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Crack tip fields and location in molecular dynamics

LEFM parameters from unstructured, noisy displacement data

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National Nuclear Security Administration

LEFM from MD (or other full field $\mathbf{u}(\mathbf{x})$)

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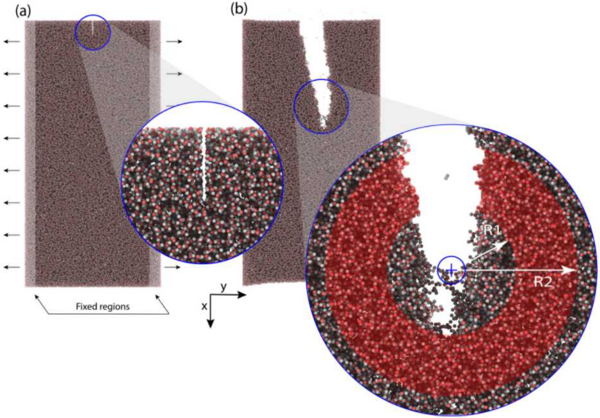
- Motivated by MD simulations of fracture in silica glass
- How to compute K_{I}, K_{II}, etc?
- How to deal with process zone on atomic scale?
- Where is the effective crack tip (center of LEFM fields)?



Solution: use boundary collocation (sort of)

- Traditional boundary collocation is LSQ fitting of LEFM parameters to $\mathbf{u}(\mathbf{x})$ at boundary
- We fit $\mathbf{u}(\mathbf{x})$ to an annular region surrounding crack tip
- Ayatollahi and Nejati (Fatigue Fract Eng Mat, 34:3, 159–176, 2011) did this using LSQ solution to an overdetermined system

$$
\begin{aligned}
u &= \sum_{n=0}^{N} \frac{A_n}{2\mu} r^{n/2} \\
&\quad \times \left\{ \left(\kappa + \frac{n}{2} + (-1)^n \right) \cos \frac{n}{2}\theta - \frac{n}{2} \cos\left(\frac{n}{2} - 2 \right) \theta \right\} \\
&\quad + \sum_{n=0}^{M} \frac{B_n}{2\mu} r^{n/2} \\
&\quad \times \left\{ \left(-\kappa - \frac{n}{2} + (-1)^n \right) \sin \frac{n}{2}\theta + \frac{n}{2} \sin\left(\frac{n}{2} - 2 \right) \theta \right\} \\
&= f_0 A_0 + \sum_{n=1}^{N} A_n f_n^{\mathrm{I}}(r,\theta) + \sum_{n=1}^{M} B_n f_n^{\mathrm{II}}(r,\theta), \qquad (3)
\end{aligned}
$$

$$
\begin{aligned}
v &= \sum_{n=0}^{N} \frac{A_n}{2\mu} r^{n/2} \\
&\quad \times \left\{ \left(\kappa - \frac{n}{2} - (-1)^n \right) \sin \frac{n}{2}\theta + \frac{n}{2} \sin\left(\frac{n}{2} - 2 \right) \theta \right\} \\
&\quad + \sum_{n=0}^{M} \frac{B_n}{2\mu} r^{n/2} \\
&\quad \times \left\{ \left(\kappa - \frac{n}{2} + (-1)^n \right) \cos \frac{n}{2}\theta + \frac{n}{2} \cos\left(\frac{n}{2} - 2 \right) \theta \right\} \\
&= g_0 B_0 + \sum_{n=1}^{N} A_n g_n^{\mathrm{I}}(r,\theta) + \sum_{n=1}^{M} B_n g_n^{\mathrm{II}}(r,\theta). \qquad (4)
\end{aligned}
$$

