# The Effect of Scale Dependent Discretization on the Progressive Failure of Composite Materials Using Multiscale Analyses

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**A multiscale modeling methodology, which incorporates a statistical distribution of fiber strengths into coupled micromechanics/ finite element analyses, is applied to unidirectional polymer matrix composites (PMCs) to analyze the effect of mesh discretization both at the micro- and macroscales on the predicted ultimate tensile (UTS) strength and failure behavior. The NASA code FEAMAC and the ABAQUS finite element solver were used to analyze the progressive failure of a PMC tensile specimen that initiates at the repeating unit cell (RUC) level. Three different finite element mesh densities were employed and each coupled with an appropriate RUC. Multiple simulations were performed in order to assess the effect of a statistical distribution of fiber strengths on the bulk composite failure and predicted strength. The coupled effects of both the micro- and macroscale discretizations were found to have a noticeable effect on the predicted UTS and computational efficiency of the simulations.**

## Nomenclature

| | | |
|---|---|---|
| $P_f$ | = | probability of failure; taken as a random number between 0 and 1. |
| $\sigma_0$ | = | Weibull scale parameter |
| $\beta$ | = | Weibull shape parameter |
| $L_0$ | = | fiber length at which $\sigma_0$ and $\beta$ were determined |
| $L$ | = | characteristic length; equal to the approximate FE length |
| $\alpha$ | = | fiber strength parameter |
| $\sigma$ | = | strength to be assigned to a subcell |

## I. Introduction

The Micromechanics Analysis Code with Generalized Method of Cells (MAC/GMC)[1] provides a computationally efficient means of modeling composite materials based on Aboudi's Method of Cells micromechanics theories[2-5]. Using this method, a doubly or triply periodic repeating unit cell (RUC) is discretized into an arbitrary number of subcells. Each subcell is assigned material properties and a constitutive law to describe the local material behavior. Continuity of displacements and tractions are then enforced along the subcell boundaries in an average sense, and all field quantities are evaluated at the subcell centroids. MAC/GMC may also be coupled to ABAQUS Standard or Explicit[6] by another code, FEAMAC. Using this coupling technique, finite element integration point stresses are mapped onto RUCs and a local MAC/GMC analysis is performed. Subsequent changes in material response are then passed back up to the finite element level and the procedure continues. This technique is graphically shown in Figure 1.

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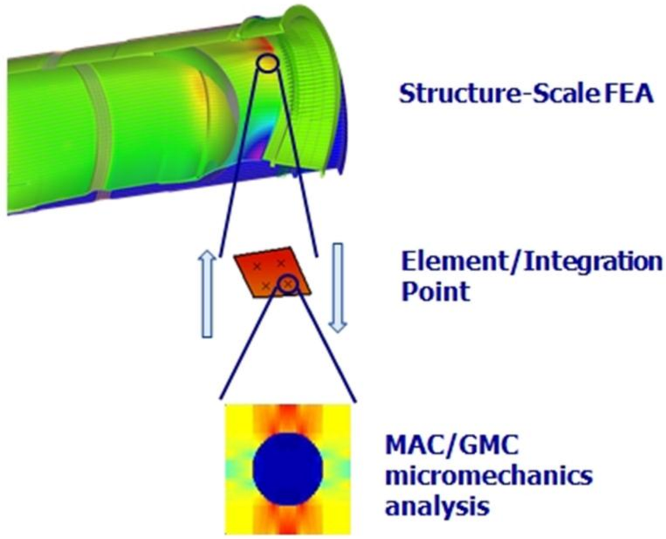
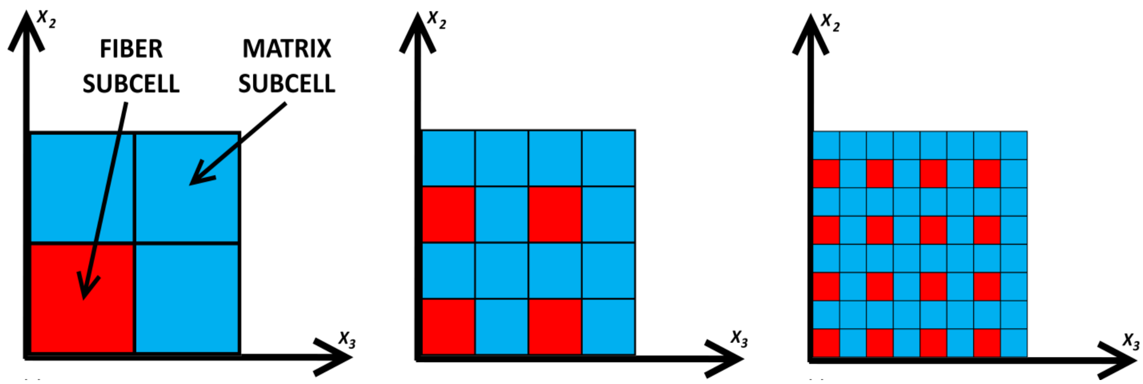



