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(U) Marker Lagrangian Simulations using Geometry From CAD Assembly Files



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Abstract The Eulerian code PAGOSA now contains an option for the forward time integration of any user selected material in the Lagrangian frame of reference. This option is accomplished using a Multifield version of Brackbill's FLIP plus Sulsky's MPM. FLIP+MPM is a Marker Lagrangian scheme that is not to be confused with well known Grid Lagrangian schemes. This Marker Lagrangian method allows materials to undergo completely arbitrary deformation, up to and including fracture and separation. Using this option makes PAGOSA into a mixed frame simulation tool such that fluids can be integrated in the Eulerian frame and solids integrated in the Lagrangian frame. Boundaries between the fields are said to be 'immersed' in the computational domain, and their nature is formulated using Multifield Theory.

Each Marker in a field of FLIP+MPM material tracks the thermodynamic state of a small (but finite) piece of mass. Initiation of the Markers using the geometry and material information from CAD Assembly files is the subject of the talk. The ease and speed with which the dynamics of the assembly can be studied is demonstrated.

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Outline

- Sketch of Marker Lagrangian vs Grid Lagrangian.
- Sketch of the Marker Lagrangian Full Stress.
- Sketch of the I1–J2 model for Macroscale Fracture.
- Step2Abaqus.py, PartsList.py, Abaqus2Pagosa.py.
- Example: Eglin's Spear Impacting Rock.

Sketch of Marker Lagrangian vs Grid Lagrangian.

- The ‘Grid Lagrangian’ finite element method uses one set of points for storing the primitive data for the thermodynamic state. A set of COLLOCATION points WITHIN the primary points are used for computation of spatial gradients needed for advancing the state on the primary points. Boundaries between different materials are defined by the faces of finite elements formed by the primitive points.
- Because the COLLOCATION points are WITHIN the primitive points the COLLOCATION grid can become seriously distorted (like in a pure shear) such that the accuracy of the integration is hopelessly poor.

- The ‘Marker Lagrangian’ finite element method likewise uses one set of points for storing the primitive data for the thermodynamic state, which includes of a FINITE MASS OF MATERIAL. The COLLOCATION points needed for computation of spatial gradients are furnished by a cartesian grid that overlies the primitive points. Using a large enough marker density on this grid produces a solution whose accuracy is controlled by the size of the grid. (As a rule of thumb, a 3x3x3 array is sufficient for convergence.) Importantly: bodies described by the primitive points can undergo arbitrary distortion with no degradation in the accuracy of the solution.
- Each Marker Lagrangian field contains the state for one material, and is user specified. Boundary conditions between the user specified fields are said to be ‘immersed’ in the domain. Forces at the boundaries are formulated by multifield theory.

Sketch of the Marker Lagrangian Full Stress

- Full stress in rate form.
- Acceleration by the mean stress.

Sketch of the I1–J2 model for Macroscale Fracture.

