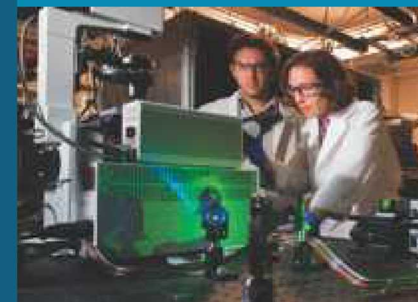
SAND2019-4784C

Continuum Stress Intensity Factors from Atomistic Fracture Simulations



MRS Spring Meeting 2019

Mathematical Aspects of Materials Science – Modeling, Analysis and Computations

April 25, 2019

PRESENTED BY

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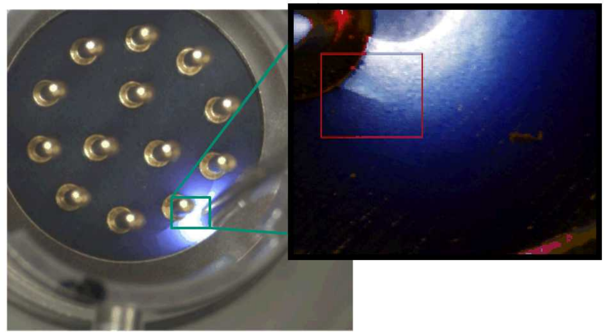
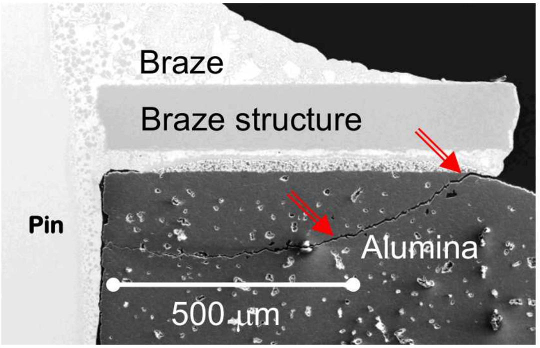
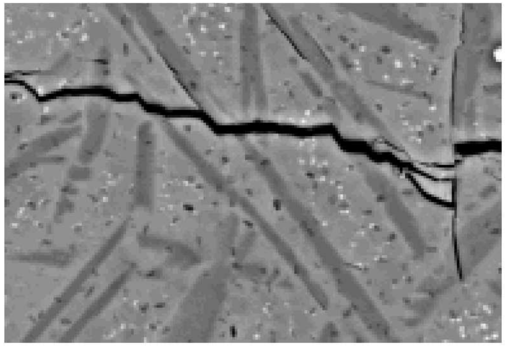
Motivation: Failure in brittle materials



