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Micromechanics-Based Structural Analysis (FEAMAC) and Multiscale Visualization Within Abaqus/CAE Environment

Steven M. Arnold and Brett A. Bednarcyk
Glenn Research Center, Cleveland, Ohio

Aquila Hussain and Vivek Katiyar
Dassault Systemes SIMULIA Corp., Beachwood, Ohio

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Glenn Research Center
Cleveland, Ohio 44135

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Glenn Research Center
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Aquila Hussain and Vivek Katiyar
Dassault Systemes SIMULIA Corp.
Beachwood, Ohio 44122

Abstract

A unified framework is presented that enables coupled multiscale analysis of composite structures and associated graphical pre- and post-processing within the Abaqus/CAE environment. The recently developed, free, Finite Element Analysis—Micromechanics Analysis Code (FEAMAC) software couples NASA's Micromechanics Analysis Code with Generalized Method of Cells (MAC/GMC) with Abaqus/Standard and /Explicit to perform micromechanics based FEA such that the nonlinear composite material response at each integration point is modeled at each increment by MAC/GMC. The Graphical User Interfaces (FEAMAC-Pre and FEAMAC-Post), developed through collaboration between SIMULIA Erie and the NASA Glenn Research Center, enable users to employ a new FEAMAC module within Abaqus/CAE that provides access to the composite microscale. FEAMAC-Pre is used to define and store constituent material properties, set-up and store composite repeating unit cells, and assign composite materials as sections with all data being stored within the CAE database. Likewise FEAMAC-Post enables multiscale field quantity visualization (contour plots, X-Y plots), with point and click access to the microscale (i.e., fiber and matrix fields).

1.0 Introduction

The use of advanced polymeric, metallic, and ceramic composites (PMCs, MMCs, CMCs) provides benefits in the design of advanced lightweight, high temperature, structural systems because they provide increased specific properties (e.g., strength to density ratio) in comparison to their monolithic counterparts. To fully realize the benefits offered by these materials, however, experimentally verified, computationally efficient, multiscale design and analysis tools must be developed for the advanced multiphased materials of interest. Furthermore, in order to assist both the structural analyst in designing ***with*** these materials and the materials scientist in designing/developing ***the*** materials,[1] these tools must encompass the various levels of scale for composite analysis, see Figure 1.

These scales are the micro scale (constituent level), the mesoscale (laminate/composite and/or stiffened panel level) and the macro scale (global/structural level), and they progress from left to right in Figure 1. Traditionally, one traverses (transcends (moves right) or descends (moves left)) these scales via homogenization and localization techniques, respectively (Figs. 1 and 2(a)); where a homogenization technique provides the properties or response of a "**structure**" (higher level) given the properties or response of the structure's "**constituents**" (lower scale). Conversely, localization techniques provide the response of the constituents given the response of the structure. Figure 2(b) illustrates the interaction of homogenization and localization techniques, in that during a multi-scale analysis, a particular stage in the

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[1] The structural engineer perspective relates to the design of structures with given materials whereas the materials scientist perspective is how to design a material for a given application. Clearly, the two perspectives are not mutually exclusive.