$$\mathbb{P}_f \doteq \sqrt{\mathbb{P}_b^2 + \mathbb{P}_s^2} ; \quad (1)$$

$$\mathbb{P}_s = \varepsilon^* \exp(\Delta \ln W_s - A^*) ; \quad (2)$$

$$\mathbb{P}_b = \delta^* \exp(\Delta \ln W_b - A^*) ; \quad (3)$$

$$A^* = A_0 L^* [q W^* \exp(1 - q W^*)] ; \quad (4)$$

$$W^* = \max(W_{bf}, W_s) / W_{su} ; \quad (5)$$

$$L^* = 1 + \ln [\max(1, \Delta x / L_\alpha)] . \quad (6)$$

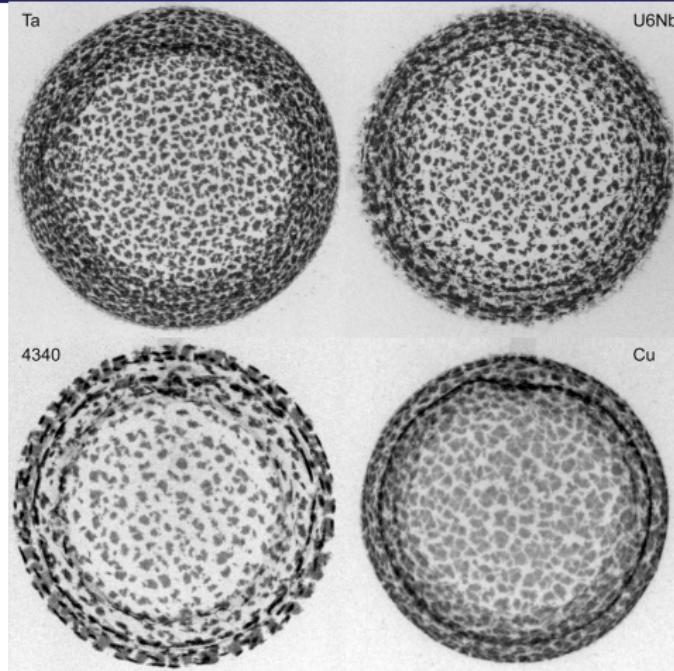
- $(\varepsilon^*, \delta^*)$ are shear and volumetric ‘Griffith’ criteria.
- (W_s, W_b) are shear and volumetric work.
- The function A^* depends on the shear work, and is new.
- The function L^* connects A^* to the microscale, and is new too.

Larry Hull's HE filled Hemispherical Shell: Verification.

Another View.

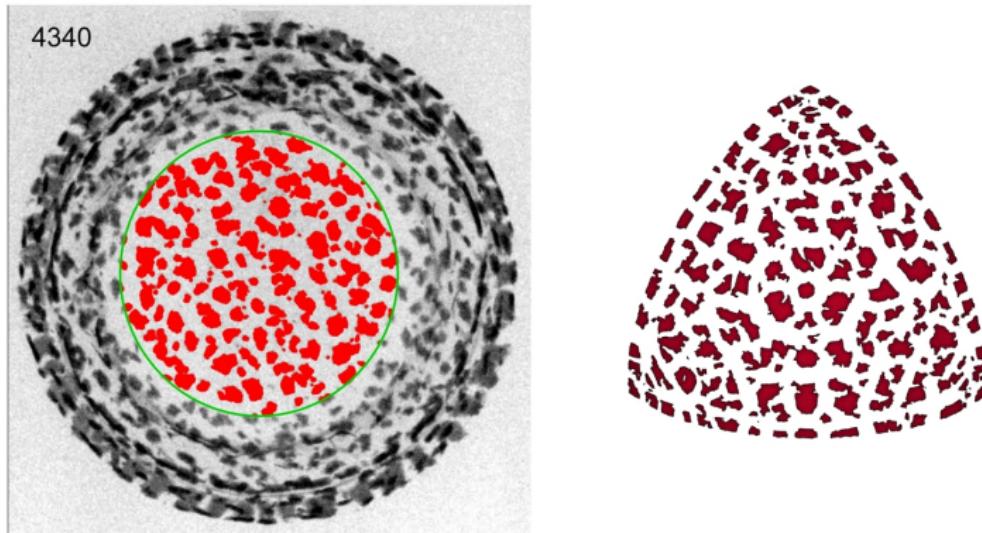
Filled Hemi Fragmentation Data¹.

Clockwise from upper left: Ta, U6Nb, Cu, 4340 annealed.