**Figure 1.** Schematic showing the coupling of MAC/GMC with ABAQUS via FEAMAC.

Recently, Ricks *et al.*[7] developed a methodology for predicting the ultimate tensile strength (UTS) and failure behavior of a TIMETAL 21S/ SCS-6 tensile dogbone specimen where a statistical distribution of fiber strengths was assigned to individual fiber subcells within an RUC prior to performing multiscale progressive failure analyses. Multiple RUCs were generated and randomly assigned in equal numbers to integration points within the finite element (FE) mesh. In general for a FE constant mesh density, increasing the RUC complexity (*i.e.*, more fiber subcells at a constant fiber volume fraction) resulted in an increase in the UTS and more randomly distributed fiber failures. The notion of a constant simulation volume was introduced to allow for a variety of micro- and macroscale discretizations for a given material volume. Of course, care must be taken to ensure that the volume of material simulated at the microscale is consistent with the macroscale representation of that same volume. Only minute differences in predicted ultimate strength and failure behavior were observed when using a finer microscale (RUC) discretization and a coarser global FE mesh versus a coarser RUC and finer FE mesh for a constant simulation volume. Additionally, it was more computationally efficient to use a finer RUC and coarser FE mesh since MAC/GMC calculations are much more computationally efficient than FE calculations for a fixed number of degrees of freedom. However, little work has been done to define the appropriate discretization at each disparate length scale in multiscale analyses. For example, a carbon fiber has a diameter of approximately 0.2 mils while the SCS-6 monofilament previously considered has a diameter of approximately 5.6 mils. More complex RUCs (*i.e.*, more fiber subcells for a given fiber volume fraction) can therefore be simulated for a given FE size in the case of carbon fiber composites (CFCs). While the SCS-6 fiber dimensions dictate the microscale discretization for a given macroscale FE mesh, CFC systems do not exhibit the same limitations. The choice in discretization at each length scale could therefore become crucial in multiscale progressive failure analyses. Over-discretization at one or more scales could lead to excessive computational costs while under-discretization could lead to an inaccurate approximation of the homogenized local material response. In this work, the effect of discretization at both the micro- and macroscales on the global composite failure response for an AS4 carbon fiber/ Hercules 3502 epoxy unidirectional polymer matrix composite (PMC) tensile specimen is investigated. Future studies will investigate more complex PMC geometries (*e.g.*, open-hole tensile) and fiber architectures (*e.g.*, woven fabric).

