

A Polyhedral Finite-Element Formulation using Harmonic Shape Functions with Applications to the Modeling of **Multi-Physics Fracture Processes**

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Outline

- 1. Pervasive fracture and fragmentation
- 2. Random meshes and a polyhedral finite-element formulation
- 3. Assessing mesh convergence in a probabilistic sense
- 4. Summary

Pervasive Fracture





blast induced structural collapse





dynamic pervasive fracture

bird strike

- crack branching
- crack coalescence
- tortuous crack paths (sensitivity to material heterogeneity)
- stochastic behavior

Geomechanics Applications





Spectrum of Fracture Problems





• enrichment methods (GFEM, XFEM, ...)

- tortuous crack paths (sensitivity to material heterogeneity)
- stochastic behavior

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How far can we extend the computational tools used for one end of the spectrum to the other?



Computational Challenges to Allowing Cracks to Grow Arbitrarily



- Do we restrict branching?
- Do we restrict initiation?
 - from surface only?
 - from crack tips only?
 - from existing cracks only?
- Constraints on turning angles?
- Constraints on crossing angles?
- Constraints on minimum fragment size?

What about 3D?

Computational Approach



- Random Voronoi tessellation (mesh)
- Polyhedral finite-elements
- Fracture only allowed at element edges.
- *Dynamic* mesh connnectivity

Pandolfi, A. and M. Ortiz, 2002, *Engineering with Computers*, **18**: p. 148-159.

• Insert cohesive tractions on new fracture surfaces (fracture energy).



Why a Random Voronoi Mesh?



Bolander, J.E. and S. Saito, 1998, *Fracture analyses using spring networks with random geometry.* Engineering Fracture Mechanics, **61**(5-6): p. 569-591.



Structured grids can result in strong mesh induced bias (nonobjective).

- need to use 'random' discretizations
- statistically isotropic (distribution of edge orientations passes KS test against the uniform distribution)

Voronoi Texture Augments Material Variability



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Voronoi Mesh Generation



Bolander, J., Saito, S., 1998, 'Fracture Analyses using Spring Networks with Random Geometry,' *Engineering Fracture Mechanics*, 61, 569-591



constraint on min. dist.

seed until 'max' packing

Poisson process



Delaunay triangulation





- Note that each Voronoi junction is randomly oriented.
- Most Voronoi junctions are triples.
- Average interior angles are 120°.



3D Randomly Close-Packed Voronoi



Equations of Motion





- Shape functions, their derivatives, and the integration points are defined in the initial configuration (Ω_0 , Γ_0).
- All integrations of the weak form are from the original configuration (total-Lagrangian formulation).

Momentum strong form

$$\frac{\partial \mathbf{P}}{\partial \mathbf{X}}: \mathbf{I} + \rho_{\mathrm{o}} \mathbf{f} = \rho_{\mathrm{o}} \ddot{\mathbf{u}}$$

- **P** is the first Piola-Kirchhoff stress tensor.
- X is the position vector of a material point.
- $\boldsymbol{x}~$ is the spatial vector.
- $\mathbf{u} = \mathbf{x} \mathbf{X}$, is the displacement vector
- ${\bf f}\,$ is the body force vector per unit mass.

Momentum weak form

$$\int_{\Omega_{o}} \rho_{o} \ddot{\mathbf{u}} \cdot \delta \mathbf{u} \ d\Omega_{o} = \int_{\Gamma_{o}} \mathbf{t}_{o} \cdot \delta \mathbf{u} \ d\Gamma_{o} + \int_{\Omega_{o}} \rho_{o} \mathbf{f} \cdot \delta \mathbf{u} \ d\Omega_{o} - \int_{\Omega_{o}} \rho_{o} \mathbf{P} : \left(\frac{\partial(\delta \mathbf{u})}{\partial \mathbf{X}}\right) \ d\Omega_{o}$$

However, most material models are hypoelastic.

deformation gradient	rate of deformation	PK1 stress	Cauchy stress	Lots of multiplications
$F = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} (3 \times 3)$	$\frac{\partial \mathbf{v}}{\partial \mathbf{x}} = \frac{\partial \mathbf{v}}{\partial \mathbf{X}} F^{-1}$	$P = J \sigma F^{-T}$ $J = \det(F)$	$\boldsymbol{\sigma} = J^{-1} \boldsymbol{P} \boldsymbol{F}^{T}$	by F and F^{-1}



Harmonic Functions

A harmonic function is a solution of Laplace's equation.

$$\nabla^2 \varphi = 0$$
 or $\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2} = 0$

Can solve efficiently using BEM, or can just use FEM.