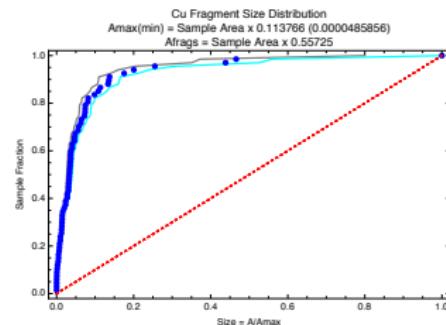
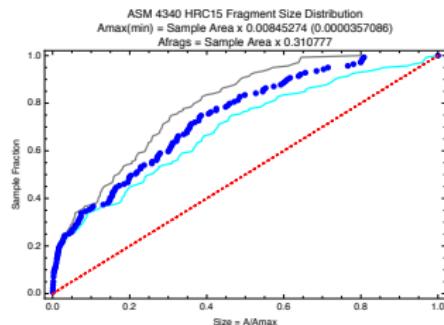
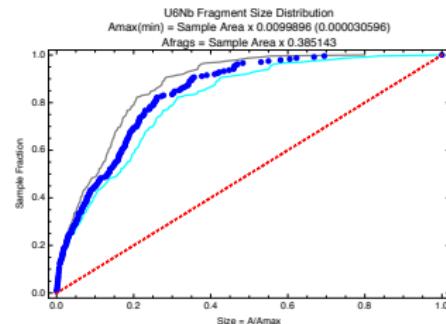
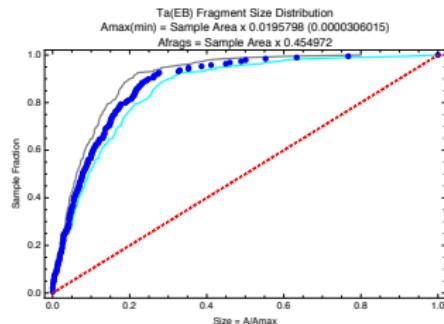
¹L. M. Hull, M. E. Briggs, G. T. Gray III, E. K. Cerreta, B. A. Kashiwa, & D. J. Alexander, Necking and Momentum Redistribution during the Expansion of Explosively Driven, U6Nb Hemispherical Shells, (2020).

Filled Hemi Fragmentation Data.



HE-filled hemispherical shell of steel alloy 4340-RC15 (annealed). Radiograph is on the left, with a region of interest drawn in green; fragments found by counting pixels in the dark regions are shown in red. Calculation on the right is shown at a scale corresponding to the experiment on the left.

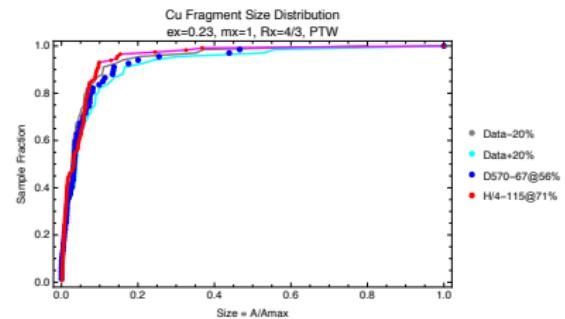
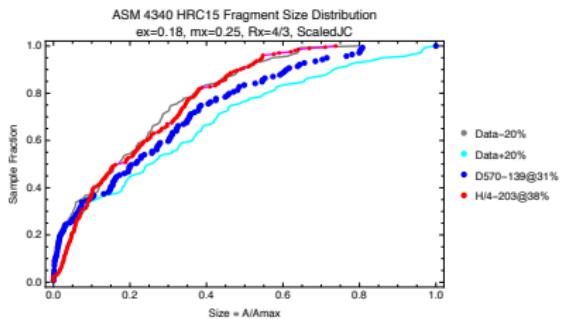
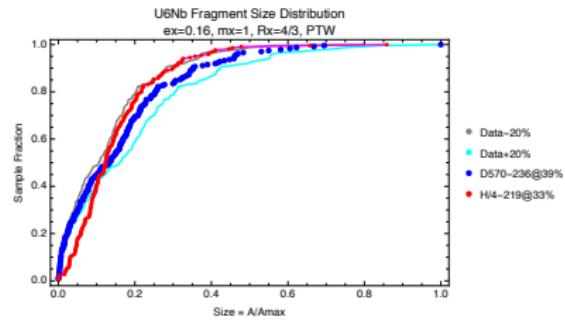
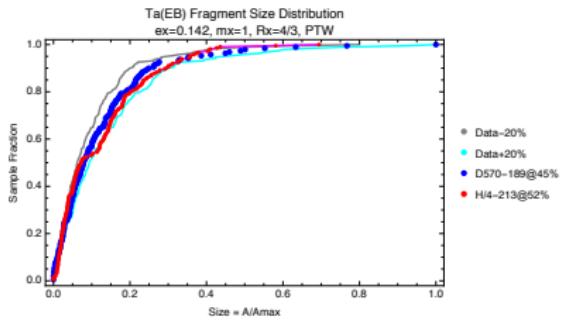
Filled Hemi Fragmentation Data.