## II. Material System

For this study, an AS4 carbon fiber/ Hercules 3502 (AS4/ 3502) epoxy material system was considered. A variety of doubly-periodic RUCs (*cf.*, Fig. 2) were used in these analyses. Different RUCs were associated with individual FEs and analyses were performed using the NASA FEAMAC software and ABAQUS FE solver. Figure 2a shows a representation of a single-fiber RUC while Fig. 2b and 2c show a four-fiber and 16-fiber RUC, respectively. Since subcell field quantities are evaluated at the subcell centroid rather, and the continuity conditions used to formulate the strain concentration matrix are enforced at the subcell boundaries in an average, integral sense, no stress concentrations are introduced by the rectangular subcell arrangement. This RUC architecture was used to approximate PMC systems where the homogenized RUC response will be determined and information regarding specific microstructural details (*e.g.*, fiber clustering) may be lost when passed up to the macroscale. A square packed architecture was specifically chosen because it yields the appropriate average, global response for PMC with a statistically varied microstructure. Both the fiber and matrix were idealized as isotropic, and linear elastic materials; inclusion of transversely isotropic fiber properties will be considered as part of a future study. The fiber has a Young's modulus of 234 *GPa* and Poisson's ratio of 0.2 while the matrix has Young's modulus of 3.8 *GPa* and Poisson's ratio of 0.36 consistent with experimental data[8-9]. A fiber volume fraction of 0.6, consistent with unidirectional AS4/ 3502 experimental data found in CMH-17[10], was used in these analyses.



a) b) c)

**Figure 2.** Microstructural representation of a unidirectional PMC for a) single-fiber RUC, b) a four-fiber RUC, and c) a 16-fiber RUC.

Prior to investigating the effects of discretization at both the micro- and macroscales, a statistical distribution of fiber strengths was assigned to individual fiber subcells within a given RUC. These strengths were determined by solving the following modified two-parameter Weibull cumulative distribution function for the fiber strength, σ:

$$P_f(\sigma) = 1 - exp\left[-\left(\frac{L}{L_0}\right)^{\alpha}\left(\frac{\sigma}{\sigma_0}\right)^{\beta}\right] \quad (1)$$

where $P_f$ is the cumulative probability of failure at $\sigma$ and is taken to be a random number between 0 and 1. The traditional two-parameter Weibull scale ($\sigma_0$ = 4493 *MPa*) and slope ($\beta$ = 4.8) parameters were determined from experimental data based upon a fiber test length ($L_0$ = 10 *mm*)[11]. The $(L/L_0)^{\alpha}$ term in Eq. 1 was added by Watson and Smith[12] and Padgett *et al*.[13] in order to characterize the fiber strength distribution across a range of fiber lengths. The fiber strength parameter, $\alpha = 0.6$, is uniquely determined from experimental data where multiple fiber lengths were tested[11]. The characteristic length, $L$, was set equal to the typical finite element length in the multiscale analyses as discussed in Ricks *et al*.[7] The introduction of a characteristic length avoids the pathological mesh dependence typically associated with brittle failure in FEM simulations. Essentially, the simulated fiber length in microscale calculations should not exceed that of the given finite element length (*i.e.*, the *macroscale* sub-volume over which *microscale* calculations are performed). Therefore, for different FE mesh densities, the strength distribution is modified accordingly. Since this distribution is based on "weakest link" theory, a shorter FE length corresponds to a shorter simulated fiber. This shorter fiber in turn would have a lower probability of having a critical flaw along the length and therefore a higher fiber strength. Based on Eq. 1, the overall distribution of local fiber strengths would then get shifted to higher strengths as the mesh density increases (*i.e.*, the FE length decreased). In these simulations, a maximum failure stress criterion was used to determine fiber failure. No matrix failure criterion was implemented in the current study; this issue will be addressed in future work.

