Modeling Discontinuities and their Evolution within Finite Elements: Application to Material Interfaces, 3-D Cracks, and Microstructures

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Outline

• Modeling Discontinuities in Finite Elements
• Extended Finite Element and Level Set Methods

• Applications
  • Material Interfaces
  • Three-Dimensional Cracks
  • Polycrystalline Microstructures

• Conclusions
Modeling Discontinuities in Finite Elements

• Classical Approach (FE)
  Crack discontinuity modeled by the mesh; use of quarter-point element leads to better accuracy

• Embedded Discontinuities
  ▪ Weak discontinuity: \( \dot{\mathbf{a}}^h = \dot{\mathbf{a}} + \dot{\mathbf{a}}^{enh} \)
    (Ortiz et al., 1987, Belytschko et al., 1988)
  ▪ Strong discontinuity: \( \mathbf{u}^h = \mathbf{u} + [\mathbf{u}]H_{\xi}(\mathbf{x}) \)
    (Simo et al., 1993)
Strong Discontinuity Approach

- Displacement consists of regular and enhanced components, where the enhanced component yields a jump across the discontinuity surface.

- Multi-field (assumed strain) variational principle is used.

- Enhanced degrees of freedom are statically condensed on each element, which introduces incompatibilities between elements.

- Discontinuity surface can only end on element edges.

- Mesh dependency exists, and extension to 3-D problems is non-trivial.
New Paradigm in Computational Mechanics

- CAD Model
  - Mesh Generation (Delaunay)

- Interfaces/Fronts
  - Level Set Methods

- Data Approximation
  - Interpolating Functions
  - Enrichment Functions

- FEM
- PU Framework
Partition of Unity Method (Melenk and Babuska, 1996)

Introduction of a function $f(x)$ in a FE space over a region $D \subset \Omega$ such that the sparsity of the stiffness matrix is retained

Classical Finite Element Approximation

$$u^h(x) = \sum_I \phi_I(x) u_I,$$

$$\sum_I \phi_I(x) = 1, \quad \sum_I \phi_I(x)x_I = x$$
PUM (Cont’d)

\[ u^h(x) = \sum_{I} \phi_I(x)u_I + \sum_{J} \phi_J(x)a_J f(x) \]

\( n_I \subset N \)  \hspace{1cm}  \( n_J \subset N^d \)

classical \hspace{2cm} enrichment

**Consequence**

- If \( u_I = 0 \) and \( a_I = 1 \) \( \forall I \):

\[ u^h(x) = f(x), \quad x \in D \]
Level Set and Fast Marching Methods (FMM)

- Numerical techniques for tracking moving interfaces, with the interface represented as the zero level contour of a function of one higher-dimension.
- Hyperbolic equation in terms of level set function \( \varphi(x, t) \) governs the motion of the interface; FMM is well-suited for propagation of monotonic fronts (Sethian, 1996)

- Advantages
  - Computed on a fixed Eulerian grid
  - Handles topological changes in the interface naturally
  - Readily extends to \( \mathbb{R}^d \)
Level Set Function

\[ \phi = 0 \]

\[ \phi < 0 \]

\[ \phi > 0 \]
Hexagonal Interface

$\varphi(x,0)$
Extended Finite Element Method (Moes et al, 1999)

- Finite element mesh is used to describe the domain
- Internal boundaries (e.g., cracks, holes, interfaces) are not part of the mesh
- Presence of internal boundaries is ensured by enriching the displacement approximation
- Single-field variational principle is used, and the stiffness matrix is sparse and symmetric
- Level set and fast marching methods are used to evolve the crack front in 3-D crack applications
- No remeshing required for crack growth simulations
Enriched Displacement Approximation (X-FEM)

\[ u^h_i(x) = \sum_{n_I \in N} \phi_I(x)u_{iI} + \sum_{n_J \in N^c} \phi_J(x)a_{ij}\Psi(x) \]

• Choice of the enrichment function \( \Psi(x) \) depends on the geometric entity (material interface, crack-tip, crack surface, etc.)

• \( N^c \) is the set of nodes whose support intersects the geometric entity of interest
Modeling Holes

Level set function for holes
Modeling Weak Discontinuities (1D Bimaterial Bar)

\[ x = -1 \quad \Omega_1 \quad \xi \quad \Omega_2 \quad x = 1 \]

\[ u = 0 \quad \Gamma_1 \quad \Omega_1 \quad \Omega_2 \quad u = 1 \]

Enrichment Function
Enrichment Functions (2D BVP)

$|\varphi|$  

Laplacian smoothing of $\varphi$
Extended Finite Element Method (X-FEM)

Crack Modeling in 2D
(Dolbow, 1999)
Enriched Displacement Approximation (3D Cracks)

\[
\mathbf{u}_i^h(\mathbf{x}) = \sum_{n_I \in \mathbb{N}} \phi_I(\mathbf{x})u_{iI} + \sum_{n_J \in \mathbb{N}^c} \phi_J(\mathbf{x})a_{ij} \Psi(\mathbf{x})
\]

- **Crack Interior Enrichment:** \(\Psi(\mathbf{x})\) is the Heaviside function and \(\mathbb{N}^c\) is the set of nodes whose support intersects the crack interior.

