University of California, Davis

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

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Collaborators and Acknowledgments

- X-FEM (3D Cracks): N. Moes, B. Moran, and T. Belytschko (Northwestern University)
- X-FEM (Material Interfaces and 3D Crack Growth) : D. Chopp (Northwestern University)
- X-FEM (Microstructure): D. J. Srolovitz, J. Prevost, and T. J. Baker (Princeton University)

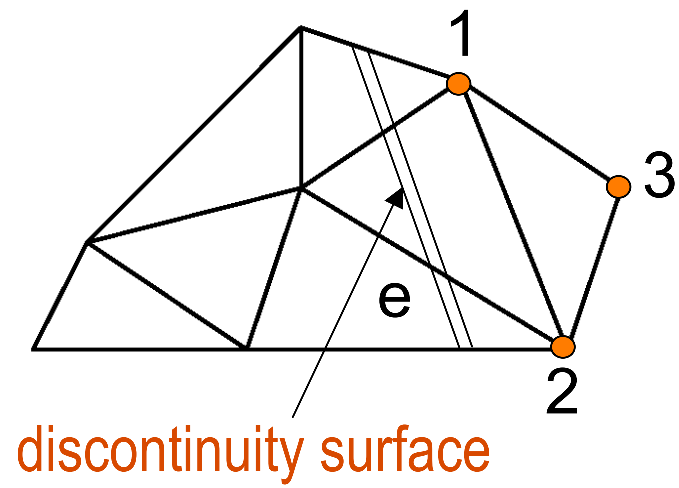
- Mark Miodownik and Elizabeth Holm are thanked for providing the Potts model code

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: $\mathring{\mathbf{a}}^{h} = \bar{\mathring{\mathbf{a}}} + \mathring{\mathbf{a}}^{enh}$
    (**Ortiz et al., 1987**, **Belytschko et al., 1988**)
  - Strong discontinuity: $\mathbf{u}^{h} = \bar{\mathbf{u}} + [\mathbf{u}] H_{\xi}(\mathbf{x})$
    (**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 → FEM
Enrichment Functions → PU Framework

Partition of Unity Method (**Melenk and Babuska, 1996**)

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

Classical Finite Element Approximation

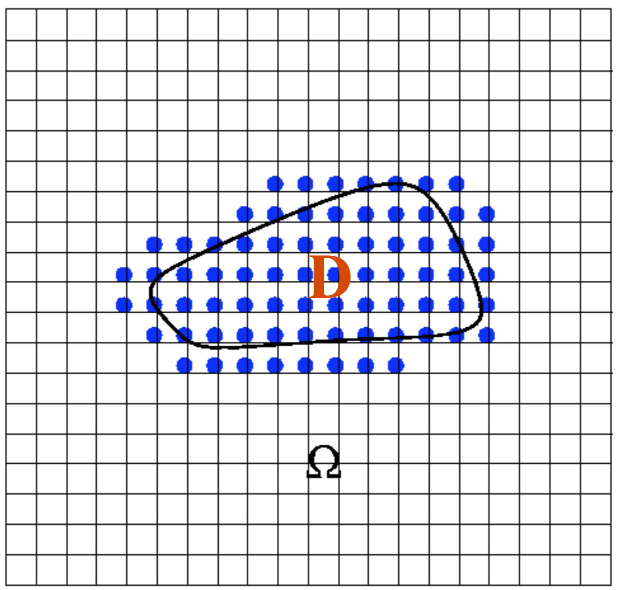
$$u^h(\mathbf{x}) = \sum_I \phi_I(\mathbf{x}) u_I ,$$

$$\sum_I \phi_I(\mathbf{x}) = 1, \quad \sum_I \phi_I(\mathbf{x}) \mathbf{x}_I = \mathbf{x}$$

PUM (Cont'd)

$$u^h(\mathbf{x}) = \sum_{\substack{I \\ n_I \subset N}} \phi_I(\mathbf{x}) u_I + \sum_{\substack{J \\ n_J \subset N^d}} \phi_J(\mathbf{x}) a_J f(\mathbf{x})$$

classical enrichment



Consequence

- If $u_I = 0$ and $a_I = 1 \; \forall I$:

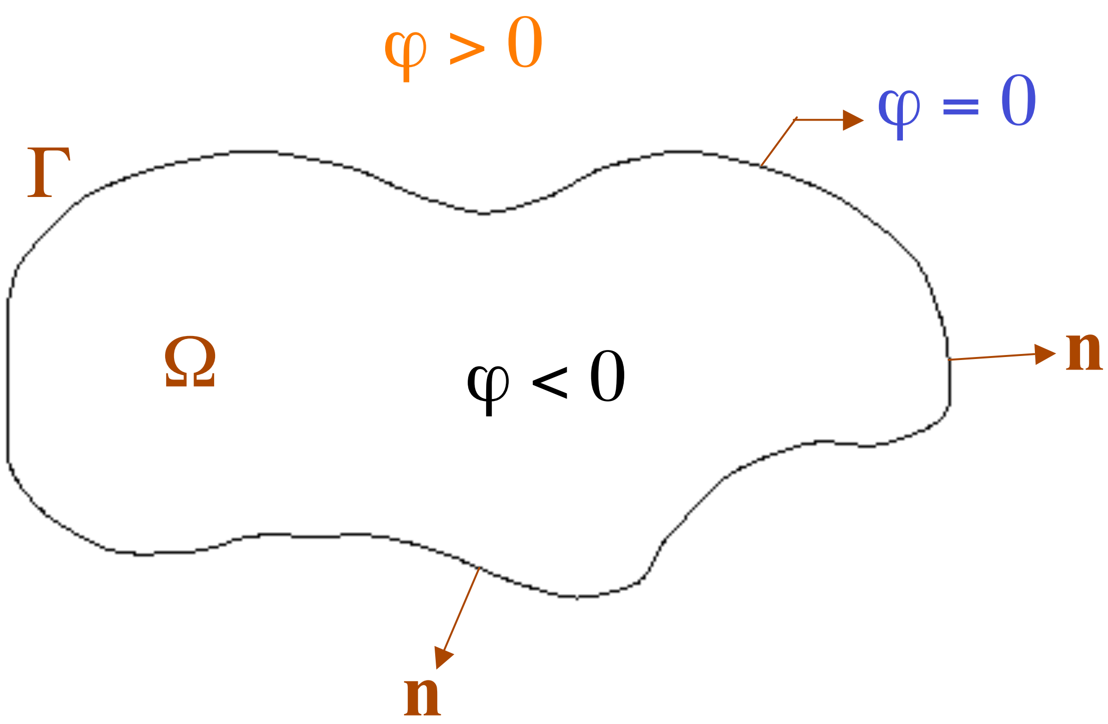
$$\boxed{u^h(\mathbf{x}) = f(\mathbf{x}), \;\; x \in D}$$

Level Set and Fast Marching Methods (FMM)

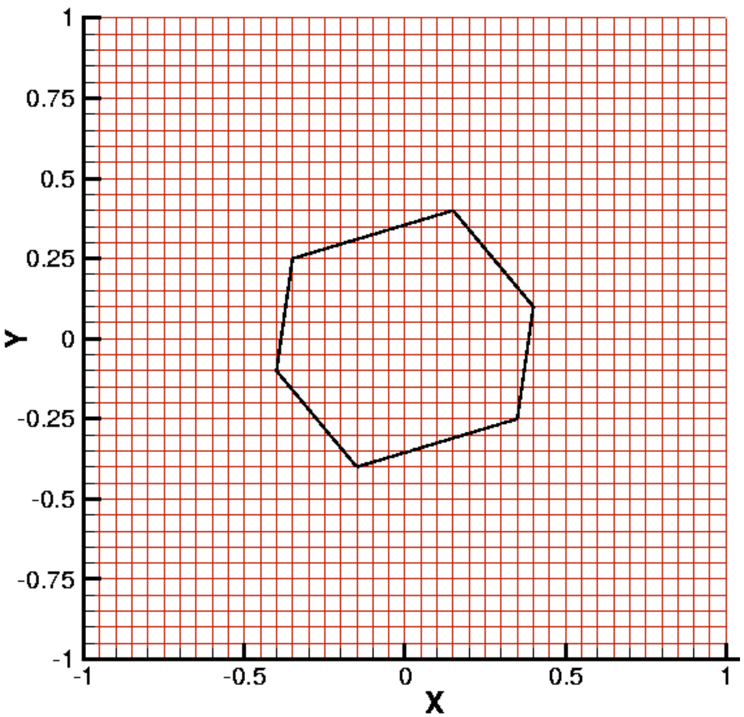
- Numerical techniques for tracking moving interfaces, with the interface represented as the zero level contour of a function of one higher-dimension
- Hyperbolic equation in terms of level set function $\varphi(\mathbf{x}, t)$ governs the motion of the interface; FMM is well-suited for propagation of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

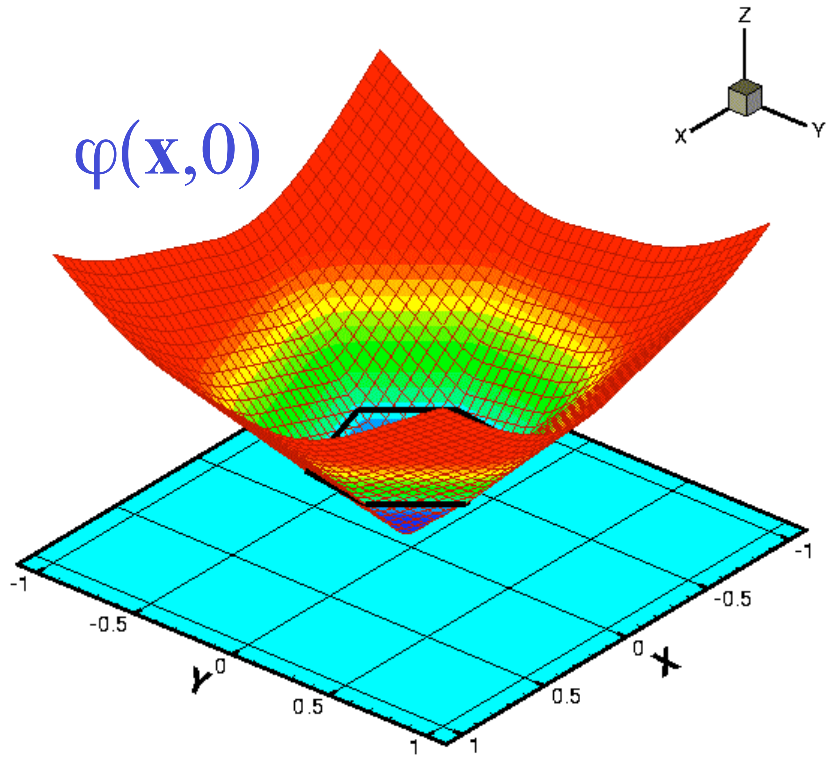
- Advantages
  - Computed on a fixed Eulerian grid
  - Handles topological changes in the interface naturally
  - Readily extends to $\mathbf{R}^d$

Level Set Function



Hexagonal Interface





Extended Finite Element Method (Moes et al, 1999)

