elements

3D:

Element Opening
($\Delta_n, \Delta_t$)
The cohesive model is defined by a potential function

\[
\Psi(\Delta_n, \Delta_t) = \min(\phi_n, \phi_t) + [\Gamma_n \left(1 - \frac{\Delta_n}{\delta_n}\right)^\alpha + (\phi_n - \phi_t)] \\
\times [\Gamma_t \left(1 - \frac{\Delta_t}{\delta_t}\right)^\beta + (\phi_t - \phi_n)]
\]

User inputs: \(\phi_n, \phi_t\) (Fracture energy) \[\sigma_n, \tau_t\] (Cohesive strength) \[\alpha, \beta\] (Softening shape parameter)

From the cohesive potential, one can determine the traction-separation relations by taking the respective derivatives.

\[
T_n(\Delta_n, \Delta_t) = \frac{\partial\Psi}{\partial\Delta_n},
\]

\[
T_t(\Delta_n, \Delta_t) = \frac{\partial\Psi}{\partial\Delta_t},
\]


The Cohesive Element Contribution in a Dynamic Setting

In a typical dynamic fracture code, the active cohesive elements contribute an additional term to the external forces acting on the model (during explicit time integration).

![Diagram of cohesive elements and traction-separation relation]

Explicit time integration for extrinsic fracture

<table>
<thead>
<tr>
<th>Step</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initialization</td>
<td>( \mathbf{u}_0, \mathbf{\dot{u}}_0, \mathbf{\ddot{u}}_0 )</td>
</tr>
<tr>
<td>for ( n = 0 ) to ( n_{max} ) do</td>
<td></td>
</tr>
<tr>
<td>Update displacement</td>
<td>( \mathbf{u}_{n+1} = \mathbf{u}_n + \Delta t \mathbf{\dot{u}}_n + \Delta t^2 / 2 \mathbf{\ddot{u}}_n )</td>
</tr>
<tr>
<td>Check insertion of cohesive elements</td>
<td></td>
</tr>
<tr>
<td>Update acceleration</td>
<td>( \mathbf{\dot{u}}<em>{n+1} = \mathbf{M}^{-1} (\mathbf{R}</em>{n+1}^{\text{ext}} + \mathbf{R}<em>{n+1}^{\text{coh}} - \mathbf{R}</em>{n+1}^{\text{int}}) )</td>
</tr>
<tr>
<td>Update velocity</td>
<td>( \mathbf{\dot{u}}_{n+1} = \mathbf{\dot{u}}_n + \Delta t / 2 (\mathbf{\ddot{u}}<em>n + \mathbf{\ddot{u}}</em>{n+1}) )</td>
</tr>
<tr>
<td>Update boundary conditions</td>
<td></td>
</tr>
</tbody>
</table>

Outline of Presentation

Dynamic Fracture with Interfacial CZMs

Unstructured Methods for 2D Dynamic Fracture Using Polygonal Finite Elements

Unstructured Methods for 3D Pervasive Fragmentation
Structured Meshes for Dynamic Cohesive Fracture

One of the primary critiques of the cohesive element method is its mesh dependency.

- The structured 4k mesh is commonly used in dynamic cohesive fracture simulation.

However, structured meshes may introduce artifacts into the fracture behavior, presenting preferred paths for cracks to propagate along.

4k meshes are **anisotropic**, but have many choices of crack path at each node.

Unstructured Meshes for Dynamic Cohesive Fracture

Alternatively, we propose using a randomly generated Centroidal Voronoi Tessellation (CVT).

Unstructured meshes produce random fracture paths with no discernible patterns.

Polygonal meshes are isotropic, but have a limited number of crack paths at each node.

Dijkstra’s algorithm is used to compute the shortest path between two points in the mesh.

The path deviation is computed as:

$$\eta = \frac{L_g}{L_E} - 1$$


A study was conducted on the path deviation over a range of 180°.

The structured 4k mesh is anisotropic, while the unstructured polygonal discretization is isotropic. However, the path deviation in the polygonal mesh is significantly higher than that in the structured mesh.

\[ \eta = \frac{L_\eta}{L_E} - 1 \]


Crack Propagation Within the Element

In order to reduce the path deviation in the unstructured polygonal mesh, we propose using an element-splitting topological operator to increase the number of fracture paths at each node in the mesh.

