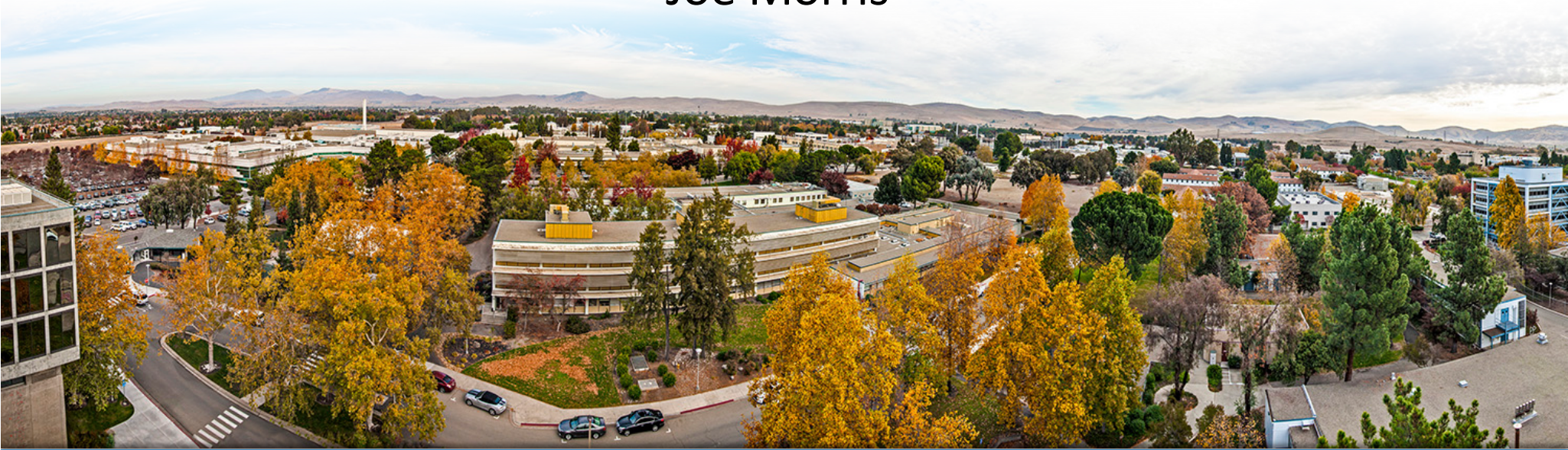


Damage Mechanics Challenge Forum

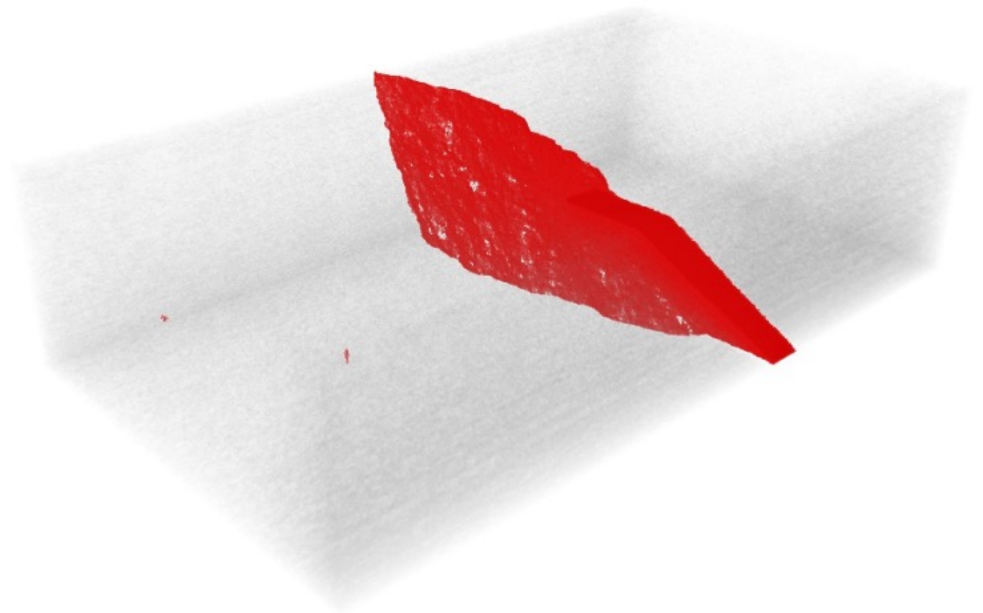
Joe Morris



This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC.
LLNL-PRES-836565

Overview

- Preparation for AGU
- Simulation results submission deadline
- Overview of submission file formats
- Q&A
- Paper timeline discussion



What I need and when...

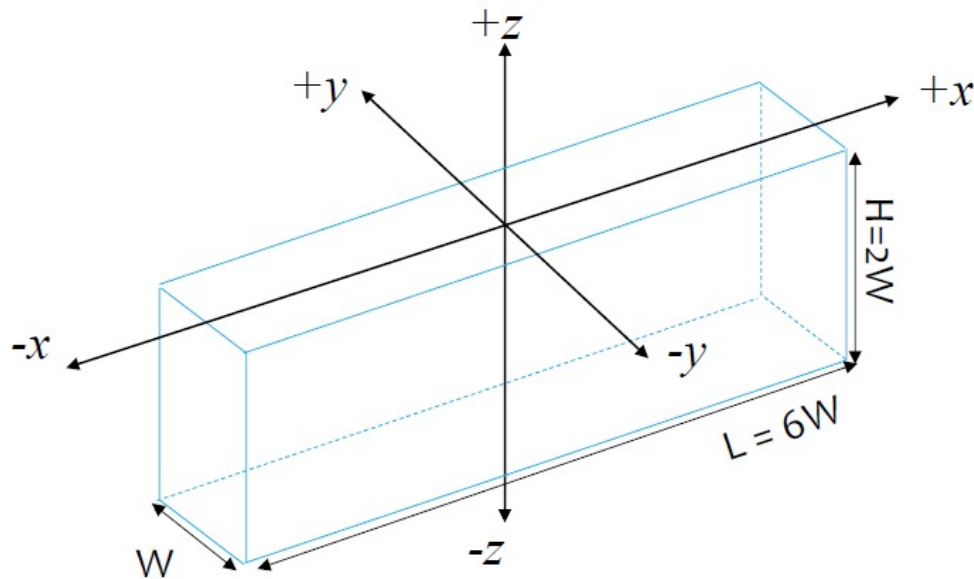
- The data / written responses for all challenge questions
- Please send me a short paragraph describing your approach
 - With my poster I want to be able to discuss the methods
 - Include a reference for me to cite
- All uploaded by Monday November 14th 23:59 Pacific Time

The purpose of the Damage Mechanics Challenge (DMC)

1. Compare computational approaches on damage evolution for predicting fracture behavior of 3D printed model rock;
2. Identify the information provided by the different simulation approaches that gives insight into the prediction and interpretation of failure in rock;
3. Identify model parameters that are currently not measured or cannot be measured in the laboratory; and
4. Determine whether there are other experimental measurements that are needed or better methods of performing measurements to monitor damage evolution.

This challenge exercise is used to determine the state of the art and future directions to improve the community's ability to simulate crack formation and evolution in natural and engineered brittle-ductile materials.

Coordinate system and other specifics



Coordinate System for Reporting

- *The coordinate system is centered on the rod on the top of the sample.
- *The top of the sample is $z = 0$.
- *The bottom of the sample is $z = -2W$.
- *The front of the sample is $y = -0.5W$.
- *The back of the sample is $y = +0.5W$.
- *The left side of the sample is $x = -0.5L = -3W$.
- *The right side of the sample is $x = +0.5L = +3W$.