## III. Coupled FE/Micromechanics Analyses

The ultimate goal of this work is to determine the effect of model refinement at the microscale (i.e., RUC level) and the macroscale (*i.e.*, FE level) on the global composite predicted ultimate strength and failure response for unidirectional PMCs. For the eight ply unidirectional AS4/ 3502 longitudinal tensile specimen considered here, a rectangular specimen of dimensions 203.2 *mm* x 12.7 *mm* x 1.12 *mm* consistent with ASTM D3039-76 was simulated. A constant fiber volume fraction of 0.6 was used and the UTS and coefficient and variation results are compared against experimental results from CMH-17[10]. Additionally, 38.1 *mm* x 12.7 *mm* x 1.57 *mm* G-10 cross-ply glass tabs were simulated with a 7° bevel angle. Tab material properties were obtained from Joyce *et al*.[14] and the tab material was oriented ±45° to the longitudinal direction in the simulations. Three different levels of FE meshes comprised of 840, 5280, and 36480 FEs, respectively were employed. Out of these totals, the specimen (*i.e.*, without the tabs) is comprised 480, 3840, and 30720 FEs, respectively. One, two, and four elements were modeled through the specimen thickness for the 480, 3840, and 30720 FE meshes, respectively. Eight-noded linear isoparametric brick elements were used to model the specimen while both eight- and six-noded linear isoparametric brick and wedge elements, respectively, were used to model the tabs. These three meshes are shown in Fig. 3 where Figs. 3a-c correspond to the 840, 5280, and 36480 FE meshes, respectively. Note that the specimen mesh (*i.e.*, without the tabs) in Fig. 3c has double the mesh density of the mesh in Fig. 3b, and Fig. 3b has double the mesh density of the mesh in Fig. 3a. Based on these meshes, $L$ was set equal to 0.2117 *cm*, 0.1058 *cm*, and 0.0529 *cm* for the 840, 5280, and 36480 FE meshes, respectively. A constant longitudinal displacement was applied to surface nodes of one grip while the surface nodes of the other grip were fixed. Contractions in both the through-thickness and transverse directions were permitted. Also note that the specimen tabs were simulated since initial simulations suggested that failure would predominately occurred at the grip regions in the absence of tabs.

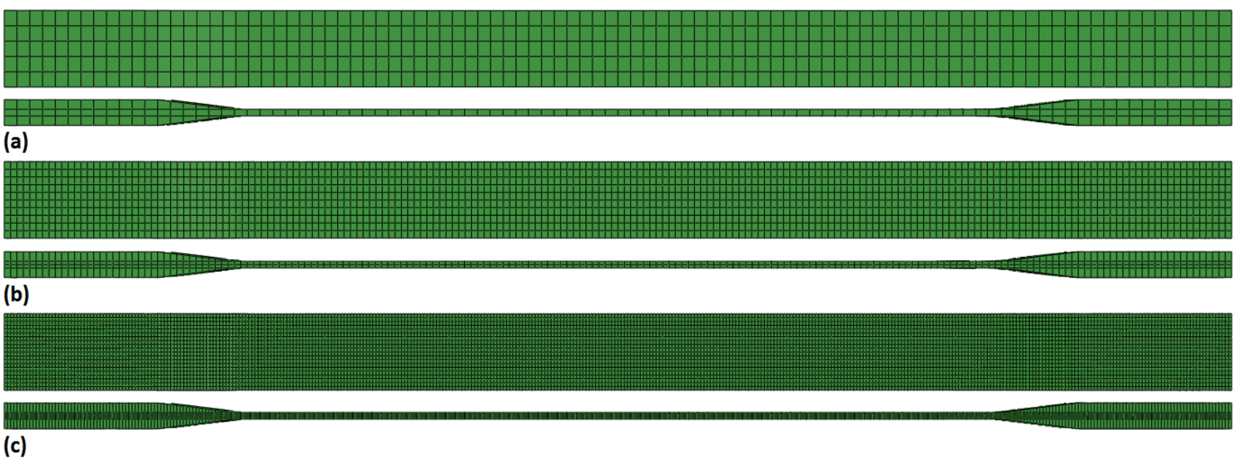



**Figure 3.** Front and side views of the three different FE meshes considered in this study: a) 840 FEs, b) 5280 FEs, and c) 36480 FEs. Note that out of these totals, the specimen (*i.e.*, without the tabs) is comprised of 480, 3840, and 30720 FEs, respectively.

It was initially assumed that a single-fiber RUC could approximate the microscale response at the finest FE discretization. In order to maintain a constant simulation volume across the two length scales, 16-fiber, four-fiber, and single-fiber RUCs were paired with the 480, 3840, and 30720 specimen FE meshes, respectively. Hence, a fixed material volume can be discretized in multiple ways at the micro- and macroscales while maintaining a constant number of simulated fibers (*i.e.*, a constant fiber to FE volume ratio). In the real material, a volume consistent with the typical FE size used in the 30720 FE simulations would contain roughly $10^3$ actual fibers. Of course, simulating every individual fiber would make the multiscale analyses intractable. However, Ricks *et al*.[7] showed that as the number of fiber subcells increases, the microscale behavior is consistent with that of the homogenized continuum. It therefore becomes crucial that the approximation of the microscale response that is passed to the macroscale is sufficiently refined to represent bulk response of the material from a statistical standpoint. To investigate this issue, additional simulations were performed in which 16-fiber and four-fiber RUCs were paired with the 5280 and 36480 FE meshes, respectively, in order to simulate more fibers for a fixed material volume. Future studies will investigate additional FE/ RUC combinations, including more refined RUCs to better estimate the microscale.

