Stochastic Framework for Predicting Microstructurally Small Fatigue Life of AA 7075-T651

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1 Introduction

This paper presents a methodology for modeling fatigue life across multiple length scales with AA 7075-T651 as the proof-test material. The paper builds on the work of DDSim [1], a next generation Damage and Durability SIMulator, which was conceived to address the limitations of current life prediction methodologies for structural components. Specifically, DDSIM was designed to address arbitrary geometry and boundary conditions of the affected component, to include the stochastics of fracture and crack growth, the physics of the damage process, and to automate the simulation process. DDSim is hierarchical: Level I provides an initial approximation of component life and identifies life limiting 'hot-spot' locations, Level II provides a high-fidelity prediction of microstructurally large life at 'hot-spot' locations, and Level III provides a high-fidelity prediction of microstructurally small life.

The ultimate goal of the micromechanical fatigue level of DDSIM, Level III, is to produce a high-fidelity reliability prediction for microstructurally small crack life for a given structural component. A high-fidelity reliability prediction is one that takes microstructural geometry and mechanics into account. The requirement of microstructural geometry and mechanics necessitates the need for multiscale analysis. Example low-fidelity reliability curves, taken from Emery [2], are shown in Figure 1. All calculations neglected any possible effects of microstructural morphology and texture. Moreover, these curves were generated using Monte Carlo methods.

It is computationally inefficient to perform the highly-detailed multiscale simulations required to account for microstructural effects to generate a high-fidelity reliability curve using Monte Carlo methods. Instead, the proposed methodology described herein builds on the plan of Emery [2], in which, during DDSIM Level I, a structure undergoes a reduced-order screening process and selects critical, 'hot-spot' locations. At these locations, detailed analyses in DDSim Level III are performed for the microstructurally small fatigue life to increase the fidelity of the reliability prediction. Improvements will be made to the prediction of the microstructurally small portion of life by augmenting an approximated reliability curve with a limited number of highly-detailed, multiscale simulations, selected to provide the greatest impact on the updated reliability curve.

Any number of microstructural realizations could be generated at a critical 'hot spot', each of which would yield a failure prediction under a varying number of cycles. However, the microstructural realizations that ultimately have the greatest impact on structural reliability are those that predict failure under a relatively small numbers of load cycles. The focus of the multiscale analyses, therefore, is on microstructural realizations that predict failures that fall in the most critical region, such as the failures occurring below about 20,000 load cycles in Figure 1. In Figure 1, this region in the low-fidelity curve has a reliability of virtually, but not exactly, 1.0. In reality, failures controlled by microstructural effects do occur at such low lives. It is of upmost importance to properly characterize this critical region to prevent premature failures.

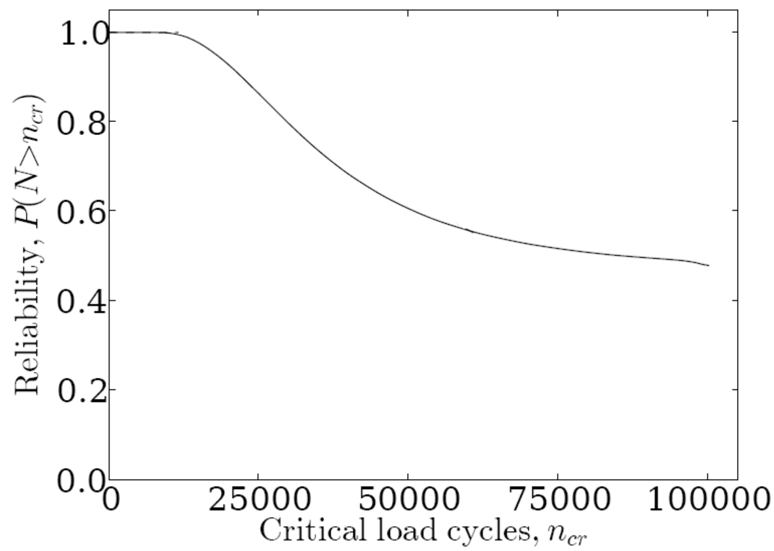

Figure 1: Low-fidelity reliability plot, taken from Emery [1], for an open-holed fatigue coupon. Critical region occurs below approximately 20,000 cycles.

