Toward High-Fidelity Multi-Scale Modeling of 3D Crack Evolution

Presented at the retirement symposium for
Professor Tony Ingraffea

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Presentation Outline

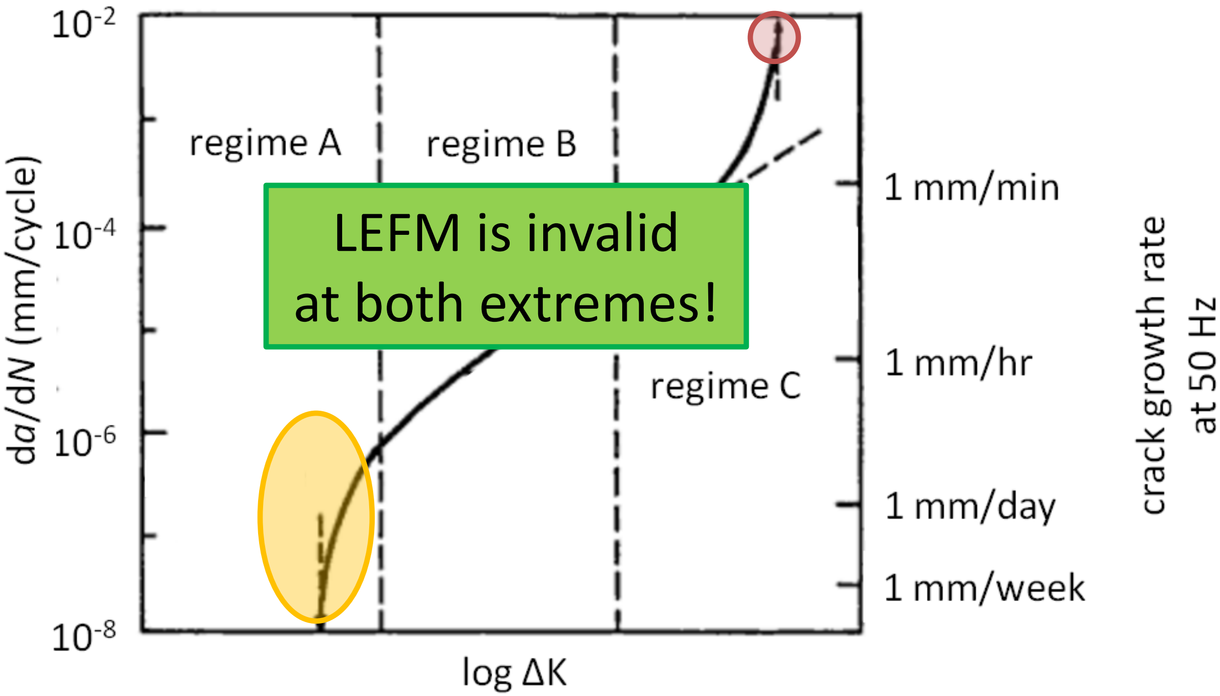
- PART I: Predicting crack propagation at the component scale
  - Toolset to simulate elastic-plastic crack growth in 3D
  - Toolset to simulate crack-shape evolution using energy-release-rate formulation
- PART II: Understanding fatigue-crack formation and early propagation at the microstructural scale
  - Study of crack nucleation in Ni-base superalloy
  - Study of crack propagation in Al-Mg-Si alloy
- Lessons learned from our time in the CFG

Overview of Work

- Generalized hypotheses:
  - *Compared to existing approaches for predicting crack evolution, more accurate predictions can be made:*
    1) *by accounting for three dimensionality of the cracked body and*
    2) *by maintaining high level of fidelity appropriate for given length scale*

<u>Micro-scale considerations:</u>
*sensitivity to microstructural heterogeneities

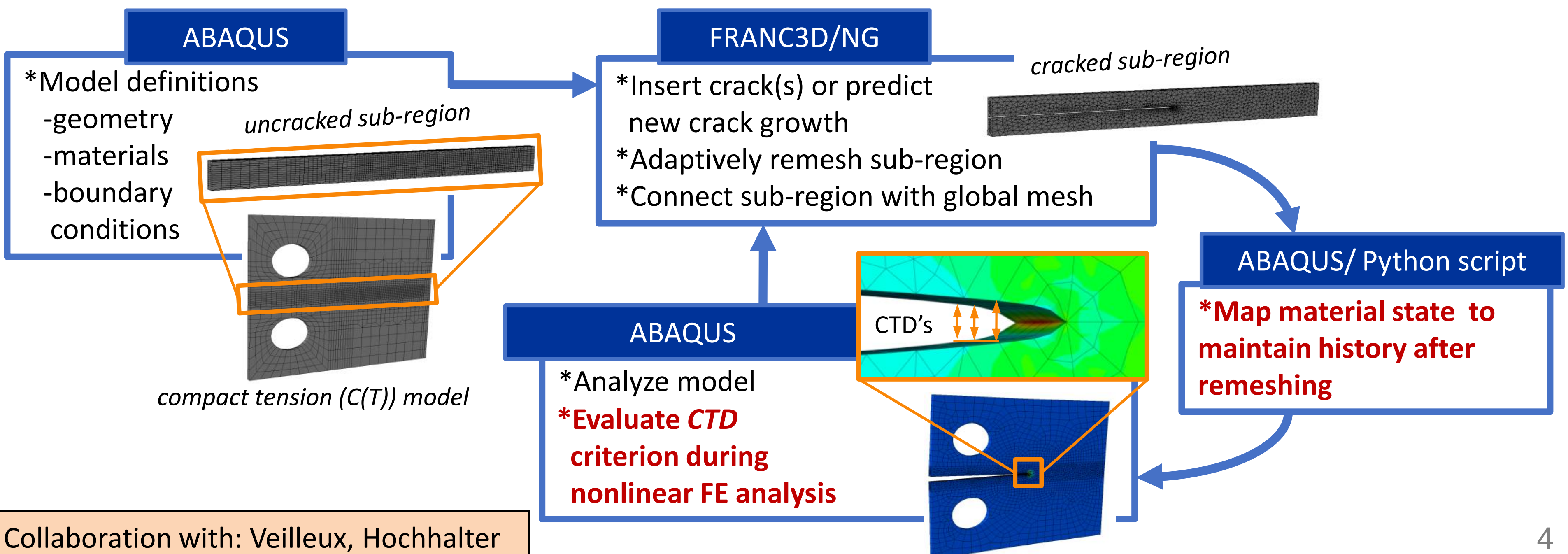
<u>Component-scale considerations:</u>
*sensitivity to constraint conditions
*tearing/fracture at limit state



schematic adopted from
Suresh, *Fatigue of Materials*

Toolset I: Generalized 3D Fracture Simulation

- Extended FRANC3D capabilities for EPFM simulations
- Applications:
  - Crack-growth predictions when material-state history is important and LEFM is not valid
- Toolset description:
  - Geometrically explicit crack representation
  - Adaptive remeshing
  - Allows prediction of crack growth direction
  - Recent **enhancements for EPFM** simulations