Reporting Roughness & Length

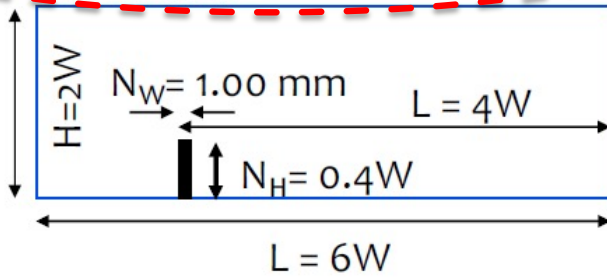
- *All length and roughness predictions should **be reported relative to the undeformed original state coordinate system** which is the distance between the crack surface and y-z plane at $x = 0$.
- *If the crack bifurcates, report multiple arrays – one for each fracture.
- *For reporting, the distance between surface roughness data points (resolution of the validation) is set to 25 micrometers.
- *The resolution of laser profilometry measurements is 0.5 micrometers.

Challenge geometry

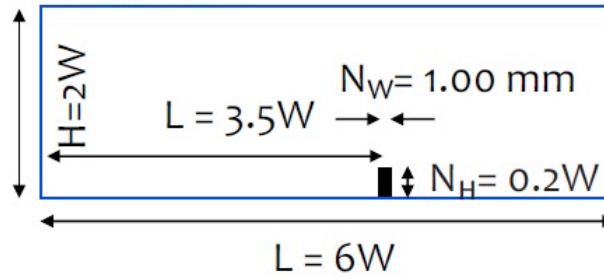
Off Center Notch - Angle

*The front of the sample is $y = -0.5W$.

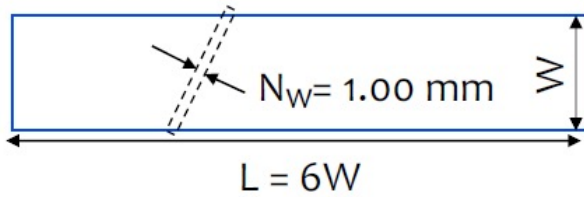
Front View



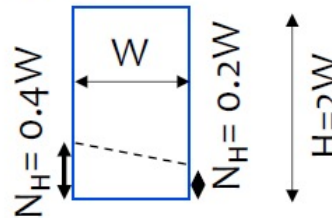
Back View



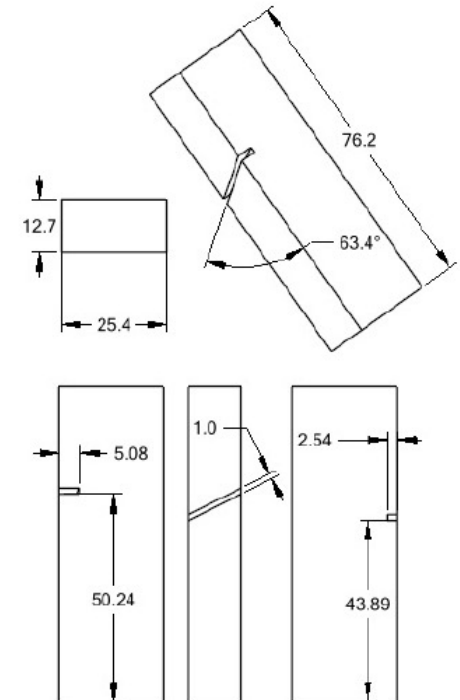
Top View



Side View



Unit: mm



Challenge Questions

Challenge Question 1: Report the best prediction of force-displacement curve from initial loading through post-peak failure. The displacement value should be the vertical (z) displacement at the contact point with the central rod. Label each load with a point number to enable linking the data reported for Question 1 to results reported for questions 2 & 3.


Challenge Question 2: Report a series of x, y, z points that define a line representing the position of the crack tip from the notch as a function of load and displacement from initial loading through post-peak . If there are multiple cracks, report the information for each crack. Data should be reported for same load points reported in Question 1 for the best estimate of the load-displacement curve. Results should be reported with at least the same level of resolution in the force/displacement increments and areal resolution based on force-displacement data that corresponds to a DIC image. Report all values relative to the undeformed original state coordinate system.