Glass to metal seals



Brazed connections



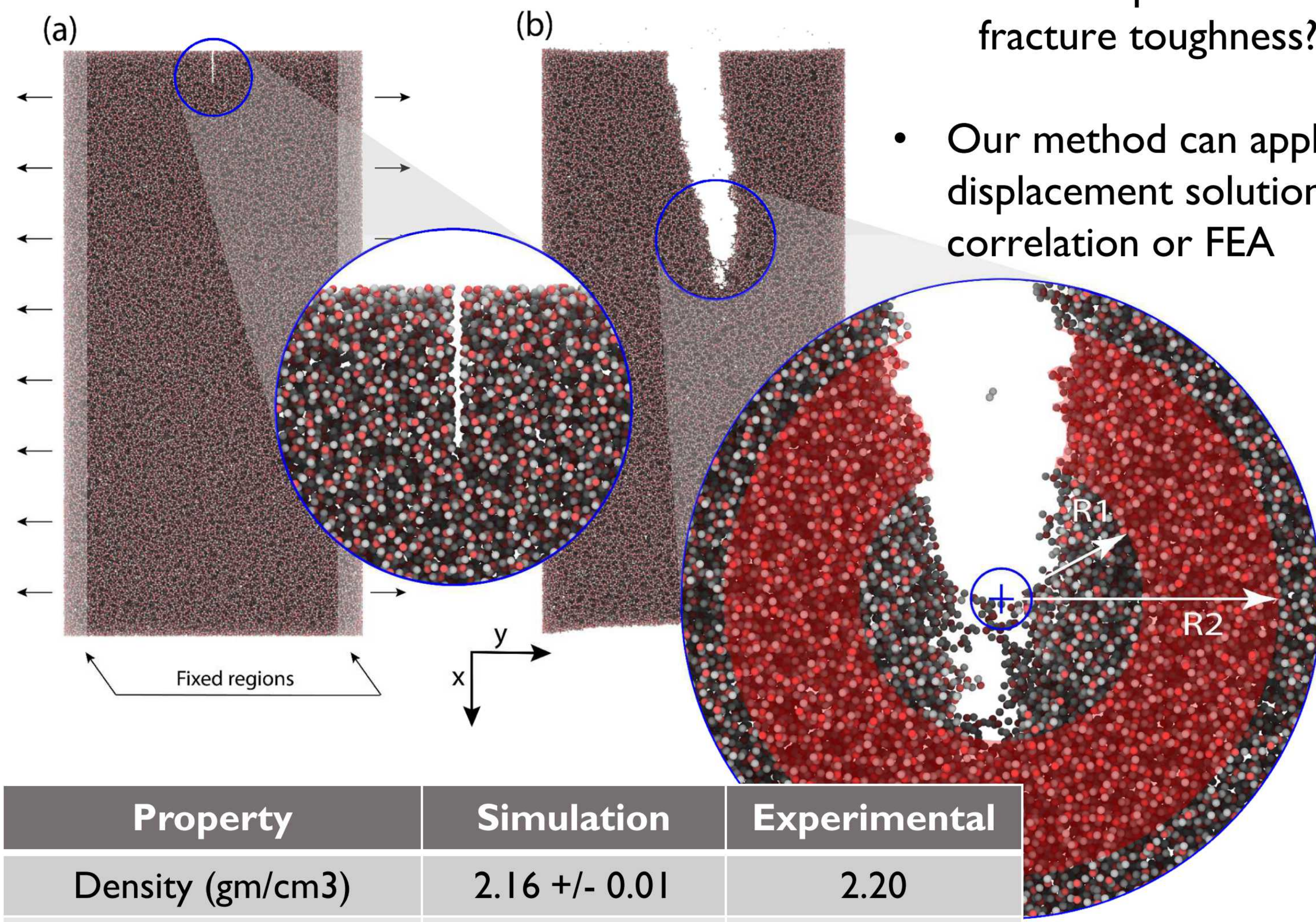
Glass-ceramics

Sandia interest: Brittle materials often fail from fracture during typical use and environmental exposure.

Challenge: Make 30 year lifespan reliability predictions for components containing brittle materials

Images courtesy of Kevin Strong (SNL) and Steve Dai (SNL).

Atomistic fracture simulations



Question:

What impact does chemistry have on fracture toughness?

- Our method can apply to any full-field displacement solution, e.g. digital image correlation or FEA

Property	Simulation	Experimental
Density (gm/cm3)	2.16 +/- 0.01	2.20
Young's modulus (GPa)	77.90+/- 2.02	72.9
Shear modulus (GPa)	25.81 +/- 0.95	31.3
Poisson ratio	0.250+/- 0.005	0.165

- *~60 X 30 X 5 nm*
- *ReaxFF potential*
- *~400K atoms*
- *540 processes*
- *~30 day computational time*

Williams expansion – LEFM fields

$$u(r,\theta) = \sum_{n=0}^{\infty}\sum_{m=1}^{2} A_m^n f_m^n(r,\theta)$$

$$= \sum_{n=0}^{\infty} A_1^n \frac{r^{n/2}}{2\mu}\left[\left(\kappa + \frac{n}{2} + (-1)^n\right)\cos\frac{n}{2}\theta - \frac{n}{2}\cos\left(\frac{n}{2}-2\right)\theta\right] +$$

$$\sum_{n=0}^{\infty} A_2^n \frac{r^{n/2}}{2\mu}\left[\left(-\kappa - \frac{n}{2} + (-1)^n\right)\sin\frac{n}{2}\theta + \frac{n}{2}\sin\left(\frac{n}{2}-2\right)\theta\right]$$

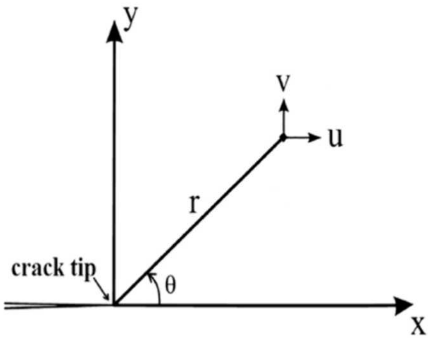
$$v(r,\theta) = \sum_{n=0}^{\infty}\sum_{m=1}^{2} A_m^n g_m^n(r,\theta)$$

$$= \sum_{n=0}^{\infty} A_1^n \frac{r^{n/2}}{2\mu}\left[\left(\kappa - \frac{n}{2} - (-1)^n\right)\sin\frac{n}{2}\theta + \frac{n}{2}\sin\left(\frac{n}{2}-2\right)\theta\right] +$$

$$\sum_{n=0}^{\infty} A_2^n \frac{r^{n/2}}{2\mu}\left[\left(\kappa - \frac{n}{2} + (-1)^n\right)\cos\frac{n}{2}\theta + \frac{n}{2}\cos\left(\frac{n}{2}-2\right)\theta\right]$$

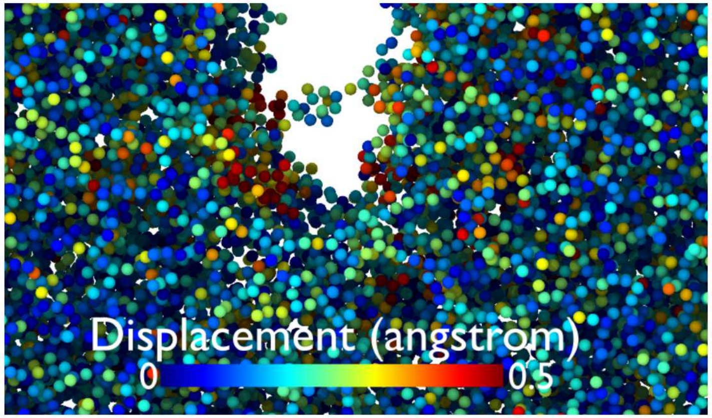
$$K_I = \sqrt{2\pi}A_1^1 \quad K_{II} = -\sqrt{2\pi}A_2^1 \quad T = 4A_1^2$$

- Solutions to the Airy stress function, in terms of displacements
- Any given observed discrete displacement about a crack tip can be described in terms of the Williams expansion



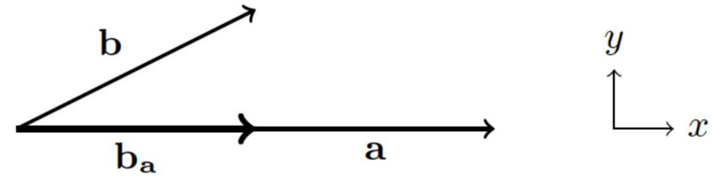
Basis set projection method

Reference t_{n-1}



- Project noisy data into the continuous space of the Williams expansion

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



$$\mathbf{u}_m^n(r,\theta) = f_m^n(r,\theta)\hat{\mathbf{e}_1} + g_m^n(r,\theta)\hat{\mathbf{e}_2}$$

