FAILPROB--A Computer Program to Compute the Probability of Failure of a Brittle Component

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Sandia National Laboratories

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Abstract

FAILPROB is a computer program that applies the Weibull[1] statistics characteristic of brittle failure of a material along with the stress field resulting from a finite element analysis to determine the probability of failure of a component. FAILPROB uses the statistical techniques for fast fracture prediction (but not the coding) from the N.A.S.A. - CARES/life[2] ceramic reliability package. FAILPROB provides the analyst at Sandia with a more convenient tool than CARES/life because it is designed to behave in the tradition of structural analysis post-processing software such as ALGEBRA[3], in which the standard finite element database format EXODUS II[4] is both read and written. This maintains compatibility with the entire SEACAS[5] suite of post-processing software.

A new technique to deal with the high local stresses computed for structures with singularities such as glass-to-metal seals and ceramic-to-metal braze joints is proposed and implemented. This technique provides failure probability computation that is insensitive to the finite element mesh employed in the underlying stress analysis.

Included in this report are a brief discussion of the computational algorithms employed, user instructions, and example problems that both demonstrate the operation of FAILPROB and provide a starting point for verification and validation.

Acknowledgment

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Introduction

Modeling and simulation are playing an increasing role in the design of nuclear weapons components. Modeling and simulation in connection with appropriate testing have the ability to provide significant advantages in cost, reliability, and design times. Over the past several years, our capabilities to analyze complex structures have improved markedly. With the increases in hardware speed and software capabilities we are able to model structures in unprecedented detail (millions of elements)[6]. In addition, recent constitutive model developments[7] have enabled increased accuracy in prediction of stress and strain fields.

Numerous nuclear weapon components (neutron generators, radars, sprytrons, strong-links, lightning arrestor connectors, etc.) depend upon the use of brittle materials, typically glass or ceramic. These materials are used in applications requiring high voltage standoff and hermetic sealing. These applications typically require joining the brittle material to a metal (direct glass-to-metal, ceramic-to-metal braze, solder, etc.) at an elevated temperature with the subsequent differential contraction during cool-down. Thus stresses arise from manufacturing operations as well as normal use and abnormal environments. Despite the advances that have been made in modeling and simulation, our ability to predict the failure of brittle components in the absence of a single, identified, dominant flaw has remained at a rudimentary level. In practice, for structures that contain a brittle component (ceramic, glass, etc.), the structure is modeled at the appropriate level of detail and the maximum principal stress in the brittle material is compared to some "rule-of-thumb" safe level of stress. This approach was quite useful in the days of crude models, large design margins, and extensive testing. However, a more accurate approach is both appropriate and required in the modern regime of detailed models, shrinking design margins, limited testing, and reliability prediction requirements.

As a first step in increasing the accuracy of our failure predictions we have obtained the CARES/LIFE package of codes from N.A.S.A. Glen Research. This package of codes provides software to produce Weibull[1] failure statistics from experimental results obtained using any type of test specimen. Numerous common specimen types are hard-coded in the software. However, unusual specimen types can be accommodated through the provision of a finite element analysis of the failure specimen along with the test results. A second module of the CARES/LIFE package uses the Weibull failure statistics to post-process finite element results of any structure to produce a probability of failure. This post-processing allows for the assessment of fast-fracture, cyclic fatigue, and slow, environmentally assisted crack growth (sub-critical crack growth). Unfortunately, the CARES/LIFE package is not particularly convenient to use in the structural analysis environment within the engineering sciences directorate at Sandia National Laboratories. Direct use of the CARES/LIFE package requires a multi-step procedure. The EXODUS II[4] finite element output data base must first be translated into a CARES/LIFE specific ASCII neutral file. For large models, translation into an ASCII format can produce excessively large files. The appropriate software from the CARES/LIFE package must then be run, producing another ASCII file. Finally, this output file must be translated into a format compatible with a plotting package for viewing. The first step of the process, the translation

from EXODUS II into CARES/LIFE neutral file format has been written and is available, but the subsequent translation to a plotting package has not been pursued. Instead, a stand-alone post-processing code, FAILPROB, has been written. FAILPROB provides the fast fracture failure prediction capability of CARES/LIFE in a traditional structural analysis post-processing environment. FAILPROB is designed to behave in a very similar manner to ALGEBRA[3], a well known and widely used post-processing code. That is, it reads and writes the EXODUS II finite element data base, thus eliminating the need for translator codes and maintaining compatibility with Sandia's entire SEACAS[5] finite element analysis post-processing environment.

A technique to accomodate the high local stresses computed for structures with material interfaces that can lead to a singularity such as glass-to-metal seals and ceramic-to-metal braze and solder joints is proposed and implemented. This technique provides failure probability computation that is insensitive to the finite element mesh employed in the underlying stress analysis. This technique includes parameters which must be experimentally verified. Reasonable values for these parameters have been set in the code and they are identified in the text. The required experimental verification is underway.

There may be some set of circumstances in which the use of the original N.A.S.A. CARES/LIFE coding is preferred to the use of FAILPROB. In this case, a translator program, EXOCAR, that reads the EXODUS II data base and produces the ASCII file required as input to CARES/LIFE has been written. The CARES/LIFE code package is available on the "JAL LAN" maintained by 9100.

Included in this report is a brief discussion of the application of Weibull Statistics to the prediction of brittle failure. Computational algorithms and their numerical implementations are presented. A set of example problems that demonstrate the operation of FAILPROB and begin the verification and validation process is included. Finally, a description of the process to execute the code and a description of the user input commands are given.

Weibull Approach to Brittle Components

McLean and Hartstok[8] have presented an excellent discussion of the application of Weibull statistics to the design of ceramic components. The brief summary presented below draws extensively from both this book and the CARES/LIFE manual[2].

The Weibull approach to failure of brittle components has its fundamental basis in weakest-link theory. As its name implies, the simplest explanation of weakest-link phenomena applies to a chain composed of discrete links. As the chain becomes longer (more links), the probability of encountering a relatively lower strength link increases. Thus, longer chains, on average, have a lower strength that shorter chains. In applying this concept to brittle materials like ceramic and glass, the chain links are transposed into volumes of material. Thus, the probability of failure increases not only with increasing applied stress but also with increasing volume of material at stress. That is, a larger volume of a brittle material will exhibit a lower average strength than smaller volume of the same material subjected to the same stress state. There is also a flavor of fracture mechanics to this approach in that the underlying assumption is that a ceramic part fails when an inherent flaw is subjected to a critical stress. The flaws in a ceramic part are assumed to be random in size and orientation, thus producing a statistical distribution in strength. As employed in the CARES/LIFE package and thus here, the failure probability (for a one dimensional stress state) can be written as:

$$P_f = 1 - e^{\left[-\int \left(\frac{\sigma - \sigma_u}{\sigma_0} \right)^m dV \right]} \tag{1}$$

where P_f is the probability of failure, σ_u is the threshold value of stress below which no failure can occur, m is the Weibull modulus, and σ_0 is the Weibull scale parameter. For ceramics, σ_u is normally taken to be zero. Since there is no generally accepted threshold stress value, this is convenient while adding a slight but unknown amount of conservatism. Both the Weibull modulus and the Weibull scale parameter may be regarded as material parameters derived from materials testing[9,10]. The Weibull modulus can be thought of as a measure of the variability in the distribution of strength. The lower the Weibull modulus the more variability in the data. The Weibull scale parameter must not be confused with the characteristic strength. The characteristic strength is specific to the specimen geometry from which it was derived. The Weibull scale parameter is more akin to a material property and can be determined from the characteristic strength given knowledge of the stress distribution and the geometry of the test specimen. Simple equations exist that permit the Weibull scale parameter to be determined from the characteristic strength for many commonly used test specimen geometries. In the simplest case, where the characteristic strength came from a tensile specimen of unit volume, the Weibull scale parameter has the same numeric value as the characteristic strength. In general, this is not the case. Characteristic strength has units of stress while, as came be seen from equation 1, the Weibull scale parameter has units of (stress) x (volume)$^{1/m}$.

Principle of Independent Action (PIA) Technique

Two common techniques were selected to expand the concept defined in equation 1 from a uniaxial stress state to a fully three-dimensional stress state. In the first technique, the PIA method, the stress tensor is transformed into its three principal stresses. Each of the three principal stresses is assumed to act independently. Thus, equation 1 is transformed into the following:

$$P_f = 1 - e^{-\left[\frac{1}{\sigma_0{}^m}\int (\sigma_1{}^m + \sigma_2{}^m + \sigma_3{}^m)dV\right]}$$

(2)

where the terms are the same as defined in equation 1. σ_1, σ_2, and σ_3 are the principal stresses. No negative (compressive) values for principal stress are allowed. If a principal stress is compressive, it is replaced by zero in equation 2. While it is not inconceivable that Weibull statistics could be applied to compressive failures, most brittle materials are very much stronger in compression than they are in tension. In keeping with this strength disparity, most test specimens are designed to determine tensile strength. Finally, all the anticipated applications involve tensile failure, not compressive failure.