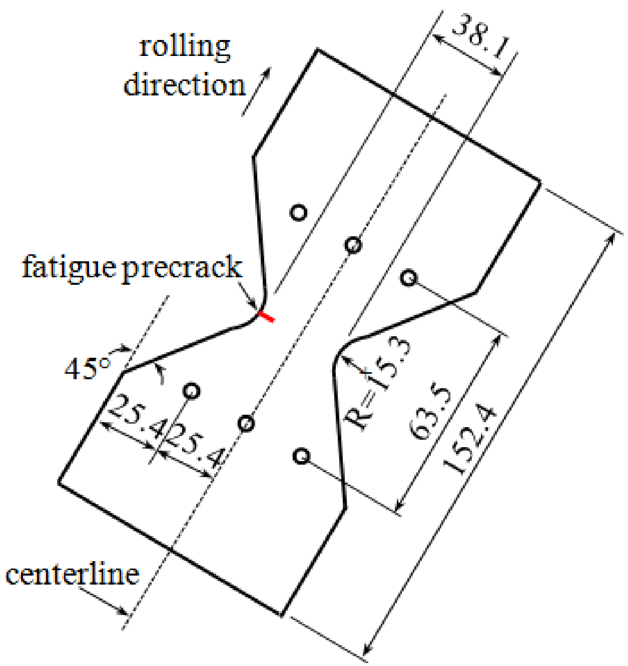


Collaboration with: Veilleux, Hochhalter

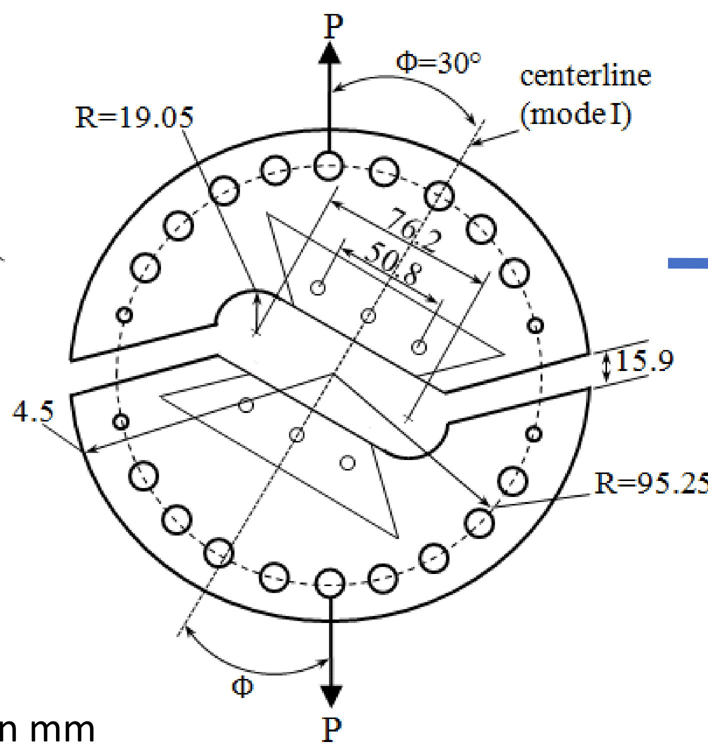
Toolset I: Validation Example

- Aluminum-alloy 2024-T3 fracture specimen in Arcan test fixture*
- 30˚ loading angle induces mixed-mode I/II crack growth