Microstructurally small fatigue crack formation includes the stages of incubation, nucleation, and microstructurally small propagation. For the purposes of this paper, incubation will be defined as the process leading to occurrence of new surface area, with nucleation defined by this first appearance of new surface area in the matrix. In AA 7075-T651, the fracture of Al_7Cu_2Fe constituent particles is the major incubation source which can lead to crack nucleation in the aluminum matrix. Propagation is the process through which surface area increases. Forsyth [3] showed that propagation can be divided into stages I and II. The hierarchy of fatigue processes, from initial material to failure, is shown in schematic form in Figure 2.

The probability framework will work along two separate paths: a detailed multiscale approach, and a simplified filter approach based on response surfaces. The multiscale approach will couple a microstructural model with a structural scale model at a 'hot-spot' location and simulate the entire hierarchy of fatigue processes. The filter approach will rely on an extensive series of finite element analyses, for each process shown in Figure 2, and on simplified geometric models, while varying pertinent material parameters. Each response surface will be used to generate statistics relating crack driving force to the surrounding material structure. The statistics will be used in turn to determine the probability of a crack advancing to the next stage in the fatigue hierarchy. The filter approach will result in an intermediate-fidelity reliability curve and the selection of a limited number of microstructural realizations to be used in multiscale simulation. The intermediate-fidelity curve will be combined with the results of the multiscale simulations to create a high-fidelity reliability prediction in the final probability framework. The rest of the paper is organized as follows: Section 2 will discuss the multiscale modeling approach, Section 3 the filtering approach and Section 4 the overall probability framework.