For each simulation, 96 distinct RUCs were generated where individual fiber subcell strengths were determined using Eq. (1). These RUCs were randomly assigned to element integration points within the FE mesh in equal numbers. Twenty separate analyses were performed for each FE mesh/ RUC combination in order to estimate the scatter in UTS and failure behavior associated with a statistical distribution of fiber strengths.

Table 1 shows the UTS results for the coupled FE/ micromechanics multiscale analyses for the different combinations of FE mesh and RUCs considered in this study. When the 840 FE mesh was paired with 16-fiber RUCs, the average predicted strength of 1765 *MPa* matches the experimental test data, while the coefficient of variation (CV) is approximately half of the experimental value of 9.39%. By simulating the 5280 FE/ four-fiber RUC and 36480 FE/ single-fiber RUC combinations, while a UTS of 1568 *MPa* (CV 6.3%) and 1537 *MPa* (CV 12.9%), respectively were obtained, these values were lower than the experimental UTS data and the 840 FE/ 16-fiber RUC simulations. This difference in UTS can be primarily attributed to the macroscale FE discretization. Note that the 840 FE mesh has only one element through the thickness of the specimen while the 5280 and 36480 FE meshes have two and four elements through the thickness, respectively. When multiple elements are used in the thickness direction, local element failures can induce out-of-plane bending in the simulated specimen leading to lower strength predictions and greater variability in the predicted strengths. This illustrates that capturing key failure mechanisms related to global deformations, instabilities, or eccentricities can be dependent entirely on the macroscale discretization. In these simulations, the microscale (RUC) response does not account for out-of-plane bending upon fiber failure. Additionally, as more fibers are simulated at the microscale, the homogenized RUC response becomes more uniform resulting in a lower CV. Other sources of variability such as local fiber volume fraction and matrix properties could potentially increase the CV and will be considered in future studies.

Alternatively, if a coarser microscale discretization is used, the material volume at the macroscale over which the microscale calculations were performed could over (or under) estimate microscale effects. When the 5280 FE/ 16-fiber RUC and 36480 FE/ four-fiber RUC discretizations were simulated, the average UTS of 1960 *MPa* and 1835 *MPa* over-estimates the experimental data (1765 *MPa*). Recall that these two cases each have the same simulation volume (*i.e.*, the same number of fiber subcells are simulated for a given element cross-section), although with another possible microscale discretization. Additionally, for the same FE mesh, more fiber subcells at the RUC level results in a higher UTS and less scatter in UTS consistent with observations by Ricks *et al*.[7] Since many fibers in a CFC could be simulated for a given FE size, one possible microscale discretization would be to use a microscale discretization that produced continuum-like behavior. Previous work[7] for a metal matrix composite system has suggested this behavior may be observed by simulating approximately 25 fibers at the microscale. In such a case, microscale calculations could be independently performed and used as a guide to determine the appropriate microscale discretization in the multiscale analyses. Ongoing work is performing these independent micromechanics calculations. Subsequent multiscale simulations will then be performed.

Additionally, as shown in Table 1, micro- and macroscale discretizations clearly influence the computational efficiency. As would be expected, when finer RUCs are used at the microscale, longer computational times result for a constant FE mesh. Similarly, for a constant microscale discretization, the computational time increases when a finer FE mesh is used at the macroscale. For example, for the 5280 FE mesh, the total clock time is 1738 *s* when 16-fiber RUCs are used at the microscale versus 623 *s* when four-fiber RUCs are used. Also, when four-fibers RUCs are used for the 5280 and 36480 FE meshes, the total clock times are 623 *s* and 4811 *s*, respectively. However when comparing results for a constant simulation volume, a fine microscale (RUC) discretization paired with a coarse macroscale (FE) discretization is more computationally efficient than a coarse microscale discretization paired with a fine macroscale discretization. Since the microscale calculations based on the generalized method of cells are more efficient than FE calculations[15], it is more computationally efficient to simulate a finer microscale discretization rather than a finer macroscale discretization.