2024-T3 fracture specimen

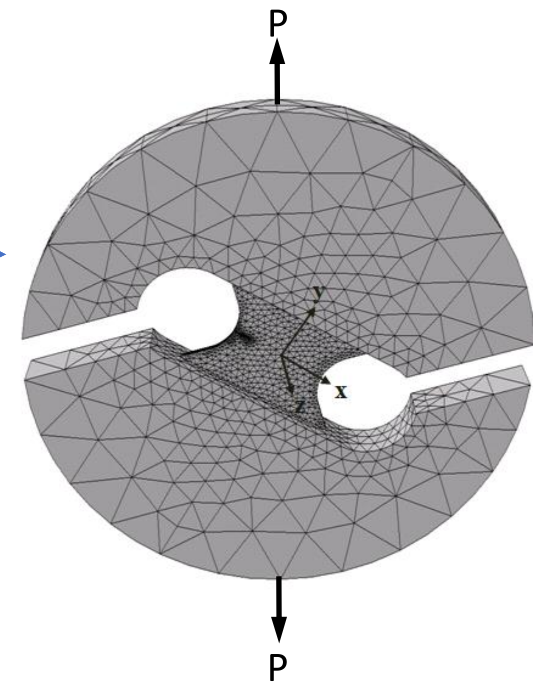


Arcan test fixture



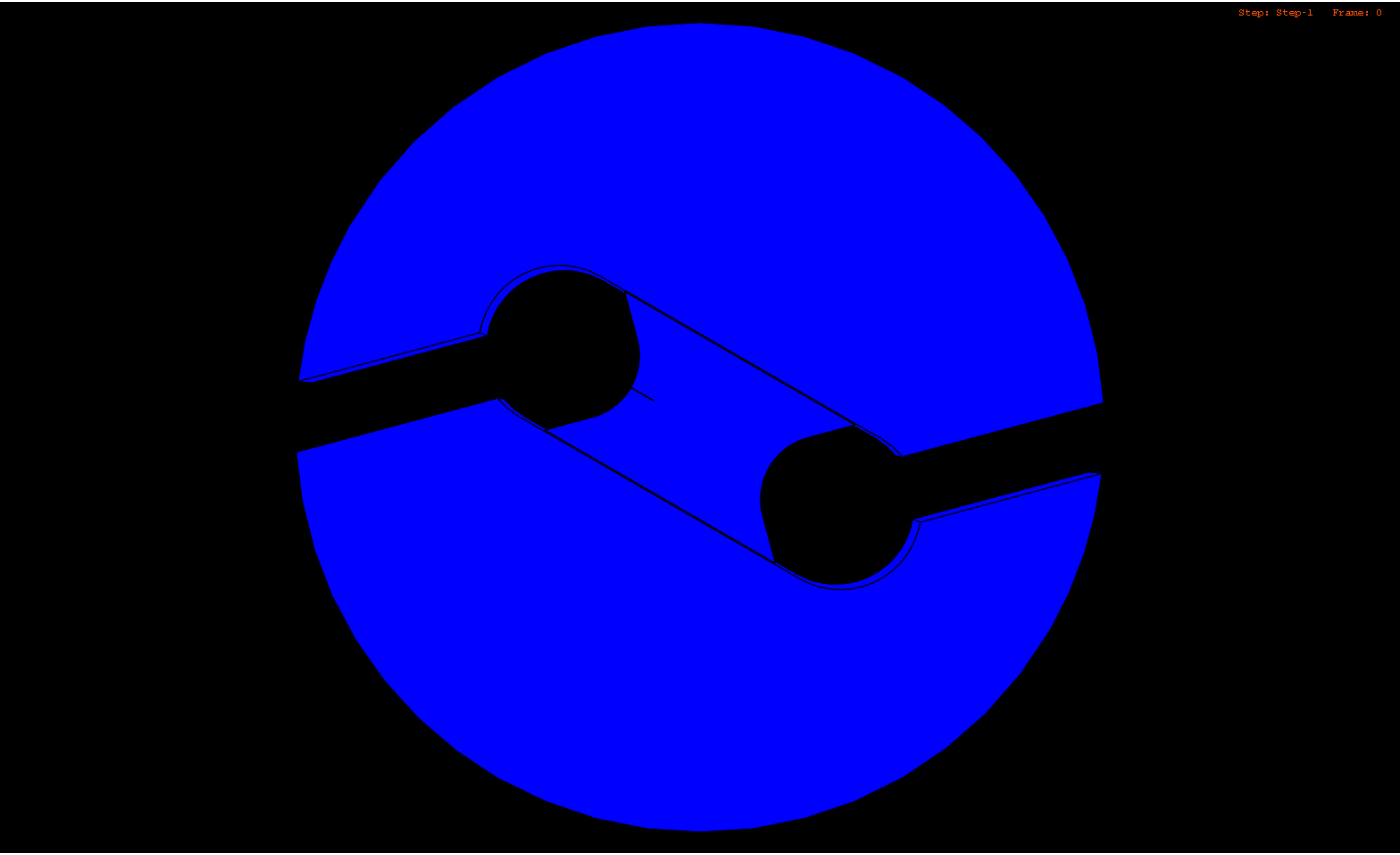
units in mm

3D FE model



*Amstutz, *et al.*, 1995 and 1997

Toolset I: Validation Example



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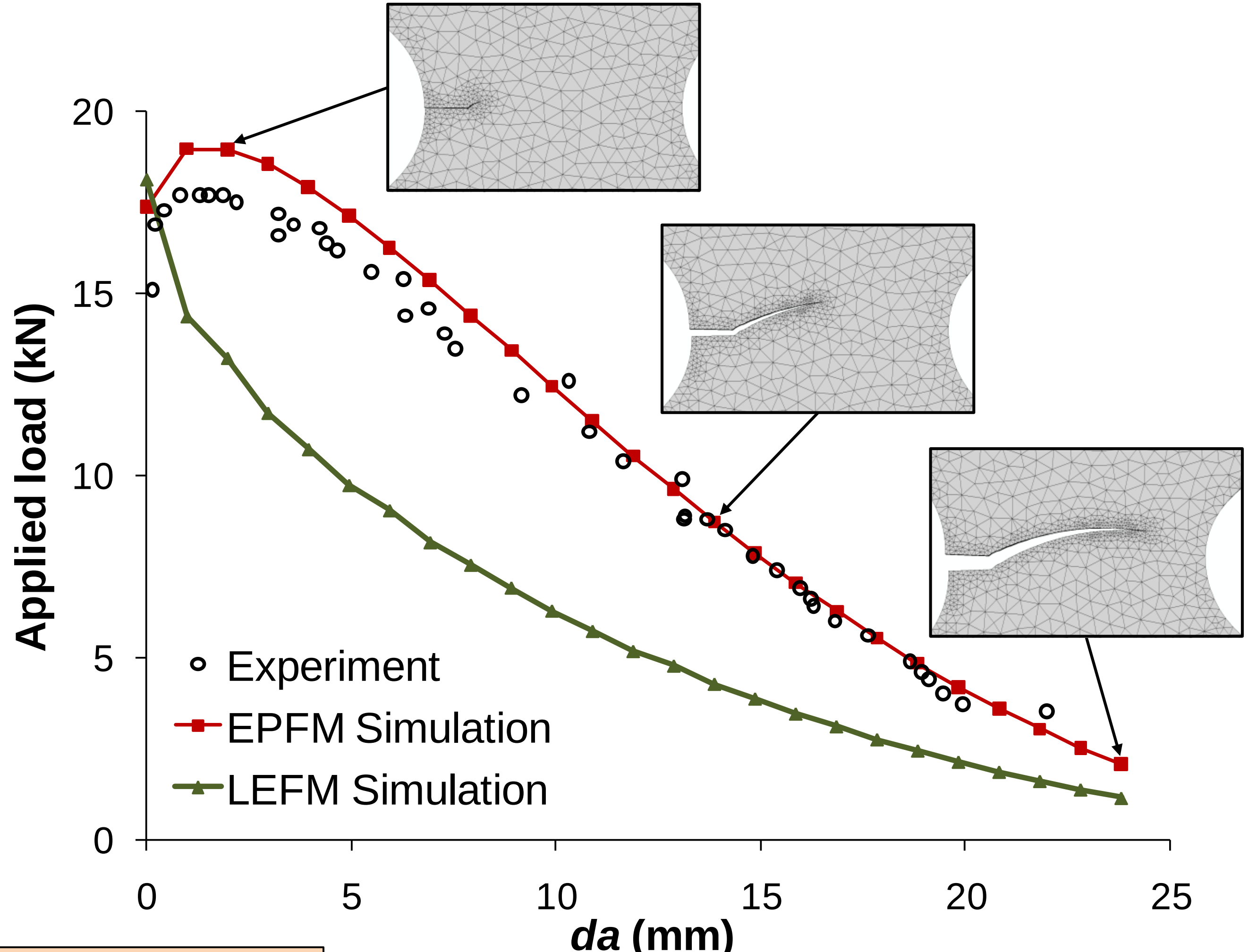
Toolset I: Validation Example

EPFM framework better predicts crack-extension response compared to LEFM framework



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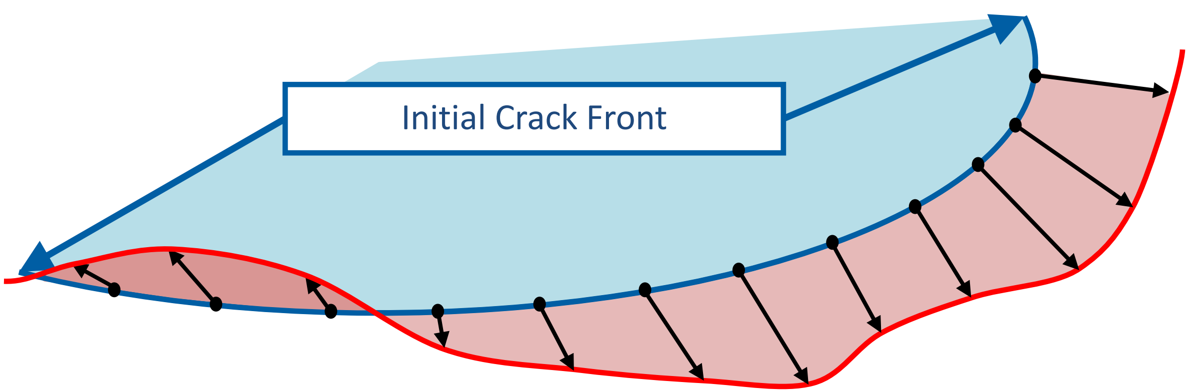
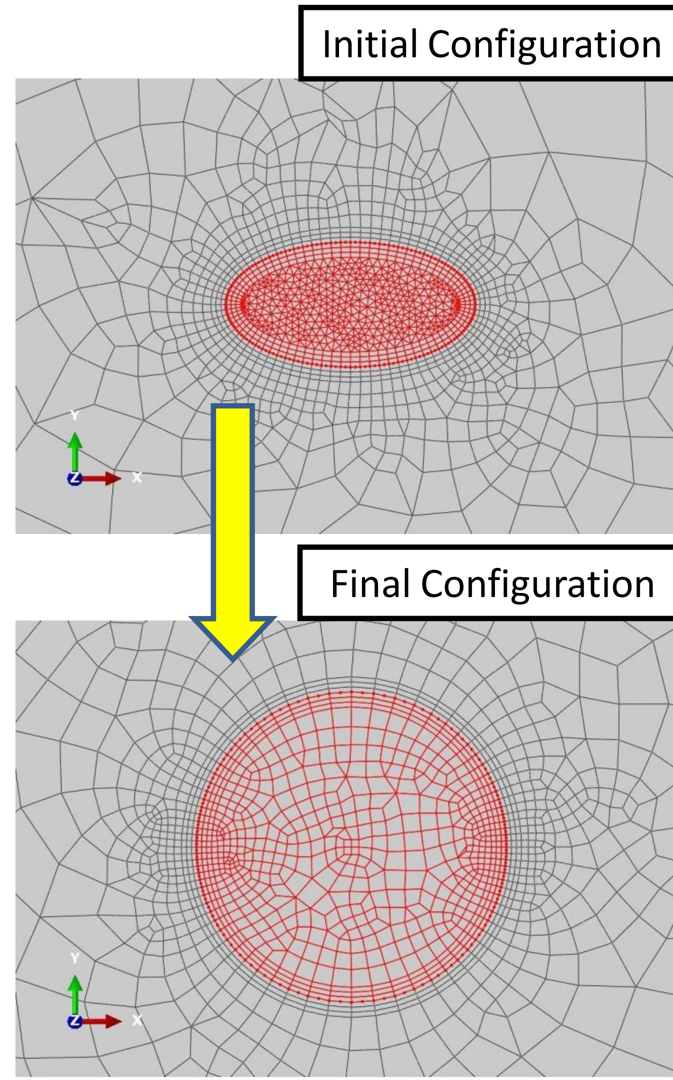
Toolset II: Energy-Based Crack Shape Evolution

- Develop simulation capability that permits arbitrary growth with unknown crack-shape evolution
  - Geometrically explicit cracks
  - Re-meshing techniques

Non-self-similar crack growth in mixed-mode bending specimen





Collaboration with: Wawrzynek, Hwang, Carter

Toolset II: Energy-Based Crack Shape Evolution

Energy Release Rate Expansion:

$$G_i^1 = G_i^0 + \frac{\delta G_i}{\delta P} \odot \Delta P_i + \frac{\delta G_i}{\delta a_j} \Delta a_j + \cdots$$

- G_i^1: Target Energy Release Rate
- G_i^0: Current Energy Release Rate
- ΔP_i: Load Increment
- Δa_j: Extension Increment

