Adaptive fracture and failure simulation

Sofie E. Leon

University of Illinois
Department of Civil and Environmental Engineering

May 14th, 2014
Acknowledgements

• Collaborators on the work in today’s presentation
  – Professor Glaucio H. Paulino
  – Daniel Spring
  – Dr. Cameron Talischi
  – Dr. Jay Foulk, Dr. Alejandro Mota and Dr. James Ostein and the Mechanics of Materials Team at Sandia National Laboratory

• Hosts of this visit
  – Professor Ivan Menezes
  – Professor Waldemar Celes

• Work funded by
  – Philanthropic Education Organization (PEO)
  – National Science Foundation (NSF)
I am from...

Sandia Internship: Livermore, CA

Grad school: Urbana, IL

Undergrad: San Luis Obispo, CA

Hometown: Ventura, CA
Complex, large-scale fracture and failure problems are computationally demanding.


What is needed to solve these problems?

Models

\[ T(\Delta_n, \Delta_t) = \nabla \Psi \]

Computational power

Solution methods
The focus of this talk will be on development of solution methods for realistic fracture simulation.

- Unstructured meshes
- Solution methods for fracture simulation
- Adaptive mesh modification
- Mapping from mesh to another
Crack patterns on structured grids may be biased by the mesh

4k structured mesh

Crack patterns on the structured 4k mesh are limited by the element facets

Adaptive mesh operators are introduced to improve fracture patterns.

Original 4k mesh

Nodal perturbation

Original 4k mesh

Edge swap

To evaluate mesh bias, we evaluate deviation in crack length

The fracture energy required to generate a crack is directly proportional to the crack length

\[ E_f = L_c G_c \]

The length of the crack should not be altered by the finite element representation such that the fracture energy artificially increases


Even with adaptive operators, structured meshes exhibit bias for crack propagation.

FEM distance measured with Dijkstra’s algorithm

Error in crack length is dependent on angle of propagation

Instead of structured meshes, we use polygonal discretizations – CVT and Near-MPS

Centroidal Voronoi Tessellation (CVT)

Near-MPS (MPS)

\[ d > r_{\text{min}} \]
Polygonal meshes provide an alternative to structured meshes that reduces mesh bias.

Crack length studies show the CVT and Near-MPS meshes are isotropic. However, error is significantly higher than the 4k mesh.

Leon, S. E., Spring, D. W., & Paulino, G. H. Submitted to *IJNME*. 
High geometric error is explained by the lack of available crack directions in a polygonal mesh.
The focus of this talk will be on development of solution methods for realistic fracture simulation.
We investigate element splitting as a means to provide more directions for the crack to propagate.

- **CVT**
  - No Splitting
  - Unrestricted Splitting
  - Restricted Splitting

- **Near MPS**
Element splitting decreases the error in crack length
Element splitting decreases the error in crack length
Element splitting decreases the error in crack length

Mean = 4.29%
Stdev = 0.018

Mean = 1.18%
Stdev = 4e-4

Mean = 3.67%
Stdev = 0.01

Mean = 1.44%
Stdev = 5e-4
Numerical investigation of polygonal meshed with Compact Compression Specimen

Crack path

$\nu(t)$

Impact velocity, $\nu(t)$ (m/s)

Time (µs)
Numerical investigation of polygonal meshed with Compact Compression Specimen
Cohesive elements aim to capture the nonlinear behavior in the zone ahead of a crack tip.

When the size of the nonlinear zone ahead of a crack tip is not negligible, for example in ductile or quasi-brittle materials, the LEFM approach may not be appropriate.

Dugdale, D. JMPS 8, no. 2 (1960): 100–104.
Cohesive elements are activated by a stress criteria

Consider a domain with an initial notch (dashed line)

Stresses are computed from displacements and extrapolated to the nodes
Cohesive elements are activated by a stress criteria

Consider a domain with an initial notch (dashed line)

Stresses are computed from displacements and extrapolated to the nodes

Nodes with stress greater than 90% of the cohesive strength of the material are flagged for further investigation
Cohesive elements are activated by a stress criteria

Compute the principle stress along the facets adjacent to the flagged nodes

If the stress is greater than the cohesive strength, insert a cohesive element
Nodes of bulk elements are duplicated when cohesive elements are inserted.