**Table 1.** Simulation and experimental results[10] for multiscale analyses for an AS4/ 3502 unidirectional PMC.

| | 840 FEs + 16-Fiber RUCs | 5280 FEs + Four-Fiber RUCs | 36480 FEs + Single-Fiber RUCs | 5280 FEs + 16-Fiber RUCs | 36480 FEs + Four-Fiber RUCs | Experimental Data |
|---|---|---|---|---|---|---|
| Average UTS (MPa) | 1765 | 1568 | 1537 | 1960 | 1835 | 1765 |
| Coefficient of Variation (%) | 4.2 | 6.3 | 12.9 | 5.1 | 3.0 | 9.39 |
| Average Total Clock Time (s) | 238 | 623 | 2535 | 1738 | 4811 | |

Figure 4 shows the distribution of failed elements for simulations where 840 FEs are paired with 16-fiber RUCs (Fig. 4a), 5280 FEs are paired with four-fiber RUCs (Fig. 4b), and 36480 FEs are paired with single fiber RUCs (Fig. 4c). In these figures, “blue” elements denote no fiber failure at the microscale while “red” elements indicate complete fiber failure at the microscale. Also recall that complete fiber failure at the microscale corresponds to 16, four, and one fiber failures for Figs. 4a-c, respectively. For Figs. 4a-b, only local fiber failures corresponding to one surface layer of FEs are shown. In Figs. 4a-c, local fiber failures are distributed throughout the FE mesh, but tend to localize at several points. As an aside, a more realistic failure behavior consistent with experimental observations can be obtained by simulating a statistical distribution of fiber strengths at the microscale. Additionally, most simulations tended to predominately fail away from the tab transition region, although some simulations showed failure at the tabs. Overall, the failure behavior is similar between these different discretizations. Failure behavior for the 5280 FE/ 16-fiber RUC and 36480 FE/ four-fiber RUC simulations are not shown. As would be expected, for a given FE mesh, if a finer microscale discretization is used, more partial fiber failures occur throughout the specimen.

