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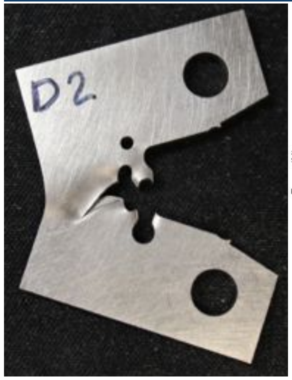

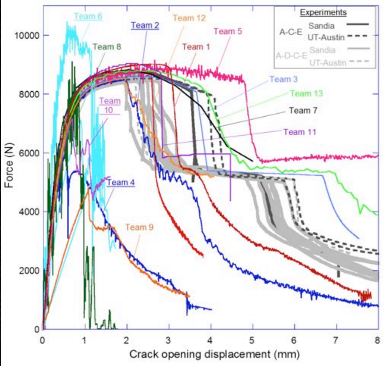

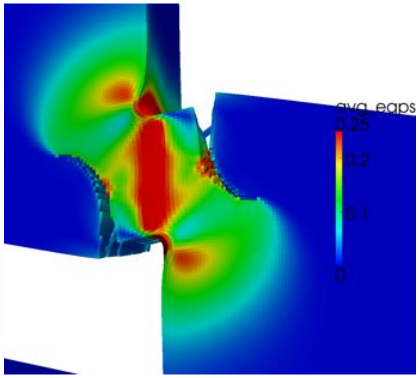

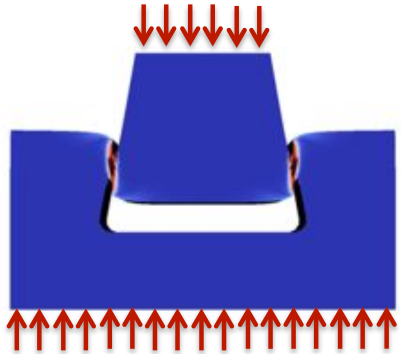

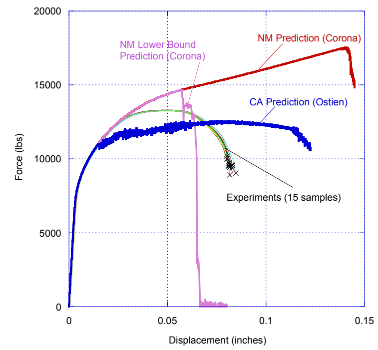

Double-Blind Assessment of Physical and Computational Simulations of Ductile Failure

Sharlotte Kramer, Structural Mechanic Laboratory

27 March 2014

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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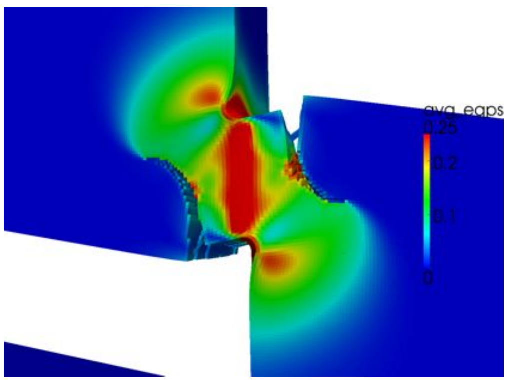
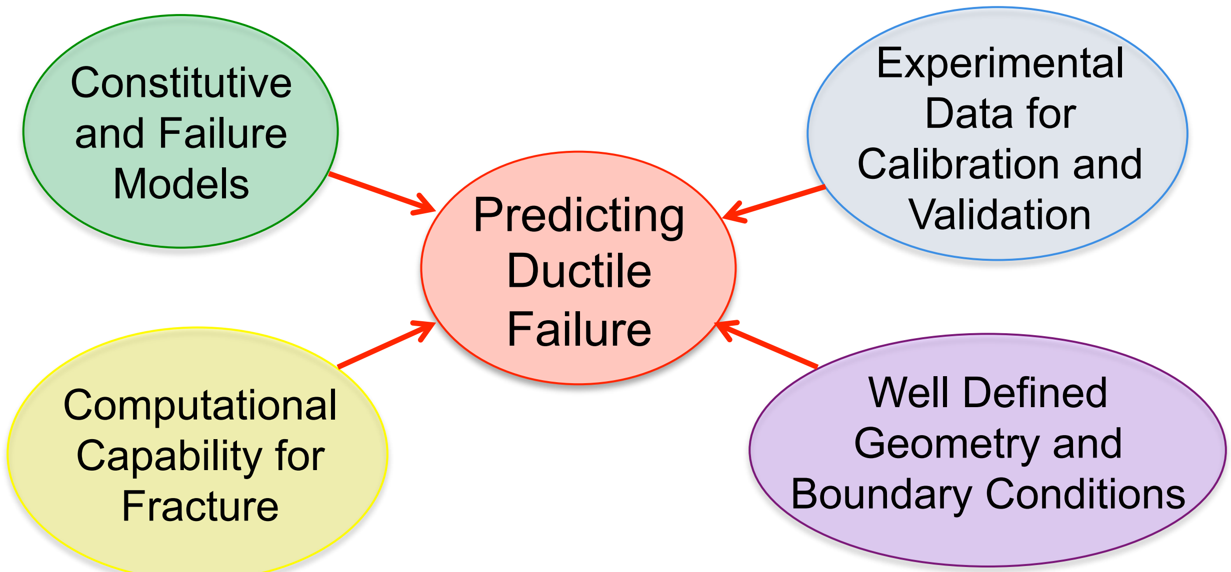
Motivation:
Predictive Capabilities of Ductile Failure

Mission Objectives:
- Reliably understand and predict complex physical behavior such as ductile failure
- Determine and improve material and component performance margins through a robust integration of theory, computations and experiments



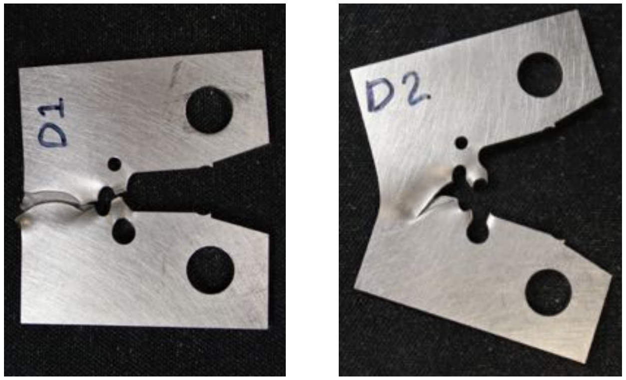
Ductile Fracture Simulation
(Courtesy of Jakob Ostien)