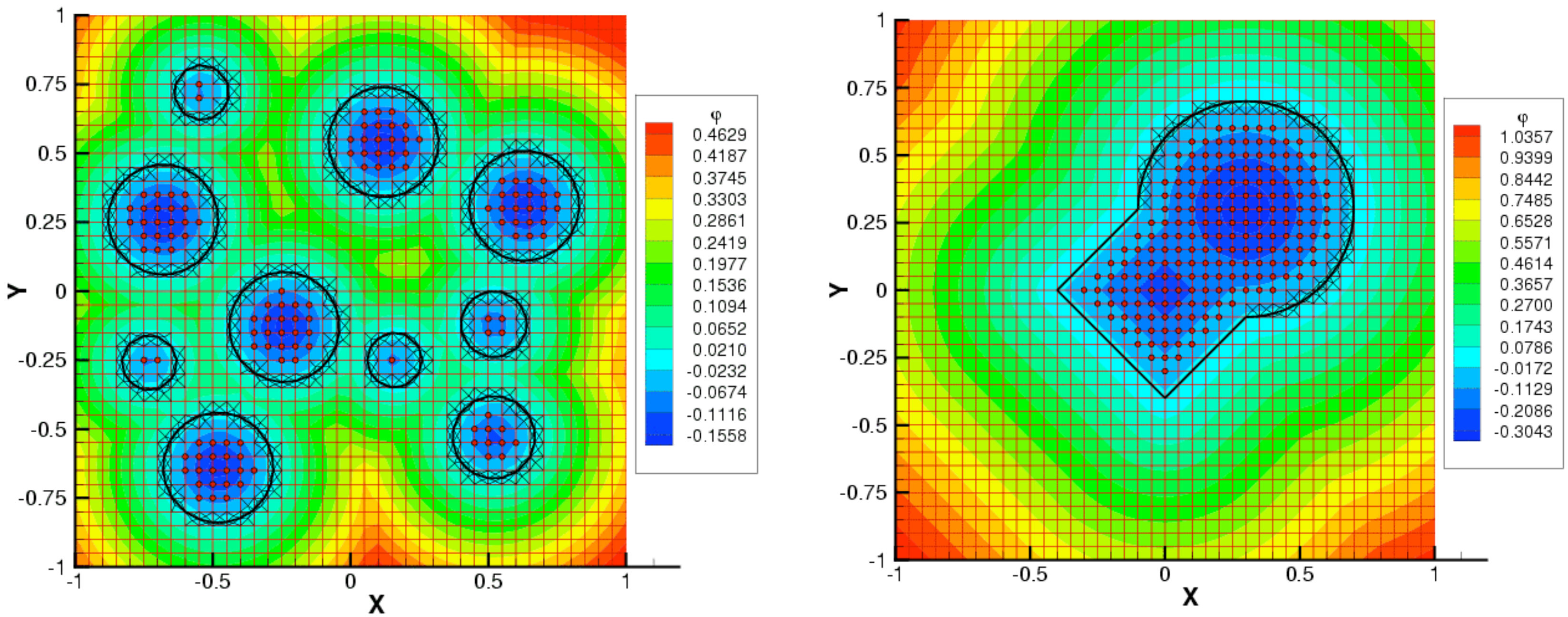
- Finite element mesh is used to describe the domain
- Internal boundaries (e.g., cracks, holes, interfaces) are not part of the mesh
- Presence of internal boundaries is ensured by enriching the displacement approximation
- Single-field variational principle is used, and the stiffness matrix is sparse 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)

$$u_i^h(\mathbf{x}) = \sum_{\substack{I \\ n_I \in \mathrm{N}}} \phi_I(\mathbf{x}) u_{iI} + \sum_{\substack{J \\ n_J \in \mathrm{N}^c}} \phi_J(\mathbf{x}) a_{iJ} \Psi(\mathbf{x})$$

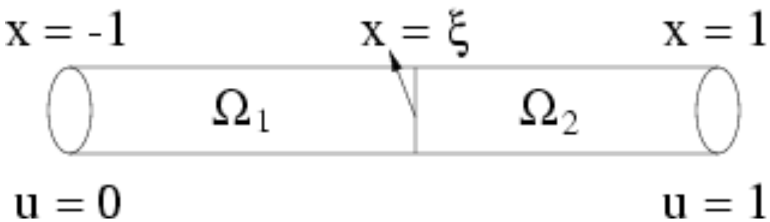
- Choice of the enrichment function $\Psi(\mathbf{x})$ depends on the geometric entity (material interface, crack-tip, crack surface, etc.)
- N^c is the set of nodes whose support intersects the geometric entity of interest

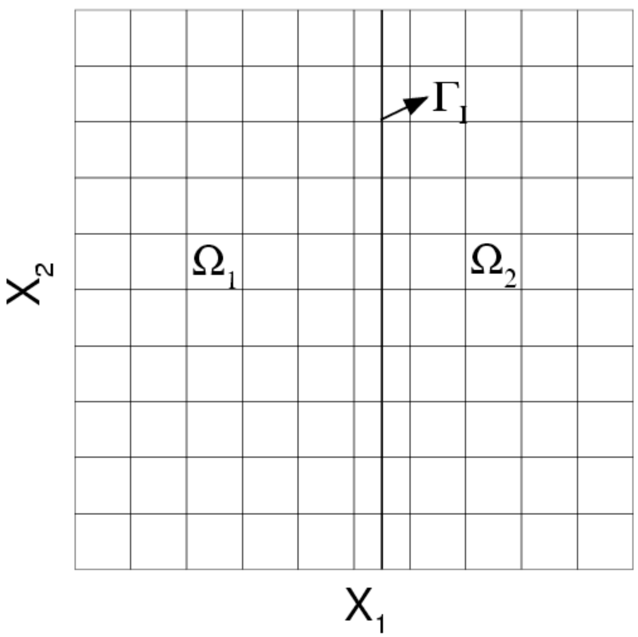
Modeling Holes

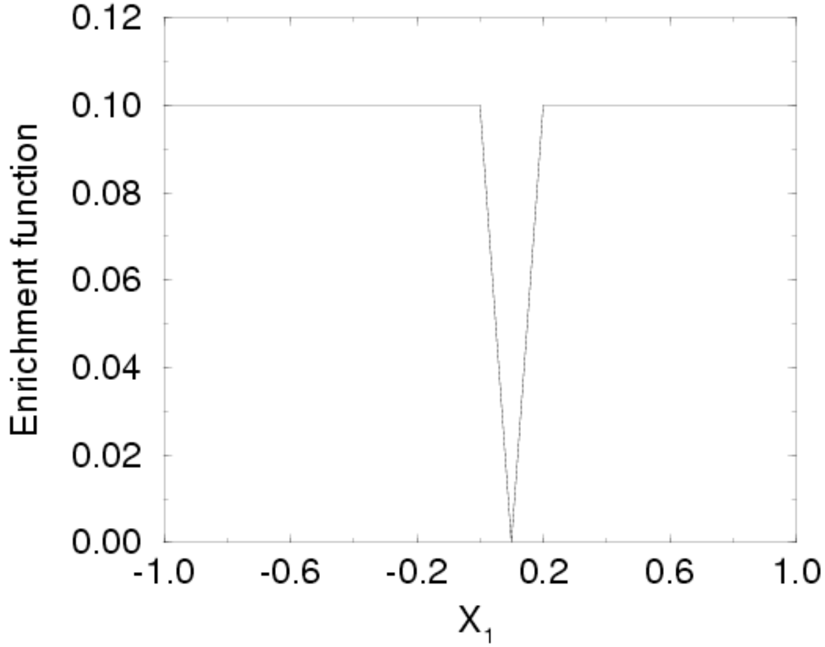


Level set function for holes

Modeling Weak Discontinuities (1D Bimaterial Bar)

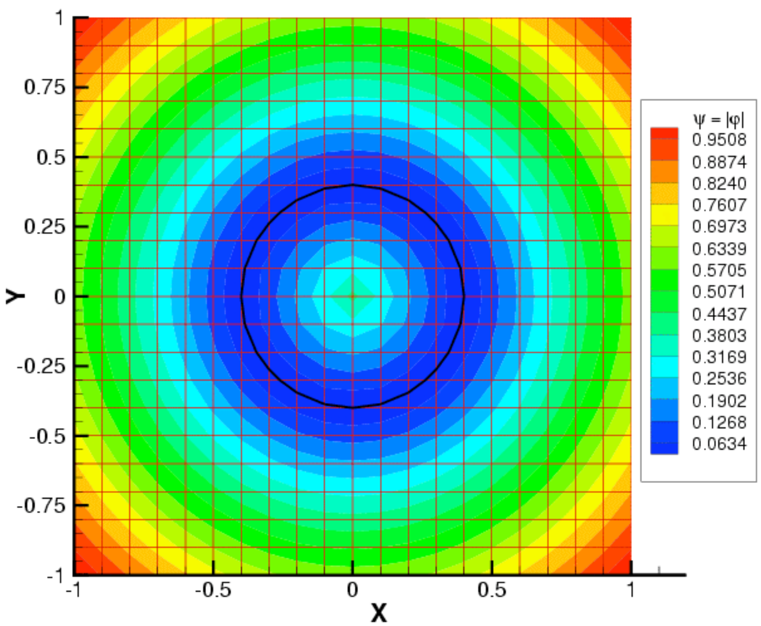




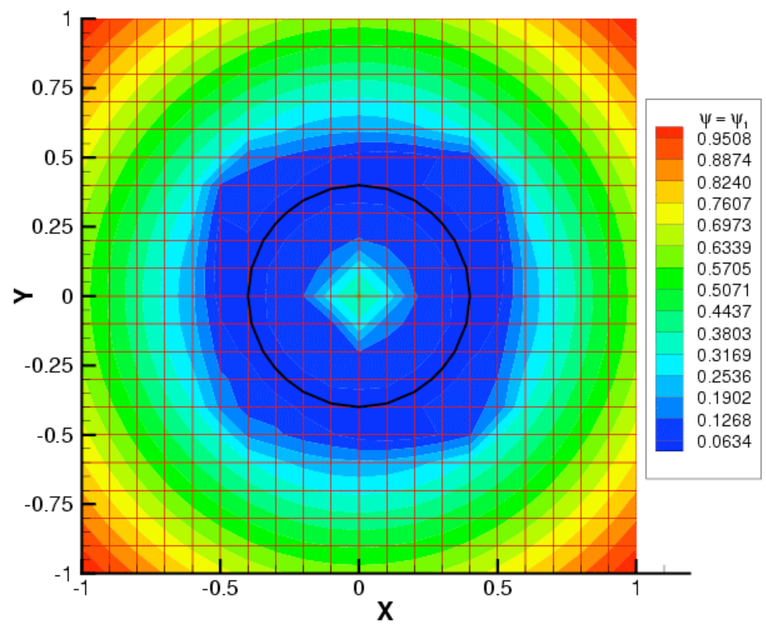


Enrichment Function

Enrichment Functions (2D BVP)



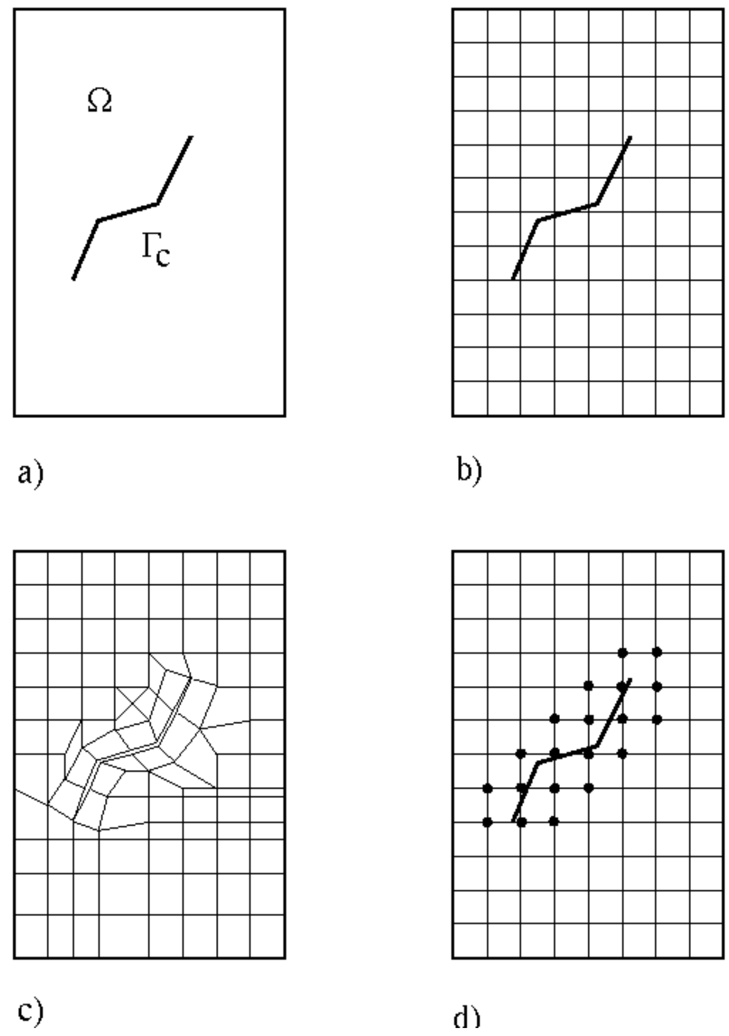
| φ |



Laplacian smoothing of φ

Extended Finite Element Method (X-FEM)

Crack Modeling in 2D
(**Dolbow, 1999**)



Enriched Displacement Approximation (3D Cracks)

$$u_i^h(\mathbf{x}) = \sum_{\substack{I \\ n_I \in \mathrm{N}}} \phi_I(\mathbf{x}) u_{iI} + \sum_{\substack{J \\ n_J \in \mathrm{N}^c}} \phi_J(\mathbf{x}) a_{iJ} \Psi(\mathbf{x})$$