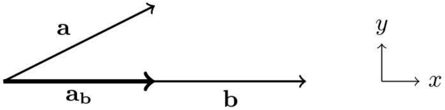
$$
\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_k \\ v_1 \\ v_2 \\ \vdots \\ v_k \end{bmatrix}
=
\begin{bmatrix}
f_1^{\mathrm{I}}(r_1,\theta_1) & \dots & f_N^{\mathrm{I}}(r_1,\theta_1) & f_1^{\mathrm{II}}(r_1,\theta_1) & f_3^{\mathrm{II}}(r_1,\theta_1) & f_4^{\mathrm{II}}(r_1,\theta_1) & \dots & f_M^{\mathrm{II}}(r_1,\theta_1) & f_0 & 0 & f_2^{\mathrm{II}}(r_1,\theta_1) \\
f_1^{\mathrm{I}}(r_2,\theta_2) & \dots & f_N^{\mathrm{I}}(r_2,\theta_2) & f_1^{\mathrm{II}}(r_2,\theta_2) & f_3^{\mathrm{II}}(r_2,\theta_2) & f_4^{\mathrm{II}}(r_2,\theta_2) & \dots & f_M^{\mathrm{II}}(r_2,\theta_2) & f_0 & 0 & f_2^{\mathrm{II}}(r_2,\theta_2) \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
f_1^{\mathrm{I}}(r_k,\theta_k) & \cdots & f_N^{\mathrm{I}}(r_k,\theta_k) & f_1^{\mathrm{II}}(r_k,\theta_k) & f_3^{\mathrm{II}}(r_k,\theta_k) & f_4^{\mathrm{II}}(r_k,\theta_k) & \cdots & f_M^{\mathrm{II}}(r_k,\theta_k) & f_0 & 0 & f_2^{\mathrm{II}}(r_k,\theta_k) \\
g_1^{\mathrm{I}}(r_1,\theta_1) & \cdots & g_N^{\mathrm{I}}(r_1,\theta_1) & g_1^{\mathrm{II}}(r_1,\theta_1) & g_3^{\mathrm{II}}(r_1,\theta_1) & g_4^{\mathrm{II}}(r_1,\theta_1) & \cdots & g_M^{\mathrm{II}}(r_1,\theta_1) & 0 & g_0 & g_2^{\mathrm{II}}(r_1,\theta_1) \\
g_1^{\mathrm{I}}(r_2,\theta_2) & \cdots & g_N^{\mathrm{I}}(r_2,\theta_2) & g_1^{\mathrm{II}}(r_2,\theta_2) & g_3^{\mathrm{II}}(r_2,\theta_2) & g_4^{\mathrm{II}}(r_2,\theta_2) & \cdots & g_M^{\mathrm{II}}(r_2,\theta_2) & 0 & g_0 & g_2^{\mathrm{II}}(r_2,\theta_2) \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
g_1^{\mathrm{I}}(r_k,\theta_k) & \cdots & g_N^{\mathrm{I}}(r_k,\theta_k) & g_1^{\mathrm{II}}(r_k,\theta_k) & g_3^{\mathrm{II}}(r_k,\theta_k) & g_4^{\mathrm{II}}(r_k,\theta_k) & \cdots & g_M^{\mathrm{II}}(r_k,\theta_k) & 0 & g_0 & g_2^{\mathrm{II}}(r_k,\theta_k)
\end{bmatrix}
\begin{bmatrix} A_1 \\ \vdots \\ A_N \\ B_1 \\ B_3 \\ B_4 \\ \vdots \\ B_M \\ A_0 \\ B_0 \\ B_2 \end{bmatrix}
$$

$$
\mathbf{U} = \mathbf{C}\mathbf{A}, \quad \mathbf{A} = \left(\mathbf{C}^{\mathsf{T}} \mathbf{C} \right)^{-1} \mathbf{U}
$$

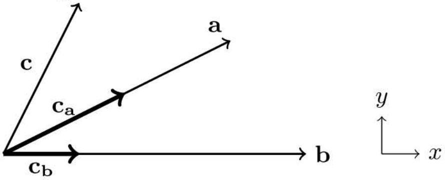
Basis projection method

- We propose to interpret the observed displacements as a noisy sampling of a real diplacement field. We project this $\mathbf{u}^{\text{obs}}(\mathbf{x})$ onto a basis of LEFM fields, $\mathbf{u}_n^s(\mathbf{x})$
- Recall that the projection of a vector $\mathbf{a}$ onto another vector $\mathbf{b}$ is given by

$$\mathbf{a}_\mathbf{b} = \frac{\mathbf{a}\cdot\mathbf{b}}{\mathbf{b}\cdot\mathbf{b}}\mathbf{b}, \qquad |\mathbf{a}_\mathbf{b}| = \frac{\mathbf{a}\cdot\mathbf{b}}{|\mathbf{b}|}$$



- But if we have $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ and want to find $\mathbf{a} = \beta\mathbf{b} + \gamma\mathbf{c}$ then single projections aren't enough information



Basis projection method

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- First approximate the observed field in a series of LEFM fields,

$$\mathbf{u}^{\text{obs}}(\mathbf{x}) \approx \sum_{n,s} A_n^s \mathbf{u}_n^s(\mathbf{x})$$