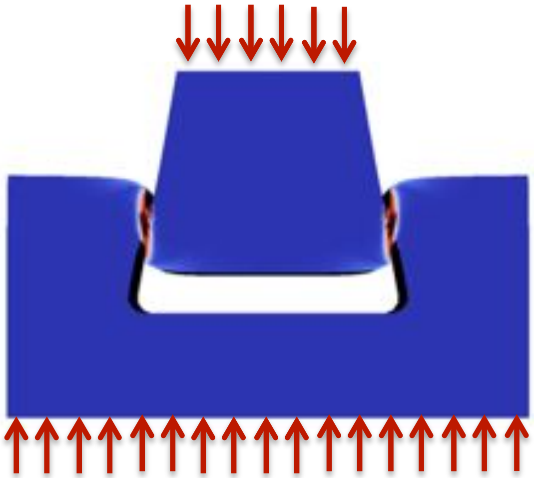
Research Goals: The Sandia Fracture Challenge
- Assess state-of-the-art capabilities in computational predictions of ductile fracture of an arbitrary geometry based on standard experimental evidence
- Assess and suggest improvements for each component of the predictive capability

Presentation Outline

- Sandia Fracture Challenge (SFC) Design and History
- Recent SFC Challenges
  - External Challenge 2012: “Crack in a Maze”
  - Sandia-Internal Challenge 2013: Shear-Dominated Fracture
- Ongoing Research
- Summary of Predictive Capabilities of Ductile Failure



External Challenge Specimens:
Crack Paths A-C-E (left) and A-D-C-E (right)



Internal Challenge Simulation

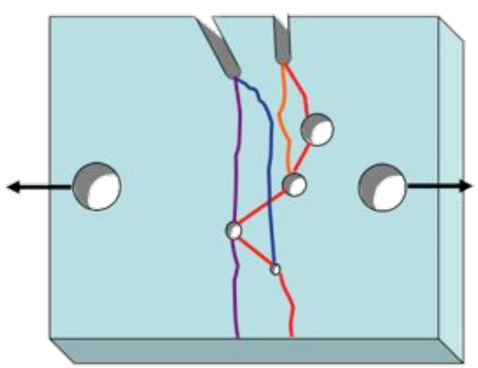
Objective Capability Assessment: The Sandia Fracture Challenge

Inspiration: X-Prize Foundation – "Revolution through Competition"

- Our Goal: "Revelation through Co-opetition" (Coined by Brad Boyce of Org. 01831)
- Blind Assessment of the entire process of ductile failure predictions: How well do modeling methods *blindly predict* metallic fracture in an arbitrary geometry?

- Challenge:
  - Given
    - Standard material calibration experiments
    - Challenge geometry and boundary conditions
  - Asked to predict:
    - Crack path
    - Load vs. Displacement curves
  - Blind experiments of Challenge geometry completed by more than one lab without collaboration on exact technique

- Challenge Geometry Criteria:
  - No obvious or closed-form solution
  - A single, repeatable solution
  - Well defined, simple boundary conditions
  - Easily measured force and displacement ranges, allowing low-cost experimental testing in at least two labs
  - Quickly and inexpensively manufactured samples with reasonable manufacturing tolerances that do not add significantly to variability in the response
  - Easily measure geometric features



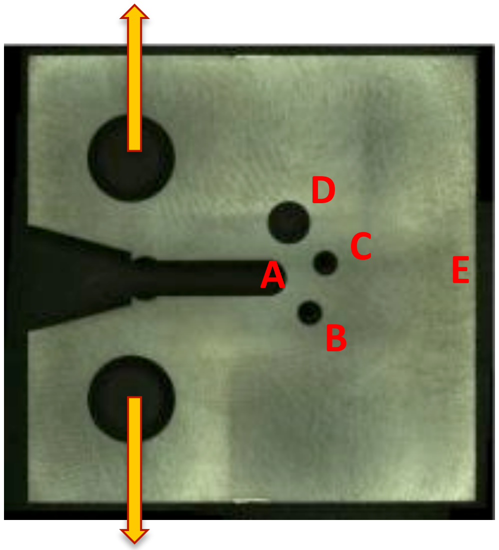
"Crack-in-a-maze" Concept

External SFC 2012: Engaging the External Mechanics Community

Sandia National Laboratories

Sandia Leadership in the External Community:

- Leading the external mechanics community in self-assessment of predicting ductile failure
- Leading cooperation between researchers around the world on the same problem through the Challenge, a subsequent symposium and workshop, and publications



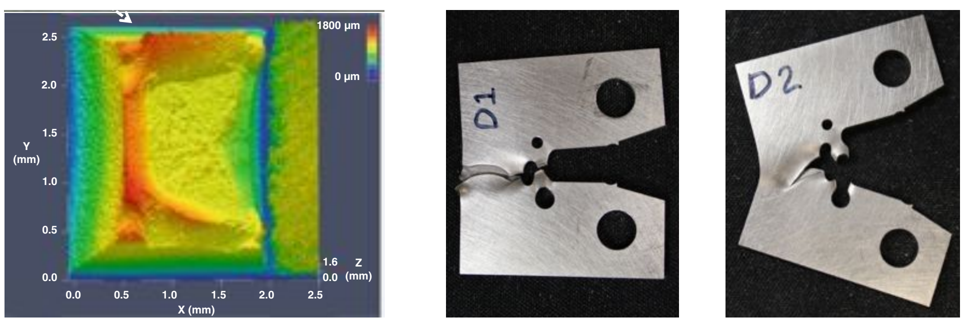
- Challenge:
  - Predict crack path and critical load and crack-opening-displacement (COD) of the first two crack initiations
  - Given tensile data in rolling and transverse plate directions, fracture toughness-like experimental data, microstructural data for the 15-5 PH plate
  - Given Challenge geometry and boundary conditions (0.0005 in/s loading rate)

Impact of External SFC:

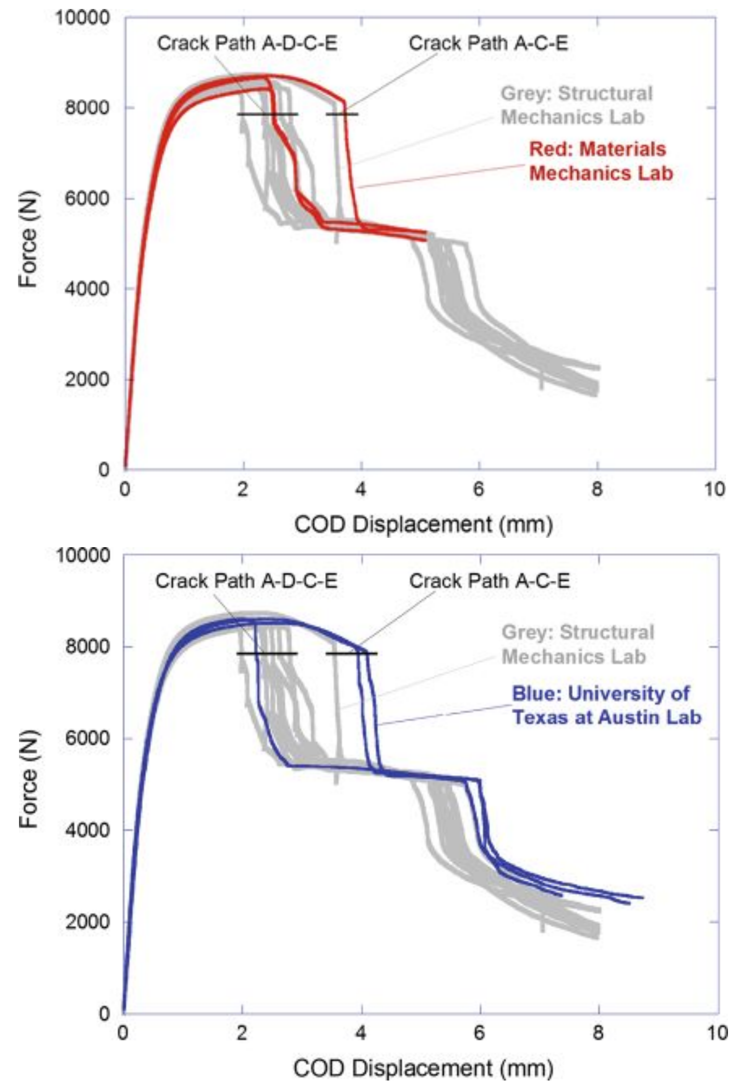
- Over 50 researchers from 14 institutions participated in the SFC.
- The variety of prediction approaches spanned from simple of complex, both for the failure models and the computational approaches. SFC provided a platform for comparing these based on the same experimental data set, never done before on a ductile failure problem.

External SFC 2012: Experimental Results

- Observation to *two* different crack paths by three independent labs
  - Bifurcation in failure solution attributed to some of the critical holes being slightly out of machining tolerances
  - Two crack paths were due to real-world machining issues, not experimental technique
  - Two crack paths led to large ranges for answers to the Challenge questions
- Subsurface cracking occurred prior to the appearance of a surface crack, suggesting mixed-mode failure: Additional experiments with shear loading may have helped the failure model calibrations



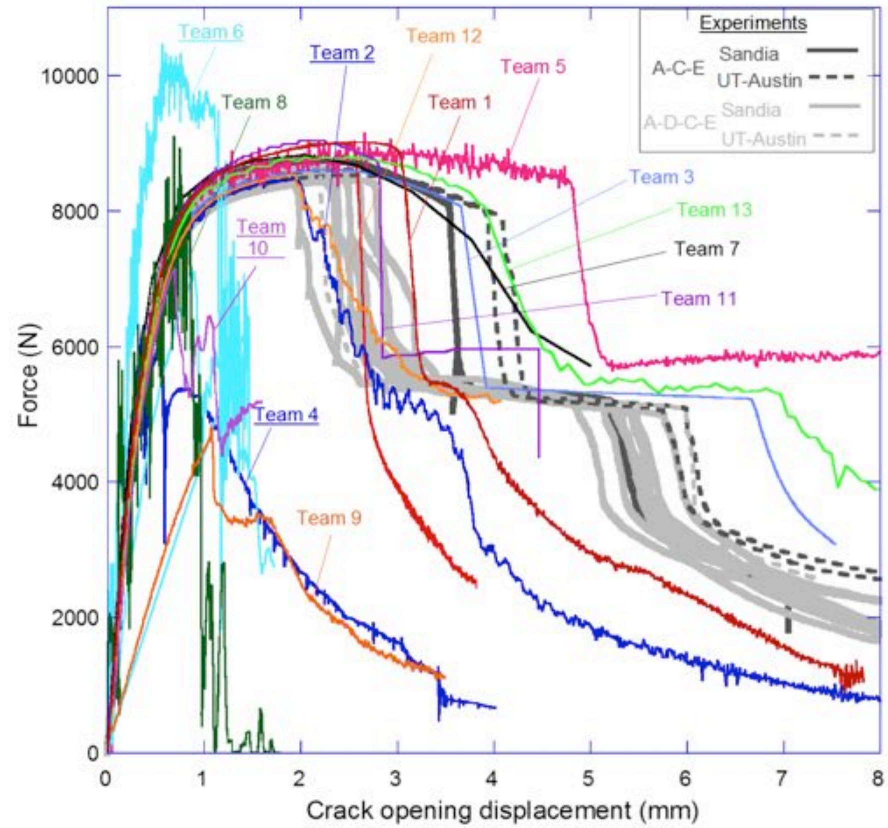
Height Profile of A-C Crack (left); Crack Paths A-C-E (middle) and A-D-C-E (right)



Overlay of Experimental Results From Three Independent Laboratories

External SFC 2012:
Wide Ranging Predictions and External Impact

- Computational Results:
  - A wide range of force-deflection curves were reported. Roughly 8 of the 14 teams predicted curves that were somewhat comparable to the scatter of experiments.
  - Most of the teams could predict *some* elements of the challenge. Sandia's Team #1 was able to predict the failure loads, but not the failure COD values.
- External Impact:
  - 2012 ASME Symposium on SFC
  - SFC Workshop held at Sandia in June 2013
  - Special Issue of International Journal of Fracture in March 2014 on the SFC
  - Requests by participants for future external challenges