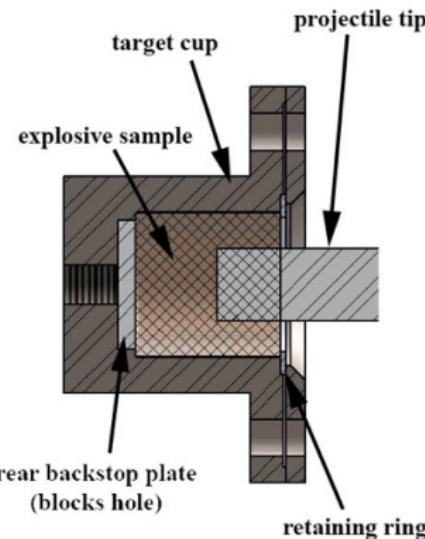
Data showing approximate total error bounds.

Filled Hemi Fragmentation Data.

Calculation compared to data.



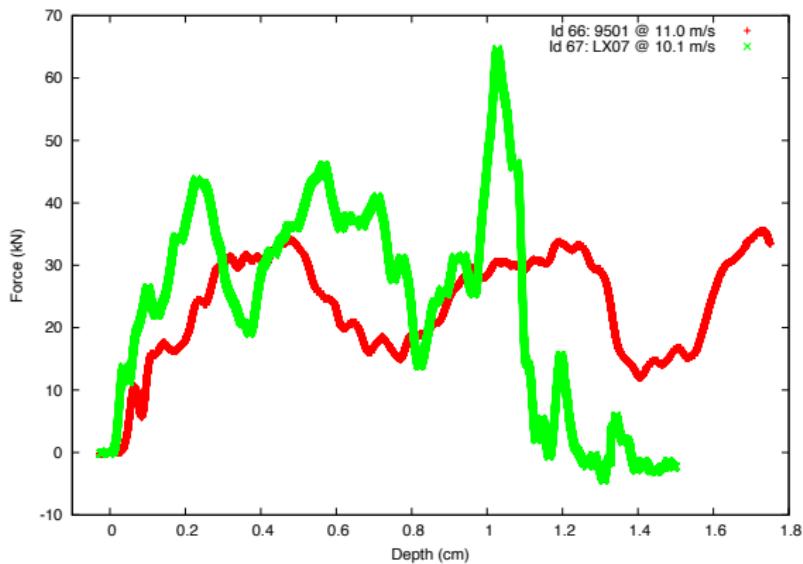
Matt Holmes *et al* Punch Gun². Target.



Target geometry, depicting projectile penetrated to full design depth of 1.1 cm.

²M. D. Holmes, P. Rae, & G. R. Parker (2018) "Viscous Heating via Low-Velocity Crushing Impact of High Explosives", LA-UR-18-25825, Presented at the 16th International Symposium on Detonation, Cambridge, MD, 07/15/2018.

Matt Holmes *et al* Punch Gun Force Data.



Force vs Penetration Depth for Test IDs 66 & 67.

Punch Gun Test 66: 9501.

Punch Gun Test 67: LX-07.

PG Test67

Pagosa FLIP+MPM Simulation Test 66: 9501.

PG Simulation of Test66

Step2Abaqus.py, PartsList.py, Abaqus2Pagosa.py.