- *Define a vector displacement function*

$$\mathbf{u}^{\mathrm{OBS}}(r,\theta) \approx \sum_{m,n} A_m^n \mathbf{u}_m^n(r,\theta)$$

- *Observed displacements can be defined in terms of the Williams expansion*

$$\langle \mathbf{u}_c^d, \mathbf{u}^{\mathrm{OBS}} \rangle = \langle \mathbf{u}_c^d, \mathbf{u}_m^n \rangle A_m^n$$

- *Project the continuous Williams functions from the left*

$$b_m^n = S_{c,m}^{d,n} A_m^n$$

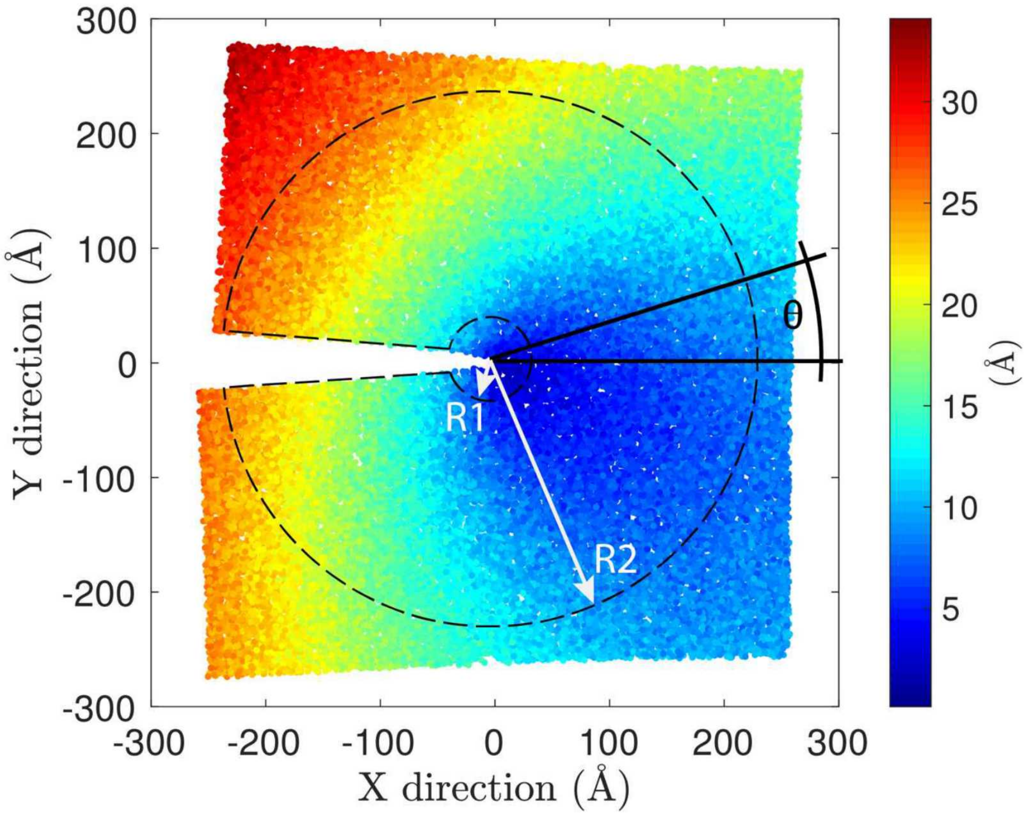
- *Considering all {m,n} combination, this results in a linear system of equations*