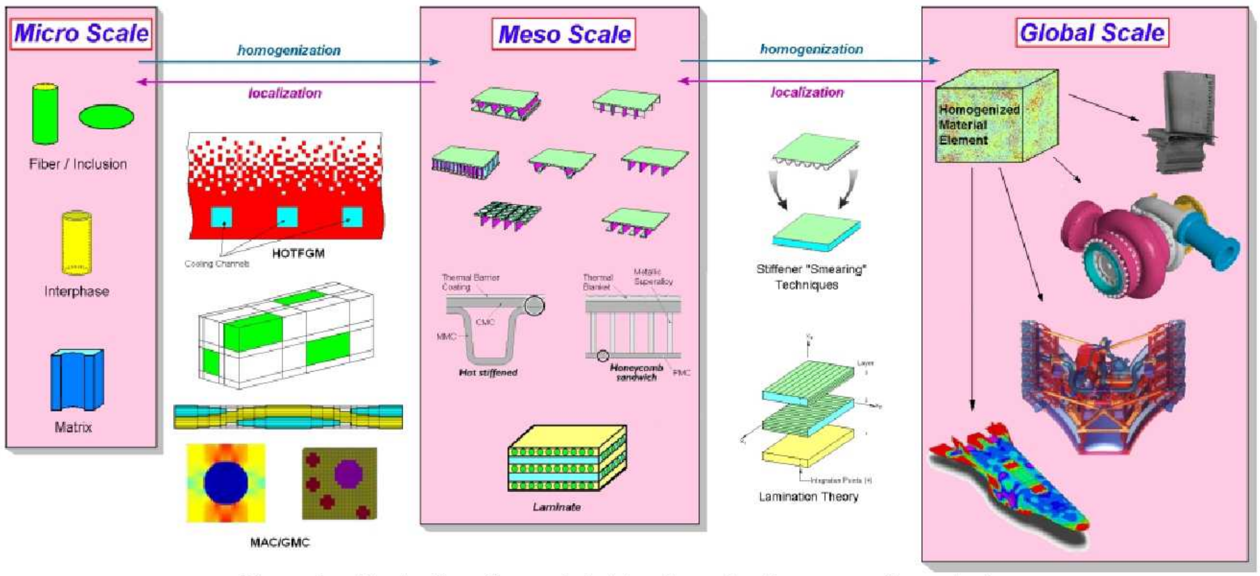


Figure 1.—Illustration of associated levels scales for composite analysis.

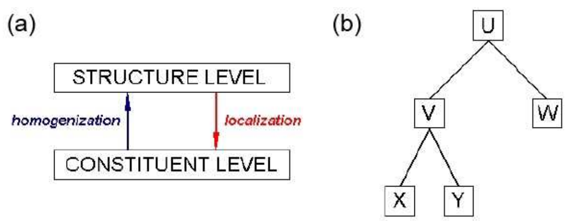


Figure 2.—(a) Homogenization provides the ability to determine structure level properties from constituent level properties while localization provides the ability to determine constituent level responses from structure level results. (b) Example tree diagram.

analysis procedure can function on both levels simultaneously.[2] For example, for the process of homogenizing the stages represented by X and Y to obtain properties for the stage represented by V, X and Y form the constituent level while V is on the structure level. However, for the process of homogenizing V and W to obtain properties for U, V is now on the constituent level (as is W). Obviously, the ability to homogenize and localize accurately requires a sophisticated theory that relates the geometric and material characteristics of structure and constituent.

Numerous homogenization techniques (micromechanical models) exist that can provide effective composite properties to a finite element package. These range from the simplest analytical approximations (i.e., Voigt/Reuss) to more accurate, yet involved methods (e.g., concentric cylinder assemblage, Mori-Tanaka, Eshelby, and Aboudi's generalized method of cells) to finally fully numerical methods that are the most general and accurate yet computationally intense (e.g., finite element, boundary element, Fourier series). Each has its realm of applicability and advantages, however, many are unable to admit general user-defined deformation and damage/failure constitutive models for the various constituents (i.e., fiber or matrix) thus limiting their ultimate usefulness, especially for high temperature analysis.

An alternative approach to micromechanics involves fully characterizing the composite material or laminate experimentally, which has the advantage of capturing the in situ response of the constituents perfectly. However, such full characterization can be expensive, and composites are almost always anisotropic

[2] This is also illustrated in Figure 1 where for example the global scale has subscales (components) within it (i.e., vehicle- engine- turbopump- blade) and the mesoscale has subcomponents (stiffened panel-laminate-ply).

on this scale. Thus development of realistic models that capture the nonlinear multiaxial deformation and failure, which are needed for use in structural analyses, can be challenging (due to the anisotropy). Clearly, the physics of deformation and failure occur on the micro scale (and below), and, by modeling the physics at the micro scale, models for the monolithic, often isotropic, constituents can be employed.