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

Representation of a Planar Crack

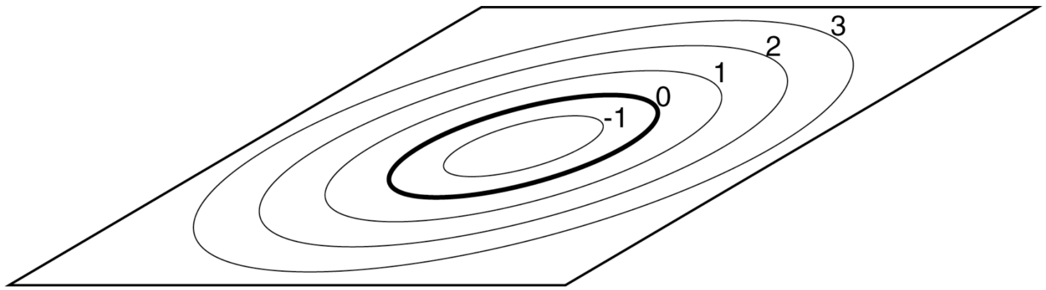
Crack Front

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

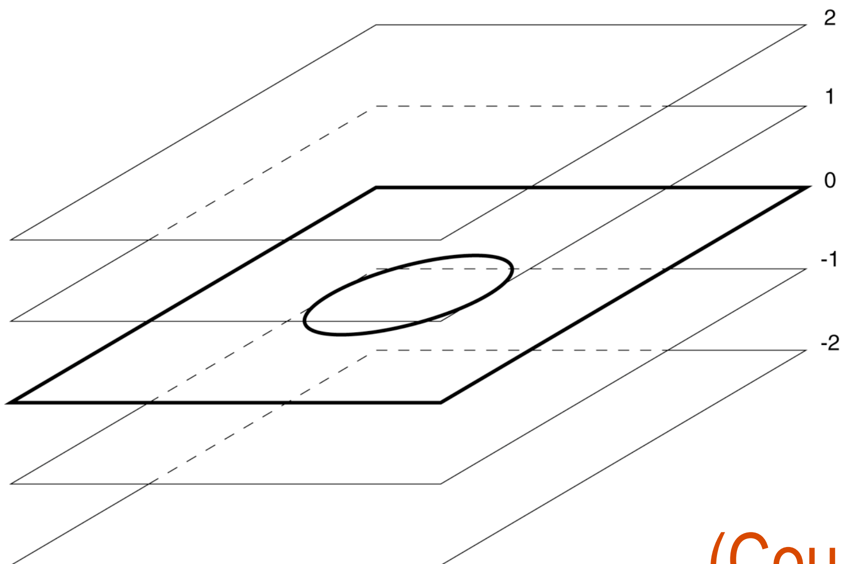
Crack Plane

Signed distance function $\varphi_2(\mathbf{x})$ is the signed distance ($+$ above and $-$ below) to the crack plane

Signed Distance Functions



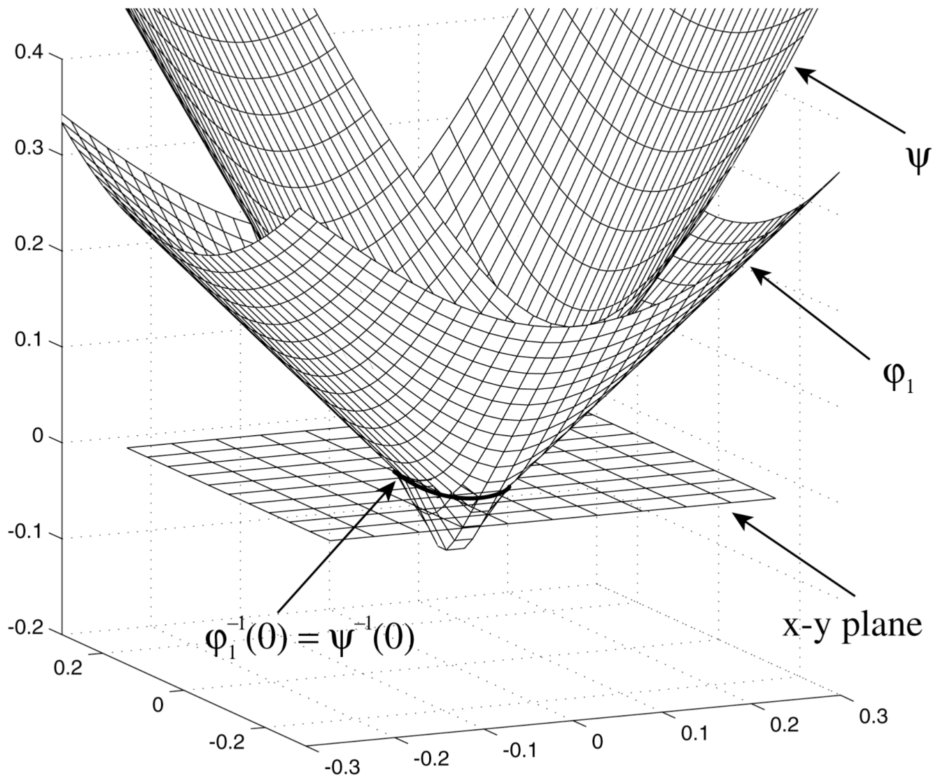
φ_1



φ_2

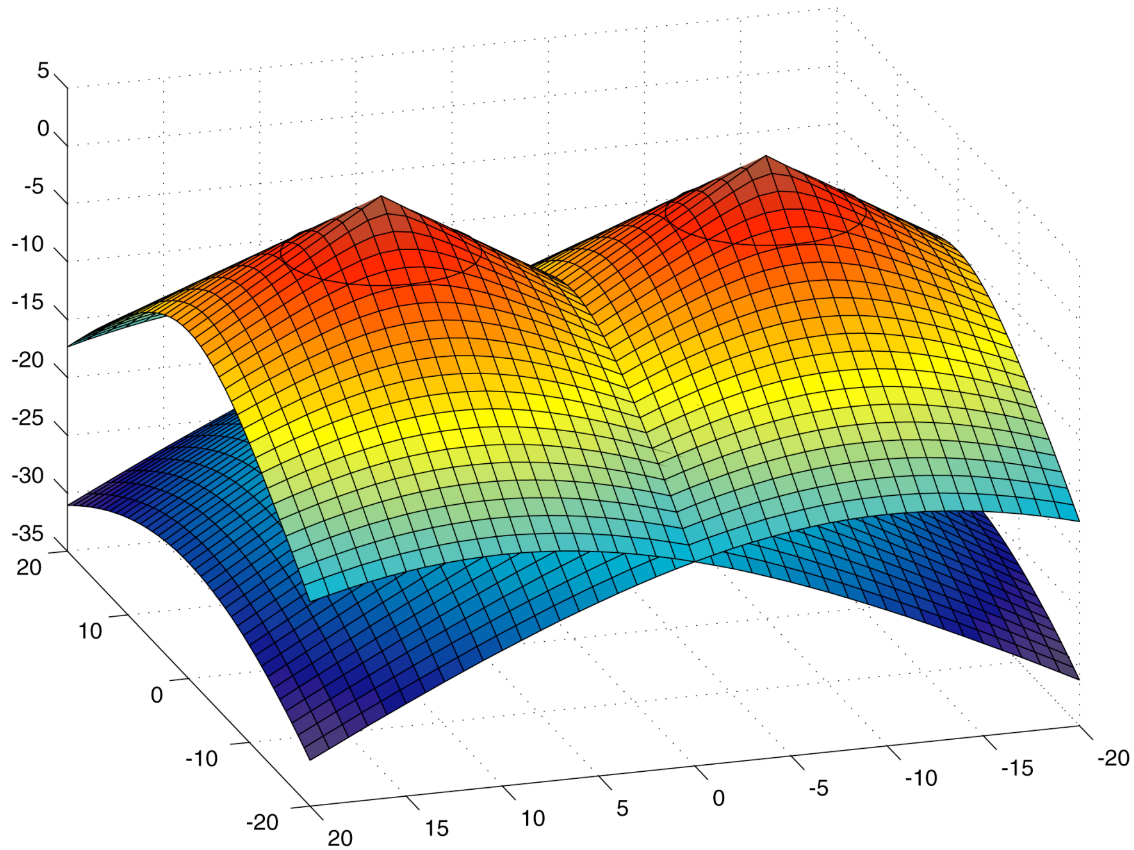
(Courtesy of **Chopp**)

Level Set (ψ) and Signed Distance Function (φ_1)



(Courtesy of **Chopp**)

φ_1 Signed Distance Function (Two Cracks)



(Courtesy of **Chopp**)

Nodal Enrichment

Selection of Nodes

Nodes are selected for enrichment on the basis of the values of the signed distance functions φ_1 and φ_2

Crack Interior Enrichment

$$H(\mathbf{x}) = \operatorname{sign}(\varphi_2(\mathbf{x}))$$

$$\operatorname{sign}(\xi) = \begin{cases} 1, \text{ if } \xi \geq 0 \\ -1, \text{ otherwise} \end{cases}$$

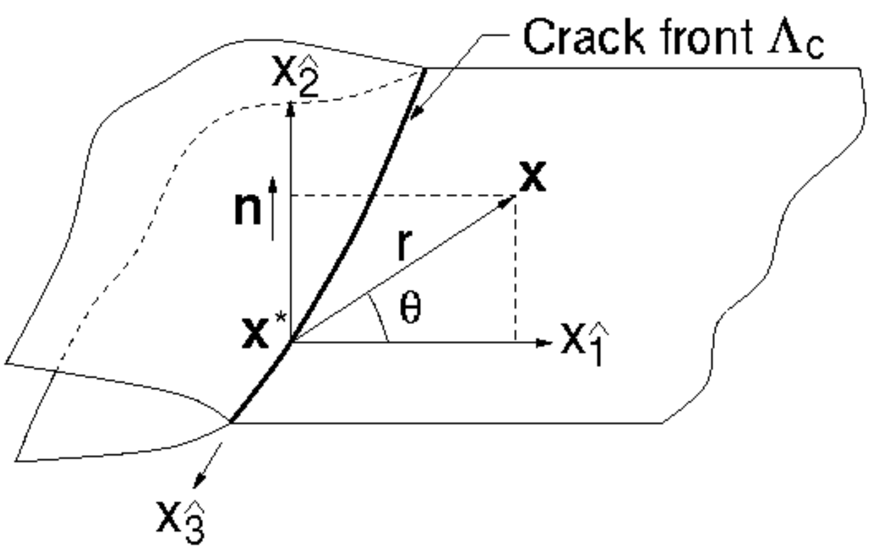
Nodal Enrichment (Cont'd)

Crack Front Enrichment

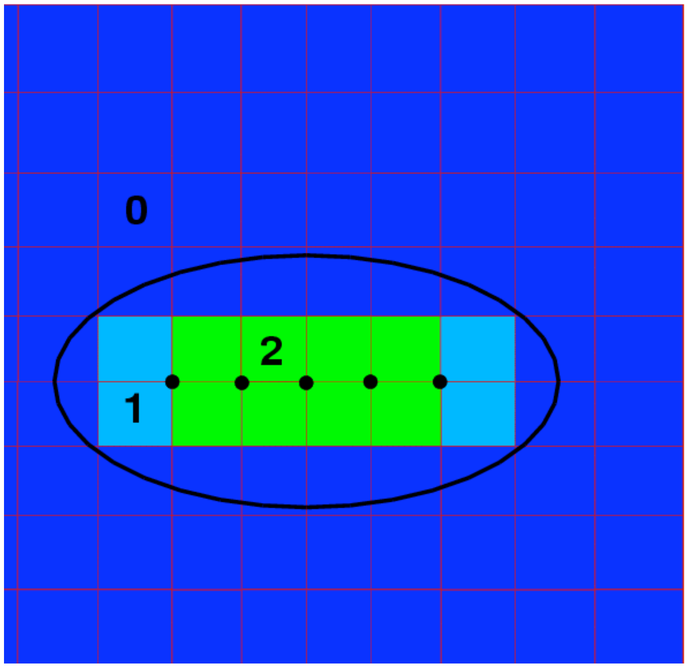
$$\psi = \left\{ \sqrt{r}\cos\frac{\theta}{2}, \sqrt{r}\sin\frac{\theta}{2}, \sqrt{r}\sin\theta\sin\frac{\theta}{2}, \sqrt{r}\sin\theta\cos\frac{\theta}{2} \right\}$$

$$r = \sqrt{\varphi_1^2 + \varphi_2^2}$$

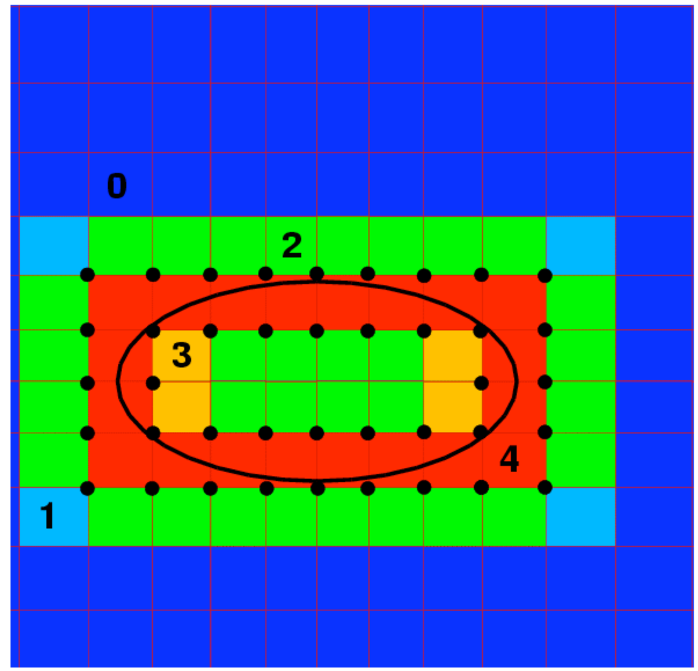
$$\tan\theta = \frac{\varphi_2}{\varphi_1}$$