Local Extension Criterion: $G_i^1 = G_{ic}$

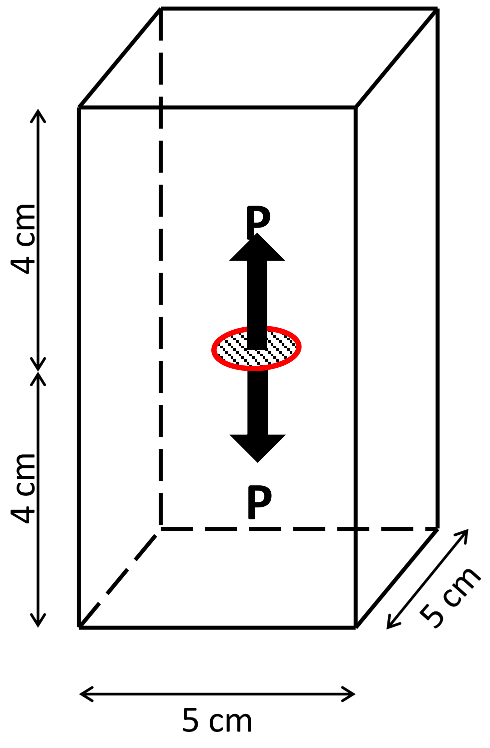
SOLVE FOR LOCAL EXTENSIONS

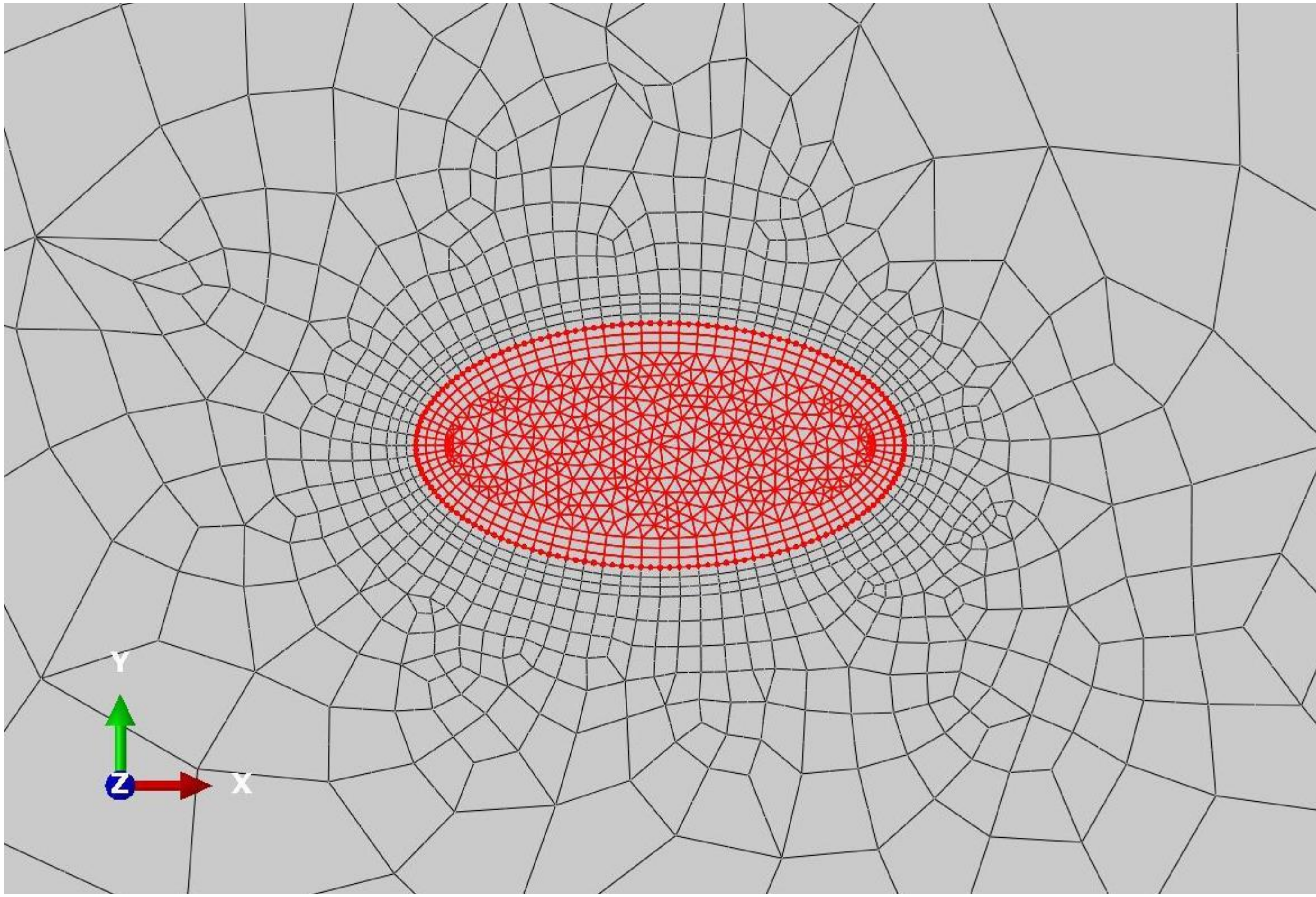
Local Extension Balance Condition:

$$G_{ic} = G_i^0 + \frac{\delta G_i}{\delta P} \odot \Delta P_i + \frac{\delta G_i}{\delta a_j} \Delta a_j$$

Collaboration with: Wawrzynek, Hwang, Carter

Toolset II: Numerical Example





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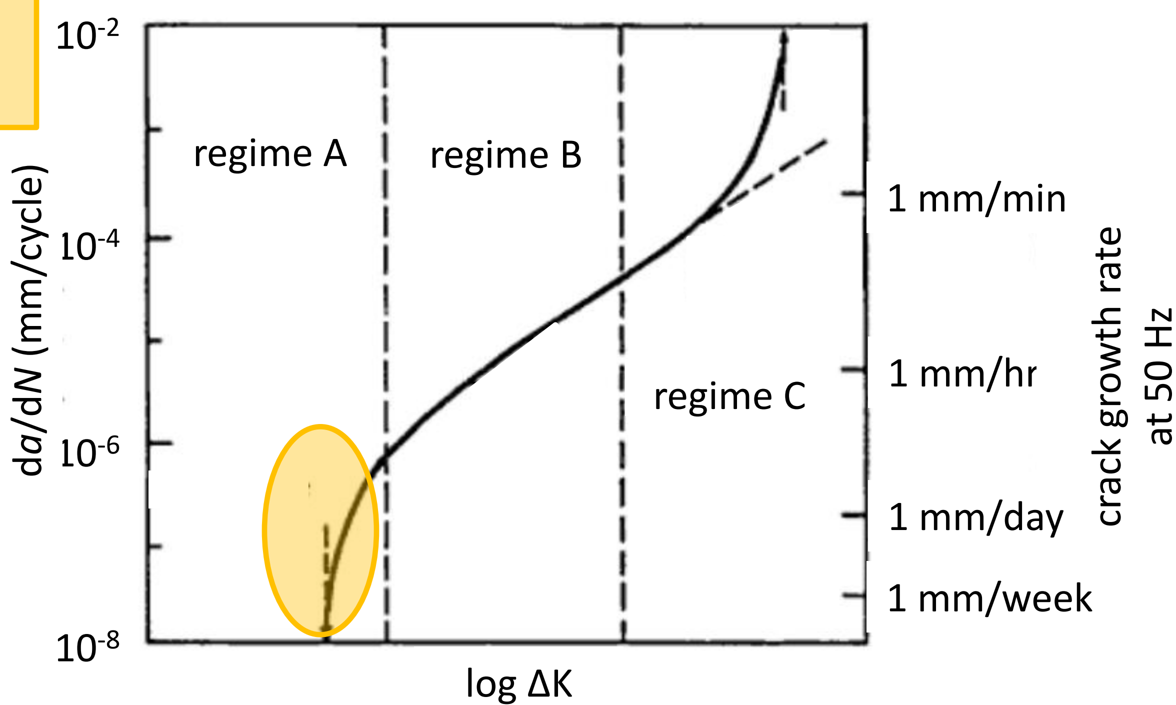
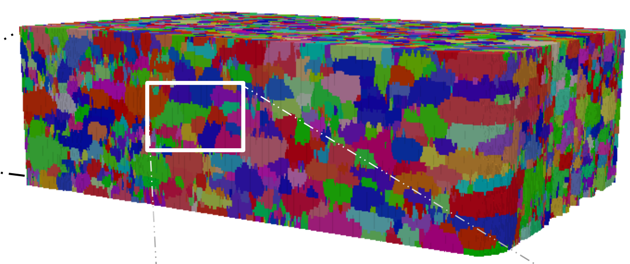
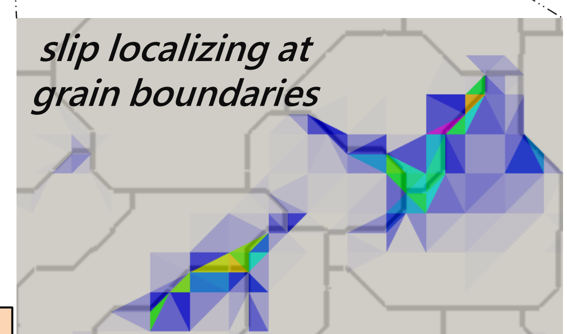
<u>Micro-scale considerations:</u>
*sensitivity to microstructural heterogeneities