Weibull Normal Stress Averaging Technique

The second method used to expand the failure probability calculation to a three-dimensional stress state is the Weibull normal tensile stress averaging technique. Here the failure probability is described by:

$$P_f = 1 - e^{-\left[\int_V k\bar{\sigma}_n{}^m dV\right]}$$

(3)

where:

$$\bar{\sigma}_n{}^m = \frac{\int_A \sigma_n{}^m dA}{\int_A dA}$$

(4)

and

$$k = (2m+1)\frac{1}{\sigma_0{}^m}$$

(5)

10

The area integration of equation 4 is performed in principal stress space over the surface, A, of a unit sphere. In the numerator of equation 4, σ_n is the stress normal to the surface of that unit sphere. As described for the PIA method, only tensile normal stresses are employed, compressive normal stresses are replaced by zero. In practice, this integration is performed numerically. A triangular finite element mesh is placed on the surface of one-eighth of a unit sphere. The area and the surface normal are computed for each triangular element. The stress tensor is resolved into its principal components and the dot product is taken with each element's surface normal unit vector. This dot product (if positive) is multiplied by the surface area of the element and then a summation is made over all the elements that make up the one-eighth sphere. The finite element mesh was refined until the error in this numerical integration was reduced to less than 0.01 percent. This procedure is much more efficient than integration using spherical coordinates. Use of a finite element mesh produces area segments of nearly equal areas whereas use of spherical coordinates results in area segments degenerating into thin slivers near the pole. It should be noted that it is the use of principal stress components that allows the integration to be limited to only one-eighth of the unit sphere. Therefore, if principal stress components are not included in the EXODUS II data base, they are computed within FAILPROB. The normalizing term, k, described in equation 5, is required to enforce compatibility between equation 1, originally derived for a uniaxial stress state, and equation 3 when equation 3 is applied to uniaxial tension.

Treatment of Singularities

The use of Weibull statistics for failure prediction of brittle components was pioneered for bulk parts, of sizes on the order of or bigger than the standard test specimens used to collect the statistics. In a typical application at Sandia, the ceramic is joined to a dissimilar material either directly (glass-to-metal seals) or through the use of a braze or solder alloy. This type of joint gives rise to a region of very high stress and stress gradient at the material interface. In elasticity theory, this interface is the location of a singularity. Thus for the class of problems of interest at Sandia, it is necessary to accommodate analytical singularities.

Singularities severely complicate the prediction of failure. Singularities introduce a mesh sensitivity issue with the computation of stress. In a singular field, the computed stress does not converge to single value with refinement of the finite element mesh. In fact, as the mesh is refined, the maximum stress computed tends to diverge. That is, for each halving of the length of an element side, the stress will typically more than double. In classical fracture mechanics, singularities are treated either through the use of a characterizing parameter (K_{Ic}) or through the use of path independent integrals (J_{Ic}). These approaches are not ideal for our applications due to the complex nature of the joints. These joints are rarely simple geometrically, making definition of contour integral paths difficult. On the other hand, the joint will typically contain a ductile material, metal part or braze alloy. Nonlinear material behavior, metal plasticity, or creep severely complicate characterization of the singularity. In addition, the use of Weibull statistics for failure prediction implies a stress value raised to some power (see Equation 1). That power can be very large, on the order of 20 or more[9,10]. Thus the use of Weibull statistics directly for failure prediction in the presence of

a singularity can result in a worse answer than the use of a simple maximum stress failure criterion.

The approach selected for implementation here is based on another classical technique for accommodating discontinuities in a finite element solution, the introduction of a length scale. A very convenient length scale for brittle materials is the critical flaw size. This can be obtained from the Weibull scale parameter and the fracture toughness of the material as:
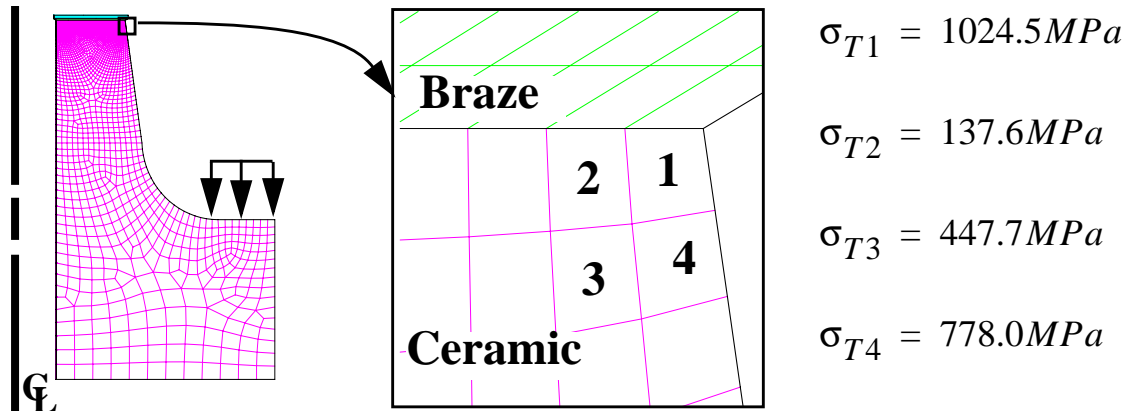
$$a_{cr} = \frac{K_{Ic}^2}{\pi \sigma_{cs0}^2} \tag{6}$$

where a_{cr} is the critical flaw size, K_{Ic} is the mode I fracture toughness and σ_{cs0} is the characteristic strength of a unit volume of the material subject to a uniform tensile stress, the same numerical value as the Weibull scale parameter but with units of stress rather than stress times volume to the power of the inverse Weibull modulus. Within an element of this size near a singularity elasticity theory is assumed to no longer apply. This is not an onerous assumption. Fracture mechanics implies that a flaw of this length, appropriately oriented, exists at the point of failure. Clearly, over the scale of an element with the assumption of the existence of a flaw the size of that element length, the material is no longer an isotropic elastic solid. Therefore, assigning a stress value to these elements using an alternate basis should not be considered a high crime against the purity of the finite element process. The selection of a_{cr} as the length scale has some effect on the computed probability-of-failure. The results of validation experiments (currently underway) are required to determine if some modification of the length scale selection will be required.

For the explanation of the singularity processing below and all the subsequent example problems in the next section, properties for an AlSiMag 771, 94% alumina,[11] are used. These are, the Weibull scale parameter, σ_0, is 325 MPa-mm$^{3/22}$, the Weibull modulus, *m*, is 22, and the critical flaw size, a_{cr}, is 0.05 mm. As discussed above, the characteristic strength of a uniform tension, unit volume specimen is 325 MPa, the same numeric value as the Weibull scale parameter.

Within the FAILPROB code, singularities are accommodated via the following procedure:

1. The singularity is detected. A singularity is defined via three criteria. First, the entire region of interest is searched for the element with the highest value of maximum principal stress (element 1 in the ceramic material shown in Figure 1). The value of maximum principal stress in this element must be greater than the Weibull scale parameter. This is a very pragmatic criterion. In Equation 1 the stress is divided by the Weibull scale parameter. If this ratio is less than one, then there is no concern with raising it to an arbitrarily large power. A problem only exists if this ratio is greater than one, in which case raising it to a very large power can completely dominate the rest of the solution out of proportion to the volume of material at this high stress. Second, the element size must be smaller than the critical flaw size. The underlying assumption

behind this criterion is that if the element is large enough, then the stresses computed within it make sense and should be used without modification. Use of the critical flaw size for this criterion is quite conservative. The final criterion is based on a stress jump. All elements of the same material surrounding the element identified above are sampled. The element with the lowest maximum principal stress is used to form a stress gradient. This largest local difference in maximum principal stress is divided by the distance between the element centroids and this result is compared to a critical jump value. This critical jump value is arbitrarily assigned the value of the uniform tension, unit volume characteristic strength divided by twice the critical flaw size for now. As experience is gained, this critical jump value can and will be adjusted for optimal performance..