Challenge Question 3: Report the displacements (Δx , Δy & Δz in millimeters – change in position relative to the undeformed state) of the front and back faces of the sample for the entire loading cycle for the same load points as in question 1 from initial loading through post-peak failure. Report values relative to the undeformed state coordinate system. Report initial undeformed position of the points (add extra files).

Discussion Question 1: Report variability of your model based on the laboratory calibration data ---does the model have any inherent variability?

Bonus Science Question: Report the x, y, and z coordinates of the two fracture surfaces (in millimeters) at the end (final load) of the simulation based on the best estimate simulation reported for Question 1. **If there is more than 1 crack, report for all.**

Challenge Question 1

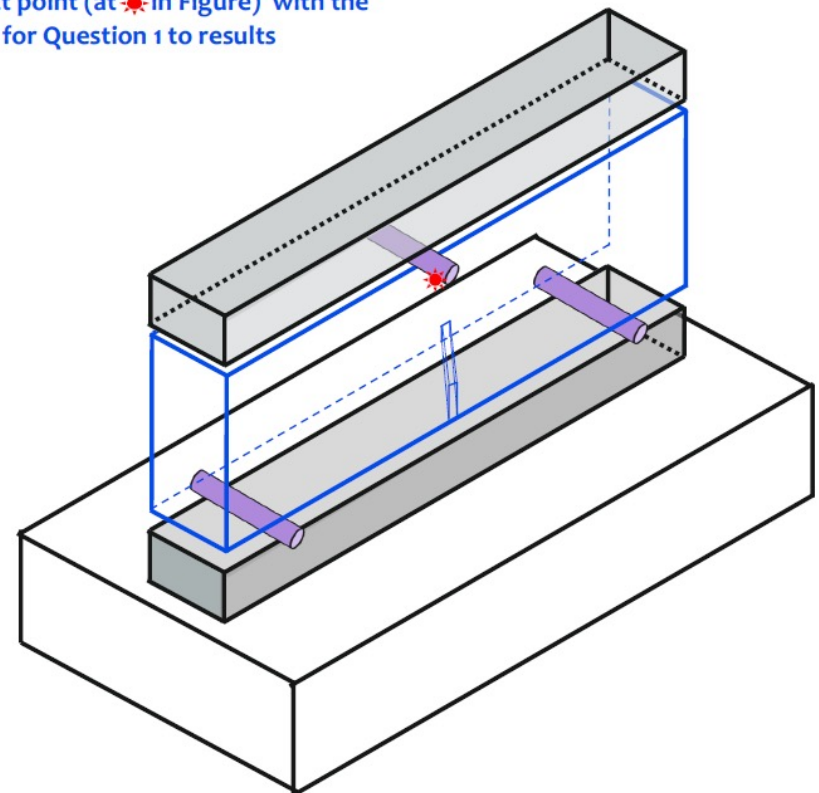
Challenge Question 1: Report the best prediction of force-displacement curve from initial loading through post-peak failure. The displacement value should be the vertical (z) displacement at the contact point (at  in Figure) with the central rod. Label each load with a point number to enable linking the data reported for Question 1 to results reported for questions 2 & 3.

Filename: "teamname_Q1.txt"

File Format: tab delimited text

Example: In columns labeled "Point Number", "Force (Newtons)" and "Displacements (mm)"

Point Number	Force (Newtons)	Displacement (mm)
1	1	0.0001
2	20	0.001
3	130	0.006
.	.	.
.	.	.
.	.	.
.	.	.
.	Peak Load	.
.	.	.
.	.	.
.	.	.
.	.	.
.	.	.