Study I: MSFC Nucleation in Superalloy

- How can we use “big data” to understand highly nonlinear microstructural phenomena?
- Case Study: Microcrack nucleation in Ni-based superalloy
  1. Develop constitutive relations and geometric representations of superalloy
     - calibrate crystal plasticity model
     - generate microstructural model for 3D crystal-plastic finite-element analysis



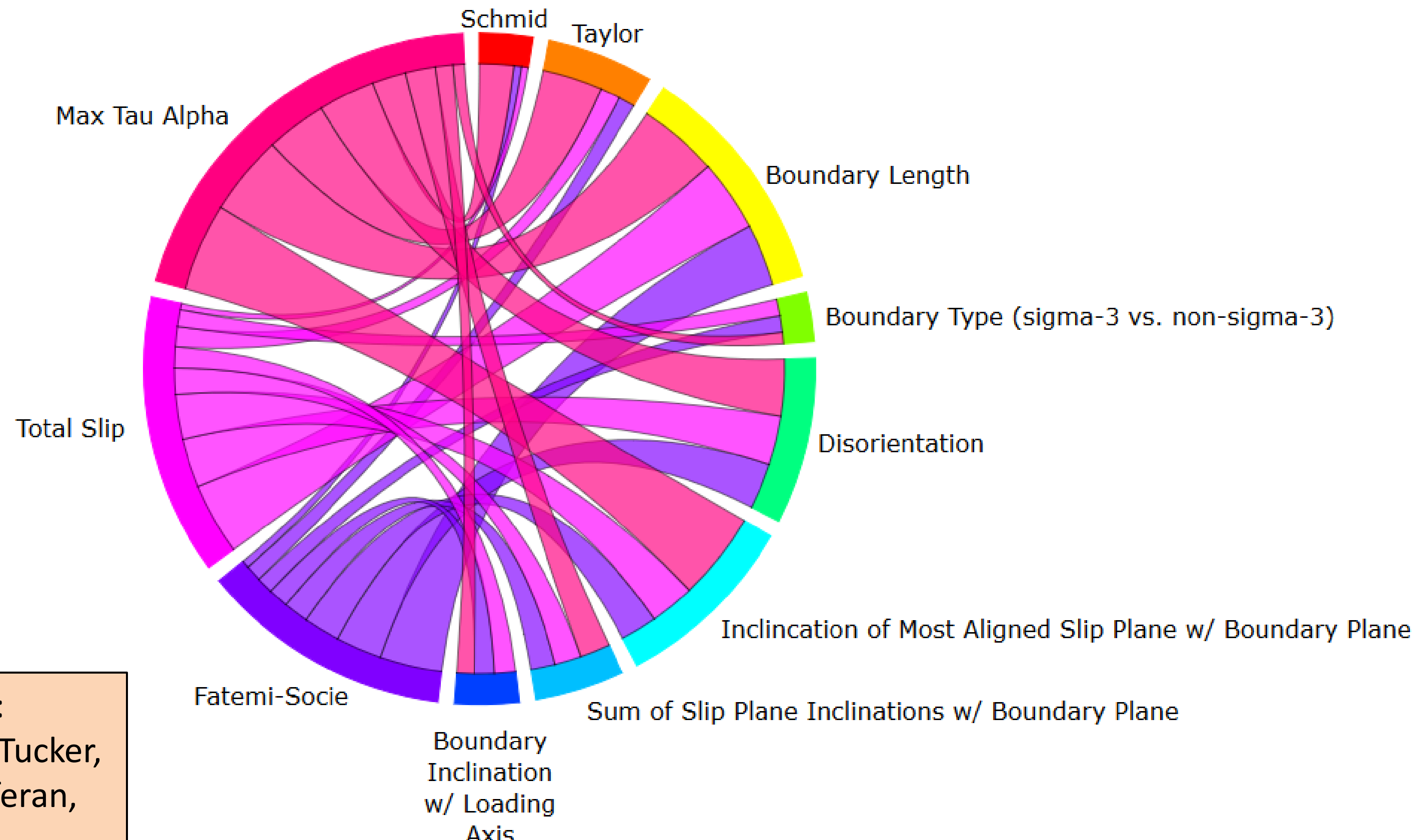


  2. Capture relevant physics related to microcrack nucleation event
  3. Correlate grain boundary character with slip localization

Collaboration with: Rollett, Stein, Tucker, Pokharel, Hefferan, Lind, Suter

Study I: MSFC Nucleation in Superalloy

- Establish correlations between microstructural attributes and fatigue indicator parameters (FIPs)
  - Analyze every grain boundary in Ni-based superalloy
  - Quantify correlation between postulated FIPs and grain boundary character
  - Determine microstructural characteristics most relevant to nucleation event



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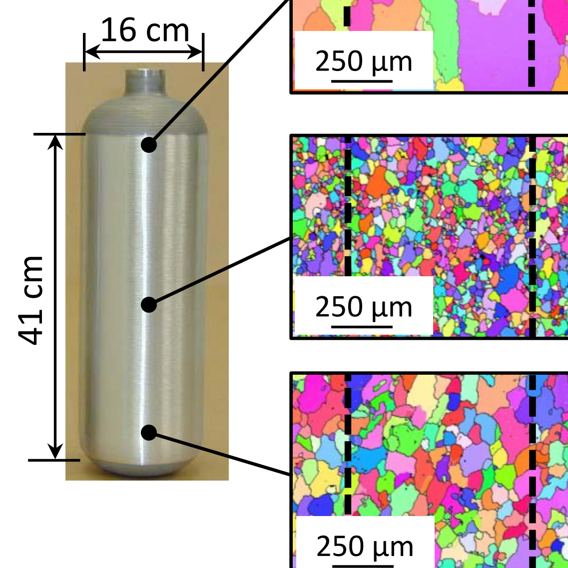
Study II: MSFC Propagation in Al Alloy

- Application: aluminum alloy used by NASA in *ultrathin* pressure-vessel components

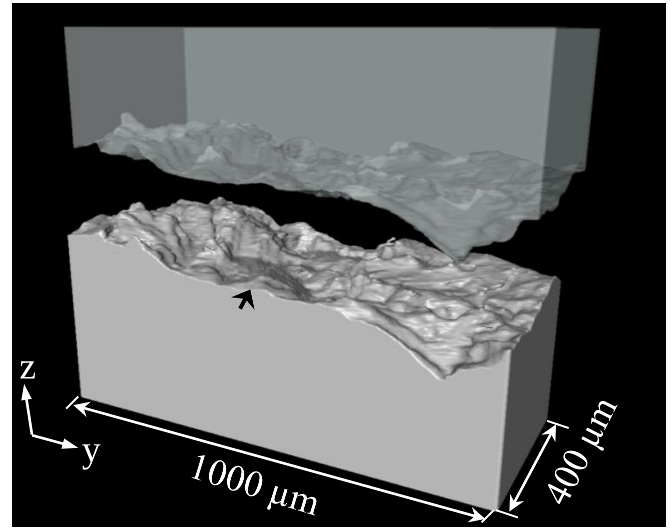
  2.5mm → <0.75mm by chemical milling
- Why do *ultrathin* liners deserve attention?
  - Consequences of crack nucleation and growth could be catastrophic
  - Effect of microstructure potentially more significant for *ultrathin* liners
  - **Real application for multiscale materials characterization and 3D modeling!**
- Little is known about how cracks propagate in 3D at microstructural length scale for polycrystalline materials