$\sigma_{T1} = 1024.5 MPa$

$\sigma_{T2} = 137.6 MPa$

$\sigma_{T3} = 447.7 MPa$

$\sigma_{T4} = 778.0 MPa$

Criteria

- The maximum principal stress in element 1 is greater than the uniform tension, unit volume characteristic strength. (1024.5 MPa> 325. MPa)

- Element 1 is smaller than the critical flaw size. (0.014 mm < 0.05 mm)

- The maximum principal stress in element 1 minus element 2 divided by the distance from element 1 to element 2 is greater than the Weibull scale parameter divided by twice the critical flaw size. (63,350 MPa/mm > 3250 MPa/mm)

All three criteria have been met, therefore a singularity has been detected.

Figure 1.   Criteria for detection of a singularity

2.   The singularity is then characterized. Using the same elements that displayed the maximum and minimum stress discussed above, a direction is defined as shown in Figure 2 from element 1 (maximum stress) to element 2 (local minimum stress). Data (stress, distance from singularity) are gathered from elements along this direction until any one of four conditions are met: a) the distance from the singularity is ten times the critical flaw size; b) a local minimum in stress (more than one element to guard against oscillations due to hour-glass deformations) is detected; c) one hundred stress/distance data pairs have been accumulated d) a material interface is encountered. This gives a

Process Until

- $d \geq 10(criticalflawsize)$

  or

- $\sigma_n > \sigma_{n-1}$ and $\sigma_n > \sigma_{n-2}$

  or

- $n = 100$

Figure 2.   Accumulate stress/distance data pairs for least squares fit

$\sigma = A(d^n)$

A = 119.1 MPa

n = -.412

cap = 507.7 MPa

Original FEM Results
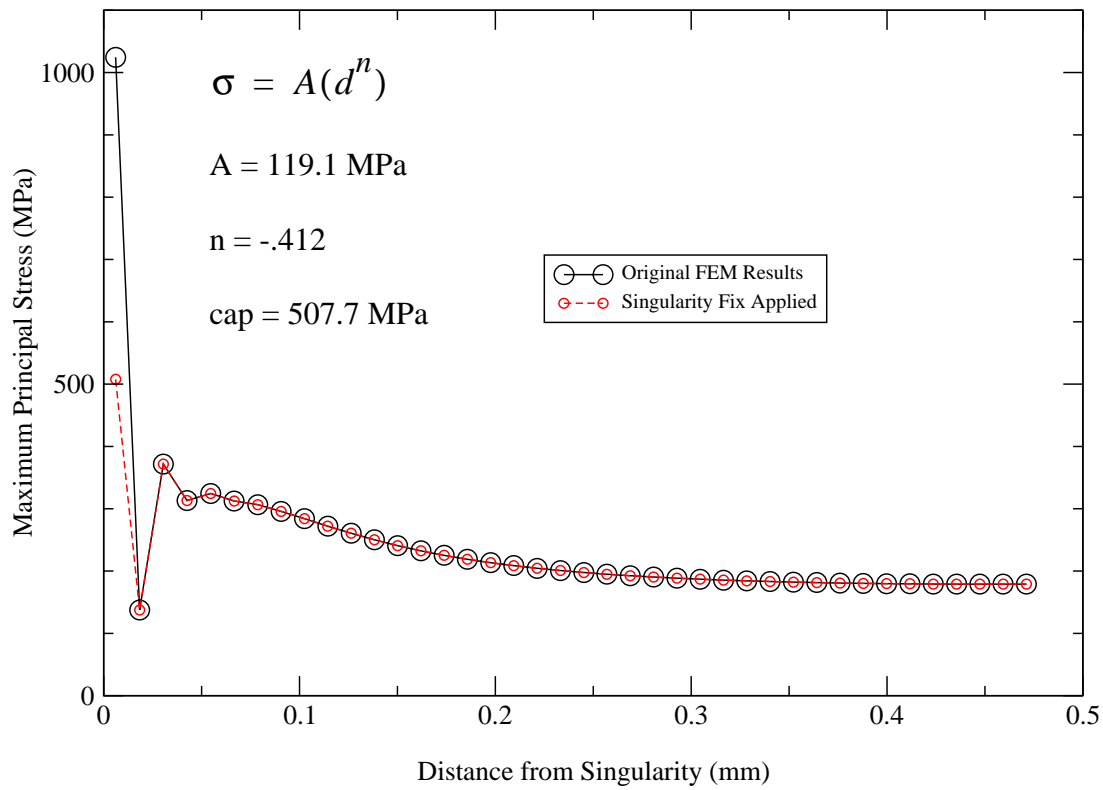Singularity Fix Applied

Figure 3.   Adjustment of stress in the vicinity of a singularity

group of stress/distance data pairs to employ to characterize the singularity. Using these values, a singular equation in stress, σ and distance, d of the following form is solved, in a least squares sense, for A and n:

$$\sigma = A(d)^n \qquad \qquad \textbf{(7)}$$

3. Using the singularity characterizing parameters, A and n, a stress cap is defined from equation 7 by substituting half the critical flaw size for the distance. Ideally, this would be the stress value computed for a mesh with an element size equal to the critical flaw size. All values of stress greater than this cap are adjusted downward to be equal to the cap. This is shown in Figure 3. This procedure is effective in producing a failure probability that is insensitive to mesh refinement. This mesh insensitivity will be demonstrated in detail for the braze tensile button in the examples section that immediately follows this section. The failure probability results are reasonable but further validation is required. The experimental background required for validation is currently underway. Various studies are measuring strength for specimens such as the braze tensile button, brazed 4-point bend bars, and 4-point bend bars with a cermet feature fired in place at the mid-point. It is important to note that in all of these studies, care must be exercised to ensure that the specimen failure is indeed a failure in the ceramic material and that the as-built local geometry is modeled.

Example Problems

Unit Volume, Uniaxial Tension

Perhaps the simplest verification specimen possible is a unit volume subjected to a uniform uniaxial tensile stress. This specimen is shown in Figure 4. One eighth of the total specimen
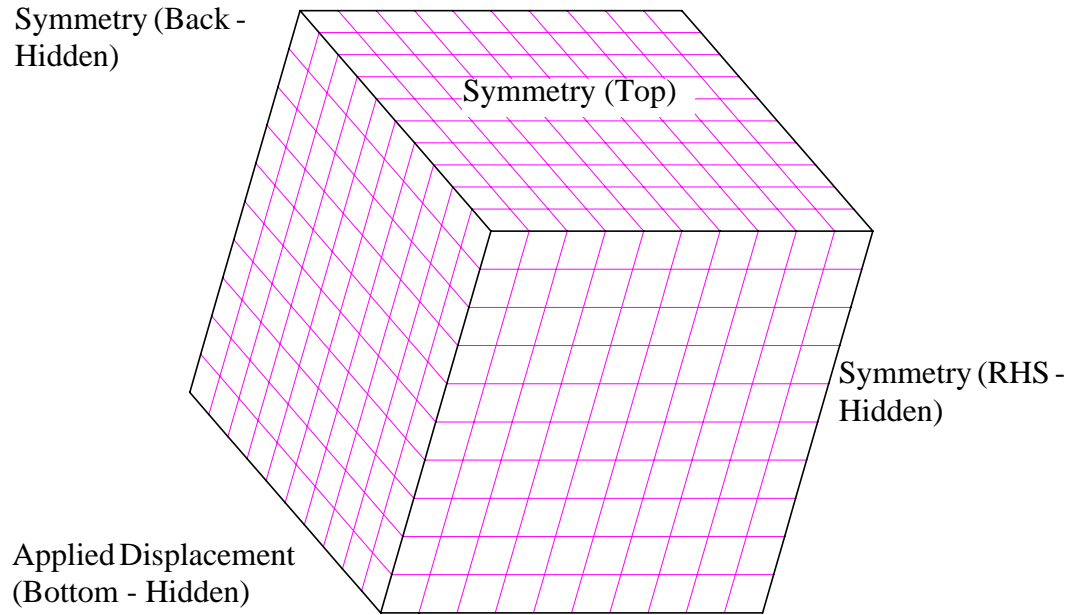

Symmetry (Back - Hidden)

Symmetry (Top)

Symmetry (RHS - Hidden)

Applied Displacement (Bottom - Hidden)

Figure 4.   Finite Element Mesh for the Unit Volume, Uniaxial Tensile Stress Example Problem

was modeled with JAS3D[13]. Three symmetry planes were employed. Thus the model has an edge length of 0.5 mm in all directions. The top, the right hand side, and the back face of the model have a symmetry boundary condition imposed that prevents displacement normal to the surface. The bottom of the model has a displacement applied normal to the surface resulting in a tensile stress. The left hand side and the front of the model are traction free surfaces. These boundary conditions give rise to a uniform uniaxial stress in the model. This is the simplest stress field attainable and is the basis for the original development of the Weibull statistics applied to ceramic failure. Given a simple uniform, uniaxial stress state acting over a unit volume, Equation 1 can easily be solved for the result, that at a stress, with a magnitude numerically equal to the magnitude of the Weibull scale parameter, the probability of failure is 63.2%, independent of the Weibull modulus. Note: for the case of a unit volume, subjected to a uniform tensile stress, the characteristic strength with units of stress has the same numerical value as the Weibull scale parameter with units of stress-mm$^{(3/m)}$. The finite element analysis of the cube was processed with FAILPROB using a Weibull scale parameter of 325 MPa-mm$^{(3/22)}$, a Weibull modulus of