Recently, a comprehensive and versatile micromechanics analysis computer code, known as MAC/GMC [Bednarcyk and Arnold (2002)] has been developed at NASA Glenn Research Center (based on Aboudi's well-known micromechanics theories, Aboudi (1991) and Paley and Aboudi(1992)) which determines the effective properties and response of composite materials and laminates based on the arrangement and properties of the constituent materials. FEAMAC (the implementation of MAC/GMC into the finite element analysis framework through user-subroutines) and HyperMAC (the implementation of MAC/GMC into the commercial structural sizing software known as HyperSizer, Collier (2009)) have begun to address the truly multiscale aspects of composite materials depicted in Figure 1. This software suite, known collectively as ImMAC, provides a wide range of capabilities for modeling continuous, discontinuous, woven, and smart (piezo-electro-magnetic) composites. Libraries of nonlinear deformation, damage, failure, and fiber/matrix debonding models, continuous and discontinuous repeating unit cells, and material properties are provided, and the software is available from NASA free of charge. The MAC/GMC core analysis modules were specifically designed to integrate with higher-scale structural analysis codes like Abaqus/Standard and Abaqus/Explicit, Simulia (2009).

It should be noted that MAC/GMC also includes a multiscale classical lamination theory module, wherein Aboudi's micromechanics theories are employed at each integration point in each ply, see Figure 3(a). Thus, once lamination theory localizes the incrementally applied laminate-level loading to the ply and then integration point, these local stresses and strains are applied to the GMC or HFGMC (High Fidelity Generalized Method of Cells) repeating unit cell. These micromechanics theories localize to the subcell level, and MAC/GMC's nonlinear deformation/damage/life models for the constituents are applied. The effects of these local mechanisms on the laminate are then captured through homogenization to the ply and laminate levels. As shown in Figure 3(c), FEAMAC is the direct implementation of MAC/GMC unit cell analyses within structural FEA. The software currently supports both standard and explicit versions of the Abaqus commercial finite element software. The coupling is accomplished utilizing the Abaqus user subroutines (see Fig. 4), which enable the MAC/GMC code to be called as a library to represent the composite material response at the integration and section points in any element within the finite element model. Two- and three-dimensional continuum elements, as well as shell elements, are supported. Any nonlinearity due to local effects (e.g., inelasticity or damage) in the fiber/matrix constituents at any point in the structure are thus captured and homogenized, and their effects on the structure are manifested in the finite element model structural response.

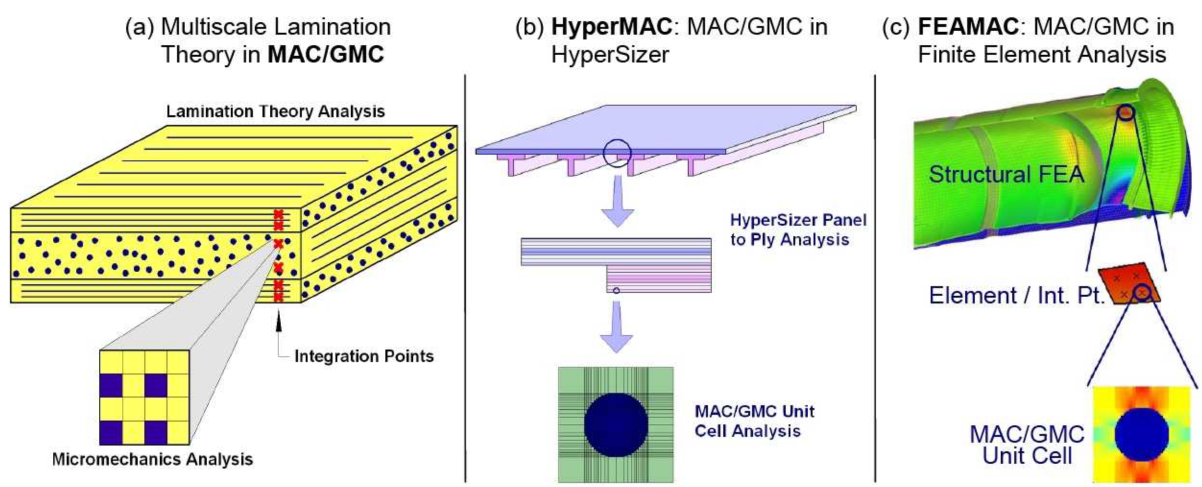


Figure 3.—(a) Multiscale lamination theory available in MAC/GMC. (b) HyperMAC coupling of HyperSizer with MAC/GMC. (c) FEAMAC coupling of MAC/GMC with finite element analysis.