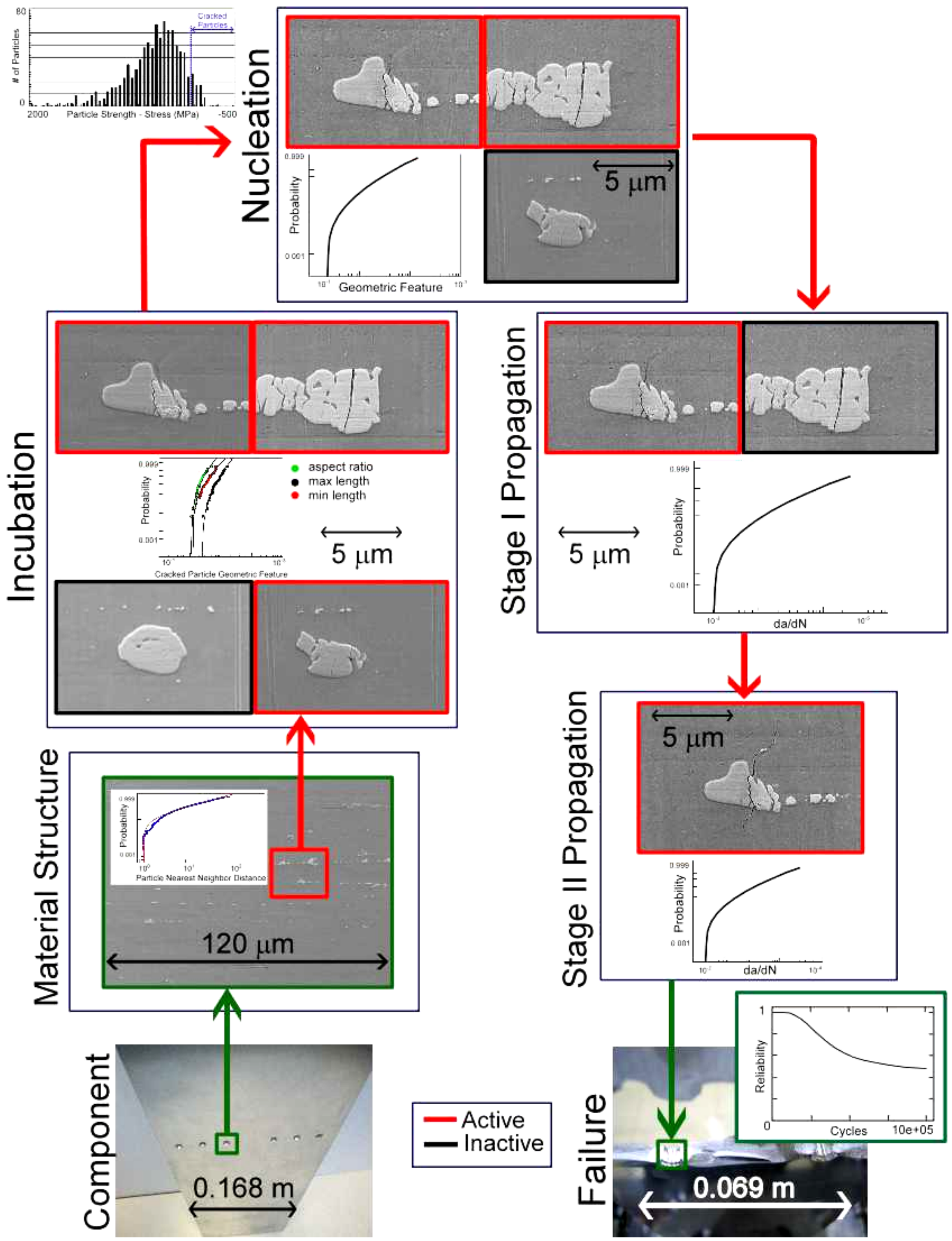

Figure 2: Schematic of overall approach from initial material damage to component failure. The response surface for each stage yields statistics relating crack driving force to surrounding material structure.

2 Multiscale Modeling

The multiscale modeling approach will combine a detailed microstructural model with a structural model at a 'hot-spot' location. Two main approaches have been extensively used for the solution of multiscale problems: superposition methods and homogenization methods. The approaches are notable for their efficiency and robustness. However, they are not sufficient for combining models with localized damage. The superposition method decomposes the solution space into global and local effects, and then superposes the two results. Solution compatibility must be enforced by prescribing homogeneous boundary conditions for the local solution at the global-local interface. The homogenization method is a multiscale expansion method that relies on three assumptions:

(i) The structure is formed by a spatial periodicity of the Representative Volume Element (RVE).
(ii) The solution is locally periodic in the statistical sense.
(iii) Macroscopic fields are constant within the RVE.

One manner in which this method is used is to calculate equivalent material properties from the local problem for the global problem. Since the method is based on a spatial periodicity assumption, the calculated material properties are inherently non-local. The non-local and uncoupled nature of these solution methods does not lend itself to coupling scales at a particular location in a structural component. Following from assumption (iii), these methods are precluded from solution at a stress riser, such as a bolt hole, a typical 'hot-spot' location.

An alternative approach, a modified multigrid method [4], Figure 3, will be used to couple the two models, structural and microstructural, instead. This procedure is designed to couple the two models so they behave coherently. The steps in the approach are: mesh and analyze the structural model, determine appropriate boundary conditions for the microstructural model, mesh and analyze the microstructural model including in it all relevant damage mechanisms, and update the stiffness of the structural model to represent the damage on the microstructural level. This approach is repeated until the boundary conditions placed on the microstructural model converge on consecutive iterations.