Nodal Enrichments for Elliptical Crack

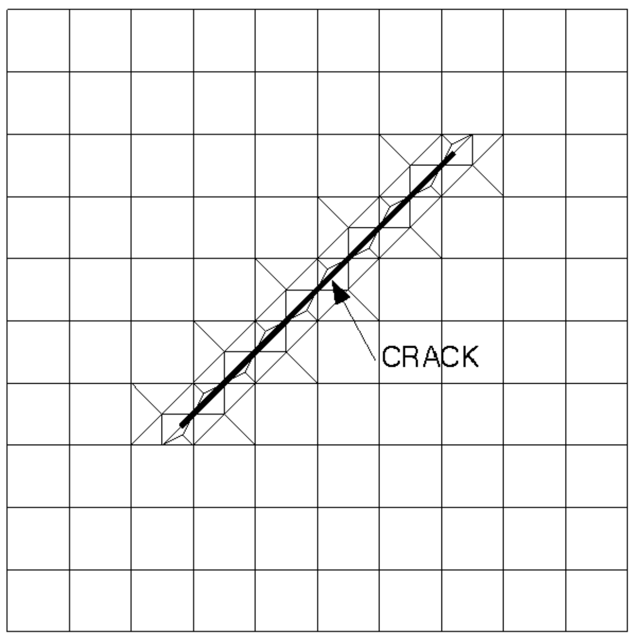


Heaviside Enrichment

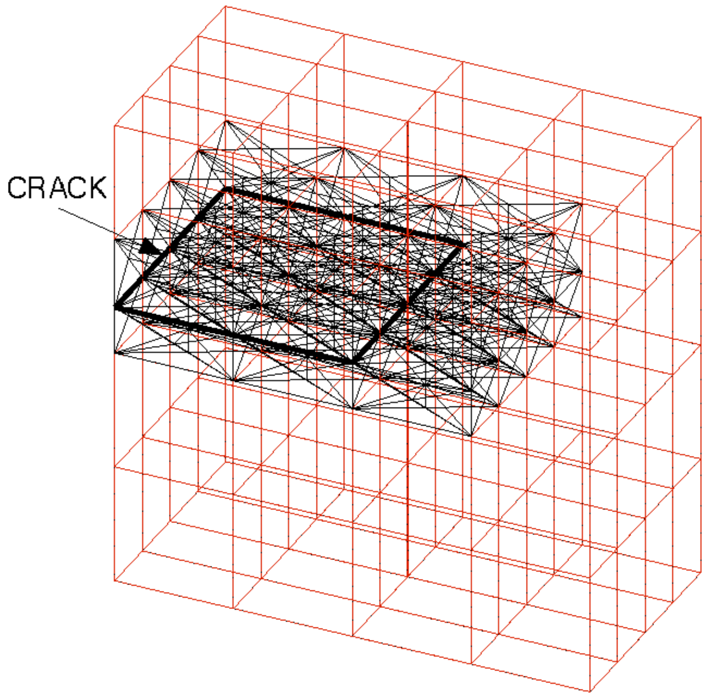


Crack-Front Enrichment

Partitioning Finite Elements



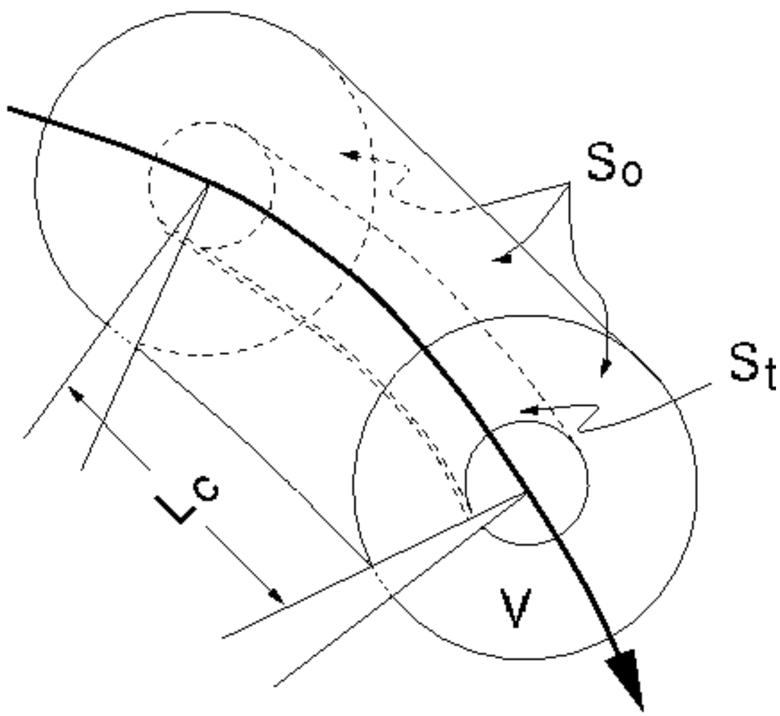
2D



3D

Computation of Stress Intensity Factors

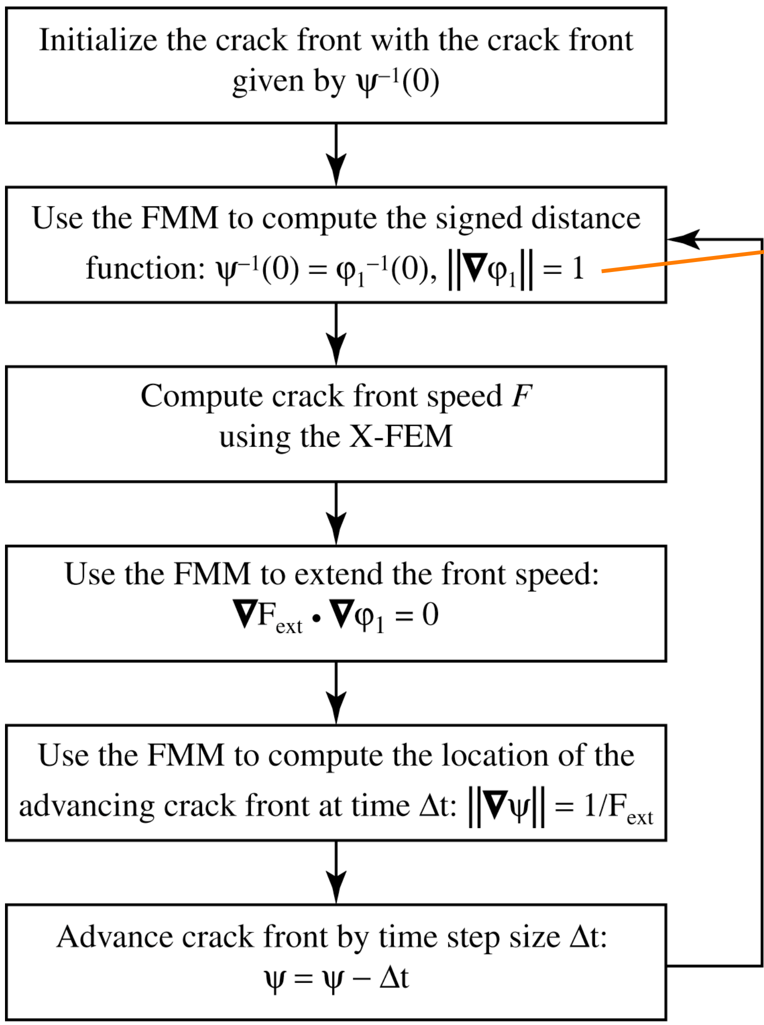
Domain Integrals (**Moran and Shih, 1987**)



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

$$J(s) = -\frac{\int_V H_{kj} q_{k,j}\, dV}{\int_{L_c} l_k n_k\, ds}$$

X-FEM/FMM Crack Growth Algorithm

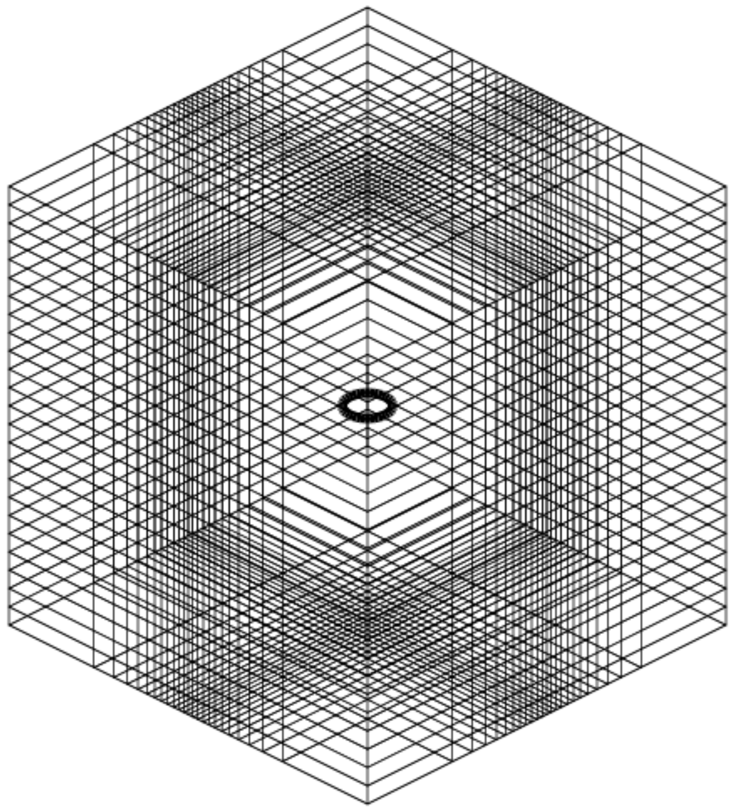


$$\frac{\partial \varphi_1}{\partial n} = 1 \Rightarrow \nabla \varphi_1 \bullet \mathbf{n} = 1$$

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

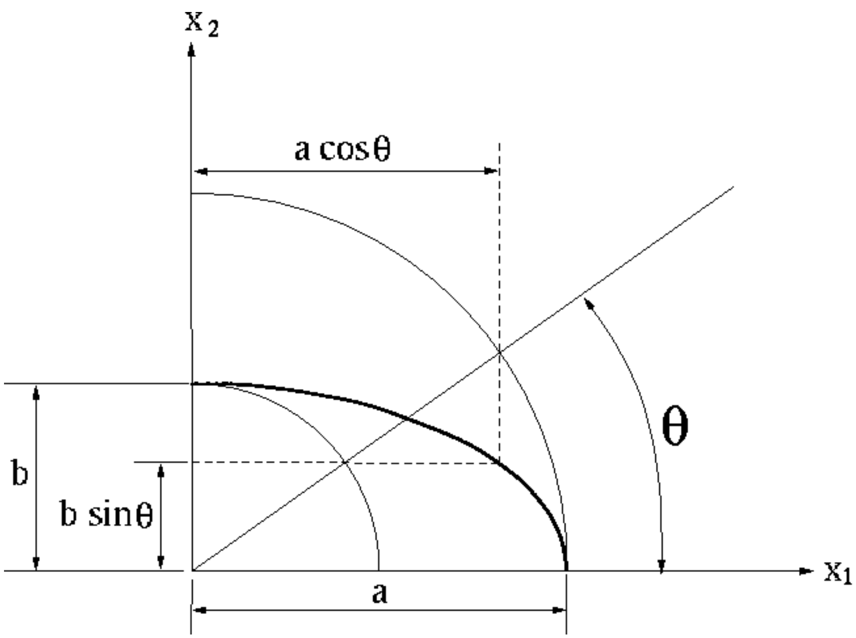
(Courtesy of **Chopp**)