- **Crack Front Enrichment:** \(\Psi(\mathbf{x})\) are the asymptotic crack functions and \(\mathbb{N}^c\) is the set of nodes whose support (closure) intersects the crack front.
Representation of a Planar Crack

Crack Front

Signed distance function $\varphi_1(x)$ is the distance of $x_p$, the orthogonal projection of $x$ on the crack plane, to the crack front

Crack Plane

Signed distance function $\varphi_2(x)$ is the signed distance (+ above and − below) to the crack plane
Signed Distance Functions

\[ \varphi_1 \]

\[ \varphi_2 \]

(Courtesy of Chopp)
Level Set ($\psi$) and Signed Distance Function ($\varphi_1$)

(Courtesy of Chopp)
$\varphi_1$ Signed Distance Function (Two Cracks)

(Courtesy of Chopp)
Selection of Nodes

Nodes are selected for enrichment on the basis of the values of the signed distance functions $\phi_1$ and $\phi_2$.

Crack Interior Enrichment

$H(\mathbf{x}) = \text{sign}(\phi_2(\mathbf{x}))$

$\text{sign}(\xi) = \begin{cases} 
1, & \text{if } \xi \geq 0 \\
-1, & \text{otherwise} 
\end{cases}$
Nodal Enrichment (Cont’d)

Crack Front Enrichment

\[ \psi = \left\{ \sqrt{r} \cos \frac{\theta}{2}, \sqrt{r} \sin \frac{\theta}{2}, \sqrt{r} \sin \theta \sin \frac{\theta}{2}, \sqrt{r} \sin \theta \cos \frac{\theta}{2} \right\} \]

\[ r = \sqrt{\varphi_1^2 + \varphi_2^2} \]

\[ \tan \theta = \frac{\varphi_2}{\varphi_1} \]
Nodal Enrichments for Elliptical Crack

Heaviside Enrichment

Crack-Front Enrichment
Partitioning Finite Elements

2D

3D
Computation of Stress Intensity Factors

Domain Integrals (Moran and Shih, 1987)

\[ K_I(s) = \sqrt{\frac{J(s)E}{1 - \nu^2}} \]

\[ J(s) = -\frac{\int_V H_{kj}q_{k,j} \, dV}{\int_{L_c} l_k n_k \, ds} \]
X-FEM/FMM Crack Growth Algorithm

Initialize the crack front with the crack front given by $\psi^{-1}(0)$

Use the FMM to compute the signed distance function: $\psi^{-1}(0) = \varphi^{-1}(0)$, $\|\nabla \varphi_1\| = 1$

Compute crack front speed $F$ using the X-FEM

Use the FMM to extend the front speed: $\nabla F_{\text{ext}} \cdot \nabla \varphi_1 = 0$

Use the FMM to compute the location of the advancing crack front at time $\Delta t$: $\|\nabla \psi\| = 1/F_{\text{ext}}$

Advance crack front by time step size $\Delta t$: $\psi = \psi - \Delta t$

$$
\frac{\partial \varphi_1}{\partial n} = 1 \Rightarrow \nabla \varphi_1 \cdot n = 1
$$

$$
\Rightarrow \| \nabla \varphi_1 \| = 1
$$

(Courtesy of Chopp)
Hexahedral Mesh

Penny crack ($24^3$ mesh)
Planar Elliptical Crack

Elliptic angle

SIFs
Fatigue Growth of One Elliptical Crack
Fatigue Growth of Two Penny Cracks
Tetrahedral Mesh

Surface mesh

Vicinity of the crack
Fatigue Crack Growth (Tetrahedral Mesh)
Fatigue Growth of Two Elliptical Cracks
Fatigue Growth of Three Penny Cracks
Modeling Brittle Fracture in Polycrystals

Lattice Spring Network Models
- Beale & Srolovitz (1988); Curtin & Scher (1990)
- Yang et al. (1990); Holm (1998)
- Zimmermann et al. (2001)

Cohesive Surface Formulation
- Zhai and Zhou (2000)
- Zavattieri et al. (2001)

Potts grain growth model
dynamic fracture
Grain Growth Model

**Ising Model** *(Ising, 1925)*

- Phase transitions (anti-ferromagnetic ↔ ferromagnetic)
- A two-spin (parallel and anti-parallel) model

