3D crack propagation analysis with PDS-FEM

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Motivation

- Necessary to consider minor local heterogeneity
  - Size and distribution local heterogeneity cannot be measured
  - Monte-Carlo simulations with randomly distributed heterogeneity
- Meshless or adaptive methods are too complicated for stochastic studies
  - Difficult to introduce heterogeneity to the numerical model
  - Sophisticated and computationally intensive
- **PDS-FEM provides simple means of modeling size and distribution of local heterogeneity with numerically efficient failure treatments**
Organization

- Discretization scheme and formulation of PDS-FEM
- Failure treatment with torsional failure as an example
- Dynamic model and kidney stone breaking as an example
Background: two models of deformable body

- Smooth, overlapping interpolation functions
  \[ u_1, u_2, u_3 \]

- Background: two models of deformable body
  - Fracture
  - Continuum
    - BVP
    - FEM / BEM / FDM
    - DEM

- Rigid-body spring
  - Equivalence to continuum is not verified and springs are mysterious

- Effort to deal with failure
  - Numerically intensive failure treatment
  - Efficient failure treatment

- Spring properties?
Discretization schemes of FEM and DEM

Ordinary FEM

Smooth and overlapping shape functions

DEM

Particles can be interpreted as non-overlapping shape functions

PDS-FEM: numerical method to solve BVP of a continuum with particle discretization
1-D particle discretization

\[ u^d(x) = \sum_{\alpha} u^\alpha \varphi^\alpha(x) \]

\( f^\alpha \) is the average value taken over the domain \( \varphi^\alpha \)

\[ \frac{df}{dx}(x) = g(x) = \sum_{\alpha} g^\beta \psi^\beta(x) \]

An average value for derivative is obtained on a conjugate geometry \( \psi^\alpha \)

Function and derivative are discretized using conjugate geometries.
2D-Particle discretization

Voronoi tessellation for function $u(x)$

Delaunay tessellation for derivative $u, i(x)$

$u^d(x) = \sum_{\alpha} u^{\alpha} \varphi^{\alpha}(x)$

$\frac{du^d(x)}{dx_j} = g^d_j(x) = \sum_{\beta} g^\beta_j \psi^\beta(x)$

Function and derivative are discretized using conjugate geometries, Voronoi and Delaunay tessellations
Particle discretization for continuum: PDS-FEM

- Boundary Value Problem for Linear Elasticity
  \[
  \begin{align*}
  \left\{(c_{ijkl} u_{k,l}(x))_{,i} + b(x)\right) & = 0 \quad \text{in } B \\
  u(x) & = \bar{u} \quad \text{on } \partial B
  \end{align*}
  \]

- Functional
  - Ordinary FEM functional
    \[
    I(u) = \frac{1}{2} \int_B u_{i,j} c_{ijkl} u_{k,l} - b_i u_i \, dv
    \]
  - Functional used in PDS-FEM
    \[
    J(u, \sigma_{ij}, \varepsilon_{ij}) = \int_B \frac{1}{2} \varepsilon_{ij} c_{ijkl} \varepsilon_{kl} - \sigma_{ij} (\varepsilon_{ij} - u_{j,i}) - b_j u_j \, dv
    \]
    First variation
    \[
    \delta J = -\int \delta u_j (\sigma_{ij,i} - b_j) + \delta \varepsilon_{ij} (\sigma_{ij} - c_{ijkl} \varepsilon_{kl}) + \delta \sigma_{ij} (\varepsilon_{ij} - u_{j,i}) \, dv
    \]
Particle discretization for continuum: PDS-FEM

1. Functional

\[ J(u_j, \sigma_{ij}, \varepsilon_{ij}) = \int_B \frac{1}{2} \varepsilon_{ij} c_{ijkl} \varepsilon_{kl} - \sigma_{ij} (\varepsilon_{ij} - u_{j,i}) - b_j u_j \, dv \]

2. Conjugate discretization

\[ b_i (x) = \sum b_i^\alpha \varphi^\alpha (x) \]
\[ u_i (x) = \sum u_i^\alpha \varphi^\alpha (x) \]

Voronoi

\[ \sigma_{ij} (x) = \sum \sigma_{ij}^\beta \psi^\beta (x) \]
\[ \varepsilon_{ij} (x) = \sum \varepsilon_{ij}^\beta \psi^\beta (x) \]
\[ c_{ijkl} (x) = \sum c_{ijkl}^\beta \psi^\beta (x) \]