- **2D**: 
  - Bulk elements
  - Cohesive element with zero initial thickness
  - Separation in cohesive element ($\delta_n, \delta_t$)

- **3D**: 
  - Bulk elements
  - Cohesive element with zero initial thickness
  - Separation in cohesive element ($T_n, T_t$)
Park-Paulino-Roesler (PPR) Model

- Potential based – Gradients of potential function give traction-separation relations
- Path dependent work of separation – energy dissipation due to fracture depends on the separation path
- Obeys cohesive interaction boundary conditions
- User has control over important model parameters

Computational implementation of the PPR potential-based cohesive model in ABAQUS: Educational perspective

Kyoungsoo Park a,b, Glaucio H. Paulino a

a School of Civil & Environmental Engineering, Yonsei University, 50 Yonsei-ro, Seodaemun-gu, Seoul, Republic of Korea
b Department of Civil & Environmental Engineering, University of Illinois at Urbana-Champaign, 203 North Mathews Ave., Urbana, IL 61801, United States

ABSTRACT
A potential-based cohesive zone model, so called the PPR model, is implemented in a commercial software, e.g. ABAQUS, as a user-defined element (UEL) subroutine. The intrinsic cohesive zone modeling approach is employed because it can be formulated within the

PPR Potential Based Cohesive Zone Model

The PPR potential based cohesive zone model was developed for mixed-mode cohesive fracture and takes into account physical parameters such as fracture energy, cohesive strength, and shape of cohesive interaction.

Learn about the features of the PPR model and how it can be applied for various materials and either intrinsic or extrinsic models. The educational page features:
- Interactive demonstration illustrating the PPR potential and its gradients
- A simple Matlab GUI and user manual available for download
- ABAQUS user subroutine (UEL)
- List of related publications

Link to PPR Educational Page
Results for CCS example without element splitting

4k

CVT

Near MPS

Too straight

Non physical branching

Crack diverges due to numerical instability
Element splitting is not suitable for the MPS mesh in dynamic fracture applications

- CVT time step = 2.5e-9 to 1e-9
- MPS time step without splitting = 1e-10 → requires over 1,000,000 steps!

Complete separation of elements is an indication of numerical instability. Element splitting would only restrict the time step requirement and worsen stability.
Element splitting is activated in the same way as insertion of cohesive elements

Flagged node with stress greater than 90% of cohesive strength

Check potential facets, if traction is greater than cohesive strength, then split the element into 2 and insert a cohesive element between them.
CVT polygonal elements with splitting provide excellent results for CCS test

Unrestricted splitting would put too great of a requirement on the time step as in the near-MPS case, but restricted splitting already provides excellent results.

The focus of this talk will be on development of solution methods for realistic fracture simulation.

Solution methods:

- Unstructured meshes for fracture simulation
- Adaptive mesh modification
- Mapping from one mesh to another
During adaptive simulation, we must map variables from the old elements to the new ones.

Element variables on original elements

Variables need to be transferred to new elements
Project element variables from one mesh to another by minimizing the error between them

$$\Phi[\varphi, \bar{z}, \bar{y}] := \int_B W(F, \bar{z}) \, dV + \int_B \bar{y} \cdot (\bar{z} - z) \, dV - \int_B \rho_0 B \cdot \varphi \, dV - \int_{\partial T_B} T \cdot \varphi \, dS$$

Certain element variables can not be projected directly – example rotation matrices

Given rotations at two points, find the rotation at some other point:

\[ R = ? \]

\[ R_1 \quad \quad R_2 \]

Polynomial interpolation of rotations does not make sense because rotations belong to a multiplicative group, specifically the Special Orthogonal, \( SO(3) \), Lie Group

\[ R \neq \frac{R_1 + R_2}{2} \]

\[ R \in SO(3) = \left\{ A \in M(n) \left| AA^T = I, \det A = 1 \right. \right\} \]

In order to produce a variable that belongs to a Lie group we can map it to its Lie Algebra where addition is admitted. The Lie Algebra of SO are skew-symmetric matrices, \( so(3) \)

\[ \log R = r \in so(3) = \left\{ B = M(n) \left| B = -B^T \right. \right\} \]
Lie group interpolation and L2 error minimizing projection

1. Logarithmic map to get Lie group variables into their Lie algebra
2. Perform the interpolation that minimizes error in the Lie algebra
3. Exponential map to get the Lie algebra variables back to their Lie group
Lie group interpolation and L2 error minimizing projection

1. Logarithmic map to get Lie group variables into their Lie algebra
2. Perform the interpolation that minimizes error in the Lie algebra
3. Exponential map to get the Lie algebra variables back to their Lie group
Lie group interpolation and L2 error minimizing projection

1. Logarithmic map to get Lie group variables into their Lie algebra
2. Perform the interpolation that minimizes error in the Lie algebra
3. Exponential map to get the Lie algebra variables back to their Lie group
Lie group interpolation and L2 error minimizing projection

1. Logarithmic map to get Lie group variables into their Lie algebra
2. Perform the interpolation that minimizes error in the Lie algebra
3. Exponential map to get the Lie algebra variables back to their Lie group
Uniaxial tension of a smooth bar is used to investigate the remeshing and mapping procedure.

- Coarse mesh, 10 elements across thickness
- Fine mesh, 20 elements across thickness
We perform numerical studies to evaluate the proposed mapping scheme.