- Step2Abaqus.py is a macro for ABAQUS CAE for reading a CAD Assembly file *.stp.
- PartsList.py is a standalone python script for reading CAD Assembly files *.dat, which contain the MATERIAL and MASS data corresponding to *.stp
- Abaqus2Pagosa.py is another macro for ABAQUS CAE for making arbitrary tet meshes on each part and writing Pagosa-readable files for Marker initialization.
- These scripts are used to write a *.csv (spreadsheet) file, used for grouping the parts into Pagosa ‘Fields’.

Example: Eglin's Spear Impacting Rock.

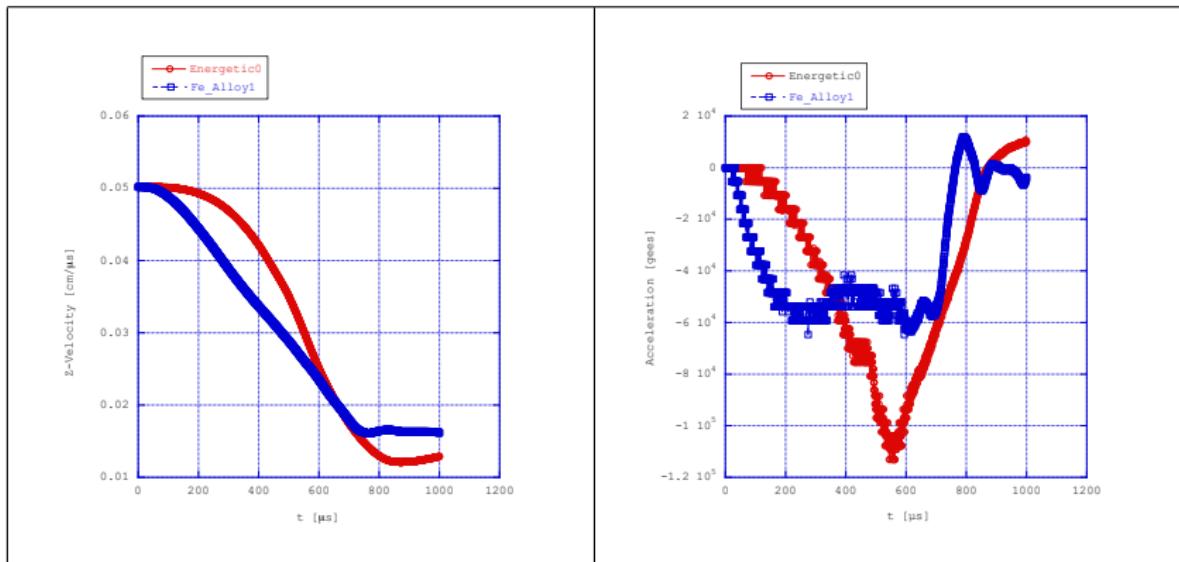
Spear Simulation 1

Eglin's Spear into STRONG basalt.

Spear Simulation 2

Eglin's Spear into Strong rock.

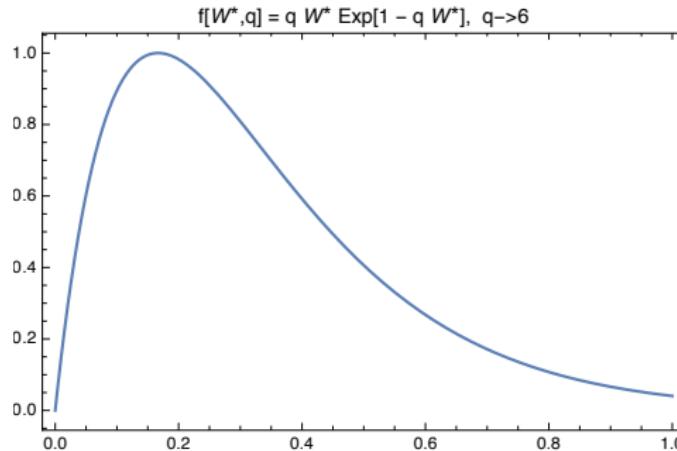
Simulation Mean Velocity and Acceleration.



Gauging the Model Coefficients.

The value of q .