Delaunay

3. determination of \( u^\alpha \)

\[ J = \frac{1}{2} \sum_{\alpha, \alpha'} K_{ik}^{\alpha \alpha'} u_i^\alpha u_k^{\alpha'} = \frac{1}{2} \sum_{\alpha, \alpha', \beta} \int_B \varphi_j^\alpha \psi^\beta \, dv c_{ijkl}^\beta \int_B \varphi_i^{\alpha'} \psi^\beta \, dv \int_B \psi^\beta \, dv \]
\[ u_i^\alpha u_k^{\alpha'} \]

4. With Voronoi and Delaunay tessellations, \( K_{ik}^{\alpha \alpha'} \) coincides with stiffness matrix of FEM with linear characteristic functions
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Failure treatment

The stiffness matrix of FEM-β is:

\[
\begin{bmatrix}
[k_{11}] & [k_{12}] & [k_{13}] \\
[k_{21}] & [k_{22}] & [k_{23}] \\
[k_{31}] & [k_{32}] & [k_{33}]
\end{bmatrix}
\]

\[
[k_{12}] = [k_{12}^{\text{direct}}] + [k_{12}^{\text{indirect}}]
\]

Spring properties are rigorously determined with material properties; \( E \) and \( \nu \)

Failure is modeled by appropriately modifying the components of element stiffness matrix
Failure treatment: modeling brittle failure

\[ b_j^{\beta\alpha} = \frac{1}{\Psi^\beta} \int_B \varphi_j^{\alpha} \varphi^\beta \, dv \]

\[ K_{ik}^{\alpha'\alpha} = \sum_{\beta} \left( b_j^{\beta\alpha} c_{ijkl} b_l^{\beta\alpha'} \right) \Psi^\beta \]

\[ \mathbf{K} = \mathbf{B}^T \mathbf{C} \mathbf{B} \]

\[ d_j^{\gamma\alpha} = \frac{1}{\Psi^\beta} \int_B \varphi_j^{\alpha} \varphi^{\gamma} \, dv \]

\[ \mathbf{B} = \begin{bmatrix}
    b_1^{\beta\alpha_1} & b_1^{\beta\alpha_2} & b_1^{\beta\alpha_3} \\
    b_2^{\gamma\alpha_1} & b_2^{\beta\alpha_2} & b_2^{\beta\alpha_3} \\
    b_2^{\gamma\alpha_1} & b_2^{\beta\alpha_2} & b_2^{\beta\alpha_3}
\end{bmatrix} - \begin{bmatrix}
    d_1^{\gamma\alpha_1} & d_1^{\beta\gamma_1\alpha_1} & 0 \\
    d_2^{\gamma\alpha_1} & d_2^{\beta\gamma_1\alpha_1} & 0 \\
    d_2^{\gamma\alpha_1} & d_2^{\beta\gamma_1\alpha_1} & 0
\end{bmatrix} \]

No new DOFs or elements are introduced to accommodate the new crack surface.
Computational overhead is almost equal to re-computation of element stiffness matrix.
Failure treatment of PDS-FEM is approximate

FEM

No new DOFs or elements are introduced to accommodate the new crack surface
Cannot guarantee the satisfaction of BCs on new crack surface

PDS-FEM

One new node and four elements are introduced

No new nodes are introduced

new crack surfaces

new crack surfaces

No new DOFs or elements are introduced to accommodate the new crack surface
Cannot guarantee the satisfaction of BCs on new crack surface
Accuracy of approximate failure treatment: problem setting

- Far field stress $\sigma_{yy}$
- Accuracy of crack tip stress field with $J$-integral

$$J = \int_{s} \frac{1}{2} \sigma_{ij} \varepsilon_{ij} - \sigma_{ij} \frac{\partial u_{i}}{\partial x} n_{j} ds$$

Far field loading

- semi-infinite crack
- circular domain
- infinite body
  - $E = 69$ GPa
  - $\nu = 0.23$
Accuracy of crack tip stress field

PDS-FEM crack tip stress filed is as accurate as the FEM solution, regardless of approximate failure treatment. The accuracy of crack tip stress filed can be improved by including rotational DOF.
PDS-FEM estimates the rotational component fairly accurately, leading to better estimation of crack tip stress field.
Example problem: torsion testing

- Problem setting: torsion testing

\[ E = 70 \text{GPa} \]
\[ \nu = 0.3 \]