We restrict elements to be split along the path which minimizes the difference between the areas of the resulting split elements.

The propagating crack now has twice as many paths on which it could travel at each node.
Additionally, we propose the use of an adaptive refinement operator, wherein each polygon around the crack tip is removed and replaced with a set of unstructured quads; which meet at the centroid of the original polygon.

The mesh is adaptively refined in front of the propagating crack-tip.
Quantification of Improvement in Path Deviation

<table>
<thead>
<tr>
<th>Meshing Strategy</th>
<th>Average</th>
<th>Standard Deviation</th>
<th>Improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polygonal</td>
<td>0.1931</td>
<td>0.0013</td>
<td>-</td>
</tr>
<tr>
<td>Polygonal with Splitting</td>
<td>0.0445</td>
<td>0.0009</td>
<td>77%</td>
</tr>
<tr>
<td>Polygonal with Refinement</td>
<td>0.0698</td>
<td>0.0021</td>
<td>64%</td>
</tr>
<tr>
<td>Polygonal with Refinement and Splitting</td>
<td>0.0171</td>
<td>0.0004</td>
<td>91%</td>
</tr>
</tbody>
</table>


Example: Pervasive Fracture and Fragmentation

Pervasive fracture of an internally impacted thick cylinder

\[ P(t) = 400e^{-(t-1)/100} \]

\[ P(t) = 400e^{-(t-1)/100} \]


When we only use a geometrically unstructured mesh, we get unbiased fracture behavior, but unrealistic fracture patterns.

When we use both a geometrically and topologically unstructured mesh, we get unbiased fracture behavior and realistic fracture patterns.

Without element-splitting

With element-splitting

Example: Dominant Crack with Microbranching

Experimental setup and results:

![Experimental setup diagram](image)

Crack Velocity

Time (μs)

Fracture Pattern

Numerical model:

![Numerical model diagram](image)

PMMA Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$</td>
<td>3.24 GPa</td>
</tr>
<tr>
<td>$\rho$</td>
<td>1190 kg/m$^3$</td>
</tr>
<tr>
<td>$\phi$</td>
<td>352.4 N/m</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>129.6 MPa</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>2</td>
</tr>
</tbody>
</table>


Adaptively refined unstructured meshes produce a smooth crack path with large macrobranches and a uniform distribution of microbranching.

The adaptively refined meshes produce results in good agreement with experiments.

Influence of Meshing Strategy on the Crack-Tip Velocity

**Numerical Results**

- Adapively Refined Mesh
- Coarse Polygonal Mesh

**Experimental Result**


## Comparison of Computational Cost

<table>
<thead>
<tr>
<th>Case</th>
<th>Elements</th>
<th>Nodes</th>
<th>Cost (min)</th>
<th>Iterations to Fracture</th>
<th>Cost/Iteration (10⁻³ s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4,000</td>
<td>7,188</td>
<td>21.5</td>
<td>28,200</td>
<td>45.7</td>
</tr>
<tr>
<td>2</td>
<td>4,000</td>
<td>7,188</td>
<td>20.8</td>
<td>23,000</td>
<td>54.3</td>
</tr>
<tr>
<td>3</td>
<td>4,000</td>
<td>7,188</td>
<td>19.1</td>
<td>21,000</td>
<td>54.6</td>
</tr>
</tbody>
</table>

Some Remarks on 2D Cohesive Fracture

- Unstructured polygonal meshes produce an isotropic discretization of the problem domain.
- Without careful design considerations, polygonal meshes are inherently poorly suited to dynamic fracture simulation with the cohesive element method.
- The newly proposed topological operators are designed to increase the number of paths a crack can propagate along, and result in a meshing strategy on par with the best, fixed meshing strategy available in the literature.
- The adaptive refinement with element splitting scheme increases the problem size, but can decrease the computational cost.
- By combining geometrically and topologically unstructured methods, the model is truly random and reduces numerically induced restrictions. Thus, reducing uncertainty in numerical simulations.


Dynamic Fracture with Interfacial CZMs

Unstructured Methods for 2D Dynamic Fracture Using Polygonal Finite Elements

Unstructured Methods for 3D Pervasive Fragmentation
Pervasive cracking and fragmentation comprises the entire spectrum of fracture behavior.