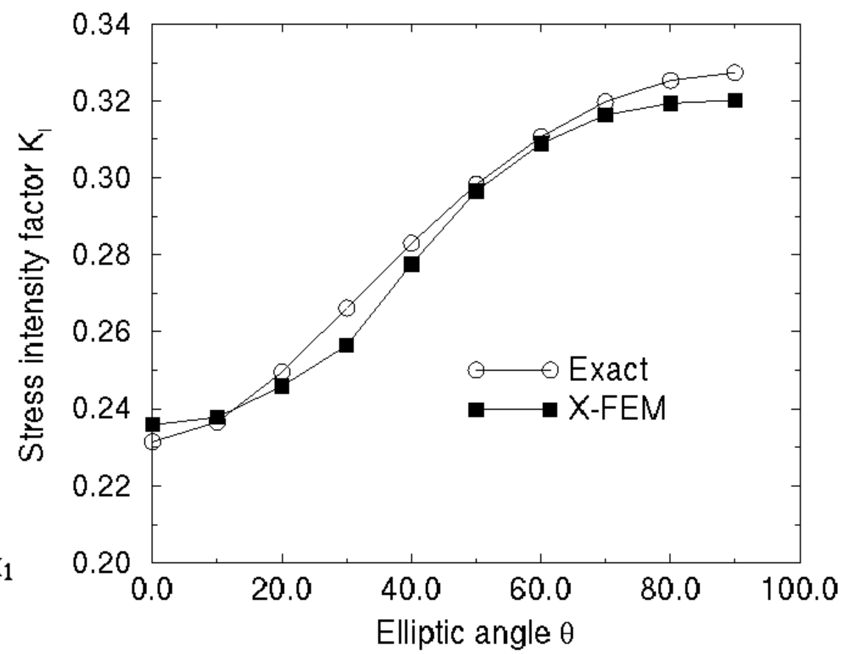
Hexahedral Mesh



Penny crack (24^3 mesh)