- The function $f[W^*, q] = [qW^* \exp(1 - q * W^*)]$ is the Poisson Distribution. It is used to 'Activate' the Fracture Propensity as the necking instability becomes intense. The function looks like this:



Gauging the Model Coefficients.

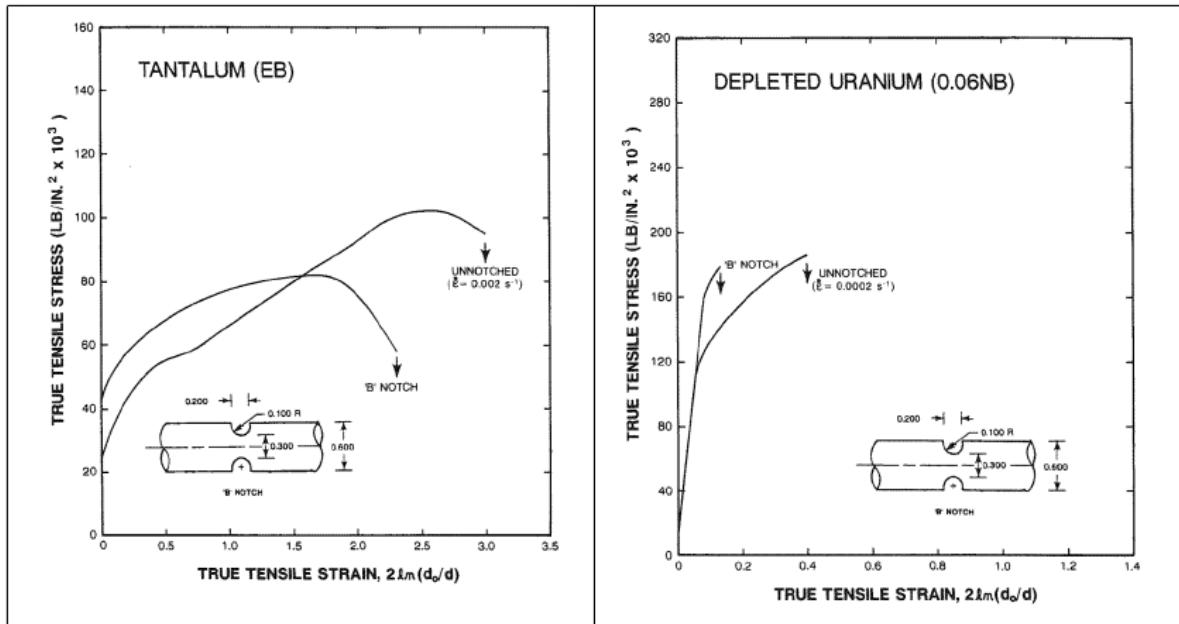
The value of q .

- In a quasistatic tensile test the onset of necking is denoted by a sudden (downward) change in the force versus displacement curve. We associate the maximum of $f[W^*]$ with the onset of necking.
- Let W_n^* be the shear work done at the onset of necking scaled by the work done at Fracture in the test. Hence