- Define an inner product as $(\mathbf{a}, \mathbf{b}) \equiv \sum_{i=1}^{k} \mathbf{a}(\mathbf{x}_i) \cdot \mathbf{b}(\mathbf{x}_i)$
- Take the inner product of the observed field with each of the LEFM fields

$$\left(\mathbf{u}_m^t, \mathbf{u}^{\text{obs}}\right) \approx \left(\mathbf{u}_m^t, \sum_{n,s} A_n^s \mathbf{u}_n^s\right) = \sum_{n,s} \left(\mathbf{u}_m^t, \mathbf{u}_n^s\right) A_n^s = \sum_{n,s,i} \mathbf{u}_m^t(\mathbf{x}_i) \cdot \mathbf{u}_n^s(\mathbf{x}_i) A_n^s$$

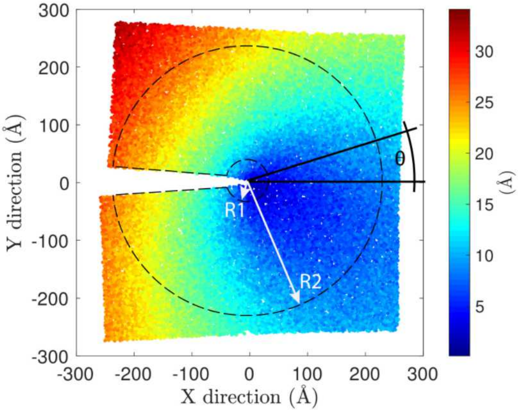
- We then get a square system to solve for LEFM parameters, $\mathbf{b} = \mathbf{SA}$
- This is equivalent to the overdetermined LSQ solution
- We can generalize the inner product definition

$$(\mathbf{a}, \mathbf{b}) \equiv \int_A \mathbf{a}(\mathbf{x}) \cdot \mathbf{b}(\mathbf{x}) w(\mathbf{x}) d\mathbf{x} \approx \frac{A}{k} \sum_{i=1}^{k} \mathbf{a}(\mathbf{x}_i) \cdot \mathbf{b}(\mathbf{x}_i) w(\mathbf{x}_i)$$

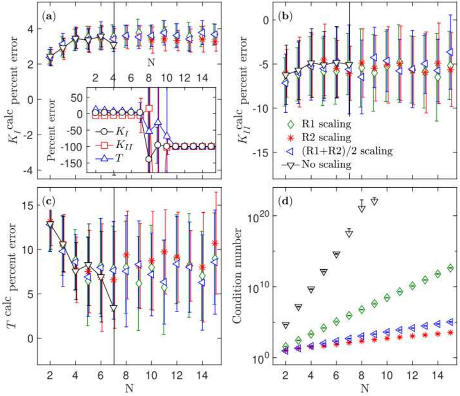
- All $\left(\mathbf{u}_m^t, \mathbf{u}_n^s\right)$ terms can be pre-computed analytically if desired

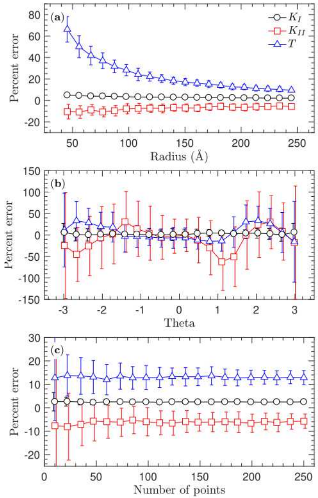
Proof of concept

- We use a toy problem to demonstrate the technique
- Form a mix of K_{I} and K_{II} LEFM fields at randomly sampled points and add some Gaussian noise
- Apply basis projection method and make sure we can extract the known K values
- This is a best case scenario: crack tip location is known, no blunting, no bridging, etc