Challenge Question 2

Report all values relative to the undeformed original state coordinate system
 = Report using Eulerian "laboratory" coordinate system

Challenge Question 2: Report a series of x, y, z points that define a line representing the position of the crack tip from the notch as a function of load and displacement from initial loading through post-peak. If there are multiple cracks, report the information for each crack. Data should be reported for same load points reported in Question 1 for the best estimate of the load-displacement curve. Results should be reported with at least the same level of resolution in the force/displacement increments and areal resolution based on force-displacement data that corresponds to a DIC image. Report all values relative to the undeformed original state coordinate system.

File Format: tab delimited text

Filename: "teamname_Q2_crack#_LD_#.txt"

Header: LD Point: (from Q1 report)

Load in Newtons:

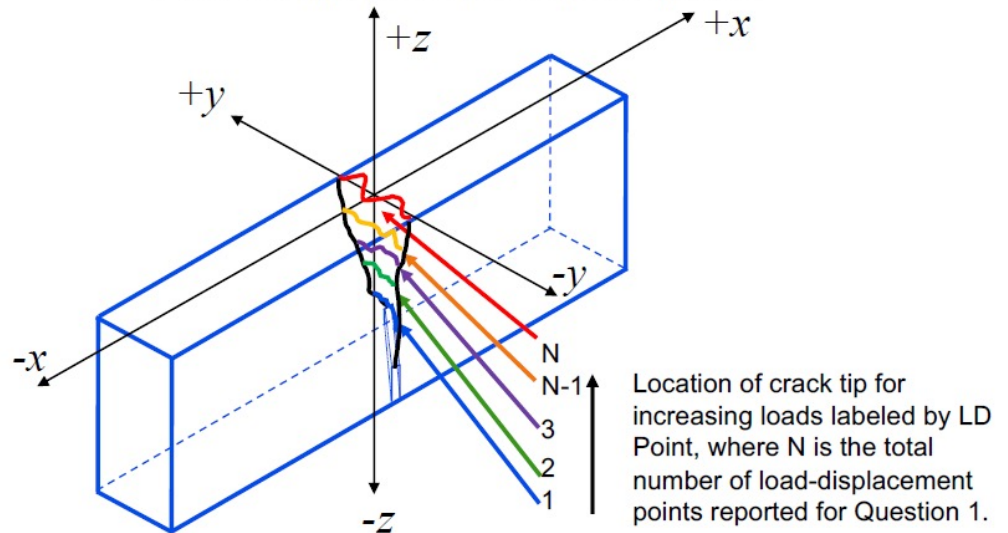
Displacement in mm:

Data: Positions in columns labeled "x (mm)", "y (mm)" and "z (mm)"

Example Files

teamname+Q2_crack1_1.txt			teamname+Q2_crack1_2.txt		
LD Point Number: 1			LD Point Number: 2		
Load in Newtons: 1			Load in Newtons: 20		
Displacement in mm: 0.0001			Displacement in mm: 0.001		
x(mm)	y(mm)	z(mm)	x(mm)	y(mm)	z(mm)
0	-11	-20	0	-11	-20
0	-10.5	-19.3	0	-10.5	-19.3
0.5	-10.1	-19.5	0.5	-10.1	-19.5
-0.1	-9.5	-19.6	-0.1	-9.5	-19.6
.
.
.
.
.
-0.2	11	-19.8	-0.2	11	-19.8

If one crack, then use crack1 in file name. If there are other cracks create additional files and increment the crack# in the filename.
 LD corresponds to the load-displacement point (from Question 1) in the file.
 One file containing the positions per load reported in Question 1.



Challenge Question 3

Challenge Question 3: Report the displacements (Δx , Δy & Δz in millimeters – change in position relative to the undeformed state) of the front and back faces of the sample for the entire loading cycle for the same load points as in question 1 from initial loading through post-peak failure. Report values relative to the undeformed state coordinate system. Report initial undeformed position of the points (add extra files).