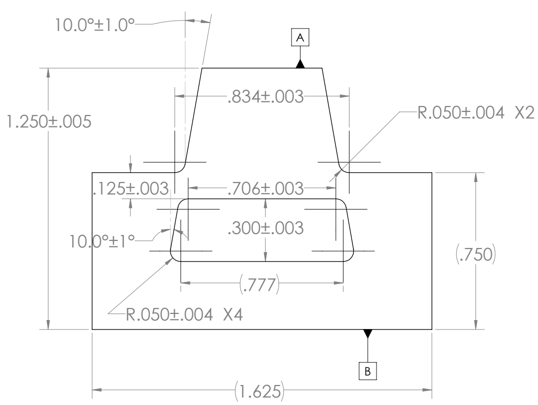
Overlay of Predictions on Experimental Results

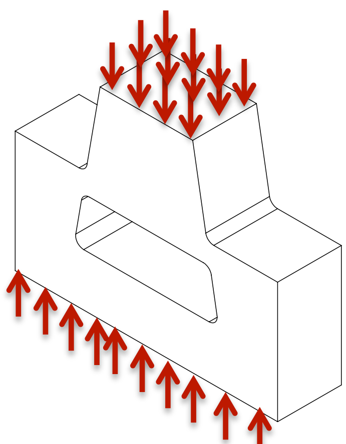
Sandia has led the mechanics community to evaluate the entire process of ductile failure predictions. There was no clear "winner" of the Challenge. The conclusion is that more research is required to find the gaps in the process and the methods that are considered "standard."

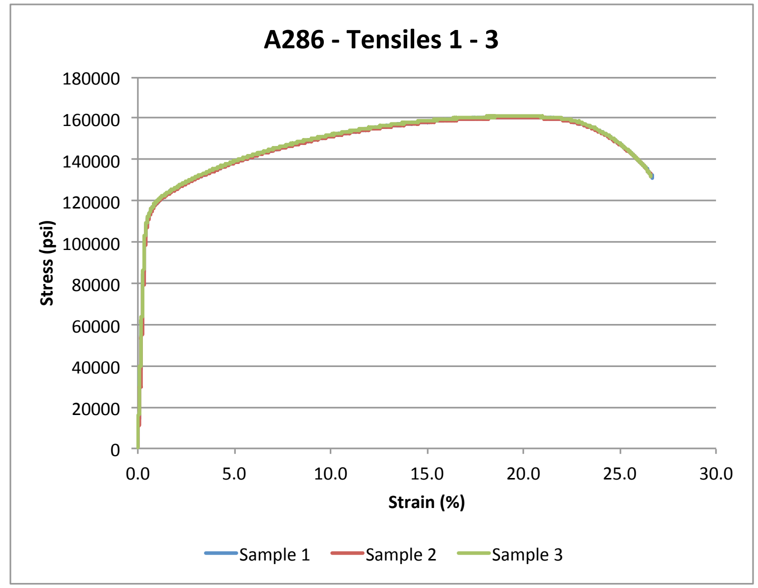
Internal SFC 2013: Shear-Dominated Failure

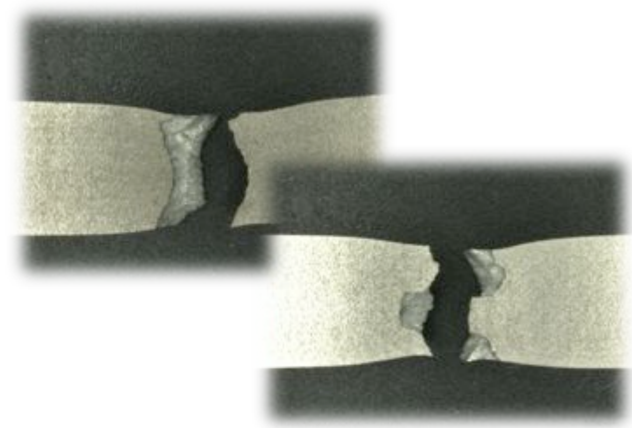
Assessment of predictive capability of a failure mode from shear, important to abnormal environments for Sandia systems

- The Challenge:
  - Predict load-displacement curve up to and through failure of a A286 steel specimen loaded in uniaxial compression at a rate of 0.001 in/s
  - Data of the base material loaded in uniaxial tension was provided for material characterization
  - Specimens tests in two experimental labs at Sandia







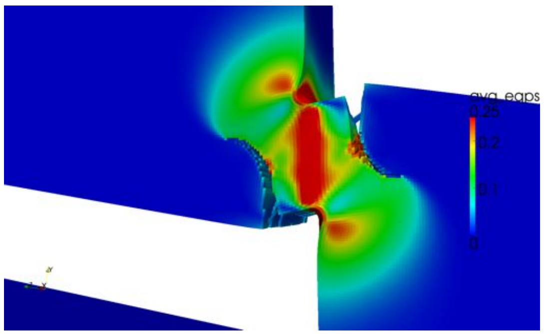


Tensile Data and Post-Test Images of A286 Steel

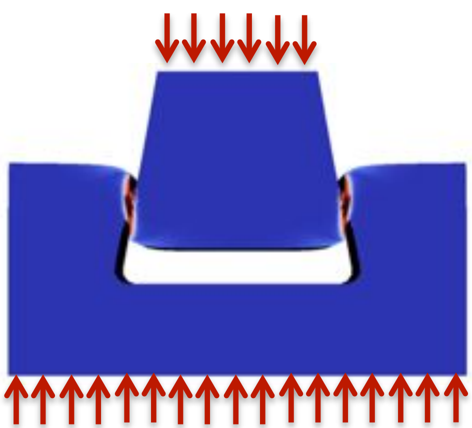
Internal SFC 2013: Experimental Results and Predictions

Predictions were far from highly repeatable experimental data: Model calibration process requires investigation to find capability gaps