Planar Elliptical Crack

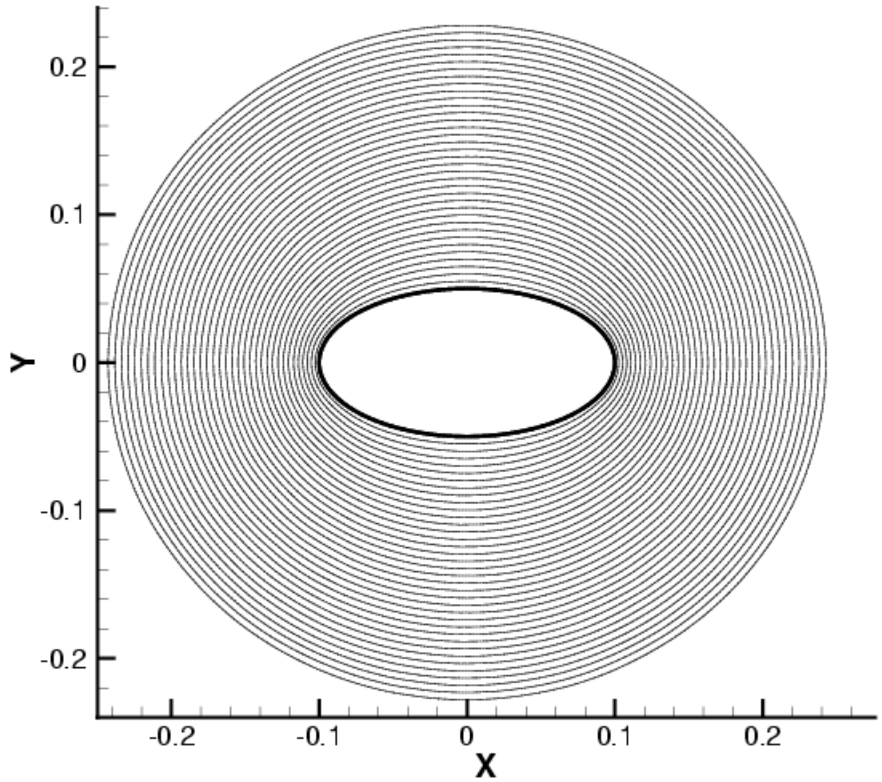




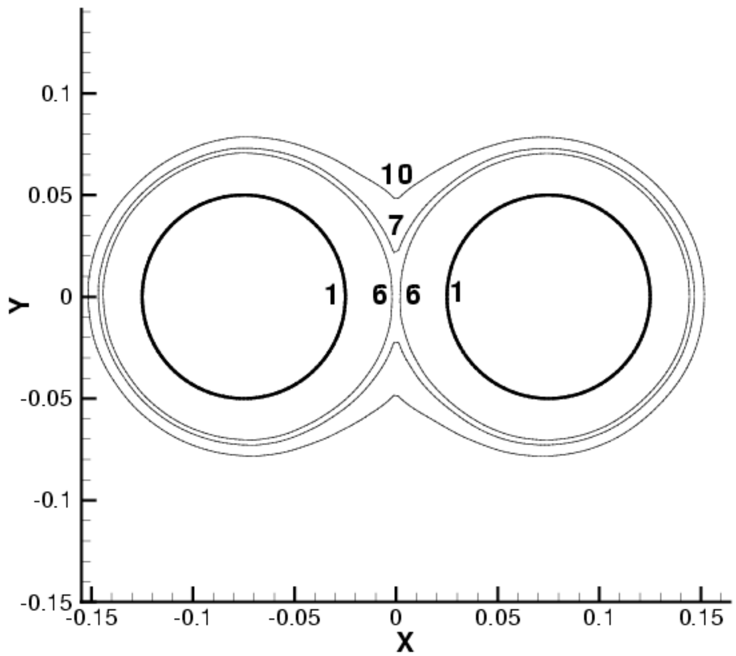
Elliptic angle

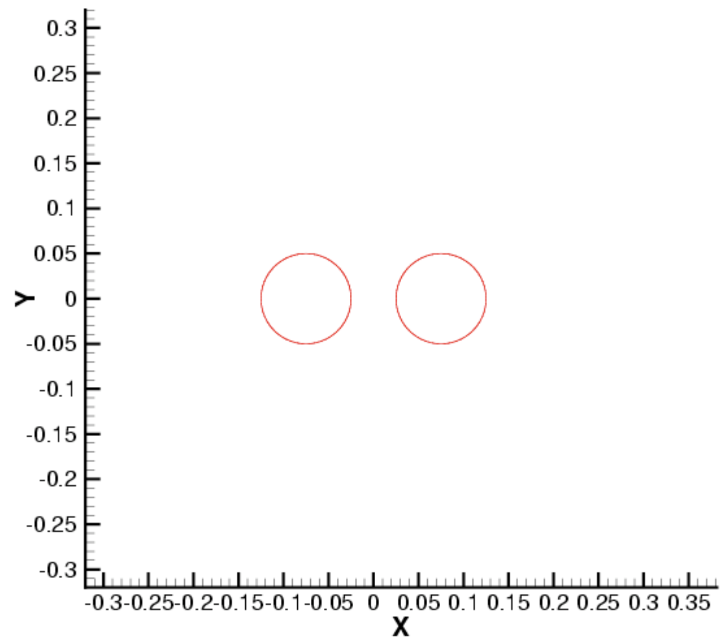
SIFs

Fatigue Growth of One Elliptical Crack

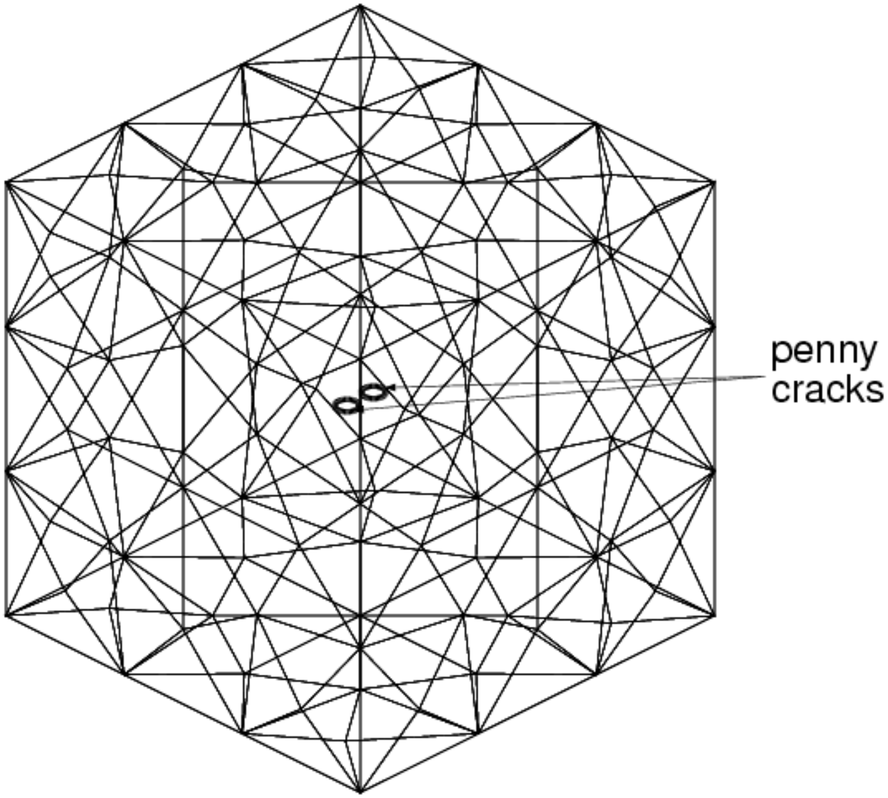


Fatigue Growth of Two Penny Cracks

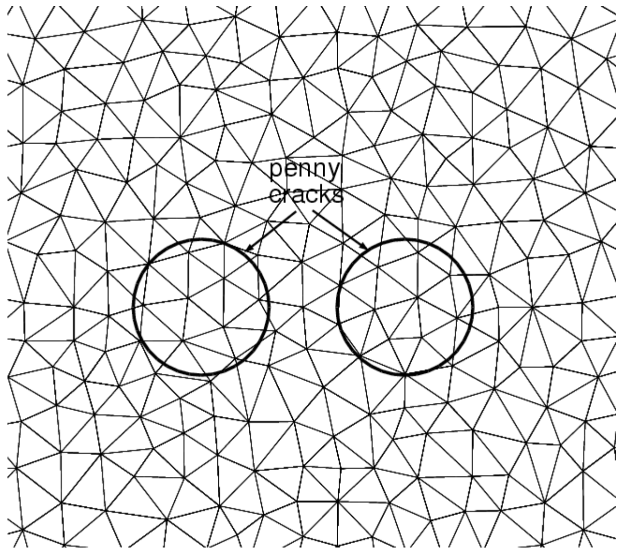




Tetrahedral Mesh

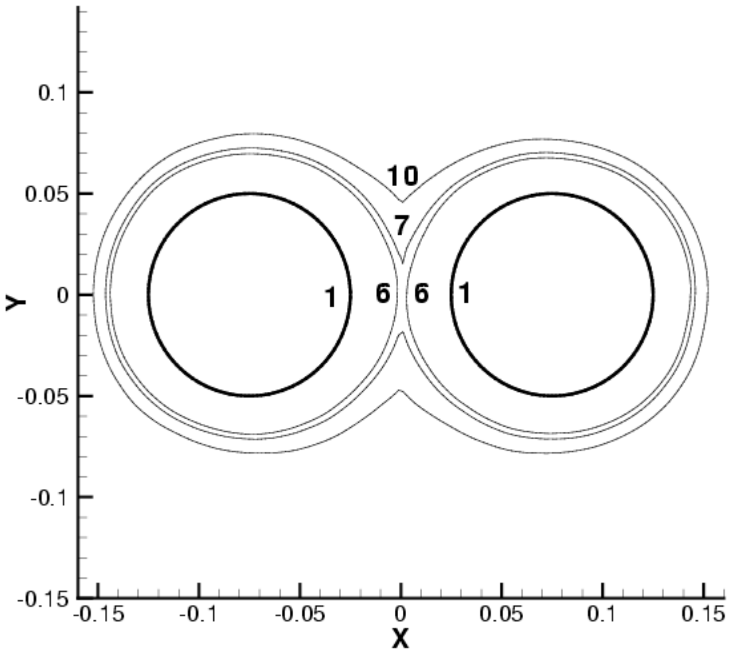


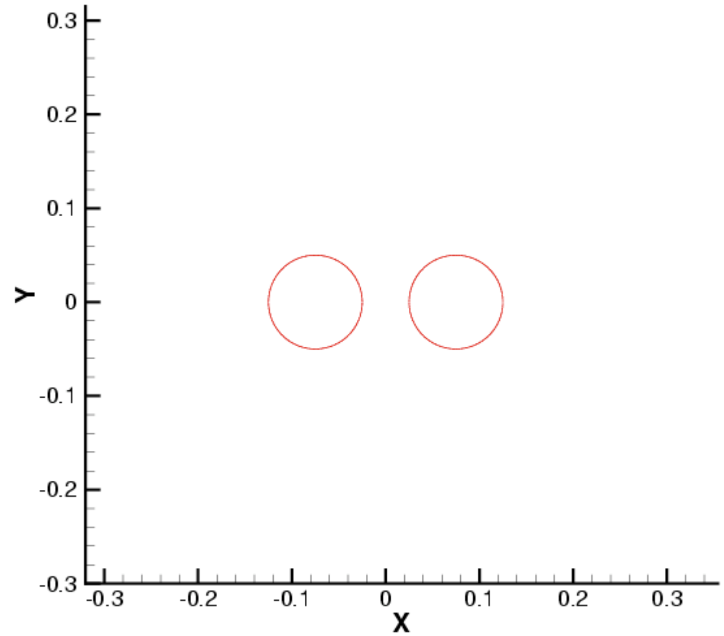
Surface mesh



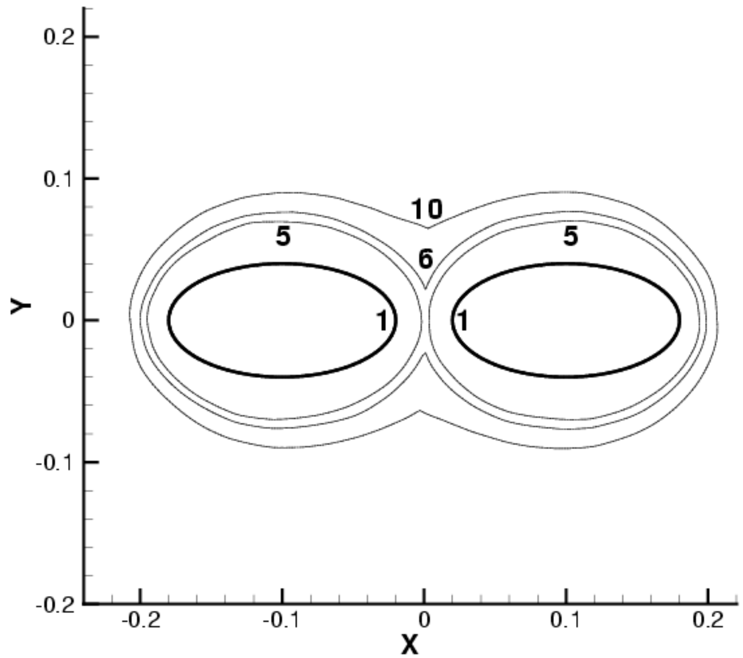
Vicinity of the crack

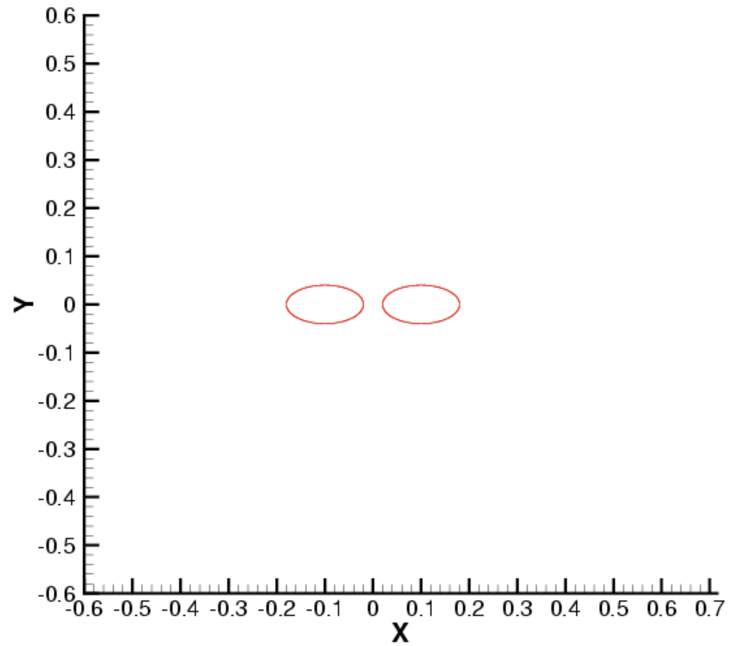
Fatigue Crack Growth (Tetrahedral Mesh)



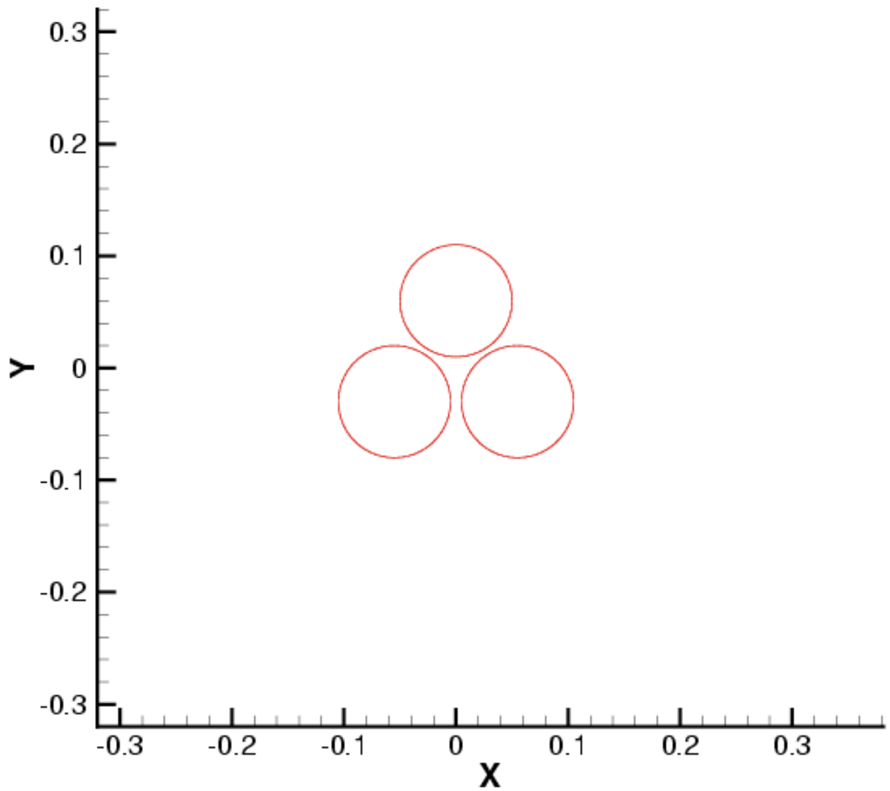


Fatigue Growth of Two Elliptical Cracks





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)**

Potts grain growth model

Cohesive Surface Formulation

- **Zhai and Zhou (2000)**
- **Zavattieri et al. (2001)**

dynamic fracture

Grain Growth Model

Ising Model **(Ising, 1925)**

- Phase transitions (anti-ferromagnetic $\leftrightarrow$ ferromagnetic)
- A two-spin (parallel and anti-parallel) model

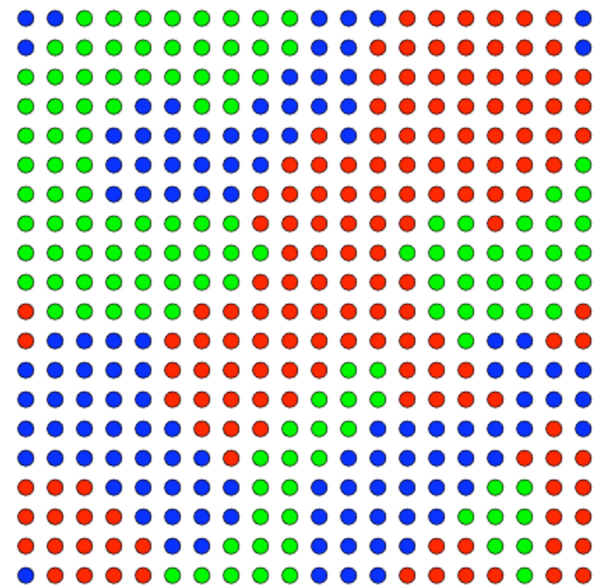
Potts Model **(Potts, 1952)**

- 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

$N = 400,\ Q = 3$



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

Potts Hamiltonian

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

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 micro-structure as well as to perform the FE analysis

Present Work

- A constrained Delaunay algorithm with smoothing is developed to mesh the microstructure

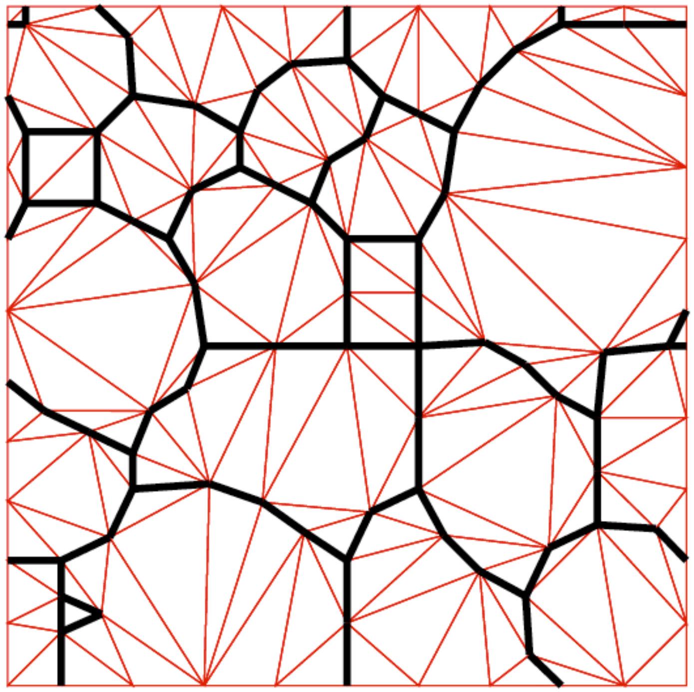
Constrained Delaunay Triangulation

Procedure

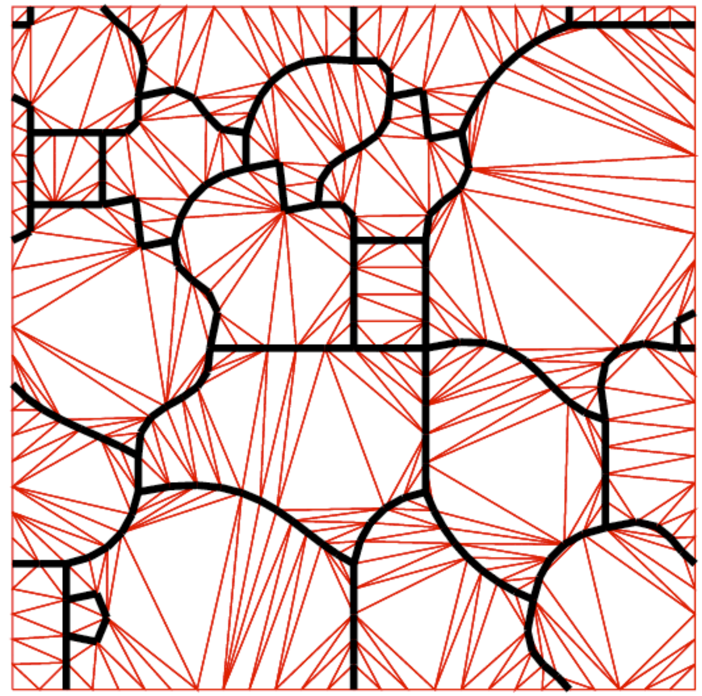
- Construct initial boundary conforming triangulation using a cubic least squares polynomial fit to represent the grain boundary edges
- Delaunay refinement using the point insertion algorithm of Rebay **(Rebay, 1993)** is implemented
- Mesh constructed for user-specified spacing ρ

