On a Nonlocal Finite Element Model for Mode-III Brittle Fracture with Surface-Tension Excess Property

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Overview

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If we linearize using the assumption of displacement gradients are small, we can approximate $E$ and $\epsilon$. Then there is no distinction between reference and deformed configuration.
Mode-III Fracture

The Mode-III fracture (or anti-plane shear fracture):
- The fracture surfaces slide relative to each other skew-symmetrically with shear stress acting as shown in the figure.
- Displacement:
  - $u_1 = 0$ and $u_2 = 0$
  - $u_3 = u_3(x_1, x_2)$
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- Also, it predicts an elliptical crack-surface opening displacement with a blunt crack-tip.

Thus, several remedies have been attempted: appealing to a non-linear theory of elasticity, the introduction of a cohesive zone around the crack tip, and non-local theories.
The problem studied here is the straight, static, anti-plane shear crack, lying on $|x_1| < a$, $x_2 = 0$ in an infinite, isotropic, linear elastic body subjected to uniform far-field anti-plane shear loading ($\sigma_{23}^\infty$). The stress-strain relations are:

$$\tau_{23} = \mu \frac{\partial u_3}{\partial x_2} \quad \text{and} \quad \tau_{13} = \mu \frac{\partial u_3}{\partial x_1},$$

where $\tau_{23}$ and $\tau_{13}$ are the relevant stress components, and $u_3$ denotes the $z-$displacement.

**Figure:** Physical description of the problem.
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$$-\Delta u_3 = 0.$$ 

Then we consider a surface tension model which depend on (linearized) curvature of the out-of-plane displacement by:

$$\gamma = \gamma_0 + \gamma_1 u_{3,11}(x_1, 0),$$

where $\gamma_0$ and $\gamma_1$ are surface tension parameters.

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where \(\gamma_0\) and \(\gamma_1\) are surface tension parameters. Then the resulting boundary condition on the upper crack-surface is give by:

\[u_{3,2}(x_1, 0) = -\gamma_1 u_{3,111}(x_1, 0)\]

Mode-III fracture BVP

\[-\Delta u_3(x_1, x_2) = 0, \quad \text{in} \quad Q\]

**Boundary conditions:**

- on \(\Gamma_0\) \(u_{3,2}(x_1, 0) = -\sigma_{23}^\infty - \gamma_1 u_{3,111}\),
- on \(\Gamma_1\) \(u_3 = 0\),
- on \(\Gamma_2\) \(\vec{n} \cdot \nabla u_3 = 0\),
- on \(\Gamma_3\) \(\vec{n} \cdot \nabla u_3 = 0\),
- on \(\Gamma_4\) \(\vec{n} \cdot \nabla u_3 = 0\).

**Figure:** Finite computational domain \(Q\).
Appealing to the BVP, the weak formulation for the problem on hand is found by integrating the PDE against a test function \( v \) over \( \Omega \). This yields

\[
\int_Q \nabla v \cdot \nabla u_3 \, dQ - \int_{\partial Q} v \left( \vec{n} \cdot \nabla u_3 \right) \, d\partial Q = 0.
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\]

There is no contribution from the second term on the left-hand side of the above equation except over the crack-surface \( \Gamma_0 \). Therefore the resulting weak formulation takes the form

\[
\int_Q \nabla u_3 \cdot \nabla v \, dQ - \int_{\Gamma_0} \nu \, u_{3,2}(x_1,0) \, dx_1 = 0,
\]
We consider the crack-surface boundary condition and rearrange the equation to obtain

\[-u_{3,111}(x_1, 0) = \frac{1}{\gamma_1} \left[ u_{3,2}(x_1, 0) + \sigma_{23}^\infty \right] \text{ on } \Gamma_0.\]
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- \(u_3(x_1, x_2)\) is an odd function in \(x_2\), therefore \(u_{3,1}(0,0) = 0\).
- Also regularization on \(\Gamma_0 \cup \Gamma_1\) requires \(u_{3,1}(1,0) = 0\).
Reformulation of the Crack-Face Boundary Condition

Then the solution to the two point boundary value problem is given by

\[ u_{3,1}(x, 0) = \mathcal{G}\{f\}(x) := \int_0^1 G(x, q)f(q)\,dq. \]
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\[
  u_{3,1}(x, 0) = \frac{1}{\gamma_1} \int_0^1 G(x, q)[u_{3,2}(q, 0) + \sigma_{23}^\infty] \, dq \\
  = \frac{1}{\gamma_1} \int_0^1 G(x, q) \, u_{3,2}(q, 0) \, dq - \frac{\sigma_{23}^\infty}{2\gamma_1} x(1 - x).
\]
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\[ = \frac{1}{\gamma_1} \int_0^1 G(x, q) u_{3,2}(q, 0) \, dq - \frac{\sigma_{23}^{\infty}}{2\gamma_1} x(1 - x). \]