80 mm

Real experiment

Helical spiral fracture surface

E = 70 GPa
\[ \nu = 0.3 \]
Example problem: torsion testing

- Ghost layer (computed using MPI)
- Helical spiral fracture surface
Organization

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Time integration approaches for PDS-FEM

FEM like continuum representation

\[ L = T - V = \sum_{\alpha} \frac{1}{2} m^\alpha \dot{u}_i^\alpha \dot{u}_i^\alpha - \sum_{\alpha} \frac{1}{2} K_{ij}^{\alpha\alpha} u_j^\alpha u_i^\alpha \]

Hamiltonian principle

\[ \delta \int_{t_0}^{t_1} L(q, \dot{q}) \, dt + \int_{t_0}^{t_1} F(q, \dot{q}) \, \delta q \, dt = 0 \]

Second order explicit algorithm

(a range of Variational integrators)

N-body problem like particle representation

\[ H = T + V = \sum_{\alpha} \frac{1}{2} m^\alpha \dot{u}_i^\alpha \dot{u}_i^\alpha + \sum_{\alpha} \frac{1}{2} K_{ij}^{\alpha\alpha} u_j^\alpha u_i^\alpha \]

Hamiltonian based

Candy’s method: 4th order symplectic

\[ p^k = p^{k-1} + b^k F(q^{k-1}) \Delta t \]

\[ q^k = q^{k-1} + a^k P(p^{k-1}) \Delta t \quad k = 1, \ldots, 4 \]

\[ F(q) = -\frac{\partial V(q)}{\partial q} \quad P(p) = \frac{\partial T(p)}{\partial p} \]

\[ q_i^\alpha = u_i^\alpha \quad p_i^\alpha = m^\alpha u_i^\alpha \]
Simulating failure of concrete wall under tsunami load

Conc. wall

Snaps of the experiment

Damaged concrete wall

Conducted at the LHC facility at the Port and Airport Research Institute, Japan
Model details

Material parameters

<table>
<thead>
<tr>
<th></th>
<th>Concrete</th>
<th>Steel</th>
</tr>
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<tbody>
<tr>
<td>$E$ (GPa)</td>
<td>30</td>
<td>210</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.2</td>
<td>0.3</td>
</tr>
<tr>
<td>$\sigma_t$ (MPa)</td>
<td>5</td>
<td>400</td>
</tr>
</tbody>
</table>

Fixed boundaries

Reinforcement mesh ($\phi 6@200\text{mm} \times 200\text{mm}$)
Input data: pressure time histories at 5 heights

Locations of pressure gauges

Pressure histories are interpolated for the intermediate points.
Crack patterns: front side of 100mm thick wall
Crack patterns: back side of 100mm thick wall

Semicircular crack patterns of the front side are reaching the back.
Shockwave Lithotripsy: kidney stone breaking

- Complete phenomena is not well explained
- Simulation of this mechanism would help further development of this technology

Typical pressure history in water induced by a single ultrasonic pulse
Current studies of Shockwave Lithotripsy (SWL)

- High speed photoelasticity and ray tracing are used to find the possible high stress regions and the locations of crack initiation.
- Predicting the crack path of this dynamic phenomena has not yet been done.
Interesting crack patterns in plaster of Paris samples

- Crack initiation and propagation is due to a dynamic state of stress
- This could be one of the toughest crack propagation problem to be simulated
Simulation of SWL: problem setting

Pressure pulse applied on this plane

Input pressure pulse


~ 6 million elements
~ 3.5 million DOFs

Plaster of Paris
- $E = 8.875 \text{ GPa}$
- $\nu = 0.228$
- $V_p = 2478 \text{ m/s}$
- $V_s = 1471 \text{ m/s}$

Water
- $K = \text{ }$
- $V_p = 1483 \text{ m/s}$
Stress waves of $\sigma_{yy}$

vertical plane

cylindrical sample

horizontal plane
Crack patterns at different sections of cylinder

Tuler and Butcher failure criterion:

\[
\int_0^t (\sigma_1 - \sigma_t)^2 dt \geq K_f
\]

\(\sigma_t\) tensile strength
Particle discretization for continuum mechanics problems

- uses a set of non-overlapping characteristic functions on conjugate geometries
- numerically efficient approximate failure treatment
- accuracy of crack tip stress field can be improved with rotational DOF
- particle physics type dynamic simulations (i.e. a simplified N body problem)

We simulated several 3D crack profiles with complicated geometries