22, a critical flaw size of 0.5 mm, and the symmetry was accounted for. The results are shown in Figure 5. These results provide the first verification of FAILPROB.
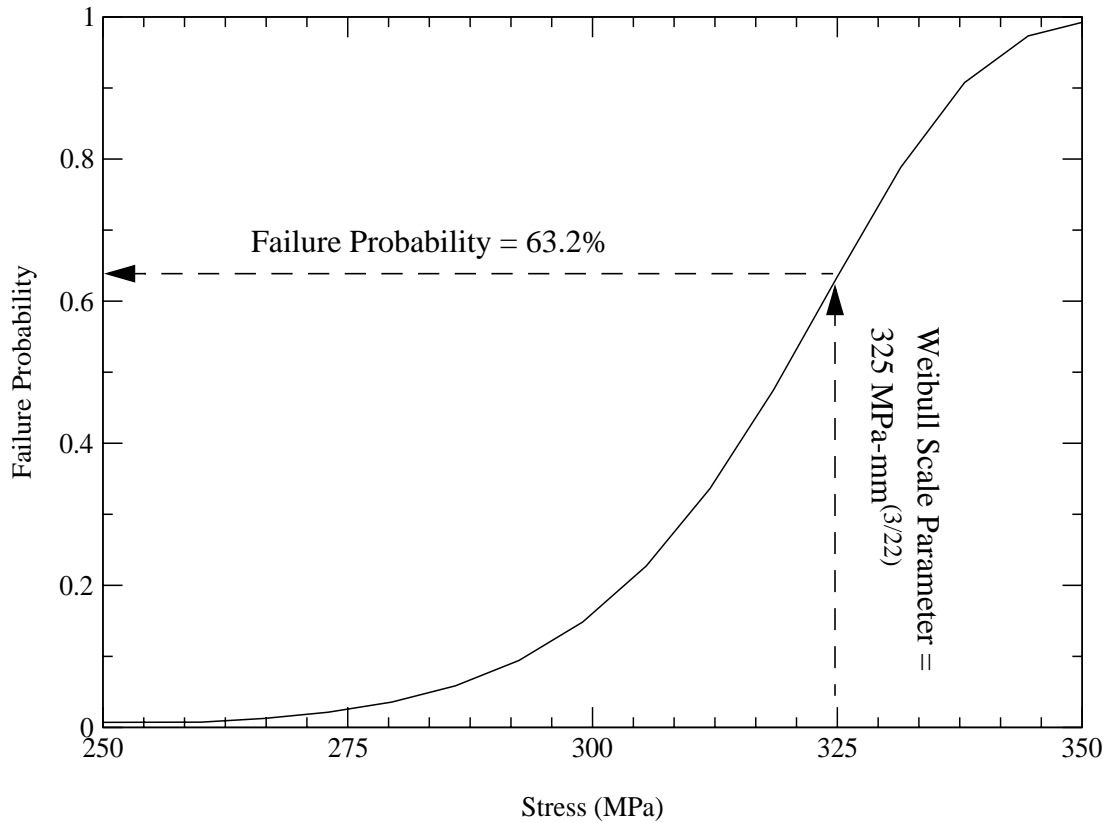

Figure 5.   Failure Probability for the Unit Volume, Uniaxial Stress Specimen

Four-Point Bend Bar

The second example has the flavor of both verification and validation. The geometry was the ASTM standard four-point bend bar[9,10]. This specimen has a height of 3 mm, a width of 4 mm and a length of 45 mm. The span between the top (inner) rollers is 20 mm and between the bottom (outer) rollers is 40 mm. This is the same specimen that was used to generate the material properties used throughout this report. In addition, mesh sensitivity issues were investigated here. The four-point bend specimen was meshed with four different densities of elements (roughly a factor of two in element size between each mesh) as shown in Figure 6. For all four mesh densities, two planes of symmetry were employed, thus one fourth of the total specimen was modeled. The left-hand-side, and the front face had symmetry boundary conditions imposed. A chord section of the loading rollers was modeled and a frictionless contact surface was applied between the roller and the specimen. The bottom roller was fixed, while the top roller had an imposed downward displacement. This combination put the specimen into bending with the maximum tensile stress along the bottom surface. The four-point loading created a region of nearly constant stress gradient between the two inner (top) rollers. As in the prior example, JAS3D was used to perform the finite element analysis.

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Top, Inner Roller -
Imposed Displacement
Downward

Symmetry -
Left Hand Side

Symmetry -
Front Face

Bottom, Outer Roller -
Fixed

Coarse Mesh
1308 Elements

Medium Mesh
6486 Elements

Fine Mesh
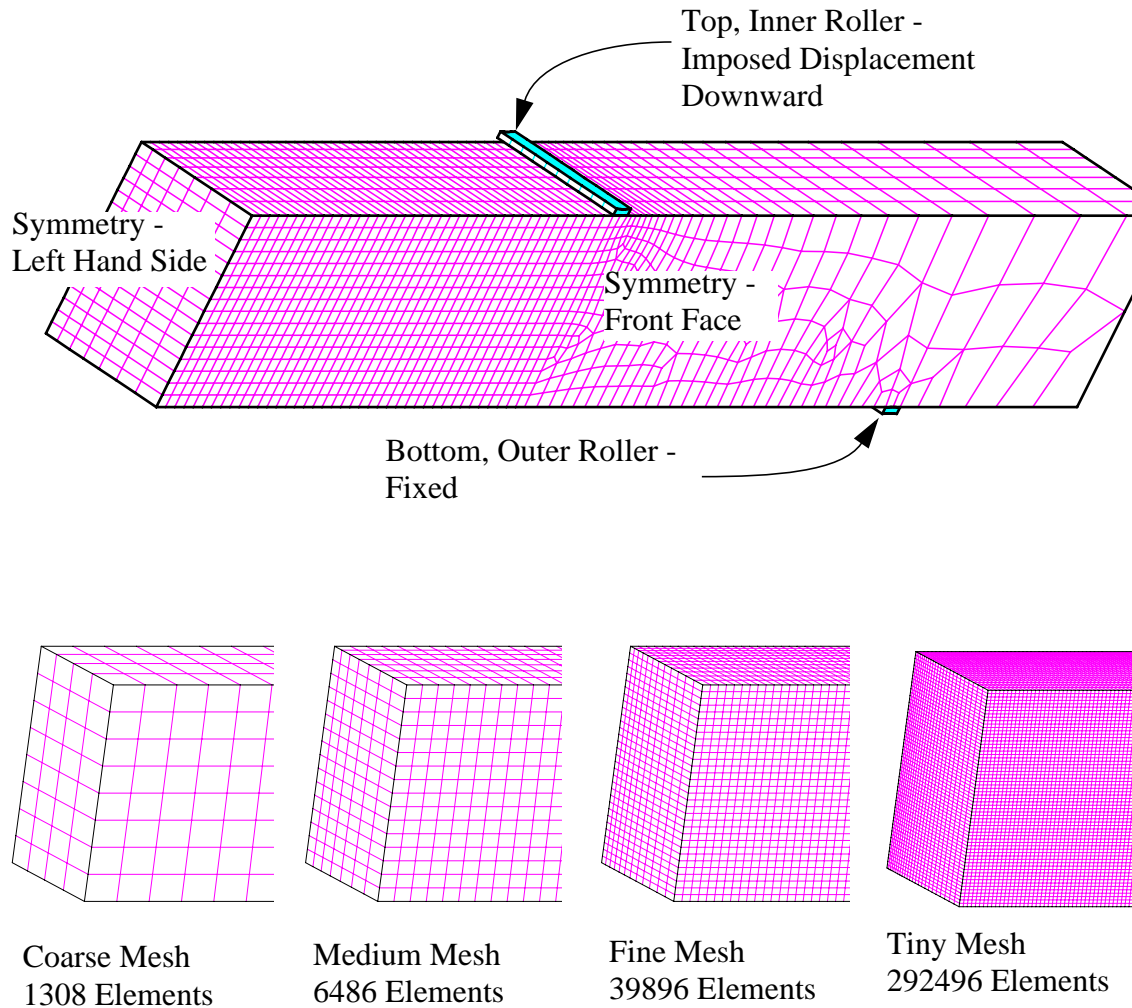39896 Elements

Tiny Mesh
292496 Elements

Figure 6.   Meshes of the Four-Point Bend Bar Specimen.