Recently, FEAMAC-CAE (which consist of two Graphical User Interfaces, FEAMAC-Pre and FEAMAC-Post) was developed through collaboration between SIMULIA Erie and NASA Glenn Research Center to enable a seamless coupling of the FEAMAC analysis module with Abaqus/CAE to provide a unified system for setting up, solving, and performing truly multiscale visualizations of the results stemming from elements which utilize the MAC/GMC defined materials. This multi-scale software package thus enables for the first time, efficient micromechanics based analysis of composite structures simply by calling a MAC/GMC library directly from Abaqus to represent the composite material within the structure. The remainder of this paper will be devoted to describing the FEAMAC-Pre (Section 2.0) and FEAMAC-Post (Section 3.0) modules of the newly developed FEAMAC-CAE suite as depicted in Figure 5. Applications (Section 4.0) and Conclusions (Section 5.0) are also described.

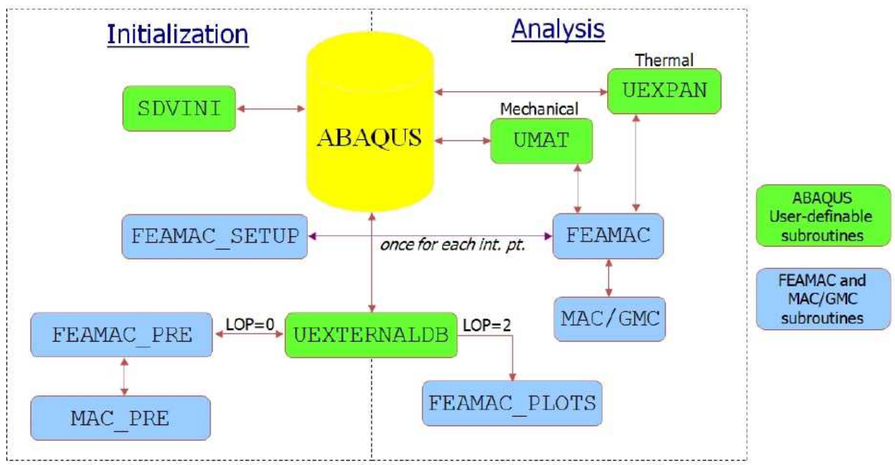


Figure 4.—Schematic showing the implementation of the FEAMAC code within the Abaqus built in UMAT framework.