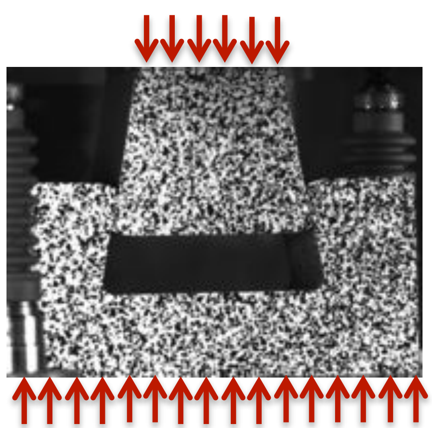
- 15 repeatable experimental failure results
- Two internal Sandia teams with very different predictions using two common failure models used at Sandia



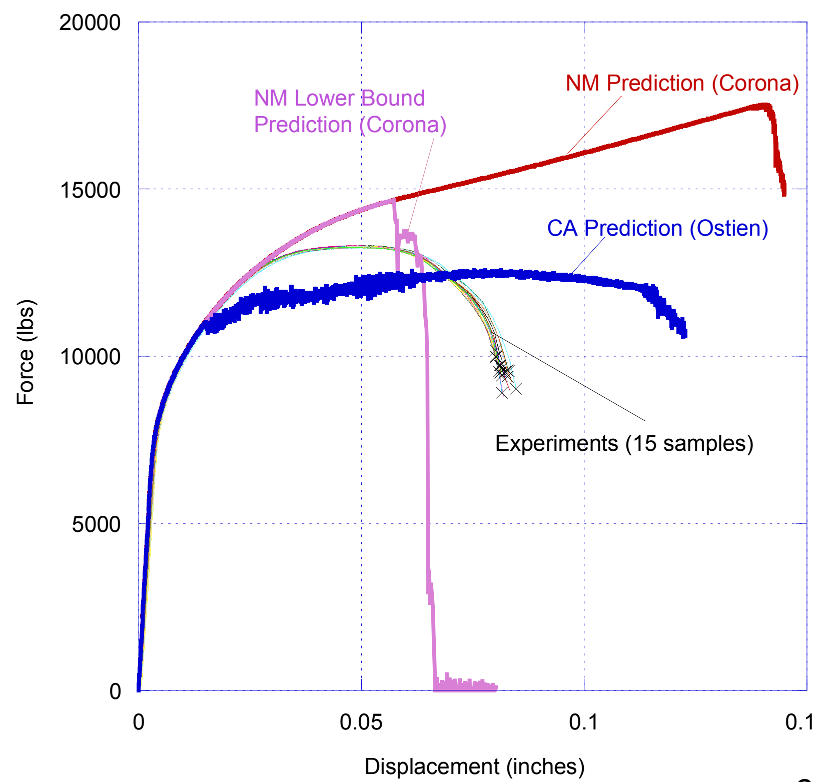
CA team *BCJ_MEM* shear damage model



NM team model prediction at failure using Wellman's Tearing parameter



Example experimental image at failure

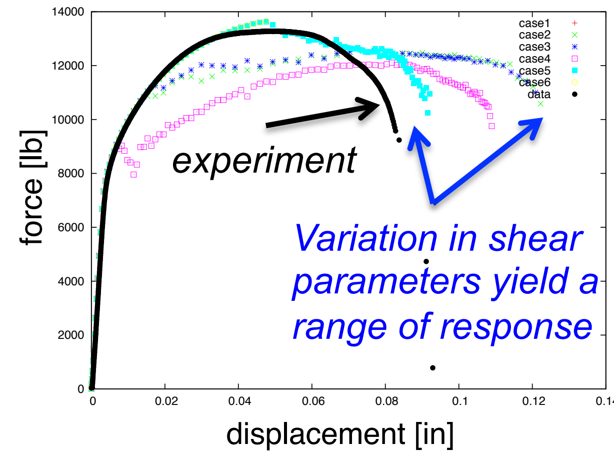


Internal SFC 2013: Assessment and Recommendation

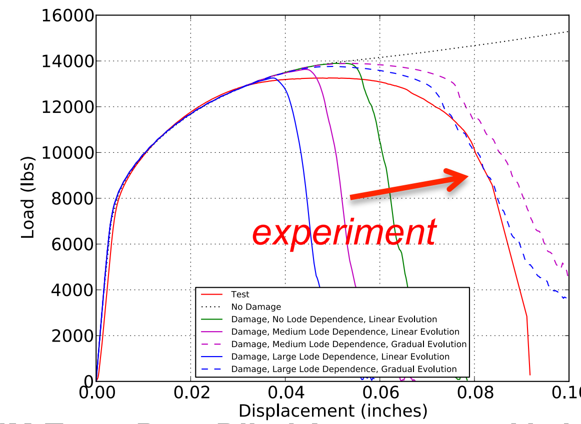
Self-assessment highlights areas of success and required improvements for predictive capabilities

- Experiment Assessment: Highly repeatable experiments, so quality Challenge geometry
- CA-Team Post-Blind Assessment: Tensile tests are insufficient to calibrate shear parameters in BCJ_MEM failure model
- NM-Team Post-Blind Assessment: Tearing parameter needs calibration using shear-dominated loading, with additional tests with different stress triaxiality and Lode parameter

Recommendation: Tensile tests are insufficient to calibrate failures models for validation geometries that have other dominant failure modes



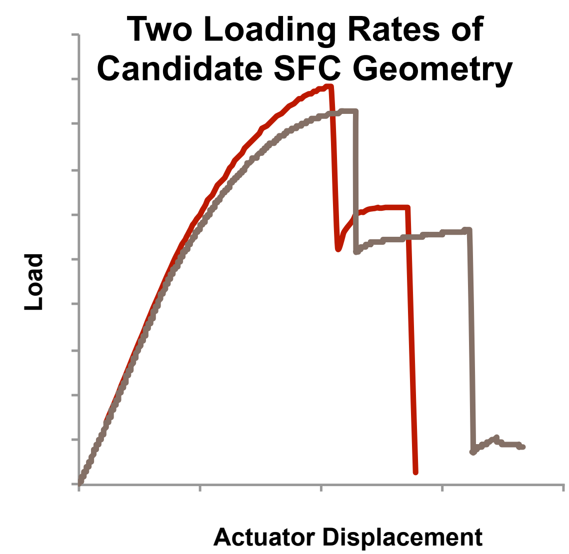
CA-Team Post-Blind Assessment: 100-fold Variation in Shear Parameters led to 30-40% range of displacements