Figure 7 shows the load versus roller displacement results of the analyses of each of the four mesh densities shown in Figure 6. Roller displacement is an imposed boundary condition and load is characteristic of the entire specimen rather than a local result such as stress at a point. Therefore, load versus roller displacement should be mesh insensitive and all four mesh densities should give the same result. The differences among the mesh densities is an indication of how the solution accuracy is affected by discretization. The four mesh densities give comparable but not identical results. Therefore, all future comparisons will be made on the basis of load rather than roller displacement. Load was chosen over the roller displacement because it is more directly related to stress, which is a primary component of the failure probability computation.
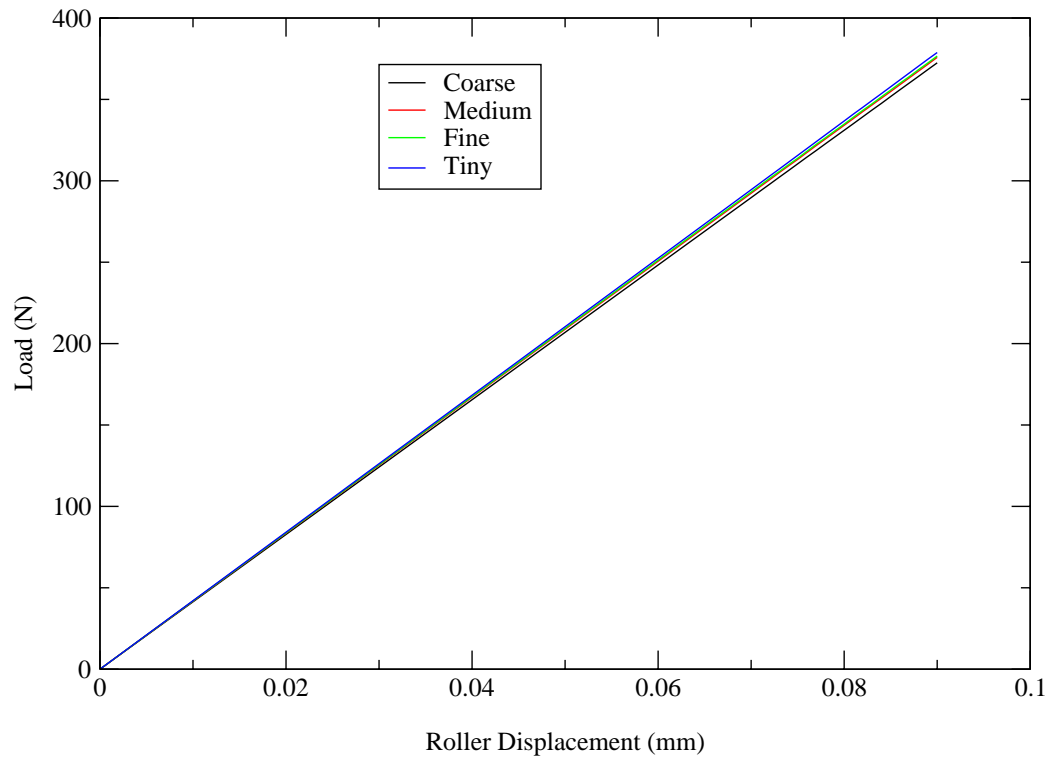
18

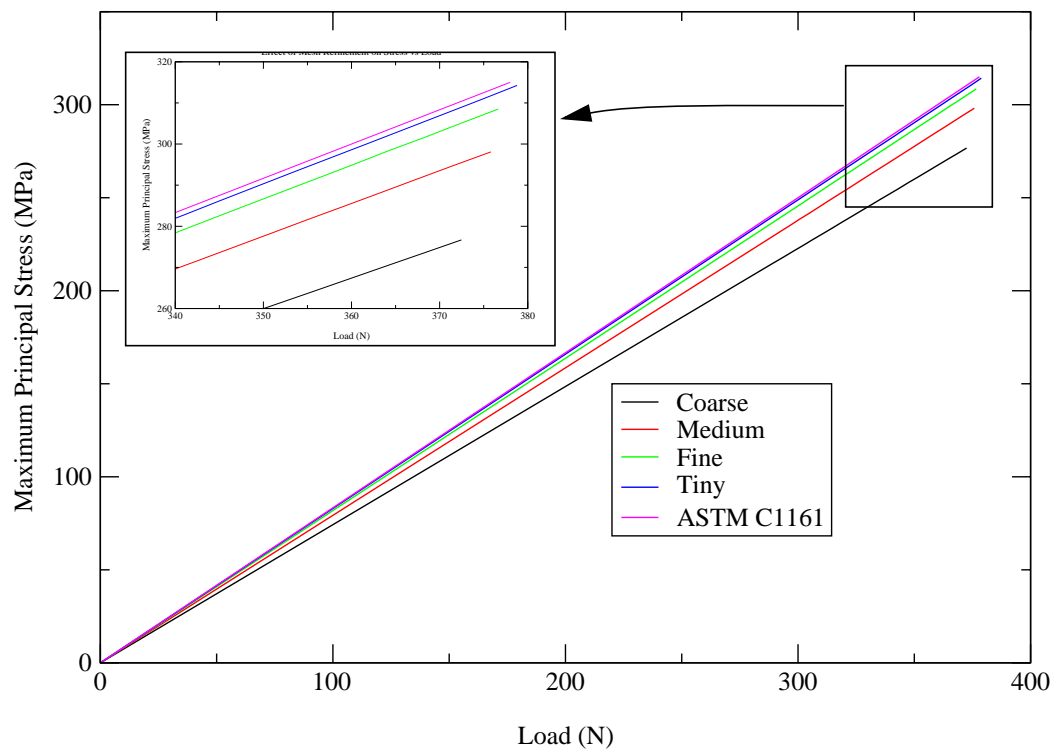Figure 7.   Load versus Roller Displacement for the 4-Point Bend Specimen