Filenames: "teamname_Q3_Front_x_LD#.txt" "teamname_Q3_Back_x_LD#.txt"
 "teamname_Q3_Front_y_LD#.txt" "teamname_Q3_Back_y_LD#.txt"
 "teamname_Q3_Front_z_LD#.txt" "teamname_Q3_Back_z_LD#.txt"

LD# is the load-displacement point number submitted in Question 1.

File Format for Displacement Data: 2D Array of displacements centered relative to the undeformed coordinate system and discretized with $\Delta x = \Delta z = 100$ micrometer

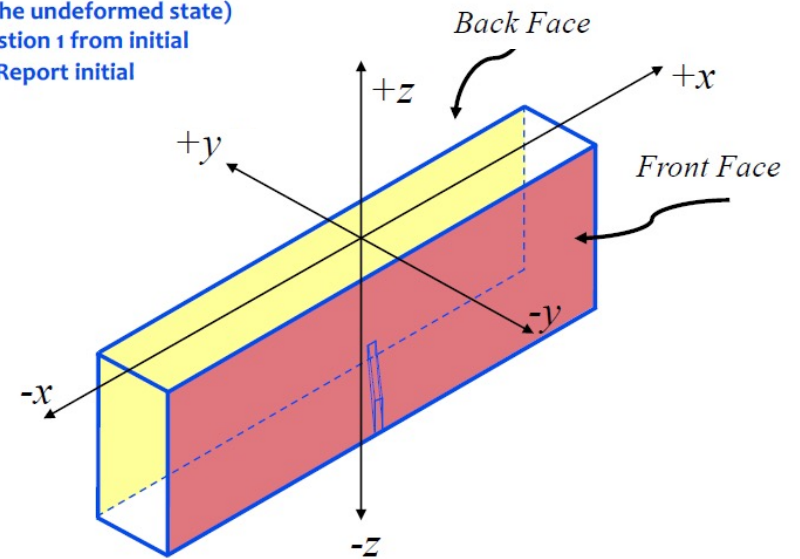
Example Files: teamname+Q3_Front_x-LD1.txt

LD Point: 1
 Load in Newtons: 1
 Displacement in mm: 0.0001

Z=0	0	0.001	0.0008	...	M
	0	0.0005	0.0007
	0.0005	0.0006	0.0007
	0.001	0.0006	0.0006

Z=-Max	N	0.0005	0.001	...	M x N
	x=-0.5L	x=0	x=+0.5LMax		

M means the number of values in the x direction
 N means the number of values in the z direction



Discussion Question 1

Discussion Question 1: Report variability of your model based on the laboratory calibration data ---does the model have any inherent variability?

Filename: “teamname_DQ1_1.txt” or “teamname_DQ1_1.docx”

File Format for Displacement Data: Provide a narrative (it can include graphs, but if you include graphs please send data used to make the graphs as tab delimited text) that addresses:

1. What is the source of the variability in the model (e.g. mesh, computation method, input, scale, calibration of model, calibration data, etc.) and why?
2. Did you calibrate your model with the data provided? If not why? If yes, what data you **used** for calibration? What other data or subject matter expert sources did you rely upon for modeling inputs?
3. If no variability, why not?
4. How was the answer to Question 1 affected by the variability?
5. How did you determine what was the “best estimate” or “best answer” for Question 1 ?
6. Provide a list of references that are most relevant for the methodology that was used.

Bonus Science Question

Potential complications:

- Comparing **stress-free** state for loose chunks not intersecting notch will be tricky
- Quantified roughness might be a more interesting question/comparison
- Who plans to submit response to this question, what are your thoughts?

Bonus Science Question: Report the x , y , and z coordinates of the two fracture surfaces (in millimeters) at the end (final load) of the simulation based on the best estimate simulation reported for Question 1. If there is more than 1 crack, report for all.

Filename: "teamname_BSQ_Surface_1_xyz_crack_1.txt", "teamname_BSQ_Surface_2_xyz_crack_1.txt"

If one crack, then use crack_1 in file name. If there are other cracks, create additional files and increment the crack_# in the filename

File Format for Displacement Data: tab delimited text containing a 2D Array of positions (in mm) relative to the undeformed original state coordinate system discretized with $\Delta x = \Delta y = \Delta z = 100$ micrometer.