NM-Team Post-Blind Assessment: Variation in Lode Dependent and Damage Evolution

Ongoing Research:
Improving Ductile Failure Prediction Capability

- External SFC 2014 on moderate strain-rate loading for ductile failure (To be Issued May 2014)
- Additional research through post-blind assessments of Challenges
  - Detailed evaluation of both experimental and computational approaches
  - Implementation of new failure models into Sierra Mechanics
- Related Research on Improved Constitutive Model Calibration:
  - Current Early Career Lab Directed Research and Development Funding on new inverse methods like the Virtual Fields Method (VFM)
  - VFM utilizes full-field experimental data without the need for inverse FEM simulations for constitutive model calibration



Rate Sensitive Response of Candidate Challenge Geometry

SFC research in future will assess the current state-of-the-art in predictive capabilities *and* push for improvements, both internally and externally.

Summary: Sandia's Predictive Capabilities of Ductile Failure

Double-blind assessment of the complete ductile failure predictive capability (both physical and computational simulations) demonstrates:

- Sandia currently has strengths and weaknesses to predict ductile failure
- The Sandia Fracture Challenge highlights areas for investing in
  - Improved experimental capabilities to support analysts with failure model calibration
  - Additional failure models into Sierra Mechanics suggested by the external community
  - New approaches for constitutive model calibration (such as the Virtual Fields Method)
- Engineering Science Research Foundation (ESRF) is ideal for research that integrates theory, computational simulation, computational code development, experimental simulation, and validation to answer engineering questions in real-world problems
- ESRF is a leader in the external mechanics community in assessing and pushing the state-of-the-art in ductile failure modeling
- ESRF is actively investing in research that may fundamentally change how ductile failure is modeled, hence increasing trust in Sandia's predictive capabilities

Acknowledgements

- Brad Boyce, Co-lead on Sandia Fracture Challenge, Sandia Materials Mechanics Laboratory
- Sandia Structural Mechanics Laboratory: Theresa Cordova, John Liang, Mathew Ingraham, Alex Hielo, Cayetano Mendoza, Jack Heister
- Tom Crenshaw, Sandia Materials Mechanics Laboratory
- Sandia Analysts: Jakob Ostien, Edmundo Corona, Jake Koester, Kristin Dion, Michael Neilson, Amy Kaczmarowski, Erin Karasz, John Emery
- Eliot Fang, Sandia Manager of Solid Mechanics
- Michael Chiesa, Sandia Manager of Multi-Physics Modeling & Simulation
- External SFC participants from Schlumberger, University of Texas at Austin, Massachusetts Institute of Technology, University of California-Los Angeles, University of Cincinnati, Ruhr-University Bochum, Northwestern University, Cornell University, NASA, Tsinghua University, Zhejiang University, University of Missouri, Dalian University of Technology, University of Arizona, Global Engineering and Materials, Naval Surface Warfare Center Carderock Division, Xi'an Jiaotong University
- Funding: Advanced Scientific Computing (ASC) and Weapons System Engineering Assessment Technologies (WSEAT) programs

Personal Research Involvement While at Sandia (Nov 2011-Now)

Sandia National Laboratories

- Research Projects:
  - 2 Principal Investigator projects
  - Support researcher on 8 projects
  - Co-lead of 2014 Sandia Fracture Challenge (with Brad Boyce)
- 4 Peer-Reviewed Journal Publications
- Reviewer of 4 articles in peer-reviewed journals
- 2 Conference Presentations at the 2012 and 2013 Society of Experimental Mechanics (SEM) Annual Conferences
- Professional Service and Involvement:
  - Session organizer for 2014 SEM Annual Conference
  - SEM Research and Education Committee member
  - SEM Optical Methods Technical Division member

Backup Slides

Components of Predicting Ductile Failure

Integration of Theory, Computational Simulation and Experimental Discovery and Validation

Constitutive and Failure Models

- Physics-Based: Void nucleation & growth
- Physics-Inspired: BCJ; Cohesive zone
- Empirical: Tearing parameter
- Non-physical: Maximum stress or plastic strain

Complexity

Experimental Data for Calibration and Validation

- Tensile base material tests
- Fracture toughness-like tests
- Other loading conditions for base material calibration
- Ideally repeatable validation geometry experiments

Computational Capability for Fracture

- Localization and X-FEM methods
- Non-local / gradient
- Cohesive zones
- Crack-Band methods
- Remeshing / Adaptivity / Multi-grid
- Element Degradation and Death

Mesh Convergence

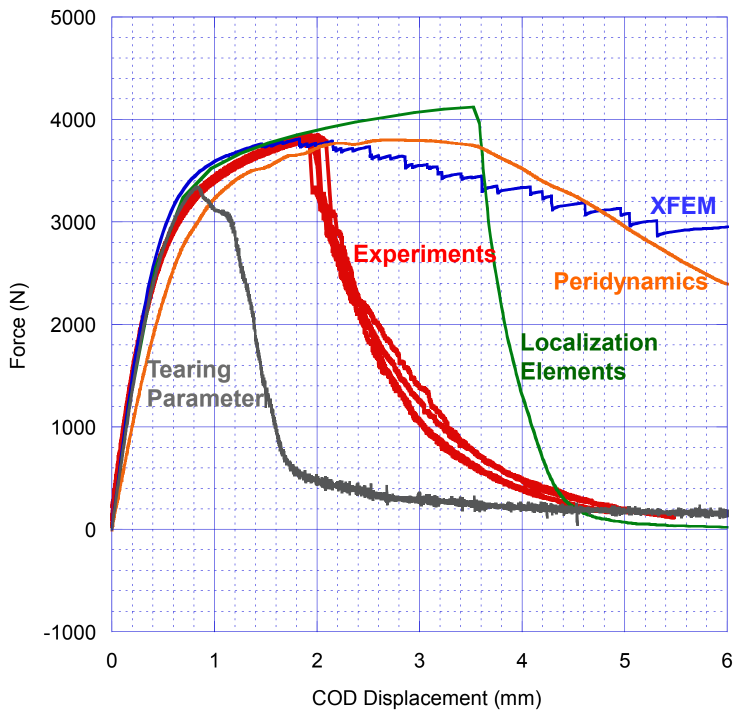
Well Defined Geometry and Boundary Conditions