Figure 8.   Maximum Principal Stress versus Load for the 4-Point Bend Specimen

Figure 8 compares the maximum principal stress versus load for the four mesh densities to the closed form solution from ASTM C1161[9]. This comparison is directly related to mesh density. The closed form solution provides the stress at the extreme fiber (the highest value for the gradient). The four finite element solutions provide the stress at the element centroid, which is removed from the extreme fiber by half the element size. Thus, smaller elements will give a stress closer to the closed form solution than bigger elements. As shown in Figure 8, the finite element solutions converge to the closed form solution as the mesh is refined, a normal and desirable trait in a finite element solution. The probability of failure computed within FAILPROB for each of the four meshes is shown in Figure 9. The average strength from the testing (same test data used throughout this report[11]) of the four-point bend specimens was 354 N. The average and median failure strength were virtually identical. For the finite element solutions using the more refined meshes, at 354 N, FAILPROB computes a probability of failure of approximately 50%. This value is consistent with the experimental data. While this result has a flavor of validation, a true validation result must utilize a specimen geometry different from the specimen used to gather the materials property data.
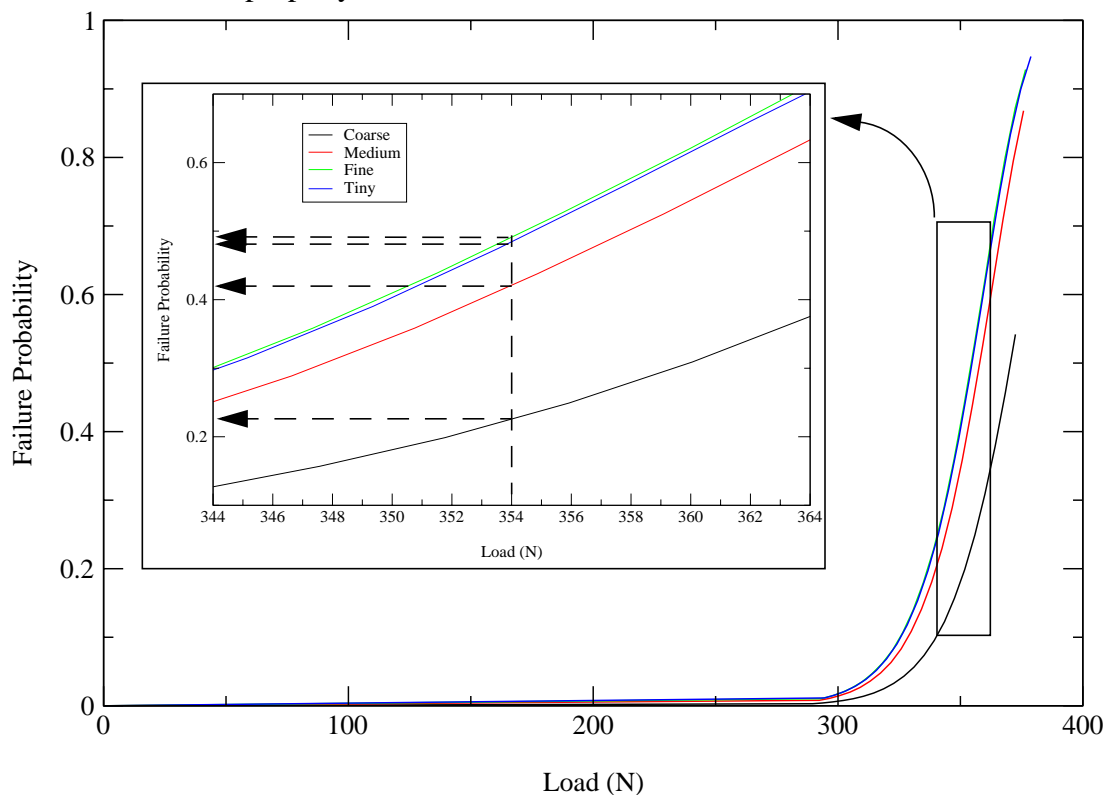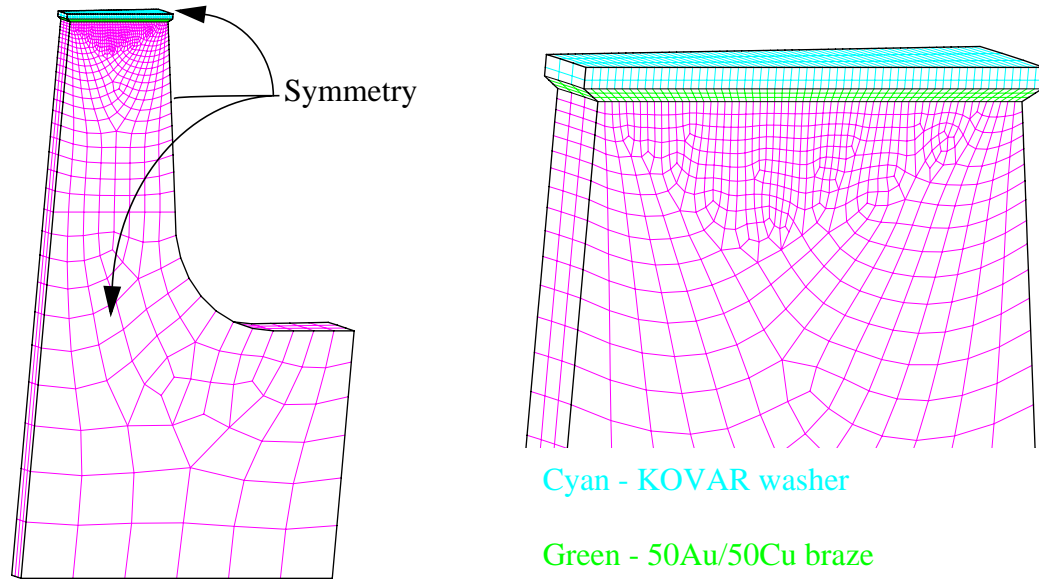

Figure 9.   Failure Probability versus Load for the 4-pt Bend Specimen

Braze Tensile Button

The braze tensile button is the standard specimen used to investigate the strength and hermeticity of braze joints[12]. This specimen consists of two ceramic "dog bone" parts that have a concentric cylindrical hole along their centerline. Each part is brazed to a central

KOVAR washer with the braze alloy under investigation. This specimen is shown in Figure 10. A five degree wedge section with symmetry planes both front and back was modeled. In addition, a symmetry plane was placed at the center of the KOVAR washer. In reality, misalignment of the parts will probably preclude the use of such symmetry planes, but for this investigation, a nominal, perfect geometry was assumed.

Symmetry

Cyan - KOVAR washer

Green - 50Au/50Cu braze

Magenta - Alumina ceramic

Five degree wedge section of the braze tensile button specimen; symmetry planes front, back, and top; center of rotation out of frame to left

Figure 10.   Braze Tensile Button Specimen Geometry

Coarse mesh - 3024 elements

Medium mesh - 12770 elements

Fine mesh - 107800 elements
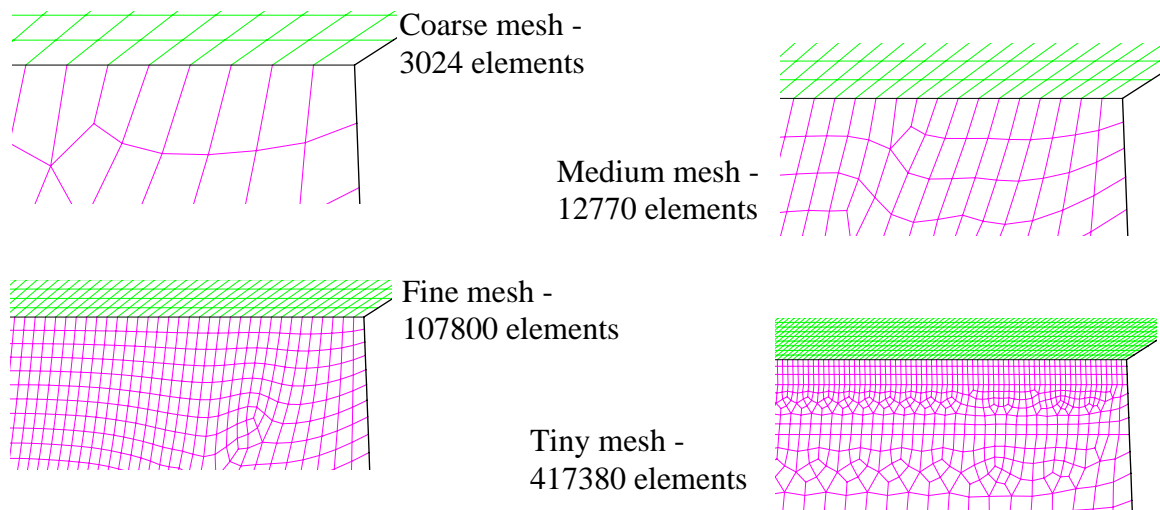
Tiny mesh - 417380 elements

Figure 11.   Meshes for the Braze Tensile Button Specimen

The entire loading cycle was simulated with JAS3D. First the temperature was ramped down from the braze solidus temperature (1223 K) to room temperature to capture the residual stress due to the braze manufacturing operation. Then external loading was applied to generate a tensile stress on the surface of the alumina wet by the braze. Because of the material property discontinuity between the alumina and the braze, there is a singularity in stress in this specimen. This singularity is shown in Figures 12 and 13 at an average tensile stress of 200 MPa over the wetted area of the alumina. It is not surprising that the character of the singularity is very similar, but not identical between sampling along a radial line versus sampling along an axial line. The oscillations in stress shown in Figure 12 are due to the incipient development of an hourglass deformation mode. These oscillations are not physical but are a numerical artifact of the under integrated (one-point) hex element used in JAS3D. These oscillations in stress are typical in regions of extremely high shear stress such as the singularity modeled here. It is possible to suppress these hourglass modes, however, suppression of the hourglass modes shown in Figure 12 adversely impacted the solution elsewhere in the mesh.
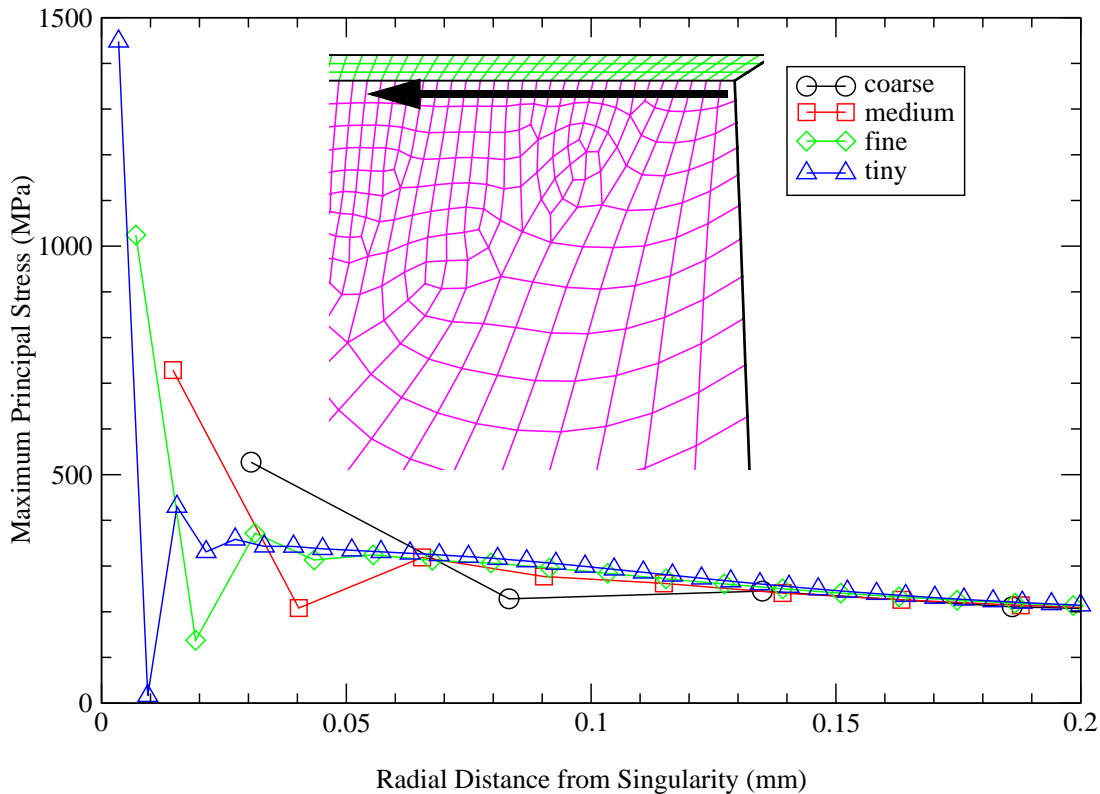