**Potts Model** *(Potts, 1952)*

- Phase transitions using $Q$-degenerate states; identical to the Ising model for $Q = 2$
- Introduced for grain growth evolution and micro-structural processes by Srolovitz et al., 1984, 1985
Potts Model

Kinetic Monte Carlo

- Square lattice with $N$ sites
- $Q$ possible spins at each site
- Spin $s_i$ at site $i$
- Periodic boundary conditions

Potts Hamiltonian

$$ H = J \sum_{i=1}^{N} \sum_{j=1}^{nn(i)} (1 - \delta_{s_i s_j}) $$

$N = 400, \quad Q = 3$
Microstructure-Meshing

**OOF (Carter et al., 1998)**
- Microstructure from micrograph or Potts model
- Construction of the FE mesh is directly based on the bonds between adjacent sites in the Potts model

**VCFEM (Ghosh et al., 1997)**
- Voronoi polygons are used to construct the microstructure as well as to perform the FE analysis

**Present Work**
- A constrained Delaunay algorithm with smoothing is developed to mesh the microstructure
Constrained Delaunay Triangulation

Procedure

• Construct initial boundary conforming triangulation using a cubic least squares polynomial fit to represent the grain boundary edges
• Delaunay refinement using the point insertion algorithm of Rebay (Rebay, 1993) is implemented
• Mesh constructed for user-specified spacing $\rho$
Boundary Conforming Triangulation

N = 400

STEP 1

$\rho = 0.1$

$\rho = 0.04$
Final Triangulation

\[ \rho = 0.1 \]

\[ \rho = 0.04 \]

STEP 2
Model Geometry and BCs

- pre-crack
- traction-free
Simulation Procedure

1. Read parameters: \( n_{\text{max}}, G_c^i, G_c^{gb}, \Delta a_{\text{max}} \)
   \[ n = 0; \bar{\varepsilon}_0 = 1 \]

2. X-FEM analysis for initial crack-tip location
   \[ \text{failure} = 0 \]

3. while \((n < n_{\text{max}} \text{ and } \neg \text{failure})\) \{

4. \[ n = n + 1 \]
   if \((x_{\text{tip}} \in \Omega_i)\)
   \[ \theta_g = \theta_{\text{hoop}}; \Delta a = \min(\Delta a_{\text{max}}, \Delta a_{gb}, \Delta a_{\text{hull}}) \]
Simulation Procedure (Cont’d)

5. if \((x_{\text{tip}} \in \Gamma_{gb})\)
   \[
   \begin{align*}
   &\text{find grain boundary directions } \theta_{gb} \\
   &\text{perturb crack along } \theta_{gb} \text{ and } \theta_{\text{hoop}} \text{ and find } \\
   &\theta_g \text{ based on } \max(G_{gb}^b / G_c^b, G_i^i / G_c^i) \\
   &\Delta a = \min(\Delta a_{\text{max}} , \Delta a_{gbv})
   \end{align*}
   \]

6. critical strain \((G = G_c)\): \(\bar{\varepsilon}_n = \sqrt{G_c^k / G} \bar{\varepsilon}_{n-1}\)

7. determine failure status

8. X-FEM analysis with \(\bar{\varepsilon}_n\) before and after crack growth

9. end
Crack Propagation Simulations (Q = 100)

\[
\frac{G_{c}^{gb}}{G_{c}^{i}} = 0.1
\]

\[
t = 10^4 \text{ MCS}
\]

INTERGRANULAR FRACTURE
Simulation 1: $t = 10000$ MCS

\[ \frac{G_c^{gb}}{G_c^i} = 0.3 \]

\[ IG = 100\% \]

\[ \frac{G_c^{gb}}{G_c^i} = 0.5 \]

\[ IG = 42\% \]
Simulation 1 (Cont’d)

\[ \frac{G_c^{gb}}{G_c^i} = 0.7 \]

\[ IG = 21\% \]

\[ R = \frac{G_c^{gb}}{G_c^i} \]
Simulation 2: \( t = 10000 \) MCS

\[
\frac{G^g_c}{G^i_c} = 0.3 \\
IG = 81\%
\]

\[
\frac{G^g_c}{G^i_c} = 0.5 \\
IG = 40\%
\]
Simulation 2 (Cont’d)

\[
\frac{G_{c}^{gb}}{G_{c}^{i}} = 0.7
\]

\[IG = 13\%\]

\[R = \frac{G_{c}^{gb}}{G_{c}^{i}}\]
Conclusions

- A numerical technique (X-FEM) that can model strong as well as weak (strain) discontinuities within finite elements was introduced.

- Level sets and fast marching methods were shown to provide a powerful complement to the X-FEM in tracking the evolution of discontinuities.

- Versatility of the X-FEM was demonstrated via various applications: material interfaces, 3-D crack growth, and brittle fracture in polycrystalline materials.