$$K_I = \sqrt{2\pi}A_1^1 \qquad K_{II} = -\sqrt{2\pi}A_2^1 \qquad T = 4A_1^2$$

Wilson et al. in review, Comp. Meth. App. Mech. Engin. 2019

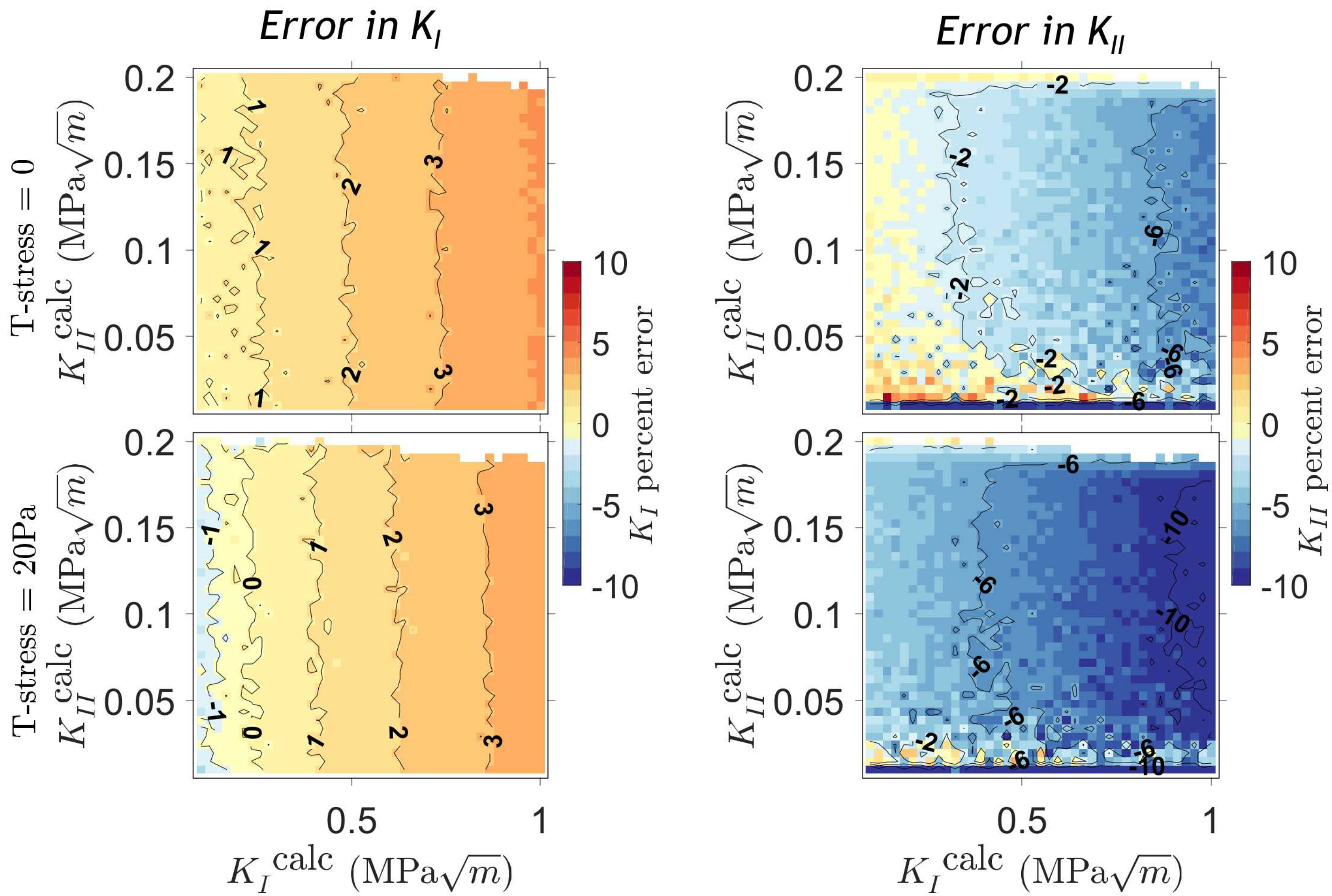
Proof of concept

- Use a simple "toy" model to demonstrate the technique
- Apply a combination of K_I, K_{II}, and T-stress fields and add Gaussian distributed noise
- The best case scenario in that,
  - crack tip location is known
  - applied field is known
  - no blunting of the crack tip



	K_I	K_{II}	T-stress
Applied	0.70	0.10	0.00
Calculated	0.713	0.108	0.00088
% error	1.86	8.34	--

