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The Sandia Fracture Challenge: How Ductile Failure Predictions Fair

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Introduction

Computational solid mechanics models are required to predict ever increasingly complex deformation and failure of structures in extreme environments. One way to build confidence in these predictions is to challenge the computational approaches with validation scenarios that can be experimentally tested for comparison. The Sandia Fracture Challenges provide the mechanics community a forum for assessing its ability to predict ductile fracture through a blind, round-robin format where computationalists are asked to predict the deformation and failure of an arbitrary geometry given experimental calibration data. These challenges were designed to (1) assess the whole prediction stream, from experiments and calibration methods to the constitutive models and numerical methods; (2) replicate real-world engineering constraints including limited calibration data and time to predict; (3) test a relatively simple, but unfamiliar "toy" problem that captures the salient features of real-world problems; (4) allow for blind participation from several computational groups with different approaches; (5) verify experimental outcomes in more than one laboratory to reduce experimental bias; and (6) use the post-blind assessment to inspire improvements. This paper overviews the three Sandia Fracture Challenges to date, with emphasis on the third, describing the Challenges, comparing the experimental results to the predictions, and identifying gaps in capabilities, both experimentally and computationally, to inform future investments. The Sandia Fracture Challenge has evolved into the Structural Reliability Partnership, where researchers will create several blind challenges covering a wider variety of topics in structural reliability. This presentation will also describe this new venture.

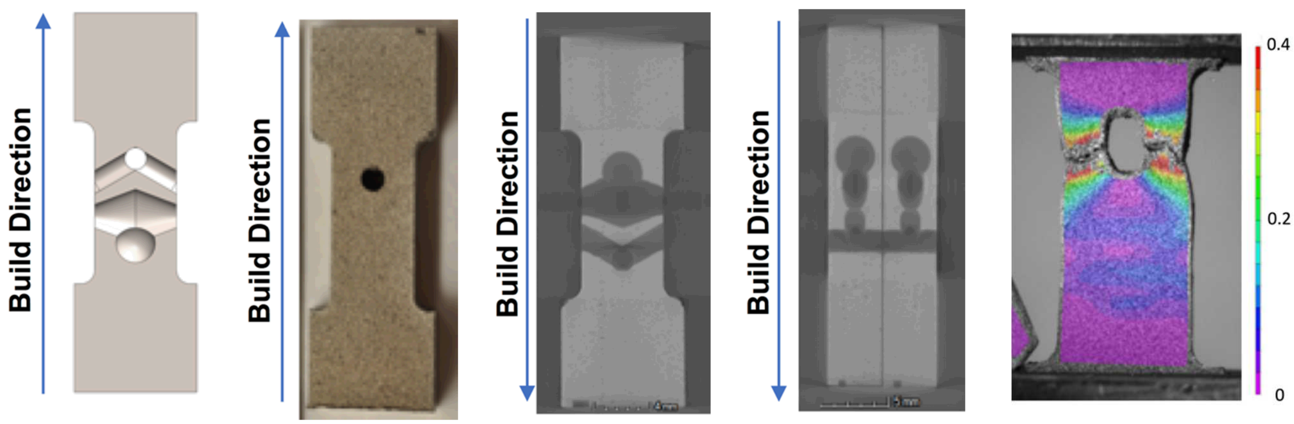
The First and Second Sandia Fracture Challenges

The first Sandia Fracture Challenge (SFC1) in 2012 was the first of its kind to provide a forum for candidly comparing different ductile failure prediction capabilities in the larger mechanics community. Here is a brief description of SFC1; a more detailed explanation can be found in a special issue of the *International Journal of Fracture* [1]. The thirteen participating teams predicted the initiation and propagation of a crack in a ductile structural stainless steel, 15-5 PH, under quasi-static room temperature test conditions. The SFC1 specimens were flat plates with a round root pre-cut slot and multiple holes influencing the crack-tip stress state. The participants were given tensile test data, sharp crack Mode-I fracture data, and some limited microstructural information. Three different experimental testing laboratories observed two different crack paths: a tensile-dominated or shear-dominated failure mode. The post-blind assessment of both experiments and computations revealed that variation in hole location led to the two different failure modes, where the out-of-tolerance geometry favored a shear-ligament crack path and the nominal geometry favored a tensile-ligament crack path. The teams expressed a desire for other calibration data in future challenges, in particular shear-dominated loading experimental data.