Harmonic Shape Function Properties

partition of unity and reproduce space

even for the discrete harmonic solution

$$\sum_{I} \psi_{I}(\mathbf{x}) = 1, \quad \sum_{I} \psi_{I}(\mathbf{x}) \ \mathbf{x}_{I} = \mathbf{x}$$
$$\sum_{I} \psi_{I}^{h}(\mathbf{x}) = 1, \quad \sum_{I} \psi_{I}^{h}(\mathbf{x}) \ \mathbf{x}_{I} = \mathbf{x}$$

- Kronecker delta property at nodes $\psi_I(\mathbf{x}_J) = \delta_{IJ}$
- shape functions defined on original configuration (no mapping to 'parent' shape)



Harmonic Shape Function Examples





Only need to store shape functions and derivatives at integration points. Discard everything else.

Accuracy of Harmonic Shape Functions?





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Comments and Questions



- 1. What accuracy is needed in the solution of the harmonic shape functions and their derivatives?
- 2. How to integrate the weak form?

These questions are intimately related!

Element Integration



- Due to computational expense of plasticity models, want to minimize the number of integration points.
- Follow approach of Rashid and Selimotec, 2006.
- Each node is associated with a "tributary" volume, connected to the centroid.
- Number of integration points is equal to the number of vertices.



Sufficient to eliminate any zero energy modes.

"Engineering" Patch Test



The patch test verifies "completeness", a necessary condition for convergence.

(Displacement field can represent rigid body motions and a constant strain state.)

Conversely, a constant stress field should be produced within each element when such a field is prescribed on the boundary surface.

and, strain field should be constant.



patch of elements



strain error ~ 20%

Element Stiffness Matrix (Linear Example) in Sandia National Laboratories



Requirements to Pass the Patch Test



(Krongauz and Belytschko, 1997)



global equilibrium equations:

$$\sum_{J} \mathbf{K}_{IJ} \mathbf{u}_{J} = \mathbf{F}_{I}$$

 K_{LJ} = global stiffness matrix

For patch test, need

$$u_{x}(x, y, z) = a_{1} x + a_{2} y + a_{3} z + a_{4}$$
$$u_{y}(x, y, z) = b_{1} x + b_{2} y + b_{3} z + b_{4}$$
$$u_{z}(x, y, z) = c_{1} x + c_{2} y + c_{3} z + c_{4}$$

to be a solution of Ku = F when applied as boundary conditions.



 $\Omega_I =$ support of node I

For interior nodes *I* need
$$\sum_{J} \mathbf{K}_{IJ} \mathbf{u}_{J}^{\text{linear}} = \mathbf{0}$$
 (**F**_{*I*} = 0)

Row *I* column *J* of K_{*IJ*} contains terms like: $\int_{\Omega_{I}} \varphi_{I,x} \varphi_{J,x} d\Omega, \quad \int_{\Omega_{I}} \varphi_{I,x} \varphi_{J,y} d\Omega, \quad \int_{\Omega_{I}} \varphi_{I,x} \varphi_{J,z} d\Omega, \quad \cdots$

For example, need $\sum_{J} \int_{\Omega_{J}} \varphi_{I,x} \varphi_{J,z} \left(a_{1}x_{J} + a_{2}y_{J} + a_{3}z_{J} + a_{4} \right) d\Omega = 0$

Requirements to Pass the Patch Test





Integration Consistency







Satisfaction of discrete form of Divergence Theorem requires "="

Approximate integration will cause failure of patch test for first-order integration.

Would need a large number of integration points and accurate shape function derivatives to satisfy patch test.