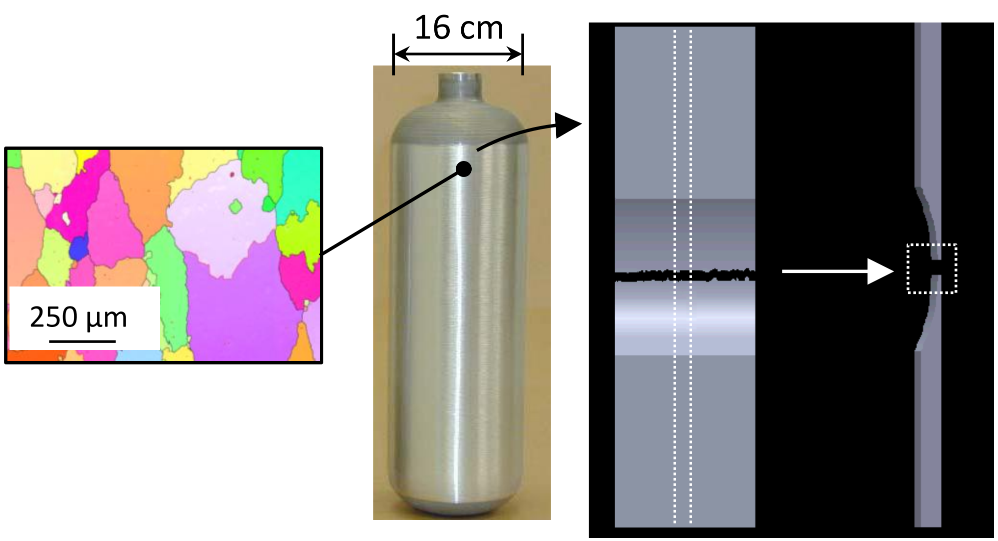


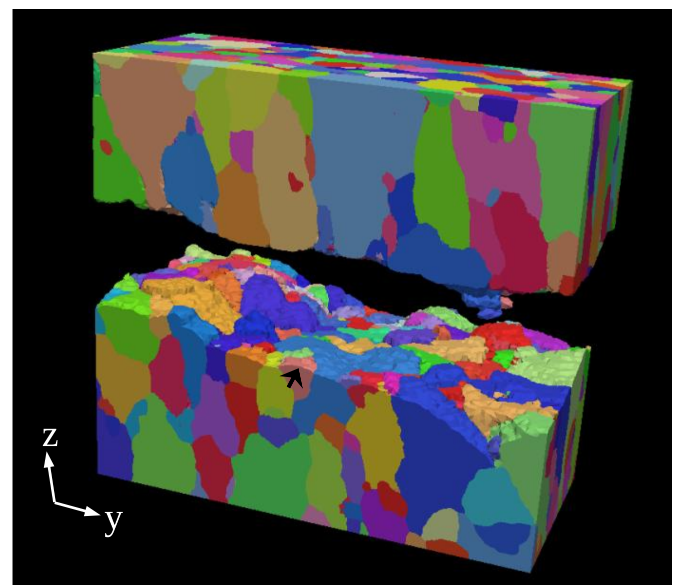
Collaboration with: Suter, Li, Lind, NASA LaRC

Study II: MSFC Propagation in Al Alloy

- Broken specimens measured using synchrotron radiation at Argonne National Laboratory
  - X-ray computed tomography (CT)
    - Highly resolved fracture surface
  - High-energy X-ray diffraction microscopy (HEDM) *
    - Grain geometries and orientations







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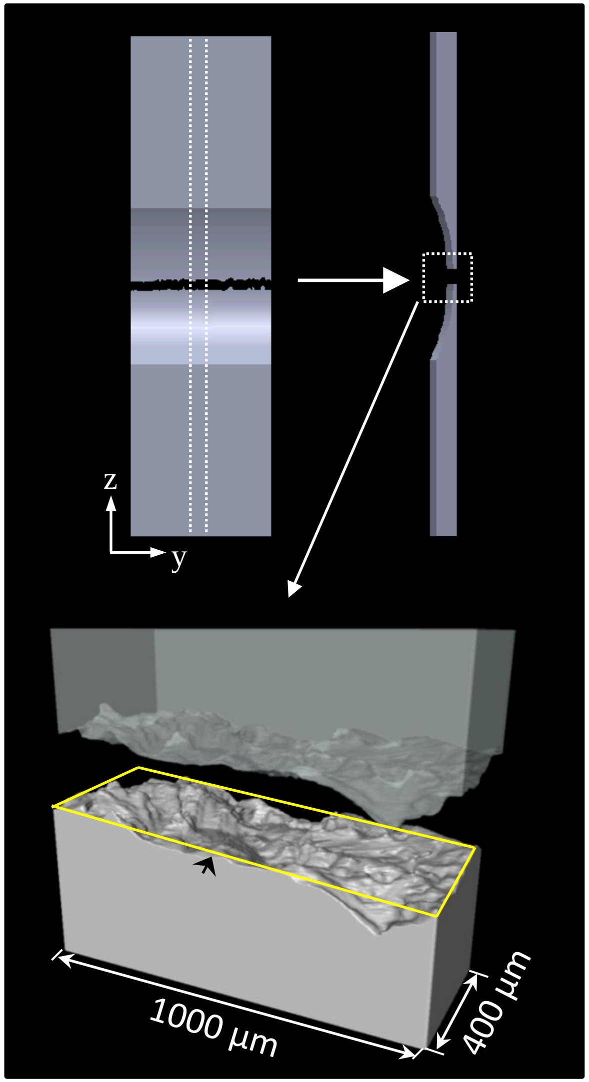
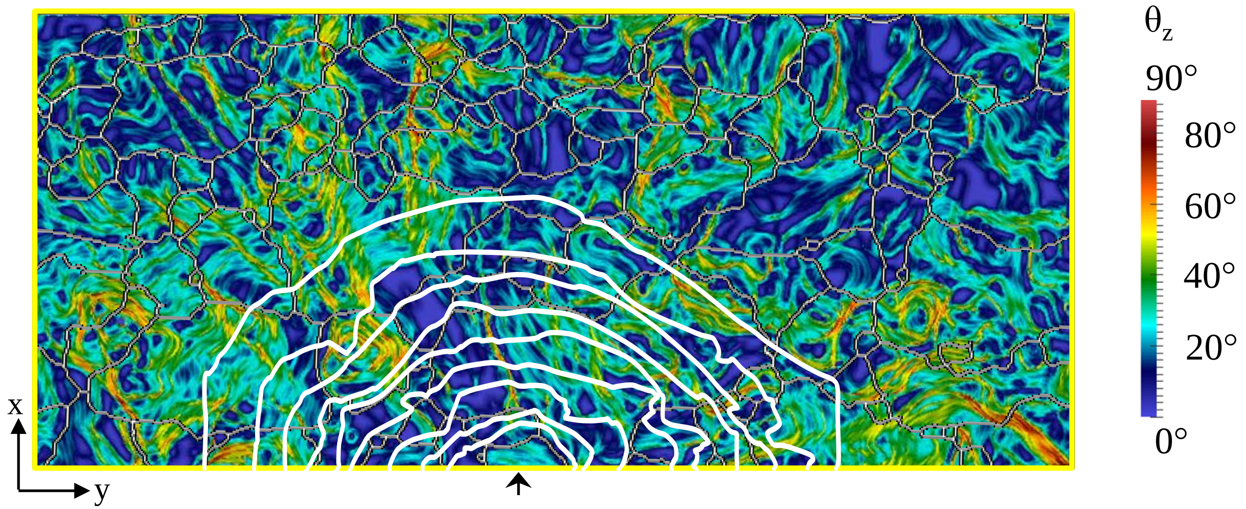
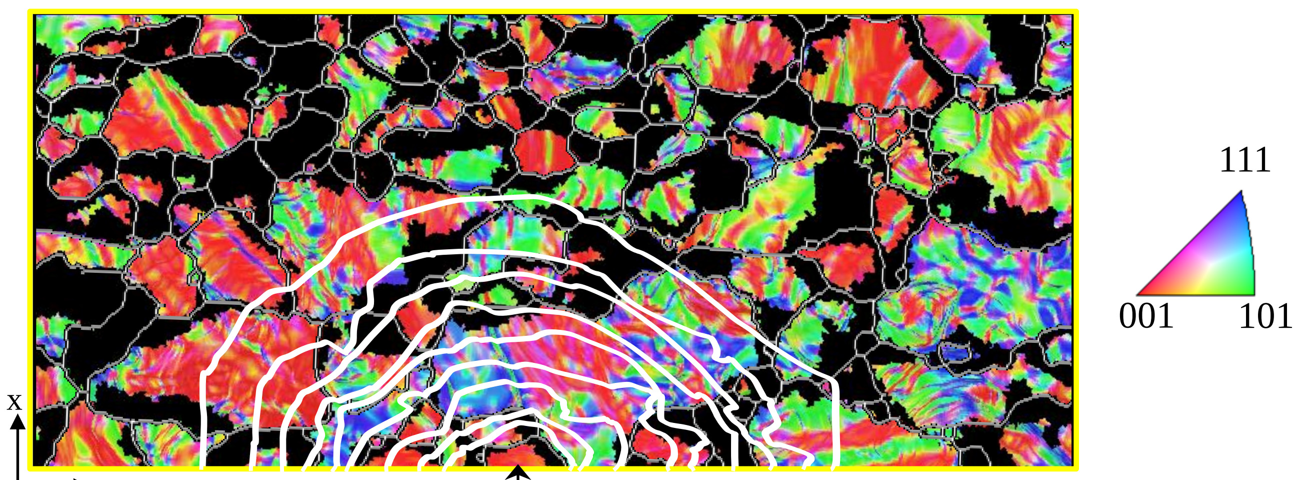
* Lienert, et al., *JOM* (2011), Suter, et al., *RSI* (2006); Li, et al., *Appl J. Cryst.* (2013)