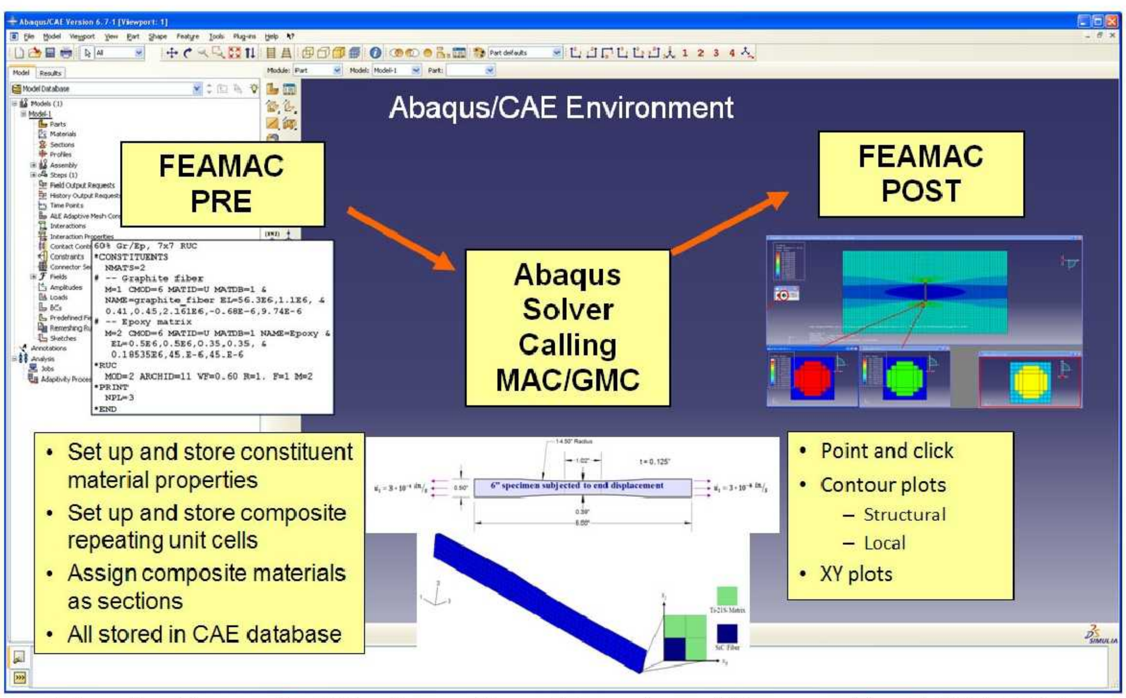


Figure 5.—Diagram identifying the specific modules and capabilities comprising FEAMAC-CAE

2.0 FEAMAC-Pre

A MAC/GMC material model consists of a geometric repeating unit cell (RUC) partitioned into different constituents of the composite where thermo-mechanical elastic visco-plastic constituent material properties, constituent damage and failure properties, composite failure and de-bonding properties are all entered in an ASCII file called a MAC input file. Constituent materials are assigned to these partitions (via subcells within the RUC), and the overall response of this RUC is used as the material response at any integration point in an Abaqus analysis. Every integration point has its own RUC response, yet each element can have only a single associated RUC definition.

Writing this MAC input file can be a daunting task for new users as MAC/GMC has 14 different predefined constitutive models including a user-definable model similar to the UMAT routine within Abaqus. Further, ten doubly-periodic (i.e., 2–D) and seven triply-periodic (i.e., 3–D) predefined fiber architectures (e.g., square pack, hexagonal pack, ellipsoidal inclusion rectangular packed, etc.) and a user-definable architecture capability exist.

Consequently, FEAMAC Pre is a simple, consistent GUI interface for defining MAC/GMC materials within the Abaqus/CAE environment, which users of Abaqus are already familiar. This is accomplished using the icons, e.g. constituent manager and RUC manager tools, on the left side of the viewport in Figure 6.

2.1 Constituents

All constituents required in the construction of a given composite must be defined, prior to creating an RUC for a MAC/GMC material. As constituent materials are not available for use within an Abaqus analysis directly, a constituent manager dialog box has been provided to enable users to create, delete, rename, copy and edit constituent materials (see Fig. 7). Constituent materials can be user-defined (see Fig. 7(b)) or pre-defined (see Fig. 7(c))—in which case the user must ensure that the pre-defined units and the units used in the analysis are identical. Commonly used metal matrix composite materials have been pre-defined as shown in Figure 7(c). Creating a user- defined constituent material requires the user to follow a multiple dialog sequence as shown in Figure 7(b) for the Classical Plasticity constitutive model. After a constituent is created the user can add advanced features to the constituent materials like strength "Allowables" (see Fig. 8(a)), one or more "Failure of Subcells" (see Fig. 8(b)), or provide "Damage" properties (see Fig. 8(c)), [Bednarcyk and Arnold (2002)].