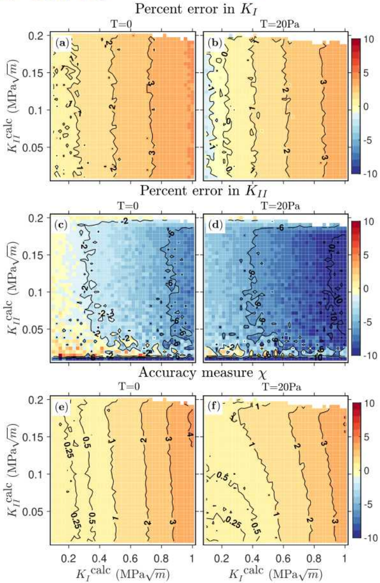
Proof of concept: results





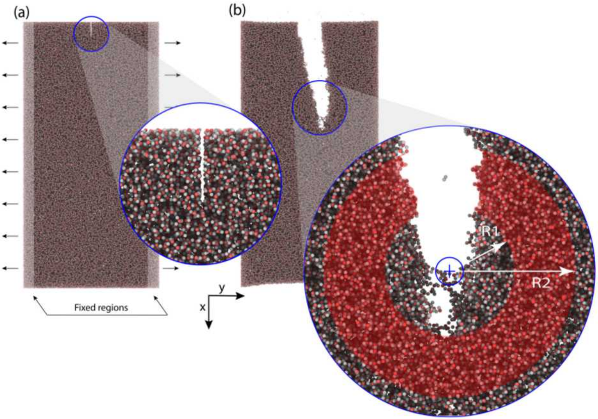
Proof of concept: systematic error

- In MD the displacements are too large for LEFM to be strictly applicable
- Can we characterize this error to correct for it?
- Error decreases with magnitude of applied fields (as expected)
- $\chi = \left[\left(\frac{\delta K_{\mathrm{I}}}{K_{\mathrm{I}}^{\mathrm{calc}}} \right)^2 + \left(\frac{\delta K_{\mathrm{II}}}{K_{\mathrm{II}}^{\mathrm{calc}}} \right)^2 + \left(\frac{\delta T}{T^{\mathrm{calc}}} \right)^2 \right]^{1/2}$
- If large K are calculated can determine error from these figures



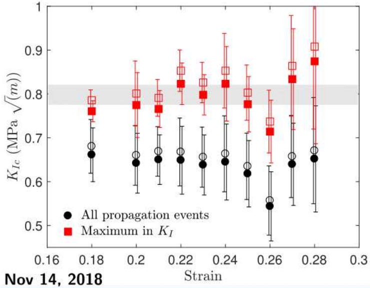
Silica glass fracture example

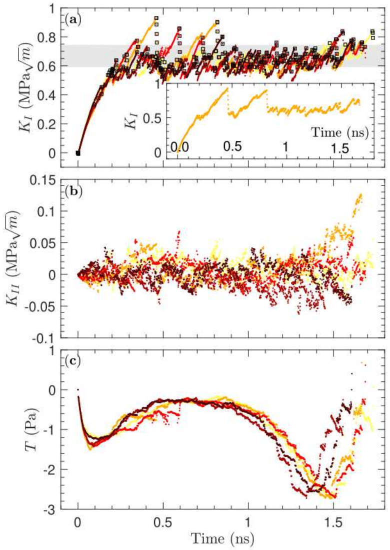
- Use ReaxFF force field with LAMMPS MD code
- Start with relaxed SiO_2 amorphous structure
- Delete atoms along a crack
- Apply affine displacement then let system relax
- Crack tip defined by last intact bond (will improve later)



Silica glass fracture example

- As system equilibrates K_I builds then plateaus as the crack begins to propagate. We can interpret the plateau as K_Ic.
- How to interpret K_Ic? Maximum or average of plateau? Something different?
- Calculated K_Ic matches well with experimental values (gray bar)