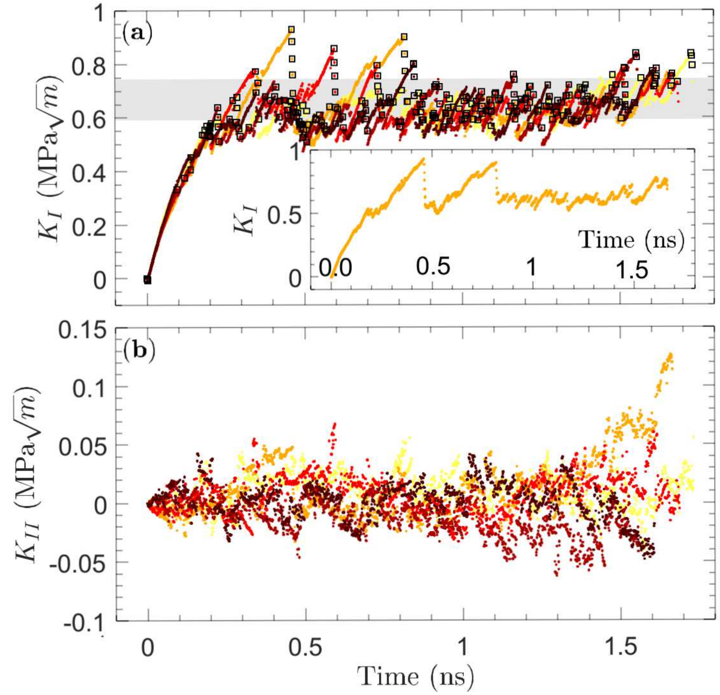
Numerical method sensitivity and errors

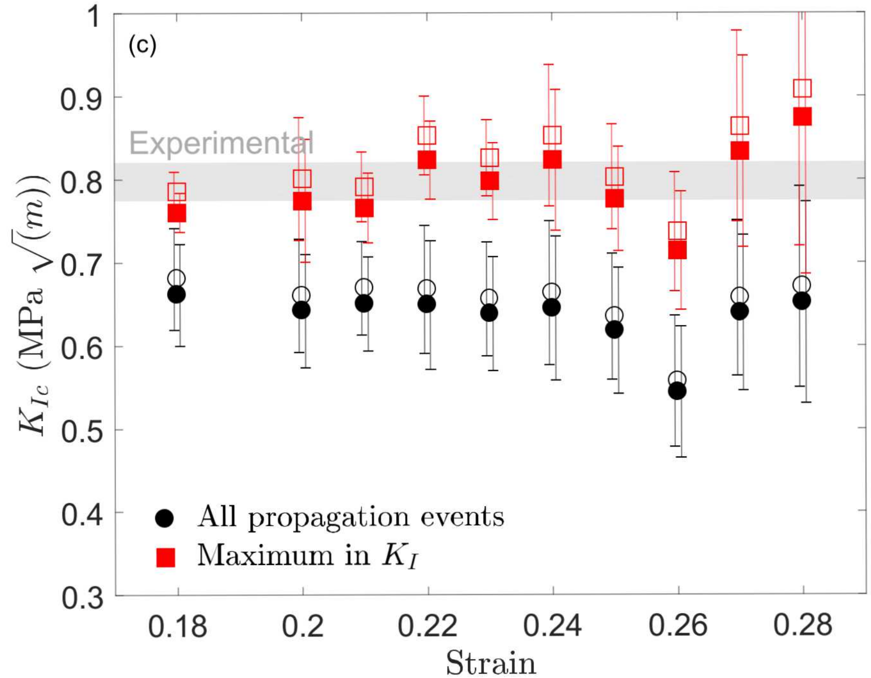


- Toy model is computationally fast and can be run hundreds of times over a range of applied fields
- Systematic errors are identified and can be utilized to estimate expected error in systems where the applied field is unknown

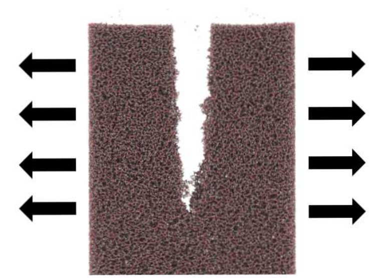
Method applied to MD fracture

Applied strain 0.22



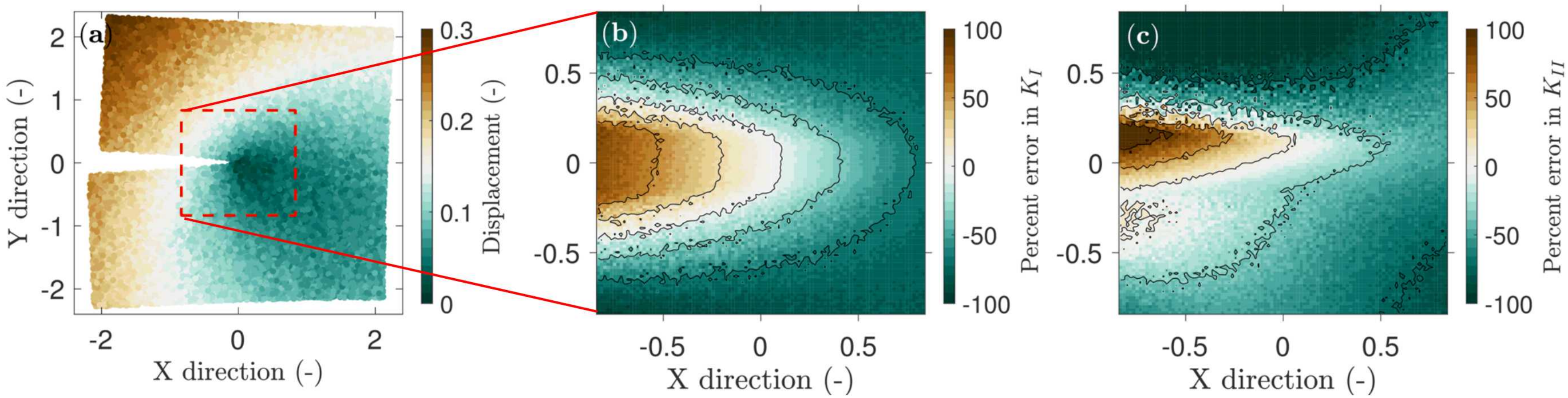


- Plateau region is representative of K_{IC}
- Systematic error in measurement can be assessed from the last slide: ~2%
- Significant strain magnitudes are due to characteristic length scale of fracture



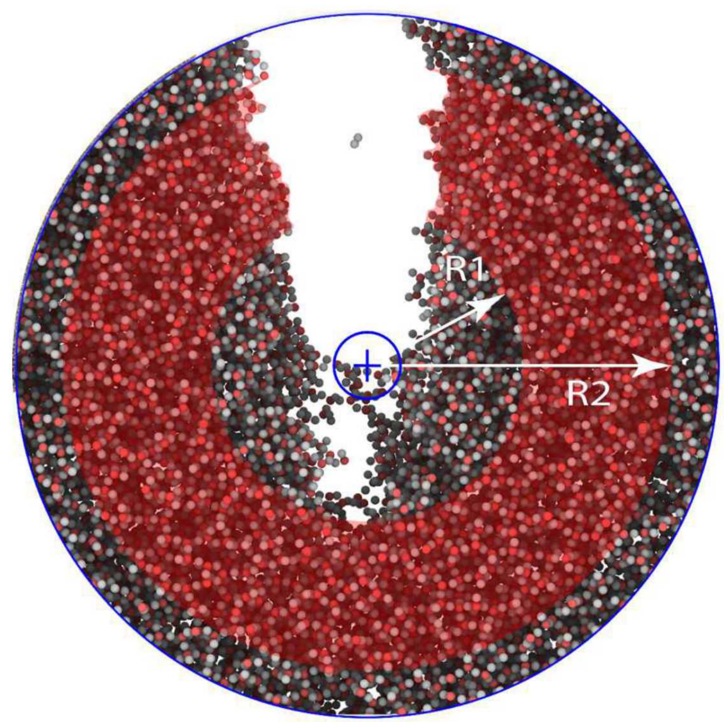
Held in constant strain

Misidentification of the crack tip



- Misidentification of the crack tip location can be important when applying the method to molecular dynamics