... too expensive!

Instead, let's "tweak" the shape function derivatives to satisfy the patch test.



Let's "tweak" the Shape Function Derivatives in Sandia Laboratories



(pseudo-derivatives)

Let
$$a_x^{I,k}, a_y^{I,k}, a_z^{I,k}$$

be the new shape function derivatives for the *I*-th shape function at integration point *k*.

How to calculate
$$a_x^{I,k}, a_y^{I,k}, a_z^{I,k}$$
?

Minimize the sum of the squares of the difference w.r.t to the original derivatives.

$$L = \sum_{I=1}^{N_{en}} \sum_{k=1}^{M} \left(\varphi_{I,x}(\mathbf{x}_{k}) - a_{x}^{I,k} \right)^{2}$$

with "integration constraints"

$$\sum_{k=1}^{M} w_k a_x^{I,k} - \sum_{j=1}^{M_{\Gamma}} w_j^{\Gamma} \varphi_I(\mathbf{x}_j) n_x(\mathbf{x}_j) = 0 \qquad I = 1, ..., N_{en}$$

solve use Lagrange multipliers



Modified Shape Function Derivatives

Introduce Lagrange multipliers λ_I , $I = 1, ..., N_{en}$ and form the augmented Lagrangian L_A

$$L_{A} = \sum_{I=1}^{N_{em}} \sum_{k=1}^{M} \left(\varphi_{I,x}(\mathbf{x}_{k}) - (a_{x}^{I,k}) \right)^{2} + \sum_{i=1}^{N_{em}} \lambda_{I} \left[\sum_{k=1}^{M} w_{k} a_{x}^{I,k} - \sum_{j=1}^{M_{T}} w_{j}^{\Gamma} \varphi_{I}(\mathbf{x}_{j}) n_{x}(\mathbf{x}_{j}) \right]$$

necessary condition for local minimum
$$\frac{\partial L_{A}}{\partial a_{x}^{I,k}} = 0, \quad I = 1, \cdots, N_{en}, \quad k = 1, \cdots, M$$
$$\frac{\partial L_{A}}{\partial \lambda_{I}} = 0, \quad I = 1, \cdots, N_{en}$$
$$\begin{bmatrix} \mathbf{A} & \mathbf{L}^{T} \\ \mathbf{L} & 0 \end{bmatrix} \begin{bmatrix} a_{x} \\ \lambda \end{bmatrix} = \begin{bmatrix} \mathbf{b}_{x} \\ \mathbf{c}_{x} \end{bmatrix}$$

same for ()_y and ()_z , only need to factor once for each element

3D Verification: Engineering Patch Test



without derivative correction

random patch



with derivative correction





Patch Test with Nonconvex Elements





Verification Test: Beam with a Transverse End-Load

3D exact linear elasticity solution, (Barber, 2010)

$$\begin{aligned} \sigma_{xx} &= \sigma_{yy} = \sigma_{xy} = 0\\ \sigma_{zz} &= \frac{F_y}{I_x} yz\\ \sigma_{xz} &= \frac{2F_y a^2}{\pi^2 I_x} \frac{\nu}{1+\nu} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \sin(\frac{n\pi x}{a}) \frac{\sinh(\frac{n\pi y}{a})}{\cosh(\frac{n\pi b}{a})}\\ \sigma_{yz} &= \frac{F_y}{I_x} \left\{ \frac{1}{2} (b^2 - y^2) + \frac{1}{6} (3x^2 - a^2) \frac{\nu}{1+\nu} - \frac{2a^2}{\pi^2} \frac{\nu}{1+\nu} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \sin(\frac{n\pi x}{a}) \frac{\sinh(\frac{n\pi y}{a})}{\cosh(\frac{n\pi b}{a})} \right\} \end{aligned}$$

From this stress field \rightarrow strain field \rightarrow integrate to get displacement field using compatibility equations.