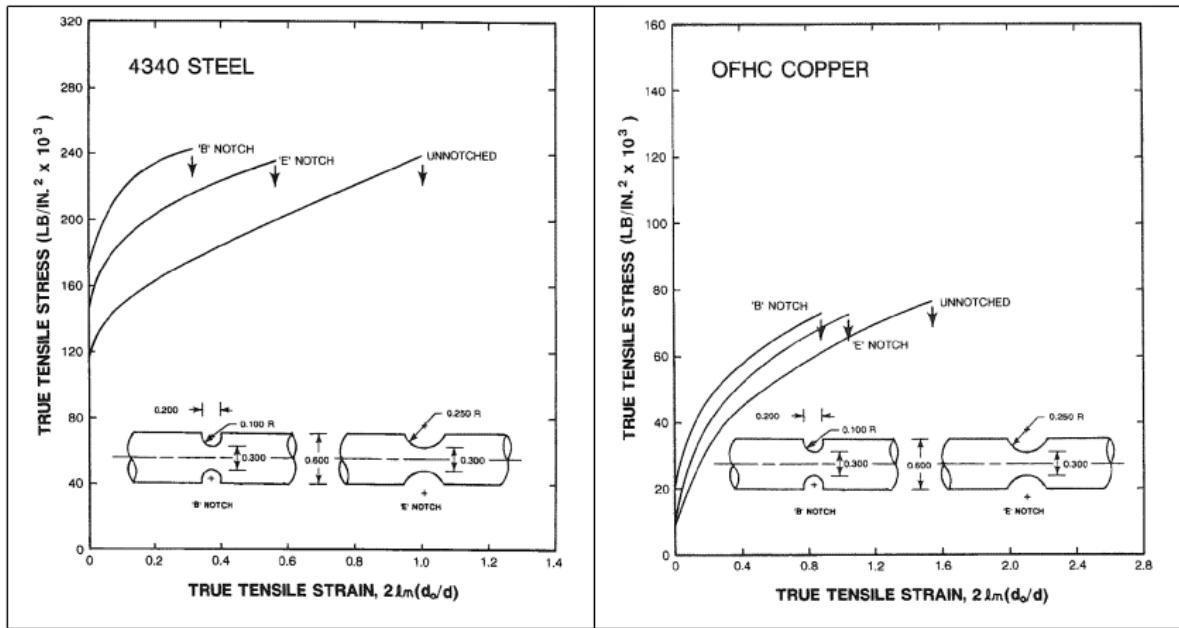
$$q = 1/W_n^* . \quad (7)$$

Quasistatic Tensile Test Data.

Data from Johnson & Holmquist (1989), LA-11463-MS.



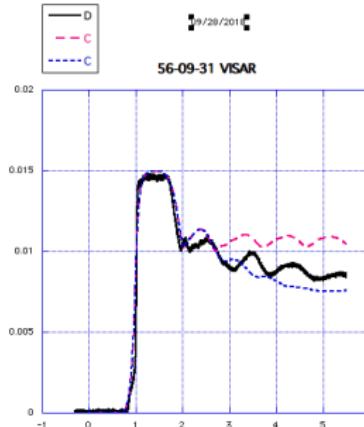
Quasistatic Tensile Test Data.



Gauging the Model Coefficients.

The value of A_0 .

- With the value of q known we can obtain the value of A_0 by using data from the well-known spall fracture test. In this the volumetric Griffith criterion reduces to $\delta^* = \sigma_{sp}/\sigma_f > 1$.
- The spall strength is estimated from the so-called velocity pull back Δu , using $\sigma_{sp} = 2\rho_0 c_b \Delta u$. The log work at spall $\Delta \ln W_{sp}$ can be computed using the measured pullback. Typical data for OFHC copper (as hot rolled) looks like this (from Ellen Cerreta, et al.)



Spall Strength Data.

Data for Ta and U6Nb, from C. E. Morris³.

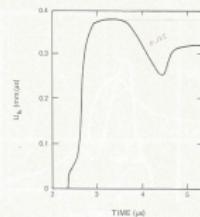
TARGET
 Material: Tantalum
 Experiment type: Pre-surface capacitor
 Experimentator: C. E. Morris
 References: R. G. McQueen, S. P. Marsh, J. W. Taylor, J. N. Fritz,
 and W. J. Carter (1970)
 Shot no.: 56-67-432 Date: February 7, 1967
 Thickness: 16.68 mm Diameter: 38.1 mm
 Density: 16.68 g/cm³
 $C_1 = 4.34 \text{ mns}/\mu\text{s}$ $C_2 = 2.16 \text{ mns}/\mu\text{s}$

IMPACTOR
 Tantalum, 1.05 mm thick, backed with low-density polyethylene
 Impact velocity: 0.590 mns/μs

TRANSDUCER Pre-surface capacitor

NOTES

Shot 56-67-432, 56-67-438, and 56-67-459 are a series of over-taking shock wave profiles at a constant impact velocity.