Characteristics
- Crack branching
- Crack coalescence
- Complete fragmentation

Issues
- Sensitivity to material heterogeneity
- Any structure introduced to the mesh will bias fragmentation behavior

The computational framework for 3D cohesive fracture is an extension of that for 2D cohesive fracture.

Issue 1: Sensitivity to Material Heterogeneity

- Most materials contain heterogeneity (or defects) at the microscale.

- Defects naturally arise in materials due to grain boundaries, voids, or inclusions.
- Defects may also be introduced through the act of processing or machining the material.
- Microscale defects constitute potential regions where stresses can concentrate and lead to damage or failure.

Constitutively Unstructured Through a Statistical Distribution of Material Properties

The material strength is assumed to follow a modified Weibull distribution:

\[ \sigma = \sigma_{min} + \lambda (-\ln(1 - \rho))^{1/m} \]

\[ \sigma_{min} = 264\text{MPa}, \ \lambda = 50, \ m = 2 \]

Issue 2: Structured Artifacts in Automatically Generated Meshes

- Automatic mesh generators often conduct additional post-processing of the mesh; to remove elements with degenerate edges and sliver elements.

- In some cases, this additional post-processing leads these (initially random) meshes to contain an underlying structure.

- To remove this structure, we propose using the technique of nodal perturbation.

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Geometrically Unstructured Through Nodal Perturbation

Nodal Perturbation:

- Nodes are randomly perturbed by a multiple of $d_{\text{min}}$:
  \[ \mathbf{X}_n = \mathbf{X}_o + d_{\text{min}} \times NP \times \mathbf{n}_{\text{random}} \]

- We conduct a set of geometric studies to quantify the effect of the magnitude of the nodal perturbation factor on the quality of the mesh.


Spring DW, Paulino GH, Achieving pervasive cohesive fracture and fragmentation in three-dimensions: Theory, computation and applications. *In Preparation*. 
First, we investigate the influence of nodal perturbation on the coefficient of variation of facet areas.

- The dynamic time step is a function of the element size.
- Small element facets reduce the size of the critical time step.


Spring DW, Paulino GH, Achieving pervasive cohesive fracture and fragmentation in three-dimensions: Theory, computation and applications. *In Preparation*. 
Geometrically Unstructured Through Nodal Perturbation

Similar trends are observed for the study on the maximum and minimum interior angles in the mesh.

Summary

<table>
<thead>
<tr>
<th>NP Factor</th>
<th>COV of Facet Area</th>
<th>Minimum Angle (°)</th>
<th>Maximum Angle (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>min</td>
<td>mean</td>
<td>max</td>
</tr>
<tr>
<td>0.0</td>
<td>0.004</td>
<td>0.130</td>
<td>0.460</td>
</tr>
<tr>
<td>0.1</td>
<td>0.004</td>
<td>0.138</td>
<td>0.470</td>
</tr>
<tr>
<td>0.2</td>
<td>0.004</td>
<td>0.157</td>
<td>0.548</td>
</tr>
<tr>
<td>0.3</td>
<td>0.003</td>
<td>0.183</td>
<td>0.628</td>
</tr>
<tr>
<td>0.4</td>
<td>0.002</td>
<td>0.210</td>
<td>0.693</td>
</tr>
<tr>
<td>0.5</td>
<td>0.004</td>
<td>0.236</td>
<td>0.790</td>
</tr>
<tr>
<td>0.6</td>
<td>0.005</td>
<td>0.259</td>
<td>0.865</td>
</tr>
</tbody>
</table>

Ex: The commercial software Abaqus qualifies elements with interior angles less than 10° or greater than 160° as distorted.

Example: Radial Fragmentation of a Hollow Sphere

Here, we consider the pervasive fragmentation of a hollow sphere with symmetric boundary conditions.

\[ E = 370 \text{ GPa} \quad \rho = 3900 \text{ kg/m}^3 \]
\[ \phi = 50 \text{ J/m}^2 \quad \sigma_{\text{min}} = 264 \text{ MPa} \]

The sphere is impacted with an impulse load, which is converted to an initial nodal velocity

\[ \mathbf{v}_0(x, y, z) = \dot{\mathbf{x}} \]

We investigate the influence of idealized surface features, namely bumps and dimples, on the fragmentation behavior of the hollow sphere.

- Alternately, surface features may be viewed as geometric defects, and investigating their impact on the global fragmentation response is equally significant.