Study II: MSFC Propagation in Al Alloy





angle (degrees) between local normal and loading direction

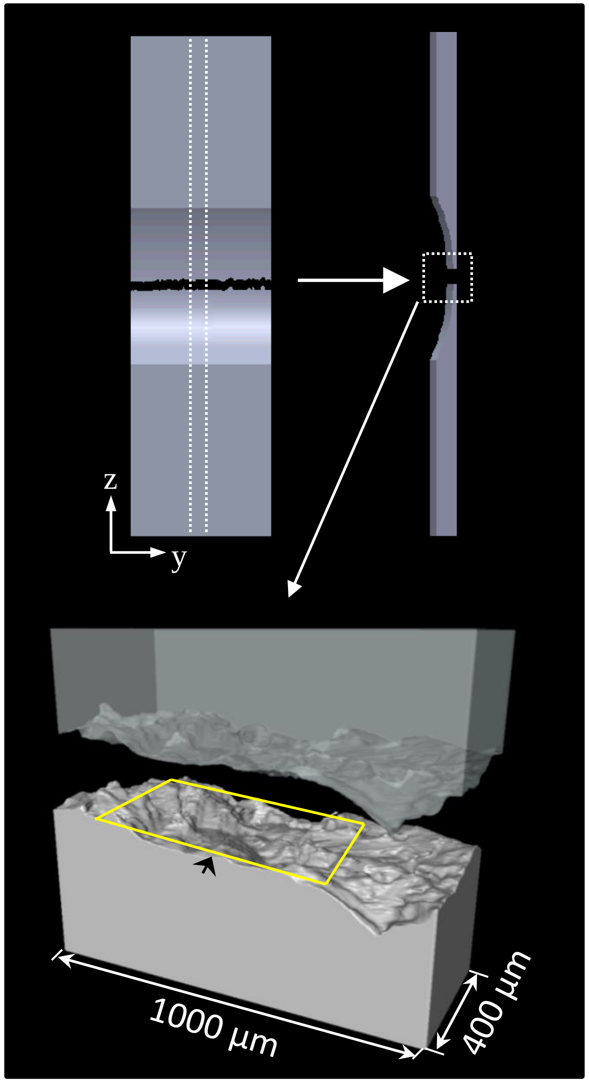


crack-plane normal in crystallographic frame

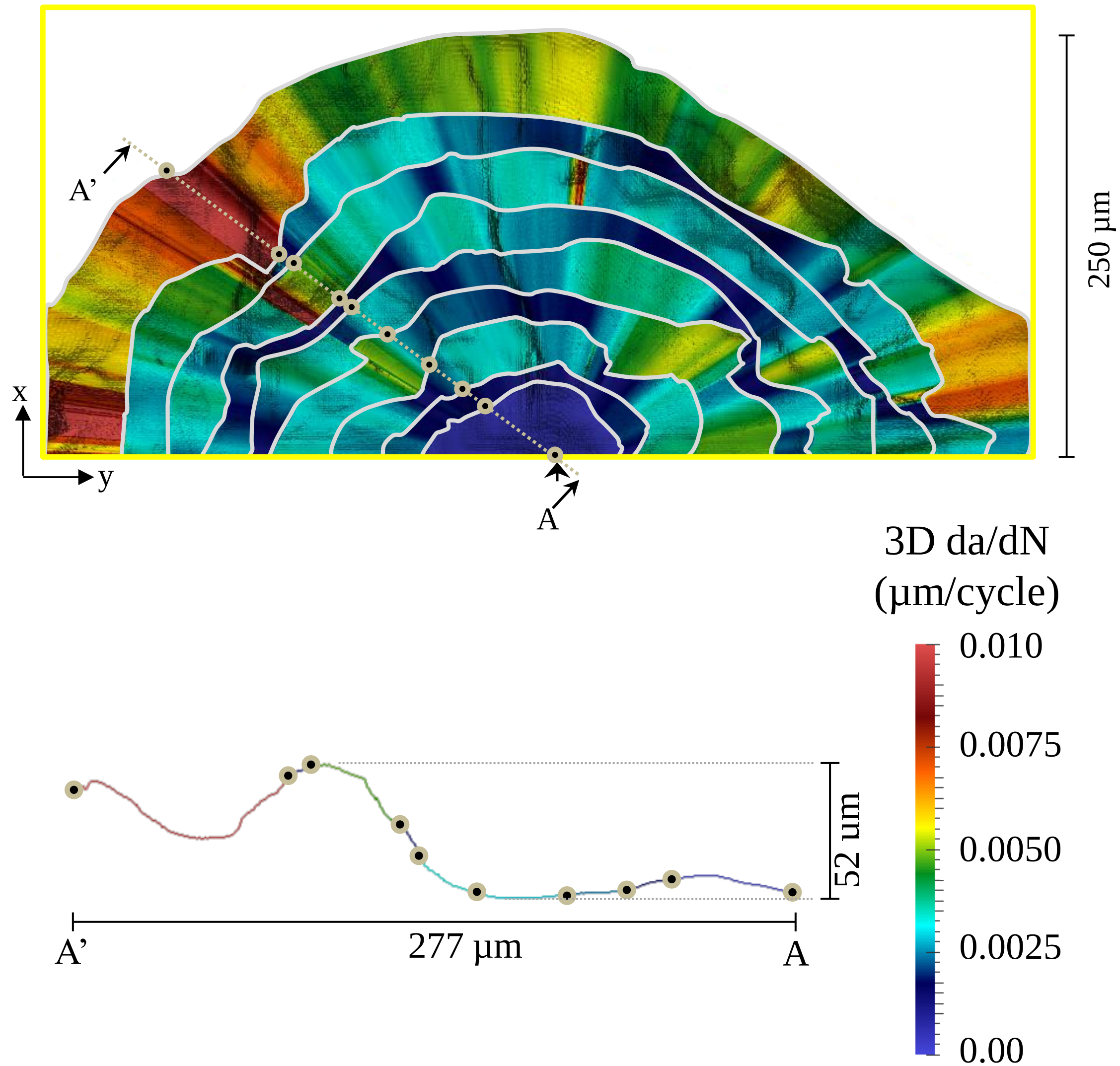
100 µm

Collaboration with: Suter, Li, Lind, NASA LaRC

Study II: MSFC Propagation in Al Alloy



observed variability in 3D crack-growth rate



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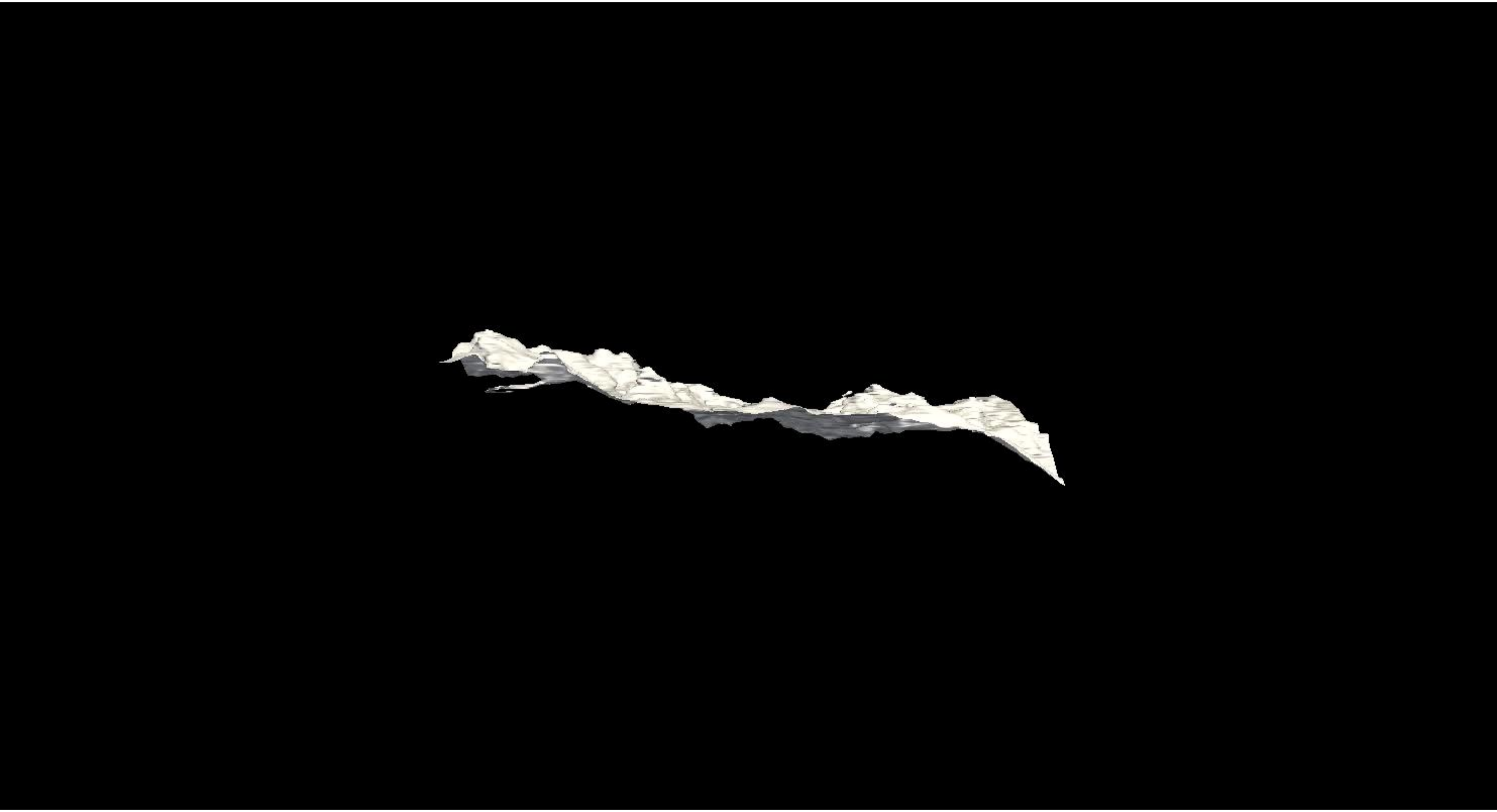

Collaboration with: Hochhalter, Cerrone

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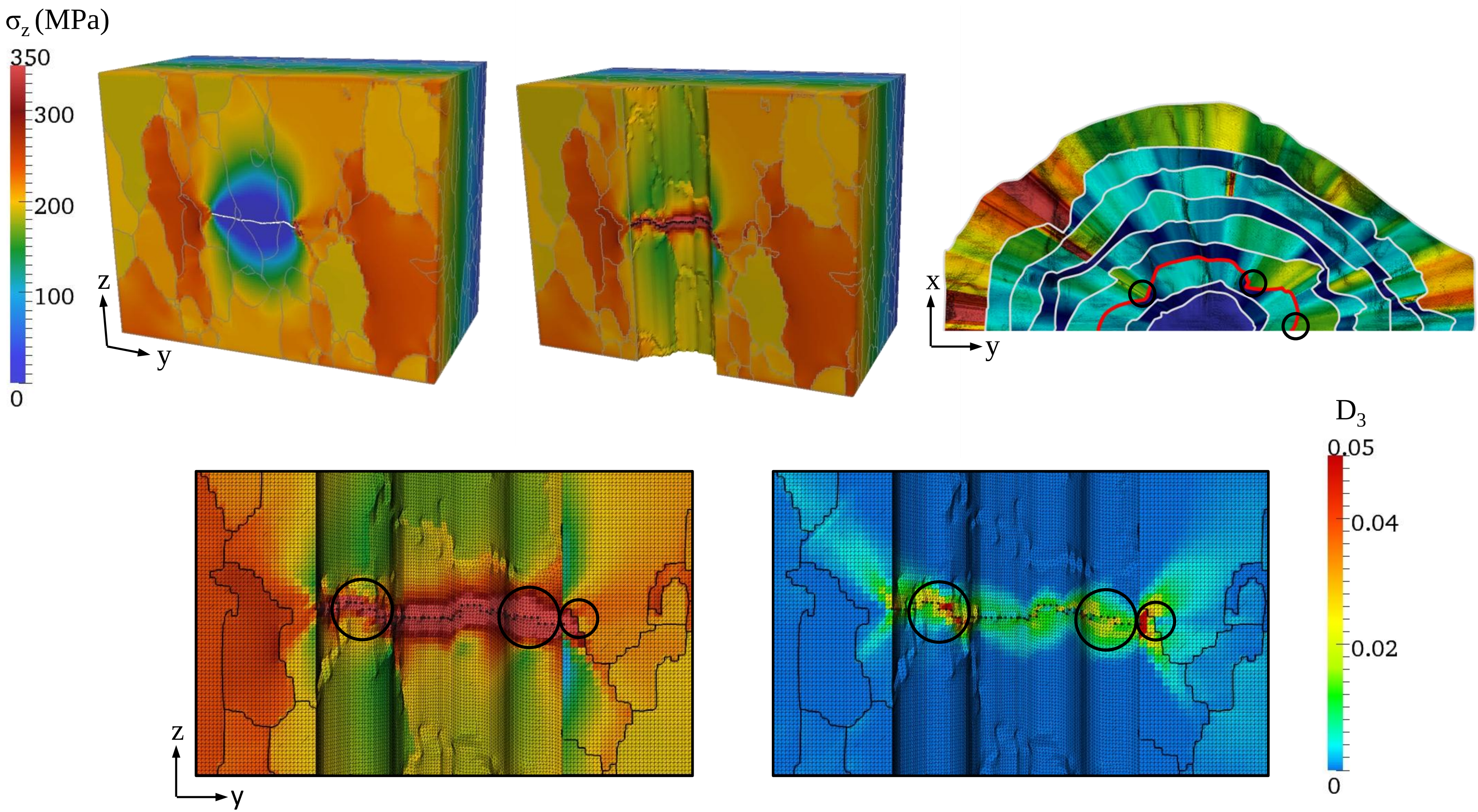

Lots of data here! Remaining need for quantitative post-processing.

Collaboration with: Hochhalter, Cerrone

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Lessons Learned from Tony and the CFG

- Collaborate (it's required to do the best job possible!)
- Be rigorous (computing time is not an excuse for not doing good work!)
- Don't forget the two most important Vs in life… (verification and validation)
- "A good leader brings good people together and makes them better." -*Brett*
- "The boss was always a big proponent of continuing education, seeking answers proactively, and never letting ignorance get in the way of scientific progress." -*Al*
- "Oh yeah, and when in doubt, ask Bruce." -*Everyone*