Figure 12.   Braze Tensile Button Singularity Sampled Radially at 200 MPa Nominal

In the absence of the singularity treatment discussed earlier, FAILPROB computes the probability of failure shown in Figure 14. Finite element analyses are routinely performed at the element sizes reflected in these meshes. For the probability of failure to vary from zero to one hundred percent due only to the element size selected for the finite element analysis is unacceptable. Ideally, a relatively arbitrary decision by an analyst such as element size should affect the computed probability of failure insignificantly.
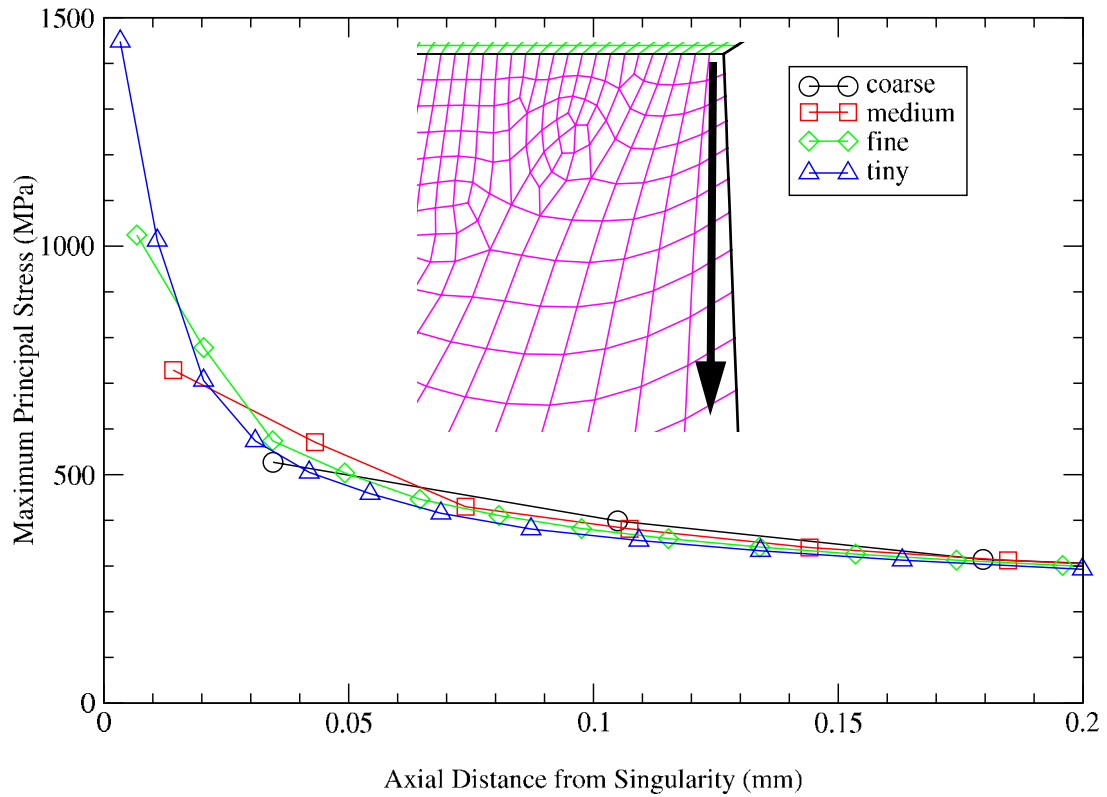
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Figure 13. Braze Tensile Button Singularity Sampled Axially at 200 MPa Nominal
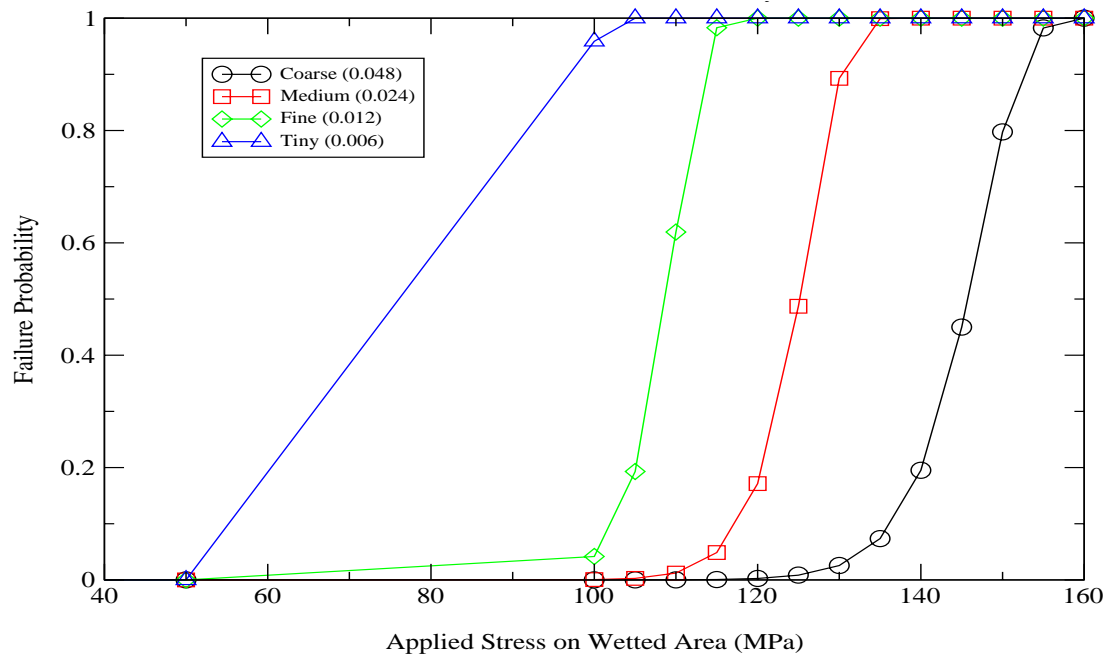

Figure 14. Mesh Sensitivity for the Computation of Probability of Failure for the Braze Tensile Button in the Absence of a Treatment for the Singularity