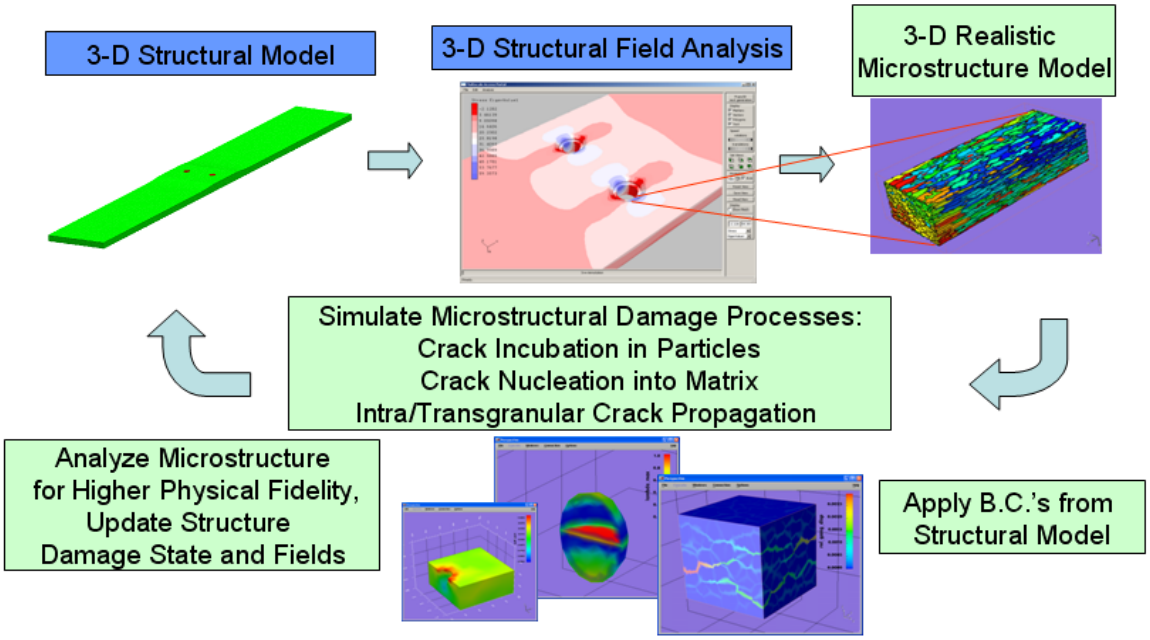

Figure 3: Schematic of modified multigrid procedure.

On each iteration, displacement boundary conditions are interpolated, using standard finite element methods, for each surface node on the microstructural model and the resulting damage on the microstructural scale is resolved onto the structural scale through modified constitutive parameters. The multiscale approach must couple the FCC polycrystal constitutive model [4] of the microstructural scale with a von Mises constitutive model on the structural scale. This means that the multiscale approach must effectively represent the slip-based damage of the microstructural scale on the structural scale. This will be accomplished by employing a volume average of the tangent stiffness tensor, $\boldsymbol{C}^{ep}$, in the volume immediately surrounding each structural scale Gauss point. The volume averaging procedure is shown in schematic form in Figure 4.

All the microstructural Gauss points within a radius, R, of a given structural Gauss point, an area indicated by the green sphere, Figure 4, will have their $\boldsymbol{C}^{ep}$ averaged to update the tangent stiffness tensor of the structural Gauss point, GP_j. This restriction operator, which is patterned after the restriction operator of Datta *et al.* [5], will be a simple arithmetic average formulated as:

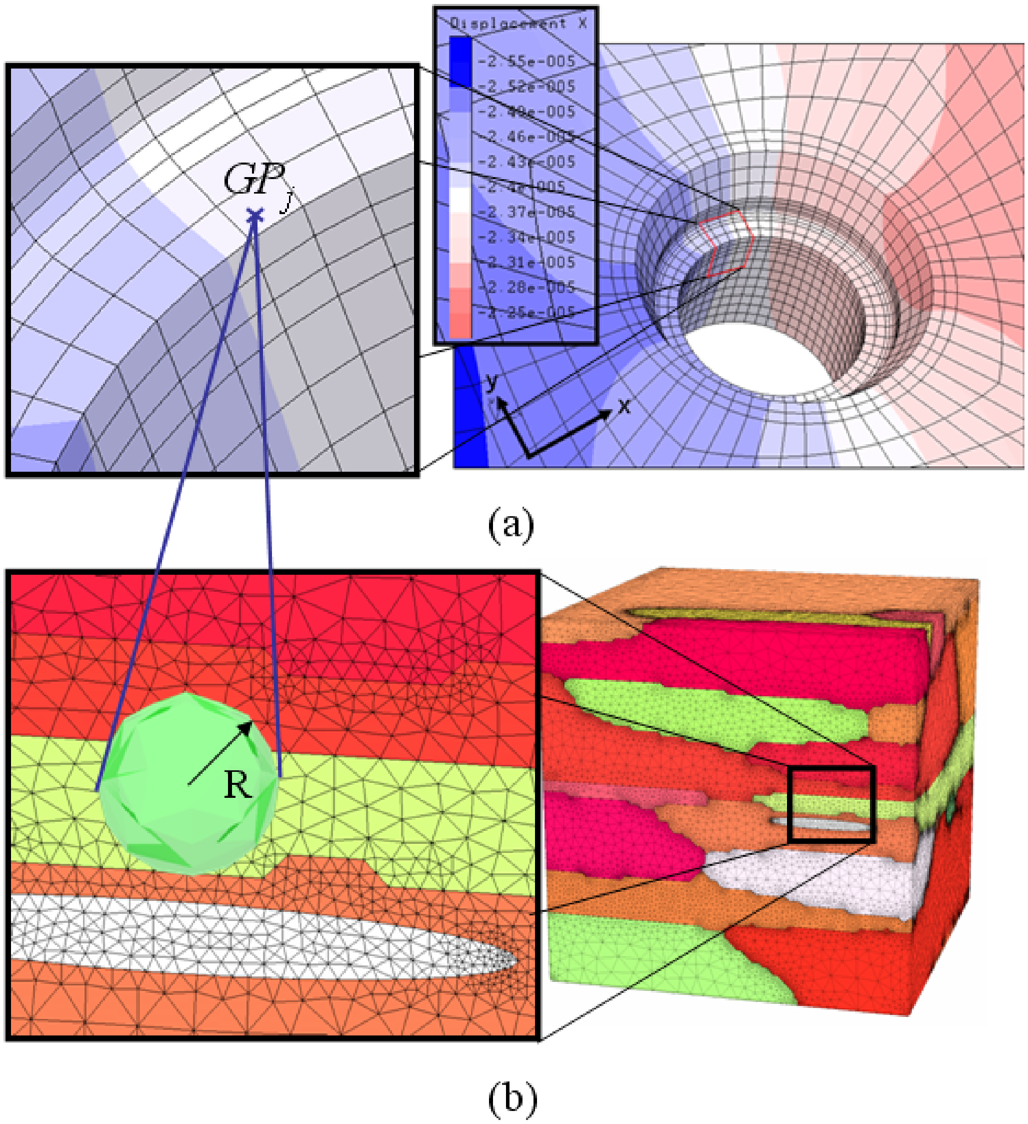

Figure 4: Schematic of multiscale approach with volume averaging for restriction. (a) Structural scale model. The location of the microstructural model is outlined in red. (b) Microstructural scale model. The tangent stiffness tensor, $\boldsymbol{C}^{ep}$, of all the microstructural Gauss points contained with the green sphere of radius, R, are restricted to a single Gauss point, GP_j, in a structural element.

$$\boldsymbol{C}^{ep\,\prime}(GP_j) = \frac{\sum_{i}^{N_{GP}} w^i \boldsymbol{C}^{epi}}{\sum_{i}^{N_{GP}} w^i} \qquad (1)$$

where C^{epi} is the tangent stiffness matrix for microstructural Gauss point *i*, w^i is its corresponding weight function based on the distance, R, away from structural Gauss point j, N_{GP} is the number of microstructural Gauss points that are being restricted to structural Gauss point j (GP_j), and $C^{ep'}$ is the resulting reduced stiffness of Gauss point j. This procedure is more computationally expensive than traditional multiscale methods, but is suitable for gaining insight into the localized damage behavior at 'hot-spot' locations.

3 Filtering Approach

A filtering procedure quickly determines which microstructural realizations will prematurely evolve a microstructurally large crack. A series of four filters - incubation, nucleation, intragranular and transgranular propagation- are introduced. The response surfaces are built by varying pertinent material properties across a series of simplified geometric models to determine the relationship between the properties and the associated fatigue stage. The incubation filter, presented in Bozek *et al.* [6], built on a particle stress response surface, was based on 1296 separate finite element simulations. The filter demonstrated the ability to predict a mean particle cracking frequency of 3.6%, comparable to the experimentally observed mean of 4.5%. The incubation response surface is able to calculate the particle maximum stress distribution based on particle aspect ratio, surrounding grain orientation and applied strain level. This stress is compared to a distribution of particle strength, based on a simplified linear elastic fracture mechanics assumption, to determine if the particle cracks.

The nucleation filter determines if, and after what number of cycles, a cracked particle will nucleate a crack into the aluminum matrix [7]. The propagation filters utilize microstructurally small crack propagation models implemented and validated by Veilleux [8] to determine which cracks propagate at a sustainable rate, that is, which cracks are likely to propagate to microstructurally large size. The finite element analyses used to populate the response surfaces are performed on physically small models in order to contain computational cost.

4 Probability Framework

As stated in Section 1, with the capability to perform only a limited number of multiscale analyses, it is imperative that the critical region of the reliability curve be properly characterized. A screening tool applies the series of four filters on a large sample of microstructural realizations. Using this methodology, crack size and number of cycles are tracked from the incubation site at particles until a crack approaches microstructurally large size without the need for any further finite element calculations. This results in a quick estimate of microstructural life for a given microstructural realization.