Case 1: Projection many times in a row onto the same mesh.

- Lie Group $\times$
- Lie Algebra $\bigcirc$

Logarithmic mapping

- Lie Algebra $\bigcirc$
- Lie Group $\times$

Exponential mapping

Same mesh
We notice some diffusion in the internal state variables when many remaps are performed.

Equivalent plastic strain in fine mesh at one integration point per element at end of analysis.

No remapping

Remap 100 times between $t = 0$ and $t = 0.25$
The dissipation is less prevalent in a fine mesh than in it is in a coarser mesh.

Coarse mesh

Fine mesh
We perform numerical studies to evaluate the proposed mapping scheme

Case 2: Remesh many times and project once at each interval

New mesh

Logarithmic mapping

Exponential mapping
Some dissipation is present in the load-displacement curve, but it reduces with mesh refinement.
Some concluding thoughts

- Despite promising geometric indicators, not all polygonal element meshes are appropriate for dynamic fracture applications.
- CVT polygonal elements with adaptive element splitting yield greater accuracy in fracture applications than structured meshes.
- The proposed Lie-group interpolation scheme ensures accuracy of adaptive remeshing.
- Development of new computational tools get us a few steps closer to large-scale failure simulation.

Thank you! Questions?
Back up slides
Explicit central difference time integration scheme

\[ M \ddot{u}_{n+1} + Ku_{n+1} = F_{n+1} \]

Updates given by the Newmark time integration scheme:

\[ u_{n+1} = u_n + \Delta t \dot{u}_n + \frac{\Delta t^2}{2} [(1 - 2\beta) \ddot{u}_n + 2\beta \ddot{u}_{n+1}] \]

\[ \dot{u}_{n+1} = \dot{u}_n + \Delta t [(1 - \gamma) \ddot{u}_n + \gamma \ddot{u}_{n+1}] \]

Parameters are chosen to arrive at the explicit central difference scheme

\[ \beta = 0 \quad \gamma = \frac{1}{2} \]

\[ u_{n+1} = u_n + \Delta t \dot{u}_n + \frac{\Delta t^2}{2} \ddot{u}_n \]

\[ \ddot{u}_{n+1} = M^{-1} [F_{n+1} - Ku_{n+1}] \]

\[ \dot{u}_{n+1} = \dot{u}_n + \frac{\Delta t}{2} [\ddot{u}_n + \ddot{u}_{n+1}] \]

Lumped mass matrix, so inversion is trivial

The time step is governed by the stability condition for the Newmark time integration scheme

\[ \omega \Delta t \leq \Omega_{\text{crit}} \quad \text{where} \quad \Omega_{\text{crit}} = \left( \frac{\gamma}{2} - \beta \right)^{\frac{1}{2}} \quad \text{then} \quad \Delta t \leq \frac{2}{\omega} \]

Where the largest natural frequency of the structure is given by the generalized eigenvalue problem

\[-Ku = \omega^2 Mu\]

Alternatively, the time step has also been approximated by

\[ \Delta t \leq \frac{l_e}{C} \quad \text{where} \quad C = \sqrt{\frac{E}{(1 - \nu)(1 + \nu) \rho}} \]

The traction-separation relation is characterized by the PPR potential-based cohesive zone model

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

Gradients of potential give traction-separation

\[ T_t(\Delta_n, \Delta_t) = -\beta \frac{\Gamma_t}{\delta_t} \left(1 - \frac{|\Delta_t|}{\delta_t}\right)^{\beta-1} \left[ \Gamma_n \left(1 - \frac{|\Delta_n|}{\delta_n}\right)^\alpha + \langle \phi_n - \phi_t \rangle \right] \frac{\Delta_t}{|\Delta_t|} \]

\[ T_n(\Delta_n, \Delta_t) = -\alpha \frac{\Gamma_n}{\delta_n} \left(1 - \frac{\Delta_n}{\delta_n}\right)^{\alpha-1} \left[ \Gamma_t \left(1 - \frac{|\Delta_t|}{\delta_t}\right)^\beta + \langle \phi_t - \phi_n \rangle \right] \]

[Park, 2009]
Failure of 304L laser weld is characterized first by necking, then free surface creation is a secondary effect.

340L is extremely tough and damage tolerant.

Hypothesis is that void size and distribution within the weld plays a large role in the necking process.
Lack of convergence in the load displacement may be due to element distortion

Remeshing would eliminate element distortion and make convergence possible
Minimization of error between source and target variables

Start with the energy functional

\[ \Phi_o [\varphi] = \int_B A(F, z) \, dV - \int_B \rho b \cdot \varphi \, dV - \int_{\partial T B} T \cdot \varphi \, dS \]

where \( A \) is the Helmholtz free energy, \( x=\varphi(X,t) \), \( F \) is the deformation gradient (\( F=\text{Grad}\varphi \)), \( z \) is the set of source internal variables, \( \rho \) is the mass density, \( b \) is the body force, and \( T \) are the external tractions.