- Samples within machine tolerances
- Repeatable and/or well measured boundary conditions in experiment
- Computational idealization of boundary conditions represent experiments
- Uncertainties of geometry and boundary conditions are quantified

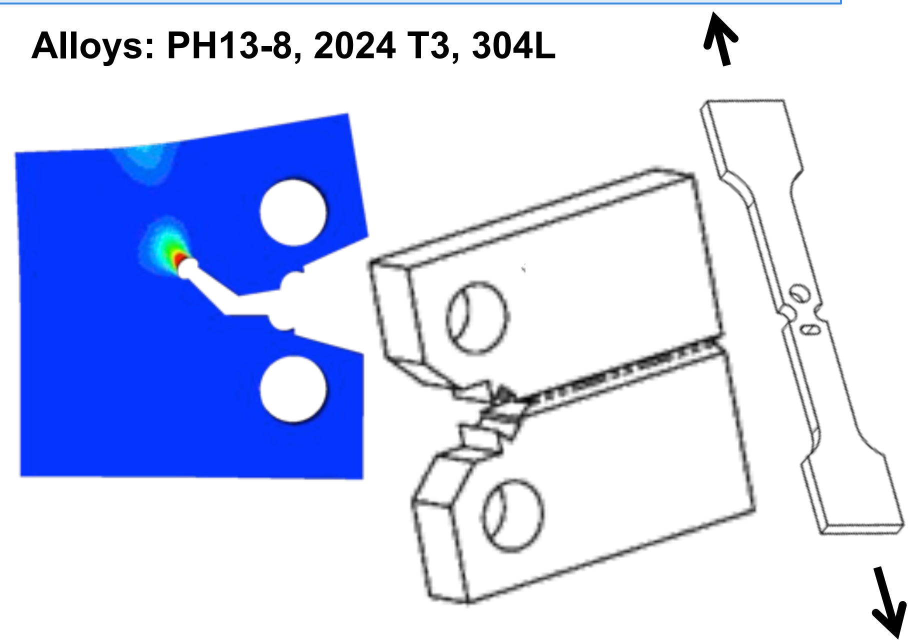
Sandia Fracture Challenge (SFC): History of the Double-Blind Assessments

Inspiration: X-Prize Foundation – "Revolution through Competition"

- Our Goal: "Revelation through Co-opetition" (Coined by Brad Boyce of Org. 01831)
- Blind Assessment of the entire process of ductile failure predictions: How well do modeling methods *blindly predict* metallic fracture in an arbitrary geometry?