Boundary Conforming Triangulation

N = 400



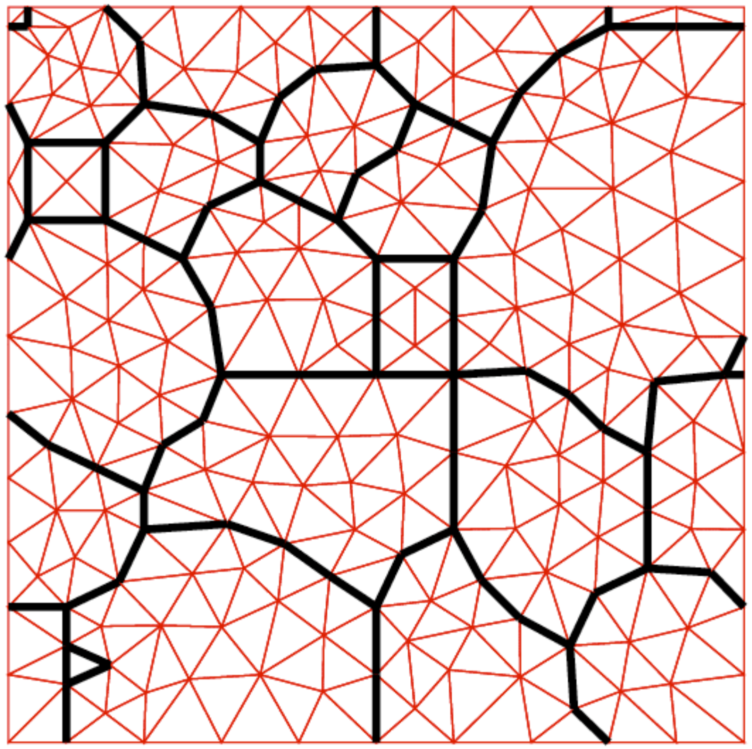
$\rho = 0.1$



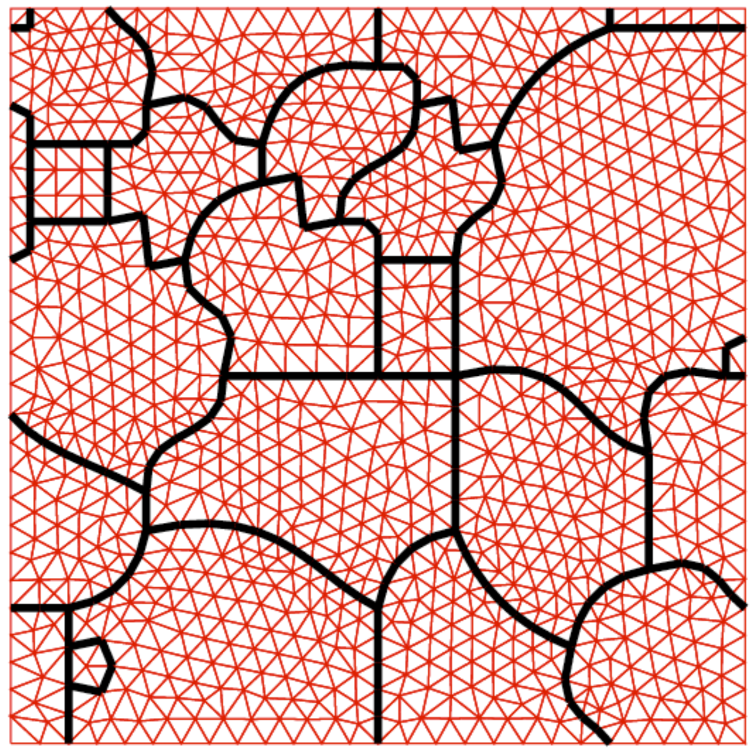
$\rho = 0.04$

STEP 1

Final Triangulation



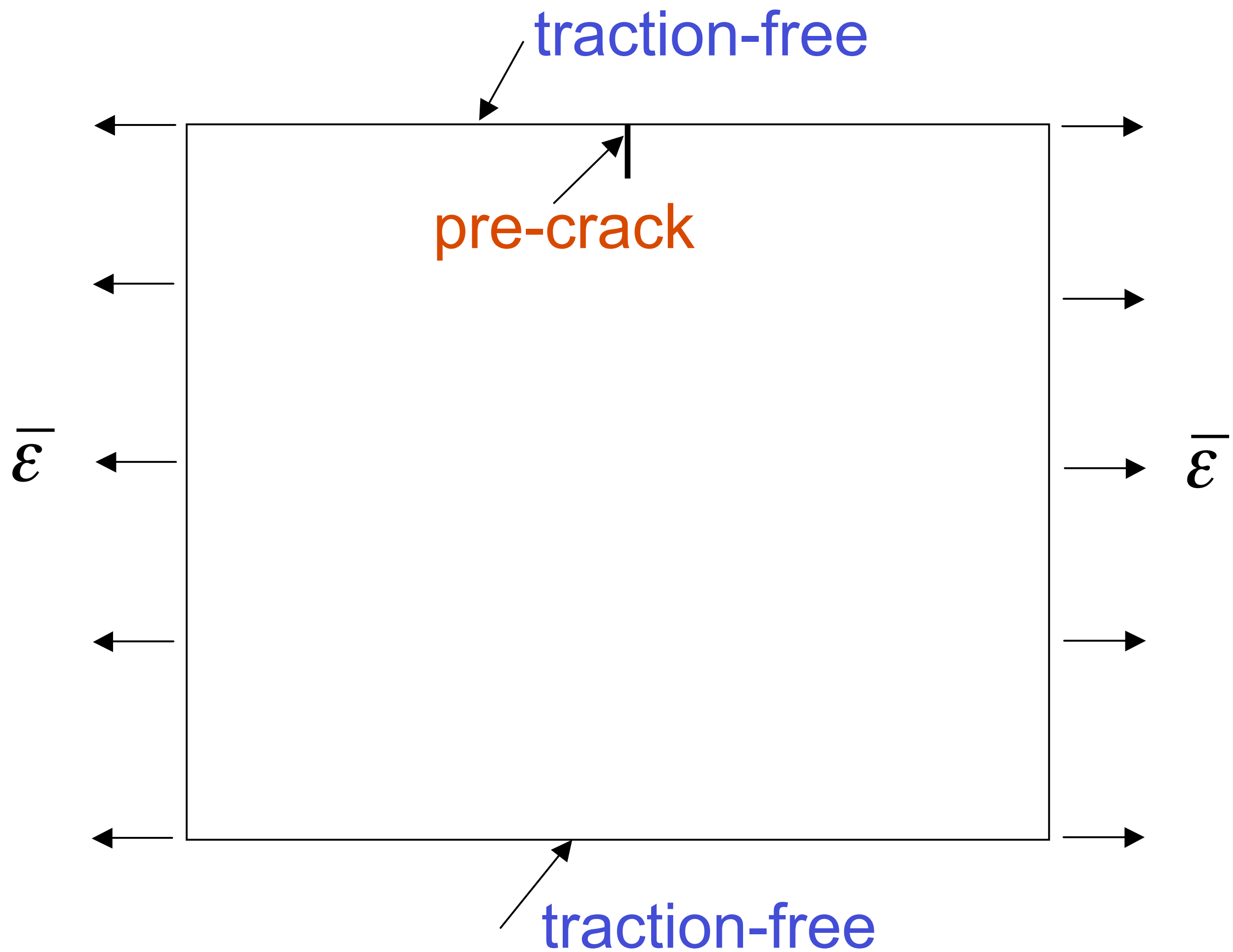
$\rho = 0.1$



$\rho = 0.04$

STEP 2

Model Geometry and BCs



Simulation Procedure

1. Read parameters: $n_{\max}, G_c^i, G_c^{gb}, \Delta a_{\max}$

   $n = 0; \bar{\varepsilon}_0 = 1$
2. X-FEM analysis for initial crack-tip location

   $failure = 0$
3. while $(n < n_{\max}$ and $!\, failure)$ $\{$

4. $n = n + 1$

   if $(\mathbf{x}_{\text{tip}} \in \Omega_i)$

   $\theta_g = \theta_{\text{hoop}}; \Delta a = \min(\Delta a_{\max}, \Delta a_{gb}, \Delta a_{\text{hull}})$

Simulation Procedure (Cont'd)

5. if $(\mathbf{x}_{\text{tip}} \in \Gamma_{gb})$

$\{$ find grain boundary directions θ_{gb}

perturb crack along θ_{gb} and θ_{hoop} and find

θ_g based on $\max(G^{gb} / G_c^{gb},\ G^i / G_c^i)$

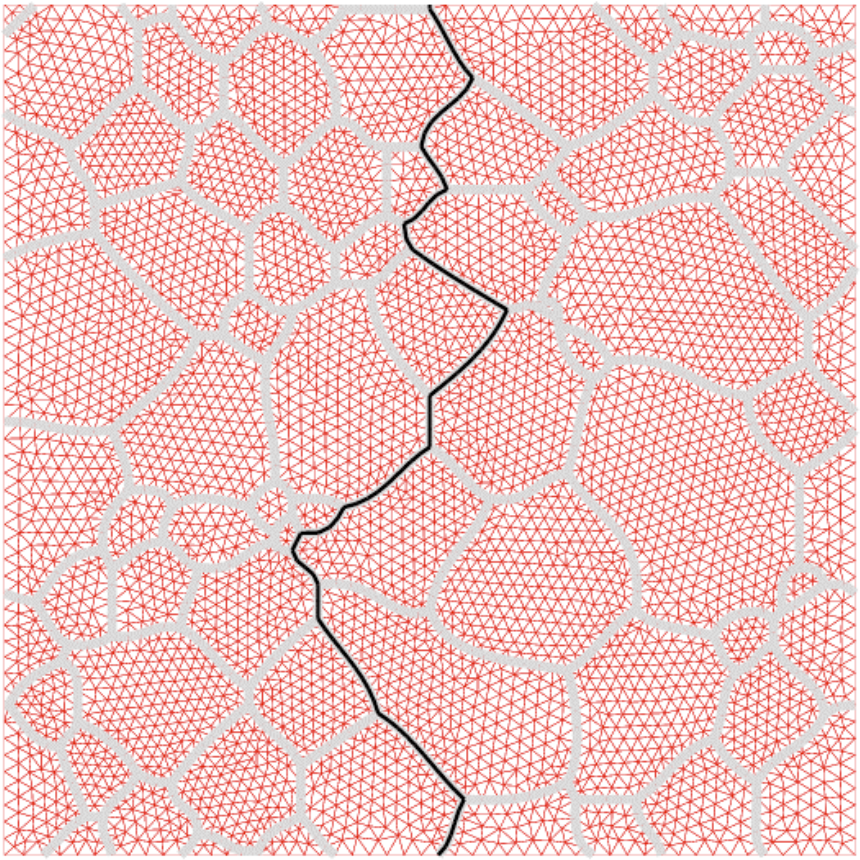
$\Delta a = \min(\Delta a_{\max}, \Delta a_{gbv})$

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

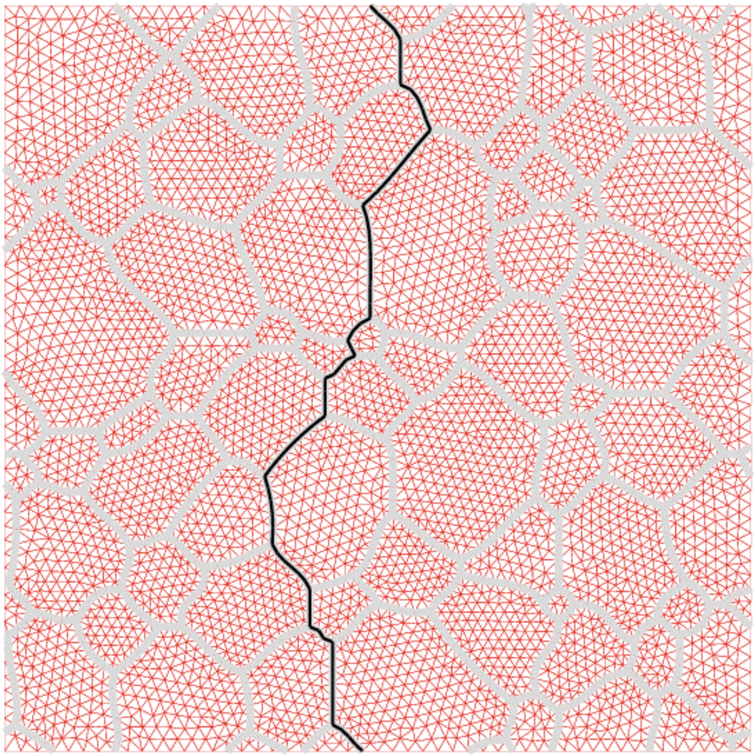
Crack Propagation Simulations (Q = 100)



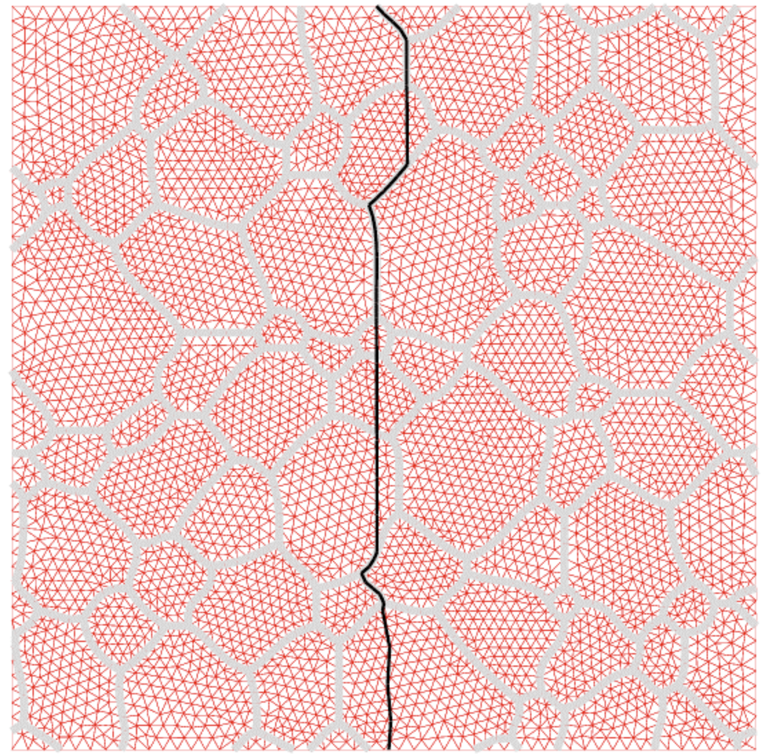
$$G_c^{gb} / G_c^i = 0.1$$
$$t = 10^4 MCS$$