Randomly Close-Packed Voronoi Meshes





median 24 nodes per element

median 14 faces per element

median 5 nodes per face

Typical FEM Solution



deformed shape, Von Mises stress



Verification Test: Beam with a Transverse End-Load





Verification Test: Beam with a Transverse End-Load





Effect of Shape Function Accuracy





Dynamic Mesh Connectivity







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(Bishop, J., 2009, Computational Mechanics, v. 44)

Time = 0.0000





CFSES: Center for Subsurface Energy Security

(www.utcfses.org)





Potential Leakage Paths for CO₂



Primary CO₂ trapping mechanism is structural.



Hydromechanical Coupling in Fractured Rock







MeshingGenie (Trilinos)

(Ebeida, M., Knupp, P., Vitus Leung, Sandia National Laboratories)

Fractured Rock







Fluid Flow in 2D Discrete Fracture Networks





Fluid Flow in 2D Discrete Fracture Networks



Solve fluid network to get nodal pressures and flow rates.





Fluid Flow in Discrete Fracture Networks



Position along link, x/L

Hydraulic Fracture Simulation









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(Bishop, J. and Strack, O., 2011, IJNME, v. 88)



Example: Explosively Loaded Cylinder











Mesh Convergence?





Review of Probability

X = random variable

(an engineering quantity of interest)

PDF

f(x) probability distribution function

 $f(x) = \frac{dF}{dx}$

CDF F(x) cumulative distribution function

$$F(x) = \Pr\left(X < x\right)$$

$$F(x) = \int_{-\infty}^{x} f(x') dx'$$







Definitions of Statistical Convergence

almost sure convergence

$$\Pr\left(\lim_{h \to 0} x_{h} = x\right) = 1$$

convergence in r-mean

$$\lim_{h \to 0} E\left(|x_{h} - x|^{r}\right) = 0$$

convergence in probability

$$\lim_{h \to 0} \Pr(|x_{h} - x| > \varepsilon) = 0$$

increasing
strength

$$\lim_{h \to 0} \Pr(|x_{h} - x| > \varepsilon) = 0$$

Example



sequence of random variables X_n , n = 1, 2, 3, ...





How to Assess Convergence-in-Distribution?



use L_{∞} norm: $L_{\infty}(F_h, F) = \sup_x |F_h(x) - F(x)|$



What about finite sampling effects?



Finite Sampling Fluctuations in CDF



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Kolmogorov-Smirnov Statistic

0.95

0.8

0.6

0.4

0.2

0

0

0.8

Z

0.4

^{1.2} 1.36 ^{1.6}

2

p(z)

$$D_{N} = \sup_{x} |S_{N}(x) - F(x)|$$
$$\lim_{N \to \infty} \Pr(D_{N} < z/\sqrt{N}) = 1 - 2\sum_{j=1}^{\infty} (-1)^{j-1} \exp(-2j^{2}z^{2}) \equiv p(z)$$

confidence bounds

$$\Pr\left(D_{N} < \frac{1.36}{\sqrt{N}}\right) = 95\%$$

$$\Pr\left(D_{N} < \frac{1.19}{\sqrt{N}}\right) = 90\%$$
• independent of distribution

• only for continuous CDFs

 $\Pr\left(D_N < \frac{1.63}{\sqrt{N}}\right) = 99\%$

(conservative to within 2% for N > 50) (tabulated for N < 50)

Kolmogorov-Smirnov Statistic



95% confidence bounds





How to use KS-statistic to assess convergencein-distribution with finite sample sizes?



$$\left| d_{i,j} - d_{N_i}, N_j \right| \le D_{N_i} + D_{N_j} = \frac{Z_i}{\sqrt{N_i}} + \frac{Z_j}{\sqrt{N_j}}$$

(Bishop, J. and Strack, O., 2011, *IJNME*, v. 88)



Summary

- 1. Presented a finite-element method for modeling pervasive fracture in materials and structures based on random meshes.
- 2. Presented a polyhedral finite-element formulation for both convex and nonconvex elements.
- 3. If engineering quantities-of-interest are extremely sensitive to initial conditions and system parameters, need to embrace a probabilistic description.
- 4. Presented a statistical-method for verifying and validating nonlinear dynamical systems in this regime including pervasive fracture.