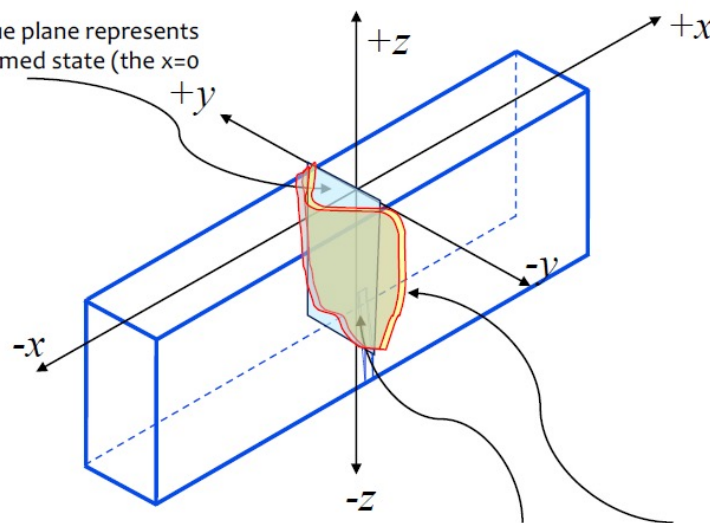
Header: Surface 1 Crack 1

Example Files

teamname_BSQ_Surface_1_crack_1.txt		
Surface 1 – Crack 1		
x	y	z
0.1	0.1	-15.5
-0.1	0.2	-15.5
-0.25	0.3	-15.5
-0.15	0.4	-15.5
0.1	0.5	-15.5
0.2	0.6	-15.5
0.35	0.7	-15.5
.	.	.
.	.	.
.	.	.
.	.	.
.	.	.
.	.	.
.	.	.

teamname_BSQ_Surface_2_crack_1.txt		
Surface 2 – Crack 1		
x	y	z
0.2	0.1	-15.5
0.0	0.2	-15.5
0.25	0.3	-15.5
0.35	0.4	-15.5
0.15	0.5	-15.5
0.22	0.6	-15.5
0.45	0.7	-15.5
.	.	.
.	.	.
.	.	.
.	.	.
.	.	.
.	.	.
.	.	.

The light blue plane represents the undeformed state (the $x=0$ plane).



Measure position of crack surfaces 1 (light gray) and 2 (yellow) & relative to undeformed state (light blue plane).

1/15/22

18

List of expected files

Please select an appropriate team name and substitute that into your filenames. Compress your prediction into one .zip named “teamname_DMC_Prediction.zip”. The zip file should include

“teamname_modelparam.txt”:

Question 1: : “teamname_Q1.txt”

Question 2: “teamname_Q2_crack#_LD_#.txt”

Question 3:

“teamname_Q3_Front_x_LD#.txt”

“teamname_Q3_Back_x_LD#.txt”

“teamname_Q3_Front_y_LD#.txt”

“teamname_Q3_Back_y_LD#.txt”

“teamname_Q3_Front_z_LD#.txt”

“teamname_Q3_Back_z_LD#.txt”

Discussion Question 1:

“teamname_DQ1_1.txt” or “teamname_DQ1_1.docx”

Bonus Science Question:

“teamname_BSQ_Surface_1_xyz_crack_1.txt”

“teamname_BSQ_Surface_2_xyz_crack_1.txt”

Questions? Clarification?

- Coordinate system
- File naming convention
- File format
- Etc...?

See you at AGU!

