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

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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*

Micro-scale considerations: *sensitivity to microstructural heterogeneities

Component-scale considerations: *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

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*Amstutz, et al., 1995 and 1997
Toolset I: Validation Example

Collaboration with: Veilleux, Hochhalter
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:

\[ \frac{\delta G_i}{\delta a_j} \Delta a_j + \cdots \]

Local Extension Criterion:

\[ G_i^1 = G_{ic} \]

Local Extension Balance Condition:

\[ G_{ic} = G_i^0 + \frac{\delta G_i}{\delta P} \Delta P_i \]

Collaboration with: Wawrzynek, Hwang, Carter
Toolset II: Numerical Example

Collaboration with: Wawrzynek, Hwang, Carter
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• PART II: **Understanding** fatigue-crack formation and early propagation at the **microstructural** scale

Micro-scale considerations:
*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

Collaboration with:
Rollett, Stein, Tucker, Pokharel, Hefferan, Lind, Suter
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Study II: MSFC Propagation in Al Alloy

• Application: aluminum alloy used by NASA in *ultrathin* pressure-vessel components
  
  2.5mm $\rightarrow$ <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
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

Study II: MSFC Propagation in Al Alloy

angle (degrees) between local normal and loading direction

Crack-plane normal in crystallographic frame
observed variability in 3D crack-growth rate

3D da/dN (µm/cycle)
Study II: MSFC Propagation in Al Alloy

Collaboration with: Hochhalter, Cerrone
Study II: MSFC Propagation in Al Alloy

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