The second Sandia Fracture Challenge (SFC2) in 2014 focused on ductile fracture in different loading rate environments since many engineering scenarios with ductile fracture involve loading outside the quasi-static regime. Again, here is a short description of SFC2, and more details can be found in a special issue of the *International Journal of Fracture* [2]. SFC2 considered a rate-dependent titanium alloy, Ti-6Al-4V, in sheet form with an unusual set of notches and holes that fostered a competition between tensile- and shear-dominated failure modes. Specimens were tested at two different loading rates, quasi-static and a modest-rate dynamic loading (failure in ~0.1 sec). Fourteen teams predicted the fracture path and quantitative far-field metrics including peak load and displacement at crack initiation, and as well as uncertainty bounds on their predictions. The teams were given measurements of the actual SFC2 geometry specimens, not just engineering drawings with tolerances as were provided in SFC1, and calibration data from standard tensile dogbone tests and modified V-notch shear tests, originally designed for testing shear in composites. The SFC2 geometry specimens were tested in three independent laboratories, observing the prevalent failure mode being the shear-dominated crack path and significant differences in the load-displacement behavior for the two different loading rates. In general, the prediction teams had more agreement with the overall far-field load-displacement data than for SFC1, which was attributed to more calibration data and experience gained from SFC1. However, the post-blind assessment revealed several shortcomings in the predictions including inconsistency in the application of appropriate boundary conditions, need for a thermomechanical treatment of the heat generation in the dynamic loading condition, and further difficulties in model calibration based on limited real-world engineering data. Despite being given material and geometric variability data, few teams provided uncertainty bounds on their predictions, showing a lack of experience in robust uncertainty quantification, particularly in limited-time-to-predict scenarios.

The Third Sandia Fracture Challenge

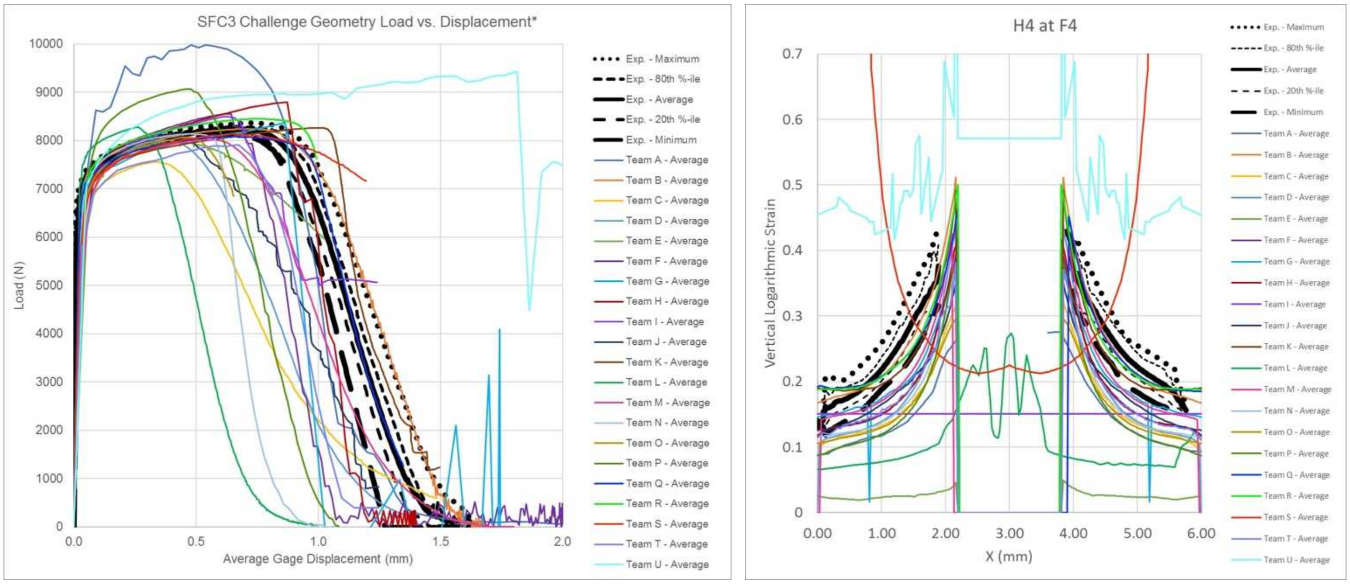
The third Sandia Fracture Challenge (SFC3), issued in 2016, asked the computational mechanics community to predict ductile fracture in an additively manufactured (AM) structure. AM is a rapidly growing fabrication process that poses many challenges for the engineering community. Many mechanics questions arise from a class of materials with generally more heterogeneity and variability than traditionally formed materials. The SFC3 geometry was an AM 316L stainless steel tensile bar with through holes and internal cavities that could not have been conventionally machined, as shown in Figure 1, going beyond our previous Challenges that were based on extruded 2D features. The prediction teams were provided extensive materials data from tensile and notched tensile tests of specimens printed on the same build tray to electron backscatter diffraction microstructural maps and micro-computed tomography (micro-CT) scans of the SFC3 geometry specimens (Figure 1c and d). Unlike previous Challenges, SFC3 took advantage of better experimental metrology, namely Digital Image Correlation (DIC), to measure surface field displacements and strains (Figure 1e) for comparison to models. The teams had to predict far-field and local quantities of interest, including predictions of variability in the resulting fracture response.