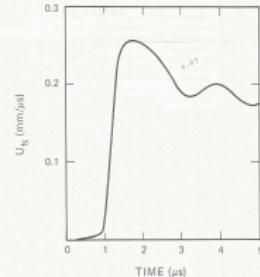


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TARGET
 Material: 94 wt% titanium with 6 wt% niobium
 Experiment type: Pre-surface capacitor
 Experimentator: C. E. Morris
 Shot no.: 56-75-20 Date: June 27, 1975
 Thickness: 12.6 mm Diameter: 41.3 mm
 Density: 17.47 g/cm³
 $C_1 = 2.39 \text{ mns}/\mu\text{s}$ $C_2 = 1.28 \text{ mns}/\mu\text{s}$

IMPACTOR OFHC copper, 4.24 mm thick, backed with low-density polyethylene foam, (rounded on 51-mm-diam titanium alloy projects)

TRANSDUCER Pre-surface capacitor
 Type: Relative

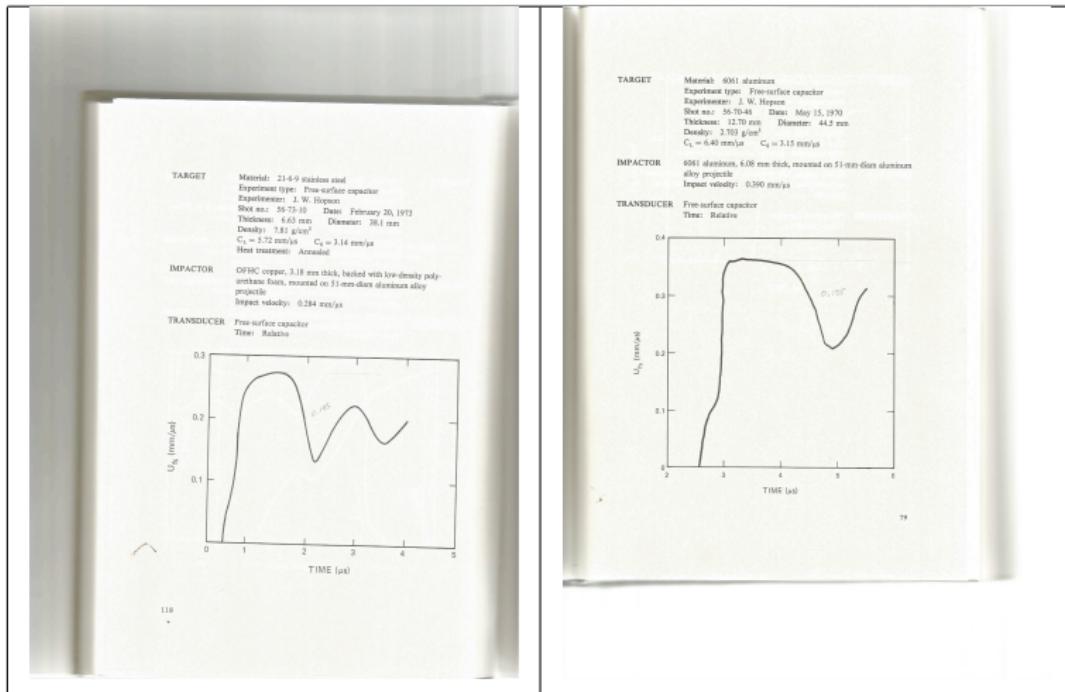


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³C. E. Morris, ed., *Los Alamos Shock Wave Profile Data*, University of California Press (1982).

Quasistatic Tensile Test Data.

Data for SS and Al-6061, from C. E. Morris[2]



Gauging the Model Coefficients.

The value of A_0 .

- Using the measured Δu we get $\Delta \ln W_{\text{sp}} = 8/5$.
- Accordingly

$$A_0 = \frac{8/5 + \ln(\sigma_{\text{sp}}/\sigma_f)}{L^*[h]f[W_{\text{sp}}^*, q]} . \quad (8)$$