- Cause of possible errors:
  - Bridging Si-O chains
  - Crack tip blunting



Numerically locating the “true” crack tip

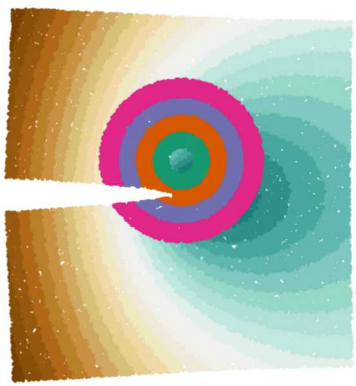
$$u(r,\theta) = \sum_{n=0}^{\infty} A \frac{r^{n/2}}{\mu} f(\theta)$$

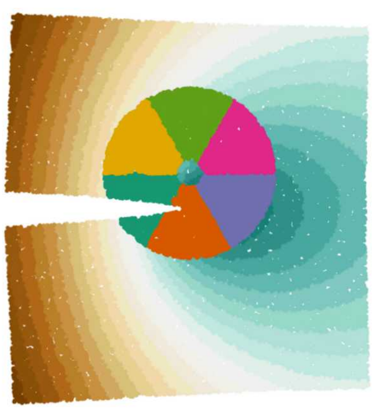
$$\Phi^R(x,y) = \frac{1}{N}\sum_{j=1}^{N} \left\| P_j^R(r,\theta) - \langle P_j^R(r,\theta) \rangle \right\|_2$$

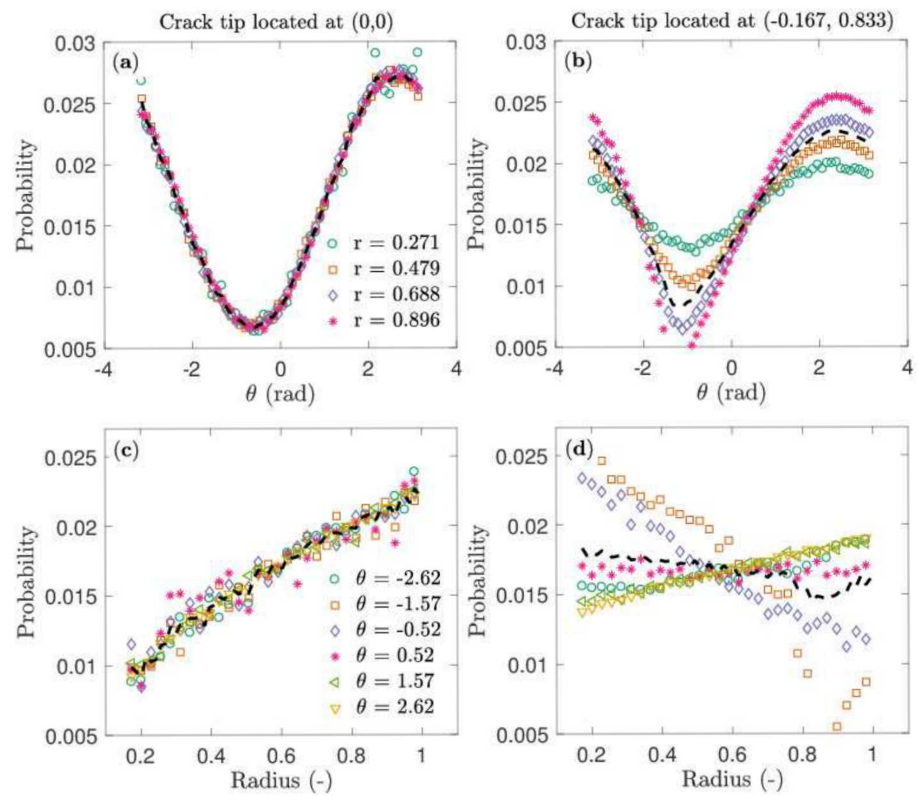
$$\Phi^\theta(x,y) = \frac{1}{N}\sum_{j=1}^{N} \left\| P_j^\theta(r,\theta) - \langle P_j^\theta(r,\theta) \rangle \right\|_2$$

$$\Phi(x,y) = \Phi^R(x,y) \cdot \Phi^\theta(x,y)$$

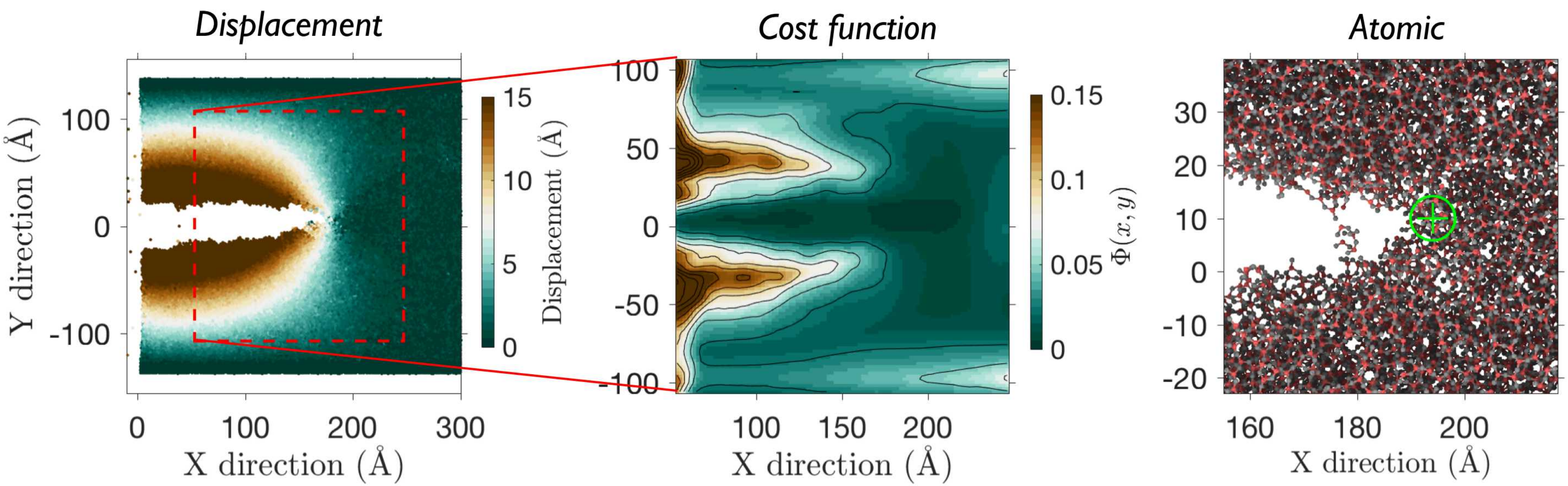
- We exploit the separability of the LEFM fields to identify the crack tip location
- A cost function can then be minimized to find spatial location