Spring DW, Paulino GH, Achieving pervasive cohesive fracture and fragmentation in three-dimensions: Theory, computation and applications. *In Preparation.*
Numerical Definition of a Fragment

A fragment is defined as a mass of bulk elements which are surrounded by a free boundary and/or fully separated cohesive elements.

**Algorithm 1** Procedure for determining the distribution of the fragments.

```plaintext
input: nBulkElems //number of bulk elements in the model
nVisited = 0 //number of bulk elements visited
while (nVisited < nBulkElems)
    Iterate over all the elements in the model
    if (element is cohesive) continue; end if
    if (element has been visited) continue; end if
    Create a new fragment structure
    Add the bulk element to the fragment, and flag it as visited
    Increment nVisited
    for (i = 0; i < number of bulk elements in the fragment; i++)
        Get current element in the fragment
        for (j = 0; j < number of adjacent elements; j++)
            if adjacent element is cohesive and not flagged as visited
                Flag cohesive element as visited
                if (cohesive element has failed completely) continue; end if
                for (k = 0; k < number of adjacent bulk elements; k++)
                    if (element has been visited) continue; end if
                    Add the bulk element to the fragment, and flag it as visited
                end for
            else
                if (element has been visited) continue; end if
                Add the bulk element to the fragment, and flag it as visited
                Increment nVisited
            end if
        end for
    end while
output: Fragments
```

Spring DW, Paulino GH, Achieving pervasive cohesive fracture and fragmentation in three-dimensions: Theory, computation and applications. *In Preparation.*
Geometric Features Can Be Used to Regularize Fragmentation Patterns

- The initial impact velocity is set at: $v_0(x, y, z) = 2500x$
- Similar trends are observed at higher impact velocities and with different statistical distributions of material strength.

Spring DW, Paulino GH, Achieving pervasive cohesive fracture and fragmentation in three-dimensions: Theory, computation and applications. *In Preparation.*
Example: Kidney Stone Fragmentation by Direct Impact

This example considers the direct impact of a kidney stone. We use this example to investigate the use functionally graded materials to regularize fragmentation behavior.


Fragmentation of a **Homogeneous Stone**

To develop a baseline, we first consider the fragmentation of a homogeneous stone with different levels of variation in material properties.

CA

CA(50)/COM(50)

COM

<table>
<thead>
<tr>
<th>Material</th>
<th>Modulus ($E$)</th>
<th>Density ($\rho$)</th>
<th>Fracture Surface Energy ($\phi$)</th>
<th>Fracture Toughness ($\sigma$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CA</td>
<td>$8.504 \text{ GPa}$</td>
<td>$1732 \text{ kg/m}^3$</td>
<td>$0.382 \text{ J/m}^2$</td>
<td>$0.5 \text{ MPa}$</td>
</tr>
<tr>
<td>CA(50)/COM(50)</td>
<td>$25.16 \text{ GPa}$</td>
<td>$2038 \text{ kg/m}^3$</td>
<td>$0.735 \text{ J/m}^2$</td>
<td>$1.0 \text{ MPa}$</td>
</tr>
</tbody>
</table>

Spring DW, Paulino GH, Achieving pervasive cohesive fracture and fragmentation in three-dimensions: Theory, computation and applications. *In Preparation.*
Next, we show that fragmentation behavior can be regularized by modelling the graded distribution of material in the stone.

Some Remarks on 3D Pervasive Fracture & Fragmentation

- The cohesive element method constitutes a framework which allows us to capture the full spectrum of fracture mechanisms.
- A statistical distribution of material properties can be used to account for microscale defects and inhomogeneities.
- A random perturbation of the nodes reduces structure created by automatic mesh generators.
- By incorporating constitutive and geometric heterogeneity in the model we can reduce numerically induced artifacts into the simulated results and increase the certainty in our simulations.
- We can use simple geometric and constitutive design features to regularize pervasive fracture and fragmentation behavior in three-dimensions.

Spring DW, Paulino GH, Achieving pervasive cohesive fracture and fragmentation in three-dimensions: Theory, computation and applications. *In Preparation.*
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Thank You, Questions?

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Additional details may be found in the related publications:

- Spring DW, Paulino GH, Achieving pervasive cohesive fracture and fragmentation in three-dimensions: Theory, computation and applications. *In Preparation*.

Daniel Spring
spring2@illinois.edu