(a) (b) (c) (d) (e)

Figure 1 – SFC3 Geometry Specimens: (a) Schematic of central cross section, revealing the internal cavities; (b) image of front surface with AM finish; (c) micro-CT scan "thick slab" view of Specimen A32 (front perspective) that essentially sums the data to show all the void and internal feature content (high contrast) through the central section of the specimens; (d) micro-CT scan "thick slab" view of Specimens A32 [left] and A15 [right] (side perspective); (e) DIC Hencky (logarithmic) vertical tensile strain field immediately after failure of Specimen A23, showing failure along the angled channels and through-hole

Two independent laboratories tested nineteen specimens that all cracked beginning at the edge of the central through-hole, emanating out along the angled channels. These specimens had relatively modest bounds in load-displacement behavior (see black lines in Figure 2a for the 20th percentile, average, and 80th percentile responses) with more variability in the surface strain response of the AM structure (see Figure 2b). Twenty-one predictions were submitted from fourteen institutions; the load-displacement data (far-field quantity of interest) are in Figure 2a, and one example of a line-scan of the surface vertical strains (a local quantity of interest) is in Figure 2b for all the teams and experiments. The post-blind assessment is currently underway; SFC3 will be fully documented in an upcoming special issue of the *International Journal of Fracture*. Here are some preliminary observations and comments regarding the SFC3 results. Unlike previous Challenges, all the teams predicted the correct crack path. The teams generally fared well when comparing to far-field quantities of interest, with two teams (B and Q) predicting a nominal load-displacement behavior within the bounds of the experimental data. The predictions of local surface strain measures tended to over-predict strains early in the deformation and then under-predict towards failure; also, experimental strain measurements tended to have larger variation than predicted. The teams took vastly different approaches to predict uncertainty bounds in their models, and there was not a straightforward, standard method to quantify those bounds for curve-type measures from the experiments. Surprisingly few teams considered the geometric variation and pore structure characteristics of AM metals, despite considerable data provided to aid that effort. There were examples of clear misinterpretations of the questions, and the post-blind assessment revealed several clerical errors in the predictions. Both of these types of mistakes are not uncommon in real engineering environments. SFC3 overall showed improved ductile fracture capabilities, particularly from teams with experience in previous Challenges, but also revealed a need for deep conversations on how computationalists should peer-review their work and quantify uncertainties.



(a) (b)

Figure 2 – Comparison of Experimental (Black) and Average Computational (Colors) Results with Experimental 20th and 80th percentile Bounds: (a) Load-displacement data and (b) surface vertical Hencky (logarithmic) strain across the horizontal line intersecting the center of the through-hole (called H4) at the load at 90% of peak load (called F4)

The Future of Blind Assessment of Structural Reliability Mechanics Predictions

The two special issues of the *International Journal of Fracture* for the first two Sandia Fracture Challenges [1-2] have been the most downloaded articles for that journal, demonstrating the vast impact these challenges have had to raise awareness in the mechanics community about the state-of-the-art in ductile fracture predictions. We anticipate such enthusiasm for SFC3, particularly because of the AM aspect. The three Sandia Fracture Challenges have spurred the formation of the Structural Reliability Partnership (SRP), spearheaded by Sandia National Laboratories, Exxon Mobil, and the University of Texas at Austin. The purpose of the SRP is to coordinate research, share best practices, and leverage investments from multiple institutions on areas of mutual interest in the domain of structural reliability. The SRP will coordinate staggered blind assessment Challenges in many different topics of structural reliability, with shared focus materials that facilitate cross-institution comparisons, knowledge transfer on "best practices", and leveraging of cross-institutional R&D investments to address shortcomings and gaps in structural reliability experiments and predictions.

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