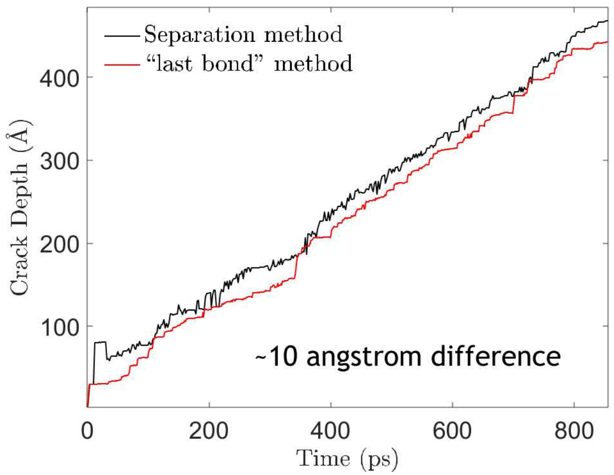


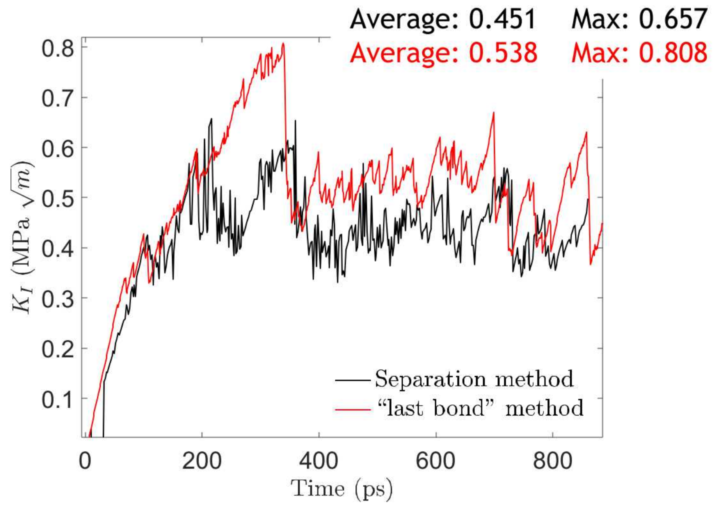




Applying method to molecular dynamics







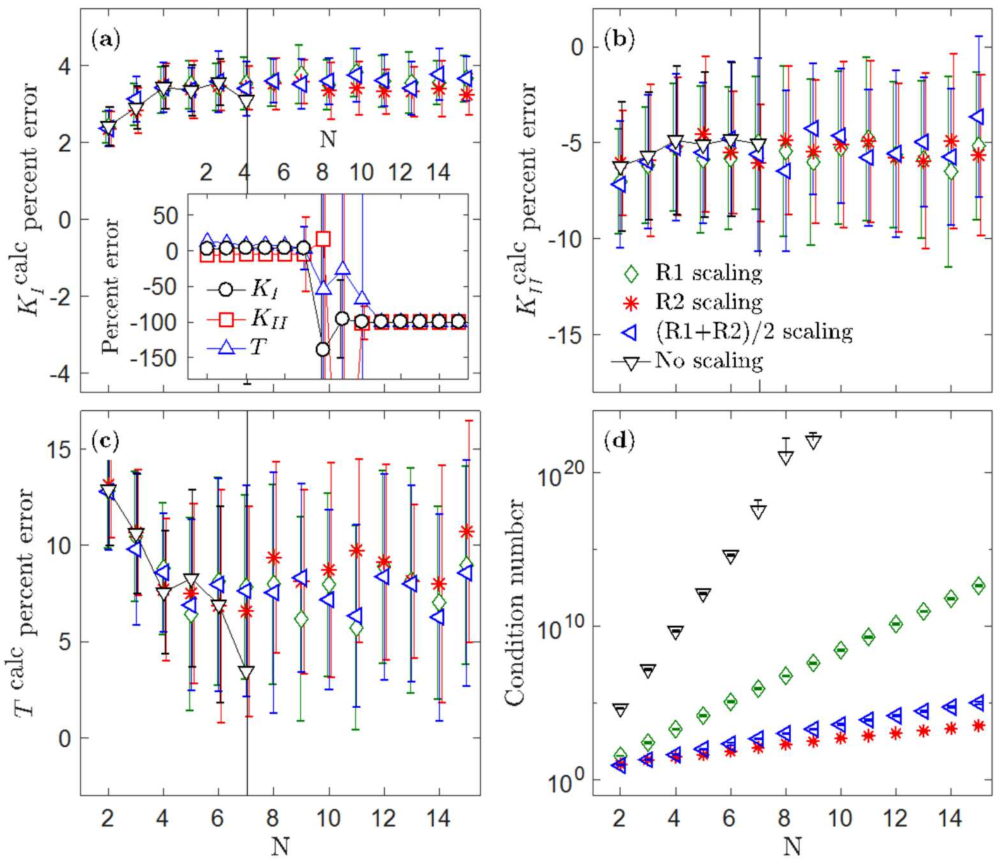
Summary

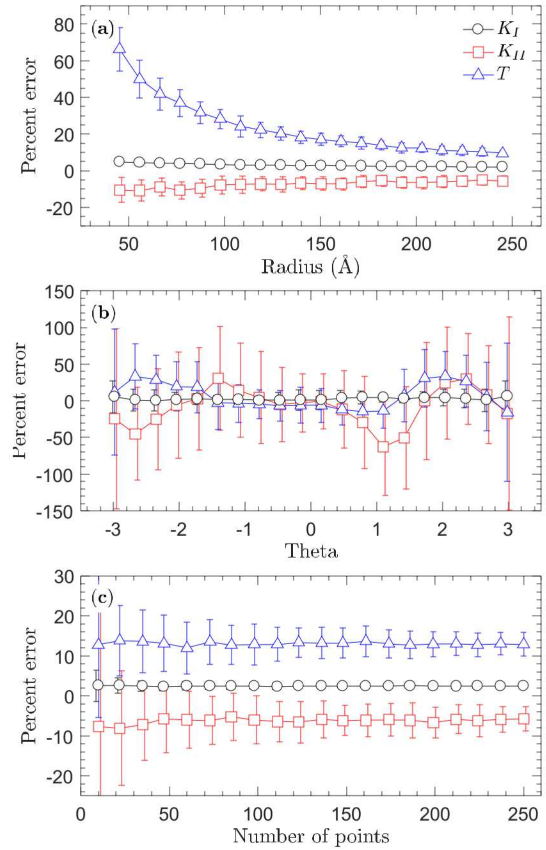
- Developed a novel computational method to determine fracture toughness from atomistic MD simulations. Results for silica glass agree with experiment
- Method maintains chemical specificity and microstructural content
- Showed that correctly identifying the crack tip location is a necessity for accuracy