Locating crack tip

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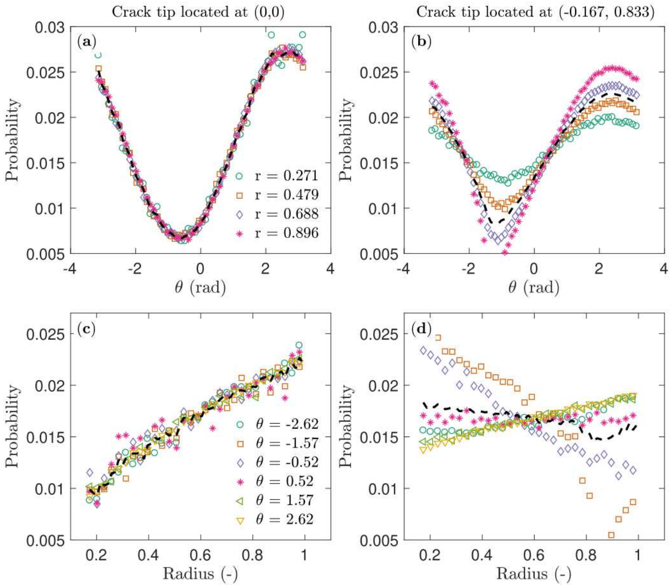
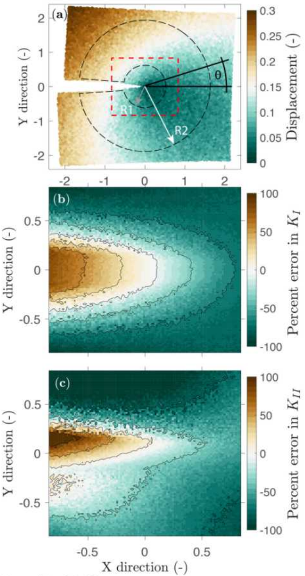
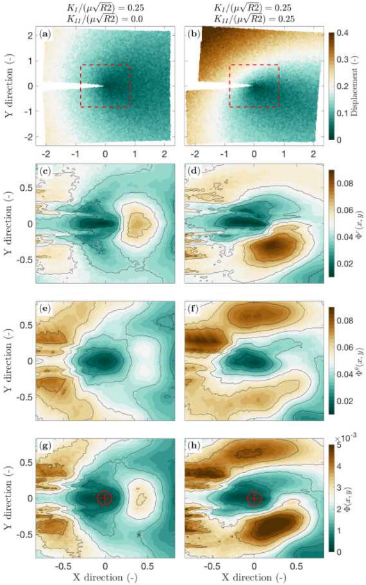
- How do we know where the correct center of the LEFM field is? There may be crack bridging. If blunting is present the singularity moves into the material from the apex of the crack.
- The elastic crack tip should make the LEFM fields separable, $u(r, \theta) = f(r)g(\theta)$
- Make a guess for crack tip position, (r_0, θ_0)
- Interpolate $\mathbf{u}^{\text{obs}}$ along circles surrounding (r_0, θ_0). If at the crack tip the circles should be sampling $g(\theta)$ only and vary from each other by a constant amount.
- Interpolate $\mathbf{u}^{\text{obs}}$ along radial lines from (r_0, θ_0). If at the crack tip the lines should be sampling $f(r)$ only and vary from each other by a constant amount.
- We form a cost function based on enforcing this separability and minimize over full field

Effect of separability



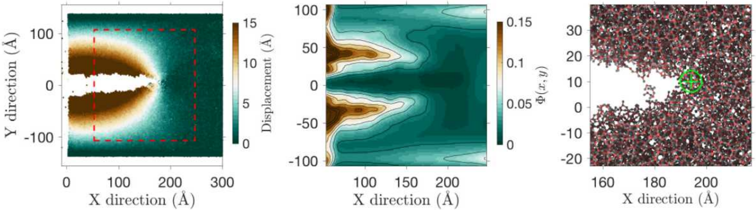
K errors and cost function





Crack locating in MD

- MD example includes crack bridging atoms and crack tip blunting
- With a "last broken bond" algorithm, crack tip is at apex
- Minimizing separability cost function places crack tip into the bulk, away from the free surface



Questions?

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Equivalency of basis projection and LSQ

- Approximate the observed field in a series of LEFM fields,

$$\mathbf{u}^{\text{obs}}(\mathbf{x}) \approx \sum_{n,s} A_n^s \mathbf{u}_n^s(\mathbf{x})$$

- Squared residual is then

$$R^2 = \left(\mathbf{u}^{\text{obs}} - \sum_{n,s} A_n^s \mathbf{u}_n^s, \mathbf{u}^{\text{obs}} - \sum_{n,s} A_n^s \mathbf{u}_n^s\right)$$

- The best fit LEFM parameters minimize this R^2,

$$\min_{A_n^s} R^2 = \min_{A_n^s} \left[\left(\mathbf{u}^{\text{obs}}, \mathbf{u}^{\text{obs}}\right) - 2\left(\mathbf{u}^{\text{obs}}, \sum_{n,s} A_n^s \mathbf{u}_n^s\right) + \left(\sum_{n,s} A_n^s \mathbf{u}_n^s, \sum_{m,t} A_m^t \mathbf{u}_m^t\right)\right]$$

- Making things stationary with respect to A_n^s we find

$$-2\left(\mathbf{u}^{\text{obs}}, \mathbf{u}_n^s\right) + 2\left(\mathbf{u}_n^s, \sum_{m,t} A_m^t \mathbf{u}_m^t\right) = 0$$

or

$$\left(\mathbf{u}^{\text{obs}}, \mathbf{u}_n^s\right) = \left(\mathbf{u}_n^s, \sum_{m,t} A_m^t \mathbf{u}_m^t\right)$$

- Thus, basis projection minimizes the residual and is equivalent to LSQ under appropriate definition of the inner product

Separability test regions