Tuesday December 13th

- NG22A Fractures, Fracturing, and Fluid Flow: Validation Data Sets, Field & Laboratory Observations, and Computational Challenges I Oral
 - 09:00 - 10:30 McCormick Place – S104b
- NG24B Fractures, Fracturing, and Fluid Flow: Validation Data Sets, Field & Laboratory Observations, and Computational Challenges II Online Poster Discussion
 - 13:45 - 14:45 Online only
- NG25C Fractures, Fracturing, and Fluid Flow: Validation Data Sets, Field & Laboratory Observations, and Computational Challenges III Poster
 - 14:45 - 18:15 McCormick Place – Poster Hall, Hall – A
 - NG25C-0399: The Damage Mechanics Challenge Results: Participant Predictions Compared with Experiment Joseph Morris

Proposed timeline for publication

- Initial method documentation due to Joe in January (see next slide)
- Targeting submission in May 2023
- Structure will be a combined review paper, led by admin team with co-authors from the participating teams
- This follows the style of previous damage mechanics challenges (see Boyce et al., 2014)

Int J Fract (2014) 186:5–68
DOI 10.1007/s10704-013-9904-6

ORIGINAL PAPER

The Sandia Fracture Challenge: blind round robin predictions of ductile tearing

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Abstract Existing and emerging methods in computational mechanics are rarely validated against problems with an unknown outcome. For this reason, Sandia National Laboratories, in partnership with US National Science Foundation and Naval Surface Warfare Center Carderock Division, launched a computational challenge in mid-summer, 2012. Researchers and engineers were invited to predict crack initiation and propagation in a simple but novel geometry fabricated from a common off-the-shelf commercial engineering alloy. The goal of this international Sandia Fracture Challenge was to benchmark the capabilities for the prediction of deformation and damage evolution associated with ductile tearing in structural metals, including physics models, computational methods, and numerical implementations currently available in the computational fracture community. Thirteen teams participated, reporting blind predictions for the outcome of the Challenge. The simulations and experiments were performed independently and kept confidential. The meth-

ods for fracture prediction taken by the thirteen teams ranged from very simple engineering calculations to complicated multiscale simulations. The wide variation in modeling results showed a striking lack of consistency across research groups in addressing problems of ductile fracture. While some methods were more successful than others, it is clear that the problem of ductile fracture prediction continues to be challenging. Specific areas of deficiency have been identified through this effort. Also, the effort has underscored the need for additional blind prediction-based assessments.

Keywords Fracture · Tearing · Deformation · Ductility · Failure · Damage · Crack initiation

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Electronic supplementary material The online version of this article (doi:10.1007/s10704-013-9904-6) contains supplementary material, which is available to authorized users.

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Required, additional documentation (January)

Please provide the following information in a **text or Microsoft Word** document with the filename “teamname_modelparam.txt” which provides the model parameters used to obtain the results reported for Questions 1-3 and Bonus Science Questions 1.

1. Team Members, institutions and email address
2. Approach (e.g. peridynamics, finite elements, particle flow code, etc.)
3. Names and version numbers of all solvers/tools used
4. Boundary Conditions
5. All element types used (including contact, cohesive laws, etc.)
6. Discretization:
 - a. In-plane element size (IP) or range of sizes (any static/dynamic refinement around crack path)
 - b. Through-thickness element size (TT)
 - c. Degrees of freedom for each individual element type and the element type totals (DOF)
7. Process coupling (E.g.: Considerations of the thermal-mechanical coupling)
8. Fracture Method (e.g. element deletion, cohesive surface, etc.)
9. Uncertainty Bounds (Methods used to characterize uncertainty, if any)
10. Material Model
 - a. Elasticity treatment
 - b. Yield surface
 - c. Hardening and/or softening laws
 - d. Use of rate dependence
 - e. Use of temperature dependence or other coupled processes
11. Fracture/Failure Model
 - a. Fracture/Failure criteria
 - b. Damage evolution
 - c. Use of rate dependence, temperature dependence or other coupled processes
12. Calibration Data that was used [e.g. longitudinal tensile, transverse tensile, notched tensile, and other literature source].
13. Any other information that you feel is relevant or important to report.



**Lawrence Livermore
National Laboratory**