Now, we know that the Hilbert transform gives the Dirichlet-to-Neumann map, ie

\[ u_{3,2}(x, 0^+) = \mathcal{H}\{u_{3,1}\} \]

\[ = \frac{1}{\pi} \int_{-\infty}^{\infty} u_{3,1}(q, 0^+) \frac{dq}{q - x} \]

\[ = \frac{1}{\pi} \int_0^1 u_{3,1}(q, 0^+) \frac{2q}{q^2 - x^2} \, dq, \]
Reformulation of the Crack-Face Boundary Condition

\[ u_{3,2}(x, 0) = \frac{1}{\pi \gamma_1} \int_0^1 k(x, q) u_{3,2}(q, 0) dq - \frac{\sigma_{23}^\infty}{2\pi \gamma_1} g(x), \quad \text{on} \quad \Gamma_0, \]
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u_{3,2}(x, 0) = \frac{1}{\pi \gamma_1} \int_0^1 k(x, q) u_{3,2}(q, 0) \, dq - \frac{\sigma_{23}^\infty}{2\pi \gamma_1} g(x), \quad \text{on} \quad \Gamma_0,
\]

where \( k(x, q) \) and \( g(x) \) are given by:

\[
k(x, q) = (q + x) \ln (q + x) + (q - x) \ln |q - x| \\
- q(1 + x) \ln (1 + x) - q(1 - x) \ln |1 - x|
\]

\[
g(x) = 1 - x(1 + x) \ln \left( \frac{1 + x}{x} \right) + x(1 - x) \ln \left| \frac{1 - x}{x} \right|
\]
Applying this result to the earlier *Weak-Form* yields the final weak form

\[
\int_Q \nabla u_3 \cdot \nabla v + \frac{1}{\pi \gamma_1} \int_0^1 v(x, 0) \int_0^1 k(x, q) u_{3,2}(q, 0) \, dq \, dx = \frac{\sigma_{23}}{2\pi \gamma_1} \int_0^1 v(x, 0) g(x) \, dx.
\]

Note that this weak form has no higher-order derivatives, thus the standard FEM can now be applied.
Parameter Determination

Theorem

The Fredholm integral equation

\[ \gamma_1 u(x) - K[u](x) = -\frac{\sigma^\infty_{23}}{2\pi} g(x), \quad \text{for} \quad 0 \leq x \leq 1, \]

where \( K \) is the integral operator

\[ K[\psi](x) = \frac{1}{\pi} \int_0^1 k(x, q) \psi(q) \, dq, \]

has a unique, continuous solution for all but countably many values of \( \gamma_1 \).

Where \( k(x, q) \) is given by:

\[ k(x, q) = (q + x) \ln (q + x) + (q - x) \ln |q - x| \]
\[ - q(1 + x) \ln (1 + x) - q(1 - x) \ln |1 - x| \]
Numerical Results: Displacement
Numerical Results: Crack-Face Displacement

![Graph showing Crack-Face Displacement](image)

- **Displacement $u_3$**
- **Nondimensionalized position ($x/l$) on the crack face**

Legend:
- Red square: Nonlocal
- Blue circle: Offline

$9 \times 10^{-5}$
Numerical Results: Near-Tip Stress $\tau_{23}$

\begin{itemize}
  \item $\frac{1}{\sqrt{1 - x}}$
  \item LEFM
  \item Surface mechanics model
\end{itemize}

Stress component $\tau_{23}$

Nondimensionalized position (x/l) outside the crack-tip
Numerical Results: Near-Tip Strain $\varepsilon_{23}$

- $1/\sqrt{(1 - x)}$
- LEFM
- Surface mechanics model

Strain component $\varepsilon_{23}$ vs. Nondimensionalized position ($x/l$) outside the crack-tip.
Numerical Results: Crack-Face Displacement

![Graph showing crack-face displacement](image)

- $\gamma_1 = 0.0$
- $\gamma_1 = 0.5$
- $\gamma_1 = 1.0$
- $\gamma_1 = 4.0$

Displacement $u_3$

Nondimensionalized position $(x/l)$ on the crack face
Numerical Results: Near-Tip Stress $\tau_{23}$

![Graph showing displacement $u_3$ versus nondimensionalized position $(x/l)$ on the crack face for different values of $\sigma_{23}$]
Numerical Results: Near-Tip Stress $\tau_{23}$

![Graph showing stress component $\tau_{23}$ vs. nondimensionalized position $(x/l)$ outside the crack-tip for different $\gamma_1$.](image)
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We showed that the two FEM implementations agree well with each other. In particular, the model predicts bounded crack-tip stresses (also strains) and a cusp-like crack opening profile with a sharp crack-tip.
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We are currently developing a corresponding implementation of both pure mode-I and mixed-mode (combination of mode-I and mode-II) fracture.
References

W. Bangerth, R. Hartmann and G. Kanschat.
deal.II – a General Purpose Object Oriented Finite Element Library,

W. Bangerth, T. Heister, L. Heltai, G. Kanschat, M. Kronbichler, M. Maier, B. Turcksin, T. D. Young.
The deal.II Library, Version 8.1, arXiv preprint,

T. Sendova and J. R. Walton.
A New Approach to the Modeling & Analysis of Fracture through an Extension of Continuum Mechanics to the Nanoscale.

L. Ferguson, S. M. Mallikarjunaiah and J. R. Walton.
Numerical simulation of mode-III fracture incorporating interfacial mechanics.

J. R. Walton.
A note on fracture models incorporating surface elasticity.
THANK YOU