The screening tool serves two purposes: it enables the selection of a limited number of microstructural realizations to be analyzed with the multiscale solver, and it allows for the creation of an intermediate-fidelity reliability curve. The probability framework is shown in schematic form in Figure 5. The results of the multiscale analyses are combined with the intermediate-fidelity reliability curve to produce a high-fidelity reliability curve. This will allow proportionally more weight to be given to the multiscale results than the lower-fidelity filter results. The results are combined through the following equations:

$$P\left(N^h < N_{cr}\right) = \sum P(N^h < N_{cr} \mid N^i \in A_i) P(N^i \in A_i) \tag{2}$$

$$P\left(N^h < N_{cr} \mid N^i \in A_i\right) = \frac{1}{N_{ms}} \sum_{j=1} I_{\left(N^i < N_{cr}\right)} \tag{3}$$

where N^h is the high-fidelity reliability curve, N^i is the intermediate-fidelity reliability curve, N_{cr} is the critical number of cycles, A_i is the sample area, N_{ms} is the number of multiscale simulations performed and I is an identity function.

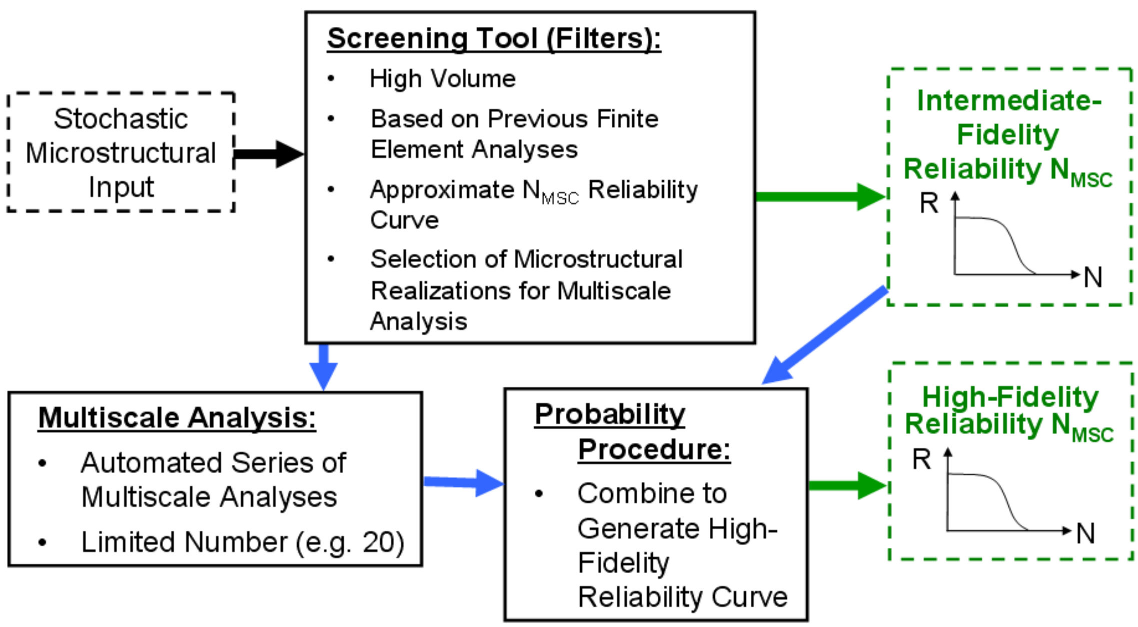

Figure 5: Schematic of Probability Framework.

5 Discussion

A methodology is presented to predict probabilistically microstructurally small fatigue life across multiple length scales. The approach is designed to address arbitrary geometry and boundary conditions and incorporate microstructural geometry and mechanics. Focus is given to accurately producing a high-fidelity reliability curve, especially in the region of the curve likely to cause premature failure. Two approaches to the problem are run in tandem: a detailed multiscale approach and a filter based approach. The filter based approach uses response surfaces to quickly approximate the microstructurally small fatigue life of a given microstructural realization. This serves two purposes: construction of an intermediate reliability curve, and selection of microstructural realizations likely to cause premature failure of a structural component. The realizations of interest are used in multiscale simulations and the results are combined with the intermediate reliability curve to achieve a high fidelity reliability curve. The two edged approach allows for both a quick estimate of microstructurally small life and the inclusion of the best available physics into the simulation process.

6 Acknowledgements

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