The functional is modified with a constraint on the target internal variables, \( z_\text{bar} \), with a Lagrange multiplier \( y_\text{bar} \), now it is a three-field functional

\[ \Phi [\varphi, \bar{z}, \bar{y}] = \int_B A(F, \bar{z}) \, dV + \int_B \bar{y} (\bar{z} - z) \, dV - \int_B \rho b \cdot \varphi \, dV - \int_{\partial T B} T \cdot \varphi \, dS \]

The independent variables belong to the following spaces

\[ \varphi \in U \quad \bar{z}, \bar{y} \in V \]

Introduce the following test functions, to perform \( \text{wrt} \) each of the independent variables

\[ \xi \in U \quad \eta, \zeta \in V \]

Minimization of error between source and target variables

The variations are

\[
D\Phi [\varphi, \bar{z}, \bar{y}] (\xi) = \int_B \frac{\partial A}{\partial F} : \nabla \xi dV - \int_B \rho b \cdot \xi dV - \int_{\partial T B} T \cdot \xi dS = 0
\]

\[
D\Phi [\varphi, \bar{z}, \bar{y}] (\eta) = \int_B \left( \bar{y} + \frac{\partial A}{\partial F} \right) \cdot \eta dV = 0
\]

\[
D\Phi [\varphi, \bar{z}, \bar{y}] (\zeta) = \int_B (\bar{z} - z) \cdot \zeta dV = 0
\]

Let \( y = -dA/dx_\text{bar} \), then introduce discretizations for the fields and test functions

\[
\varphi_h (X) = N_\alpha (X) \varphi_\alpha \in U_h \subset U \quad \xi_h (X) = N_b (X) \xi_b \in U_h \subset U
\]

\[
\bar{y}_h (X) = \lambda_\alpha (X) \bar{y}_\alpha \in V_h \subset V \quad \eta_h (X) = \lambda_\beta (X) \eta_\beta \in V_h \subset V
\]

\[
\bar{z}_h (X) = \lambda_\alpha (X) \bar{z}_\alpha \in V_h \subset V \quad \zeta_h (X) = \lambda_\beta (X) \zeta_\beta \in V_h \subset V
\]

where \( \lambda \) and \( N \) are interpolation functions

Minimization of error between source and target variables

Now the variations become

\[ \int_B \frac{\partial A}{\partial F} \cdot \nabla N_\alpha dV - \int_B \rho b N_\alpha dV - \int_{\partial T B} TN_\alpha dS = 0 \]

\[ \tilde{y}_h = \lambda_\alpha \left( \int_B \lambda_\alpha \lambda_\beta \mathbf{I} dV \right)^{-1} \int_B \lambda_\beta y dV \]

\[ \tilde{z}_h = \lambda_\alpha \left( \int_B \lambda_\alpha \lambda_\beta \mathbf{I} dV \right)^{-1} \int_B \lambda_\beta z dV \]

Projection of internal variables from source, \( z \), to target, \( \bar{z} \_\text{bar} \)

Lie-group interpolation

- Certain internal variables do not admit the additive property, thus it does not make sense to use polynomial interpolation to transfer values from one mesh to another. For example, rotations should not be added as demonstrated below:

  ![Diagram](image)

  \[ R_1 \quad R = ? \quad R_2 \]

- Given \( R_1 \) and \( R_2 \), and we want to find \( R \)
- \( R \neq (R_1 + R_2)^2 \) so polynomial interpolation on \( R \) does not make sense
- \( R \) belongs to a multiplicative group, i.e. \( R = R_2 R_1 \), more specifically \( R \) belongs to the Lie group \( SL \) (special linear group)

  \[ R \in SL(n) = \{ A \text{ is a matrix} \mid \det A = 1 \} \]

Ensure internal variables remain in the appropriate space

- Transform R from its Lie group to its Lie algebra by the logarithmic map
- Addition is the operation on the Lie algebra, so polynomial interpolation works
- Finally we transform back to the Lie group by means of the exponential map

- To combine both procedures for recovery of internal variables
  - 1. Logarithmic map to get the variables into the Lie algebra
  - 2. Perform the interpolation that minimizes error
  - 3. Exponential map to get the variable back to the Lie group

Coming into equilibrium after each consecutive remap reveals that the mesh is not converged after remapping.

Maximum equivalent plastic strain appears to converge.

However, the residual reveals that remapping pulls the system out of equilibrium.

The system comes back into equilibrium rapidly, i.e. only a few iterations.

The residual after remapping may be an indication of the discretization error. Further investigation into different levels of refinement are needed.