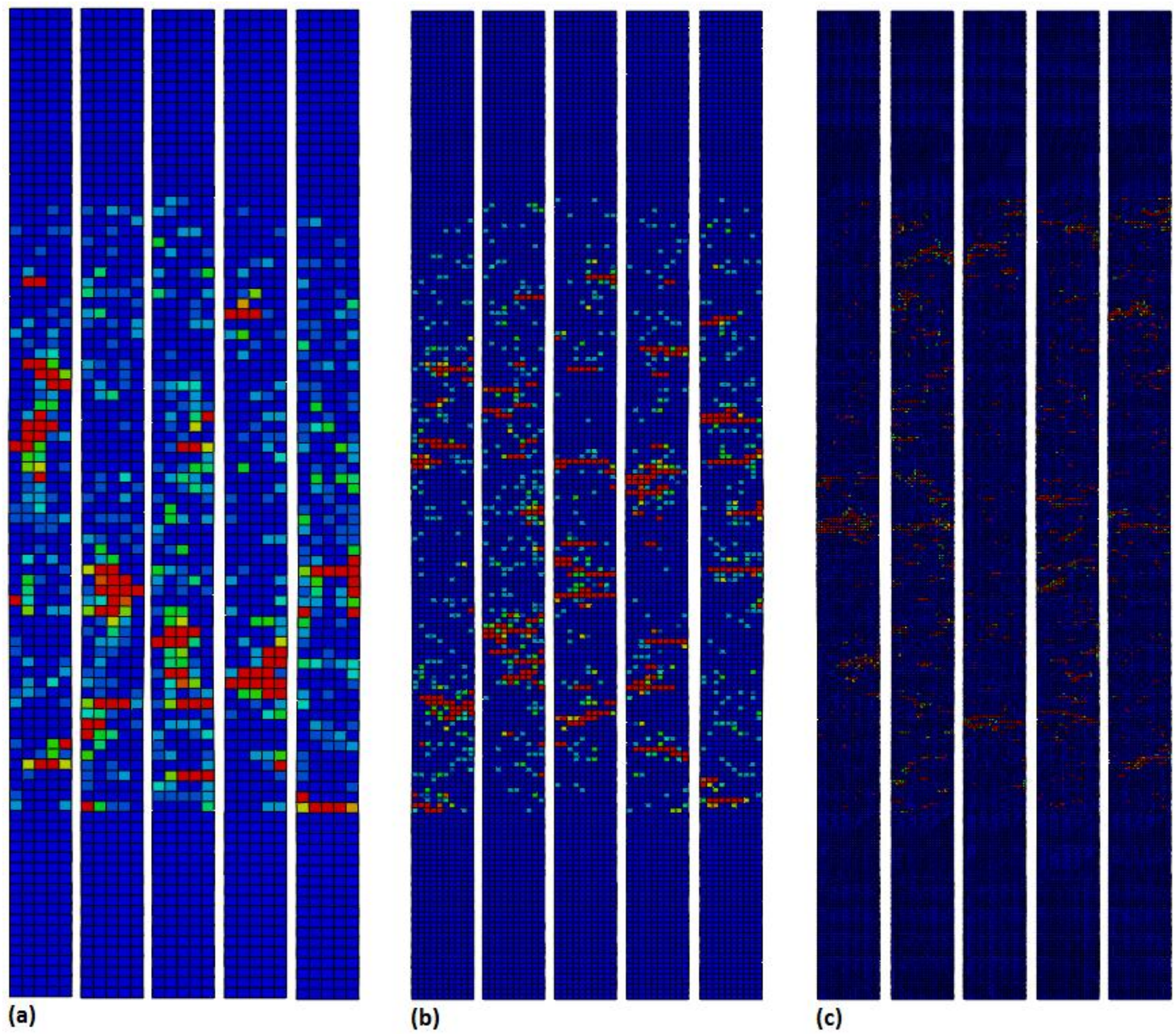



**Figure 4.** Distribution of fiber failures within the FE mesh after the onset of localization for a) 840 FE/ 16-fiber RUC, b) 5280 FE/ four-fiber RUC and c) 36480 FE/ single-fiber RUC combinations where blue represents no fiber subcell failure and red represents complete fiber subcell failure. Each group represents five distinct simulations.

## IV. Summary and Conclusions

In this work, coupled finite element (FE)/ micromechanics multiscale progressive failure analyses were performed in order to investigate the effect of mesh discretization both at the micro- and macroscale on the predicted ultimate tensile strength (UTS) and global composite failure behavior for a unidirectional AS4/ 3502 longitudinal tensile specimen. A statistical distribution of fiber strengths was embedded at the microscale and simulations were performed using the commercial FE solver ABAQUS and NASA code FEAMAC. Recognizing that a given material volume can be discretized a variety of ways at the micro- and macroscales, noticeable differences in predicted UTS were observed when these micro- and macroscale discretizations varied. The discretization at a particular length scale should therefore accurately capture failure mechanisms and approximate the local, continuum-averaged material response while attempting to avoid excessive computational costs associated with over-discretization. It was found that for a constant macroscale discretization, increasing the microscale discretization increased the computational time. A similar increase was observed when the macroscale discretization increased for a constant microscale discretization. However, since the microscale computations were more efficient than the macroscale computations, a finer microscale discretization coupled with a coarser macroscale discretization results in a more computationally efficient simulation. Therefore, length scale(s) with more computationally efficient calculations should be more highly discretized. Ongoing work is investigating more complex micro- and macroscale discretizations, other material systems, and specimen geometries (*e.g.*, open-hole tension). By investigating the effects of discretization at the micro- and macroscales, more accurate and computationally efficient multiscale analyses can be performed.

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