When the singularity is treated as discussed in the earlier section of this report, the resulting probability of failure is shown in Figure 15. The results of the singularity treatment at an
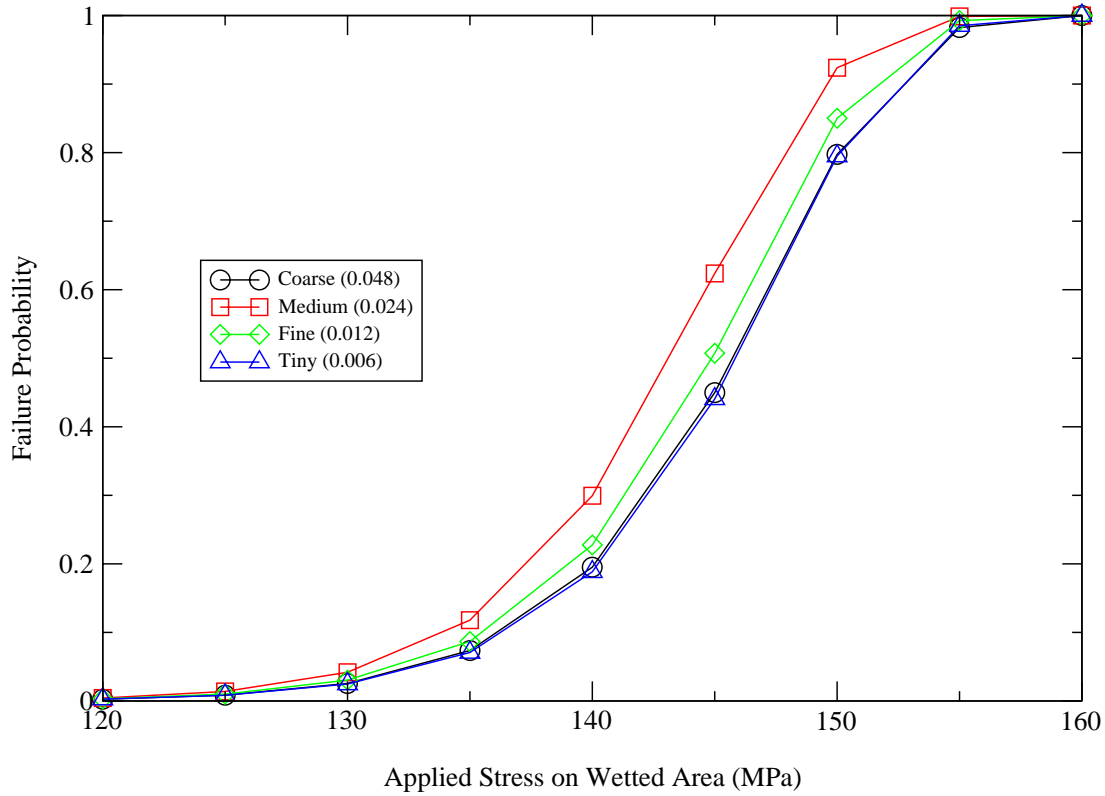

Figure 15.   Mesh Sensitivity for the Computation of Probability of Failure for the Braze Tensile Button with the Singularity Treated as Described

applied stress of 200 MPa on the face of the ceramic wetted by the braze are shown in Table 1. Note, the coarse mesh results did not meet the singularity criteria. Therefore, no modifications were performed on the results generated from the coarse mesh.

Table 1.   Results of Singularity Fix for Braze Tensile Button at 200 MPa

Mesh	Leading Constant (A)	Exponent (n)	Stress Cap
Coarse	n.a.	n.a.	n.a.
Medium	114.241 MPa	-0.400305	500.191 MPa
Fine	119.091 MPa	-0.412360	507.685 MPa
Tiny	108.611 MPa	-0.421071	513.398 MPa

There are several experimental programs currently underway using variations of the four-point bend and the braze tensile button specimens. When the results of these experimental programs are available, they will be used in the validation effort for FAILPROB. The author believes that FAILPROB can be considered verified but not validated.

Conclusions

- The N.A.S.A. CARES/LIFE fast fracture Weibull statistics technology has been implemented as a post-processing code, FAILPROB, for the EXODUSII finite element database. FAILPROB interfaces conveniently with both analysis and post-processing codes of the SEACAS system, which is used extensively at Sandia and throughout the weapons complex.

- FAILPROB provides an unambiguous probability of failure, based on Weibull statistics for brittle materials such as ceramics and glass. This is an advance over recent practice in which performance was predicted based on the comparison of the maximum principal stress to a rather arbitrary (experience based) value.

- A technique has been proposed and implemented to deal with the high local stresses that can be computed for structures with singularities such as glass-to-metal seals and ceramic braze joints. This technique provides relatively mesh insensitive results (mesh sensitivity on the order expected from analyses without singularities). This is a new capability unavailable in the N.A.S.A. CARES/LIFE technology or, to the author's knowledge, in the literature of Weibull statistics applied to failure of brittle materials.

- The materials testing to obtain the required materials properties (σ_0 and m) is well established (ASTM standard methods). This testing is routine in the materials organizations, 1800, and the materials property data are available for many glasses and ceramics in common use at Sandia.

- The example problems in this report can aid in code verification.

- Code validation awaits the results of experimental programs in progress.

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Appendix A: Executing FAILPROB

Execution Files

FAILPROB requires two files, an EXODUSII database and an input command file. The EXODUSII file is the results database of a finite element analysis and must contain either the principal stresses or the full stress tensor or both. The input command file contains the required commands and material properties for the post processing operation. These commands are presented in Appendix B.

FAILPROB produces two files, a new EXODUSII database and a text output summary. The new EXODUSII database contains everything from the input EXODUSII database plus a global variable of the probability of failure and an element variable of the probability of failure density for each material processed. The text output file provides a formatted echo of the input commands, a description of the solution path within FAILPROB, and a summary of the treatment of any singularities found.

The files used by FAILPROB are summarized in Table A-1.

Table A-1. Execution Files in FAILPROB

File	FORTRAN Unit Number	Default Extension	Type	Comment
command input	fort.6	*base*.cmd	ASCII	required
input database	fort.11	*base*.e	EXODUSII	required
output database	fort.12	*base*.a	EXODUSII	created/overwritten
output text file	fort.7	*base*.o	ASCII	created/overwritten

Execution Script

If justified by sufficient usage, the intent is to include FAILPROB in the SEACAS system. However until that has been accomplished, a script to aid in the proper connection to the necessary files and in the definition of the output file names has been made available. This script currently resides at:

sass2248-atm:/u10/gwwellm/bin/failprob

This script can either be run directly from this location or can be copied to a more convenient location. If the script is copied the path to the executable will need to be changed. The executable currently resides at and the script points to:

sass2248-atm:/u10/gwwellm/cares/FAILPROB/new/failprob

Contact the author if you encounter any problems with access to the code.

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The script to execute FAILPROB operates in three modes; appended argument list, response to prompts, or appended basename. An example of each of these three modes producing an identical result is shown below. Black text indicates data entered via the keyboard while bold red text indicates a prompt from FAILPROB.

failprob basename.cmd basename.e basename.a basename.o

failprob

Enter the input command filename >basename.cmd

Enter text output filename >basename.e

Enter EXODUS input filename >basename.a

Enter EXODUS output filename >basename.o

failprob basename

Special Software

FAILPROB is written in ANSI FORTRAN-77[14] with the exception of the following:
- EXODUSII file opening
- SUPES[15] library for dynamic memory allocation and free field reader/input parser
- netcdf calls to EXODUSII

Appendix B: Command Summary

FAILPROB was designed to be run from a command input file identified by the execution script. The input syntax is keyword driven. Commands may be entered in any order except that the material definition must be grouped together preceded by the "mat" command. In the summary of the available commands that follows, bold capital letters indicate the required portion of the keyword. If the keyword requires an additional value, this is indicated by pointed brackets enclosing the type of data required. A command summary follows:

STEp <int or **ALL**> - Defines the time step <int> to be processed or alternately selects all the time steps. Default = last time step in ".e" file.

TIMe <real or **ALL**> - Provides the same functionality as the **STE**p command but utilizing times rather than time steps. Default = last time step in ".e" file.

MATerial <int> - Defines the material to be processed. All three material properties (**WEI**bull **SCA**le parameter, **WEI**bull **MOD**ulus, and **CRI**tical flaw size) must immediately follow this command. If any of the material properties are omitted, or if any other keyword is encountered before all three material properties are entered, an error message is written and the run is terminated. Multiple material block specifications are allowed. No Default.

WEIbull **SCA**le Parameter <real> - Define the material property for this material block. No Default

WEIbull **MOD**ulus <real> - Define the material property for this material block. No Default

CRItical flaw size <real> - Define the material property for this material block. No Default.

THIck <real> - Defines the thickness used to compute volume for 2-D or shell elements. Default = 1.

AXIsymmetric - Defines axisymmetric processing for 2-D elements. Default = not set.

COMpute <int> - Defines the computation scheme to be used.

        1 - PIA method

        2 - Weibull normal stress averaging (Default)

FRAction <real> - Defines the fraction of the actual structure that has been modeled. For example, if one plane of symmetry is used in the analysis, **FRA** 0.5 should be entered. If a 5 degree wedge is modeled, **FRA** 0.139 should be used. Default = 1.

END - Terminates the input deck and initiates computations.

QUIt - Terminates the input deck and initiates computations.

EXIt - Terminates the input deck and initiates computations.

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MS 0310	P. Yarrington, 9230
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MS 0516	G. L. Laughlin, 2564
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