INTERGRANULAR FRACTURE

Simulation 1: t =10000 MCS

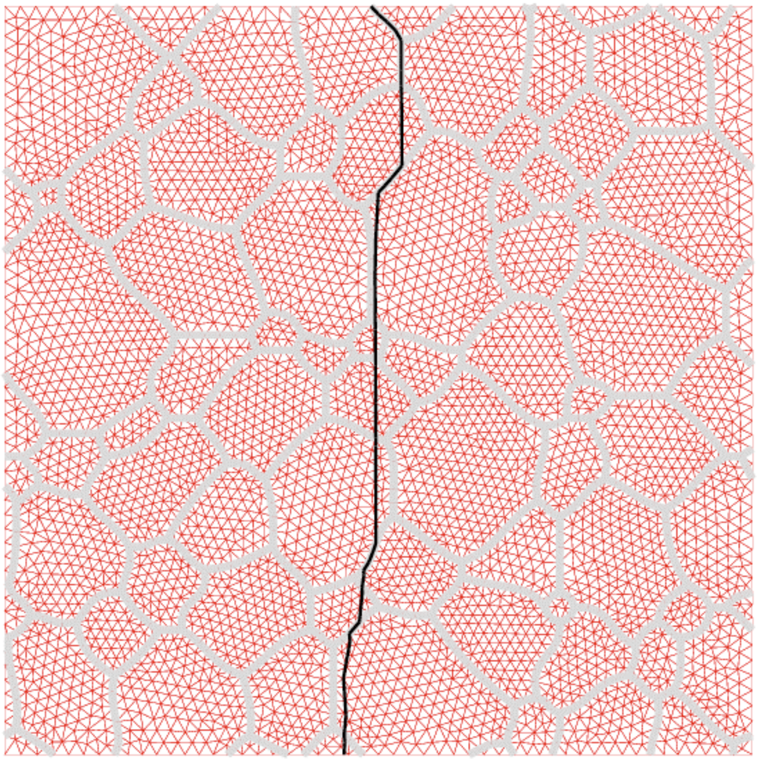


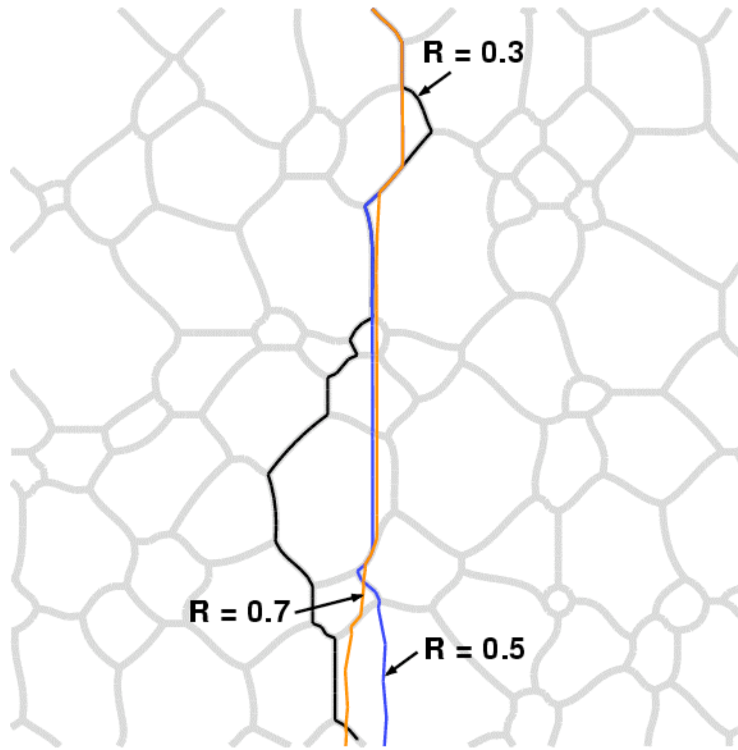
$$G_c^{gb} / G_c^{i} = 0.3$$
$$IG = 100\%$$



$$G_c^{gb} / G_c^{i} = 0.5$$
$$IG = 42\%$$

Simulation 1 (Cont'd)

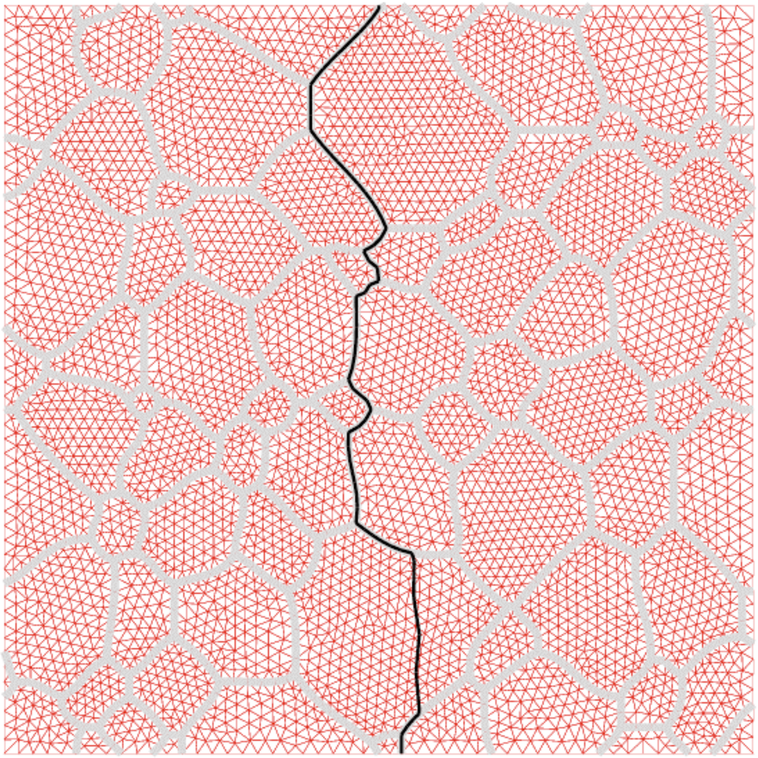


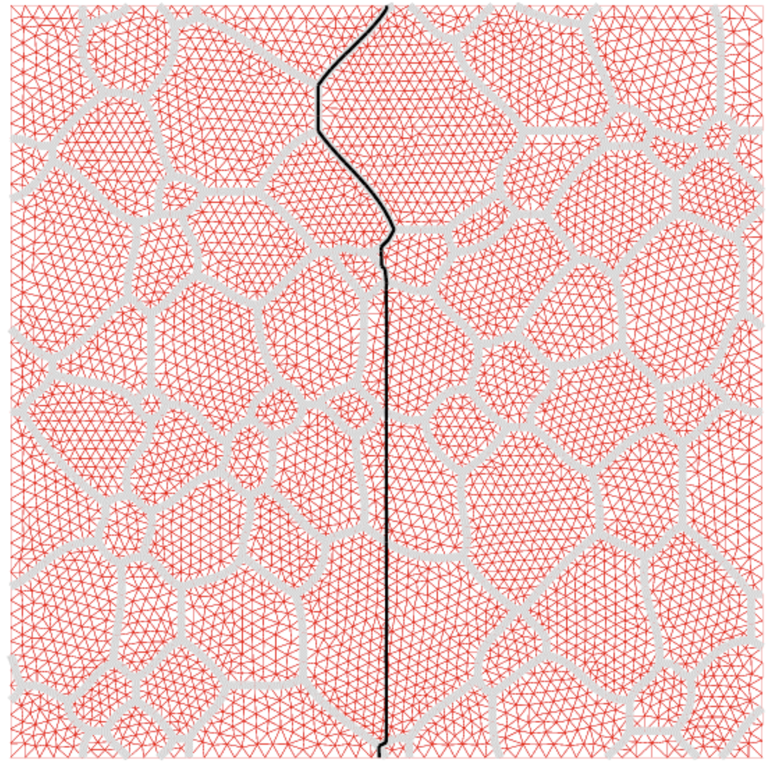


$$G_c^{gb} / G_c^{i} = 0.7$$
$$IG = 21\%$$

$$R = G_c^{gb} / G_c^{i}$$

Simulation 2: t = 10000 MCS

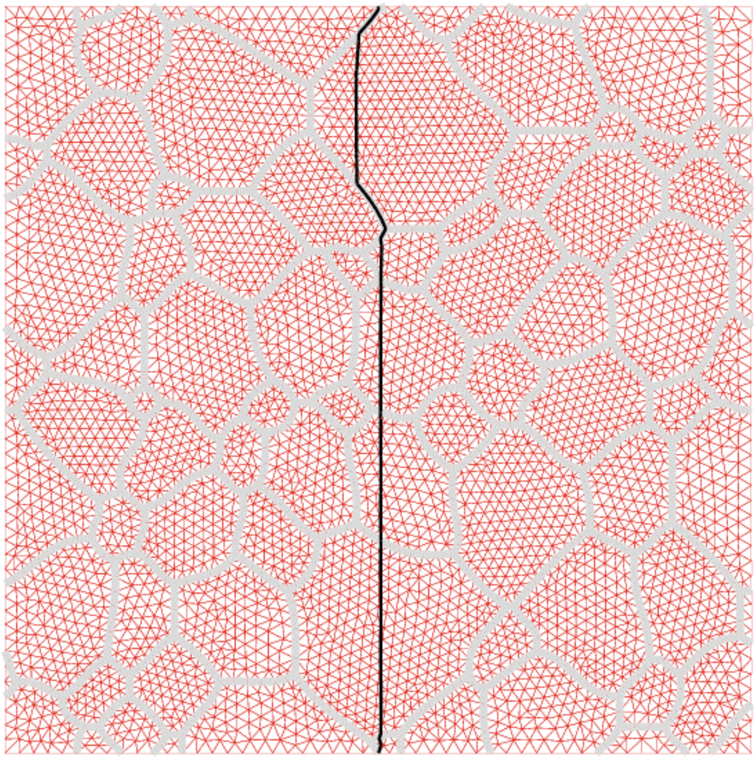




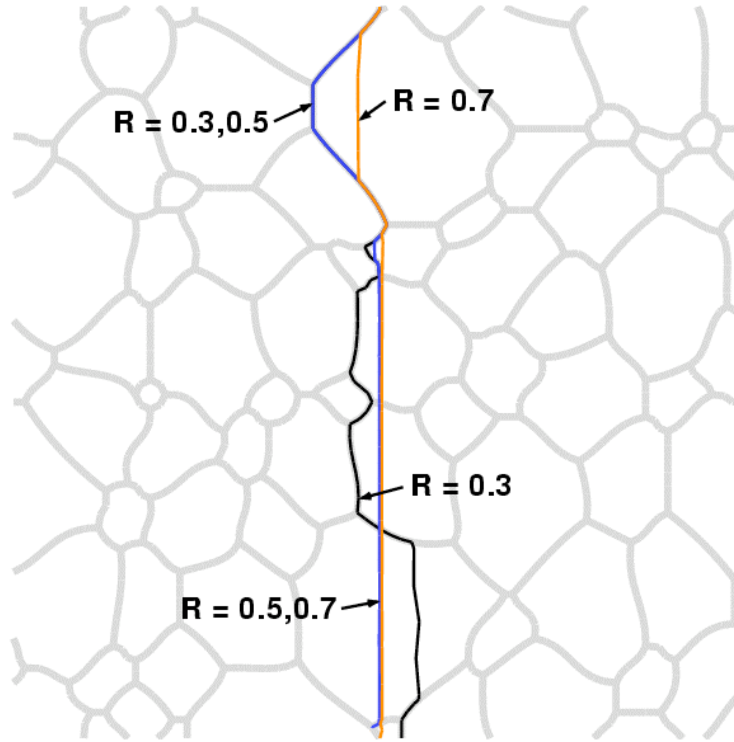
$$G_c^{gb} / G_c^{i} = 0.3$$
$$IG = 81\%$$

$$G_c^{gb} / G_c^{i} = 0.5$$
$$IG = 40\%$$

Simulation 2 (Cont'd)



$$G_c^{gb} / G_c^i = 0.7$$
$$IG = 13\%$$



$$R = G_c^{gb} / G_c^i$$

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