- **Impact:** Developed the capability to study the atomic origins of intrinsic material properties; important for understanding influence of chemistry on fracture toughness and impact of corrosive agents

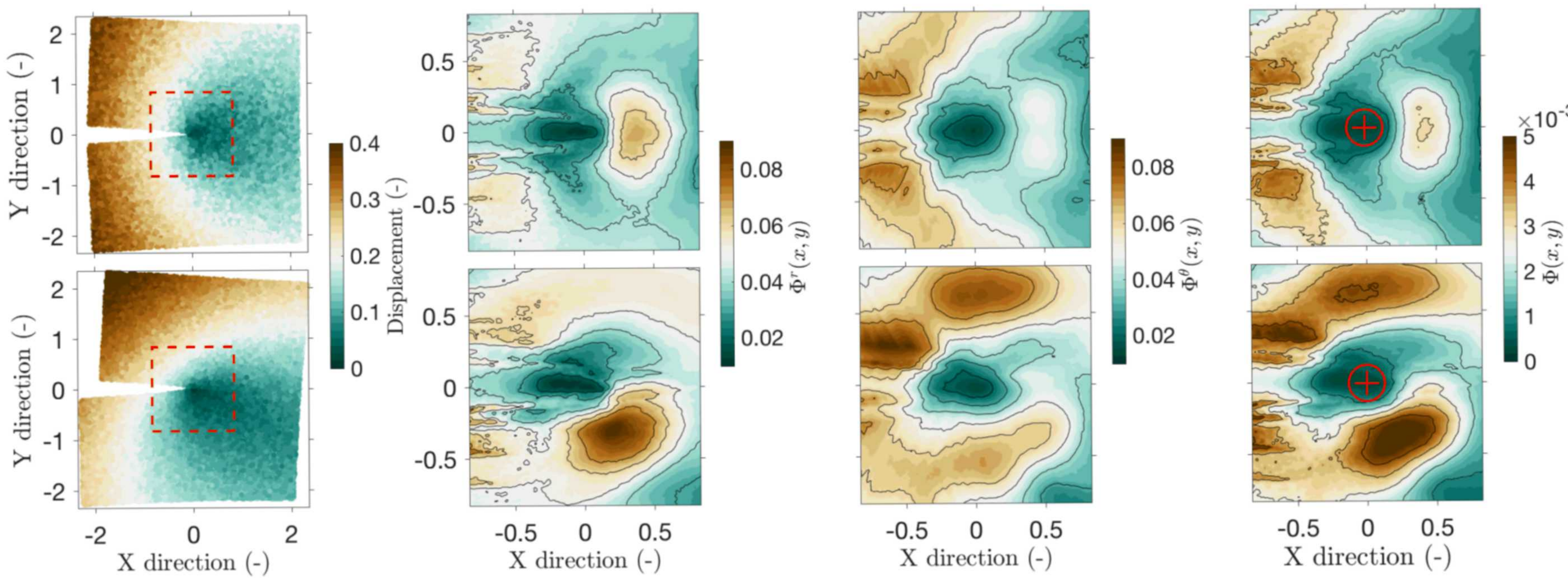
Thank you for your time and attention!

Extra slides

Numerical method sensitivity and errors






Y direction (-)
X direction (-)
Displacement (-)
$\Phi^r(x,y)$
$\Phi^\theta(x,y)$
$\Phi(x,y)$
$\times 10^{-3}$