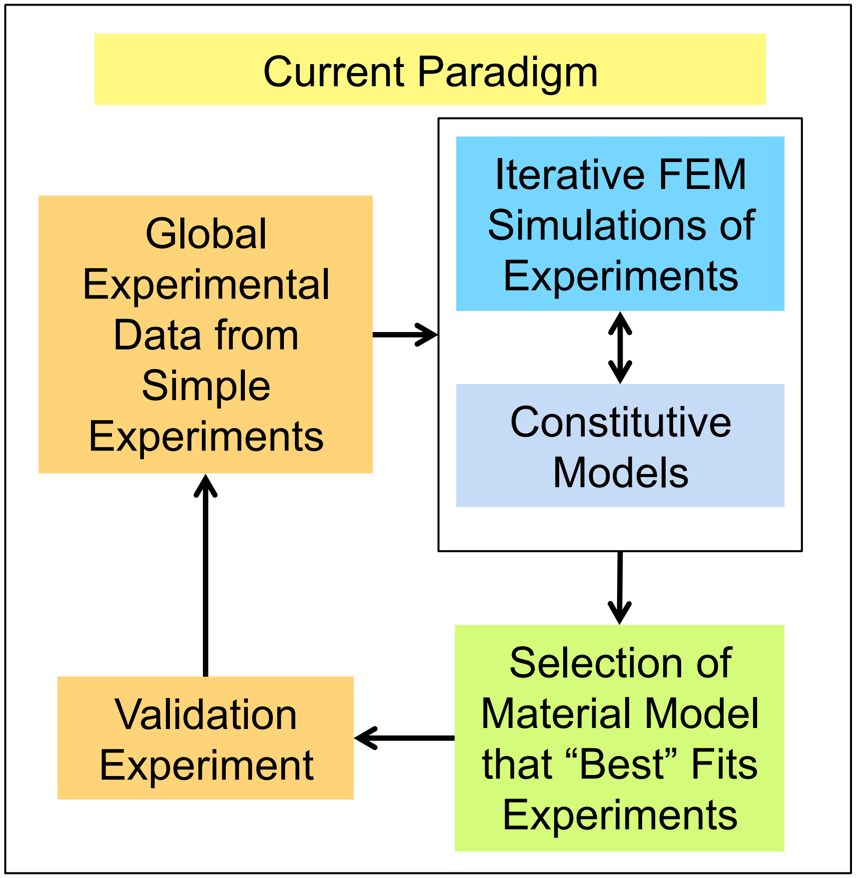
Alloys: PH13-8, 2024 T3, 304L

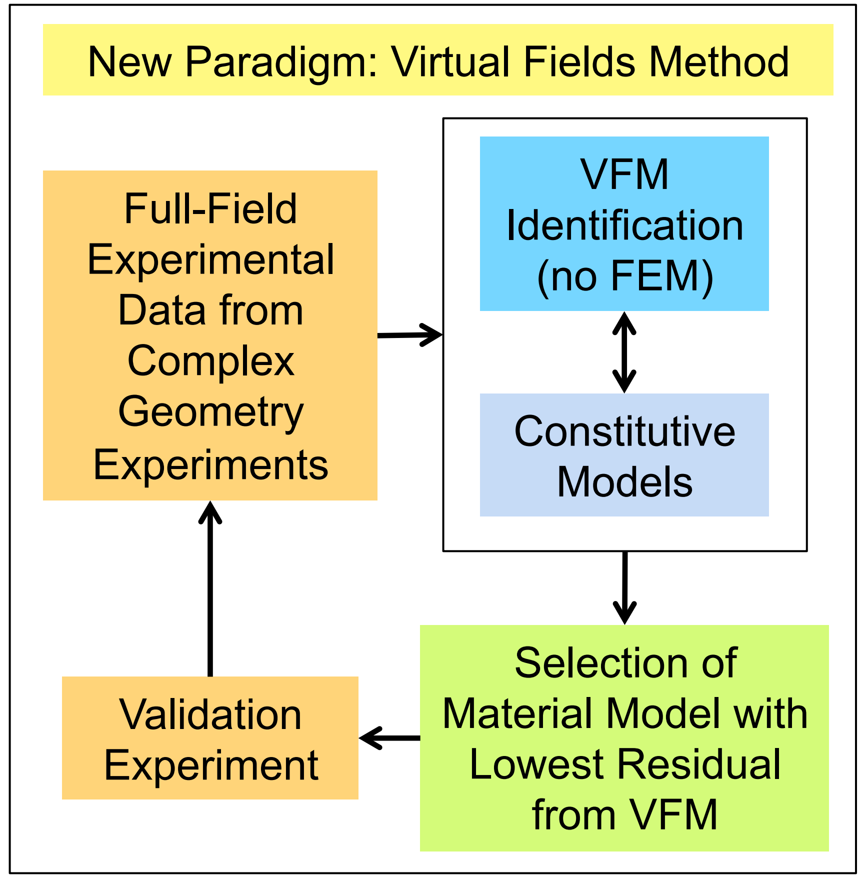


Internal Challenges (2010-2012) involved prediction of Necking, Crack Initiation, Crack Propagation

These assessments repeatedly revealed difficulties in predicting crack initiation and crack propagation for ductile tearing scenarios

Ongoing Research: Improving Constitutive Model Calibration





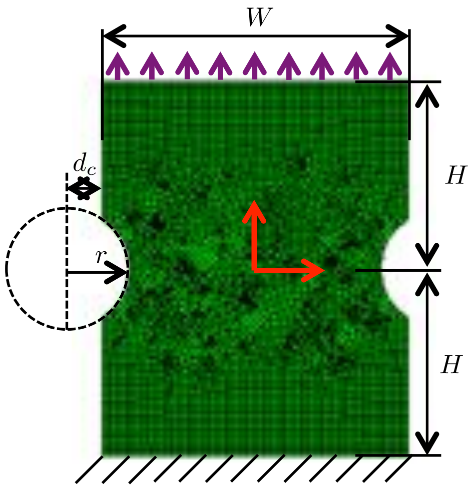
Investment in new inverse methods for constitutive model calibration (Currently LDRD funding):

- Integration of theory, advanced experimental methods, code development, and computations
- Improving material and component performance margins through improved constitutive modeling
- External collaboration with VFM research community

Ongoing Research: Virtual Fields Method Example

- Simulated Experimental Data to Demonstrate Technique
- 304L Stainless Steel Nominal Material Properties for a BCJ model: $\bar{\sigma} = \sigma_y + \kappa(\bar{\varepsilon}^p)$

$$\kappa(\bar{\varepsilon}^p) = \frac{H}{R_d}\left[1 - \exp(-R_d\bar{\varepsilon}^p)\right]$$



Inputs:

Principle of Virtual Work (PVW)

$$-\int_V \sigma_{ij}\epsilon^*_{ij}\,\mathrm{d}V + \int_S T_i u^*_i\,\mathrm{d}S + \int_V b_i u^*_i\,\mathrm{d}V = \int_V \rho a_i u^*_i\,\mathrm{d}V \quad \forall\, u^*_i\ \mathrm{KA}$$

Constitutive Model
$\sigma_{ij} = Q_{ijkl}\epsilon_{kl}$

Simulated Experimental Data
ϵ_{kl} T_i

User-Defined Virtual Fields
u^*_i ϵ^*_{ij}

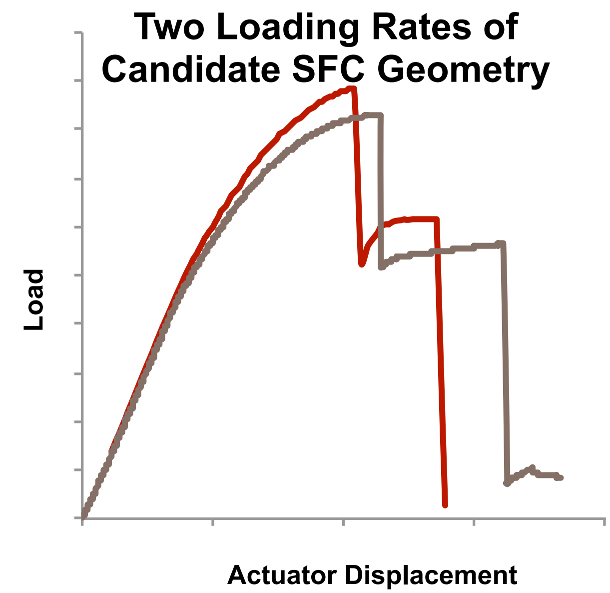
Output: Constitutive Parameters

Model Parameters	Ref.	VFM	Percent Error
E (GPa)	200	200.6	0.28
ν	0.249	0.2471	−0.76
σ_y (MPa)	193	193.9	0.44
H (GPa)	2.280	2.288	0.37
R_d	1.1	1.112	1.08

Goal:
Robust Approach for Constitutive Parameter Identification Using The Virtual Fields Method and Full-Field Experiments

Ongoing Research: The Next SFC

- External SFC 2014 on moderate strain-rate loading for ductile failure (To be Issued May 2014)
  - Two loading rates: Quasi-static and upper end of MTS-type load frames
  - Given tensile *and* shear-dominated base material experimental data at two loading rates
  - Given Challenge geometry and loading rate information
  - Asked to predict load-displacement curves for two loading rates and crack path
- Goals of External SFC 2014:
  - Assess ability to predict ductile failure in a strain-rate dependent material and for non-quasi-static loading rates
  - Assess if shear-dominated base material tests help with failure model calibration
- Additional research through post-blind assessments
  - Detailed evaluation of both experimental and computational approaches to improve Sandia's predictive capabilities
  - Implementation of new failure models into Sierra Mechanics



SFC research in future will assess the current state-of-the-art in predictive capabilities *and* push for improvements, both internally and externally.