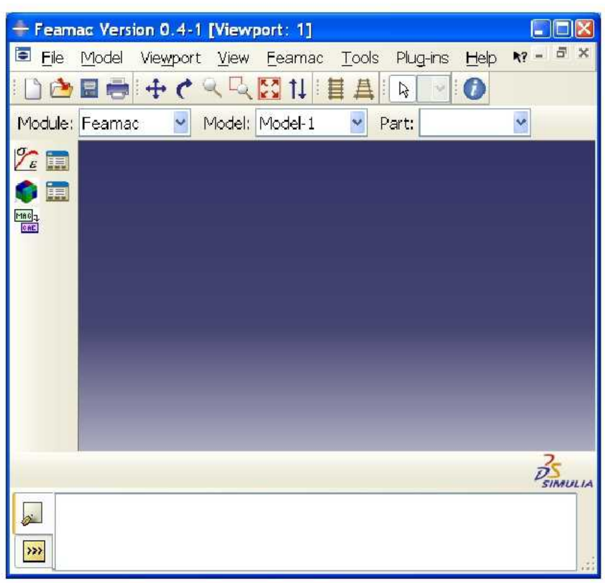


Figure 6.—FEAMAC-Pre module within Abaqus/CAE

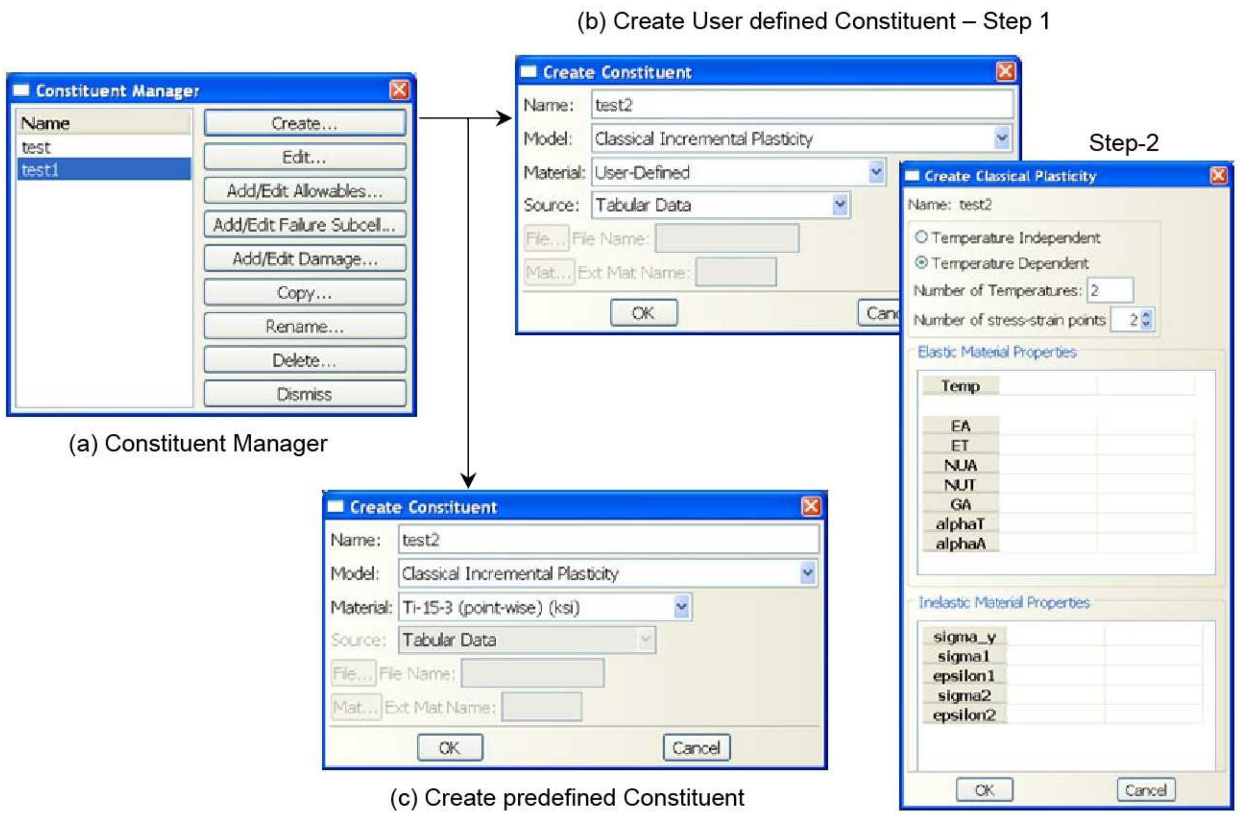
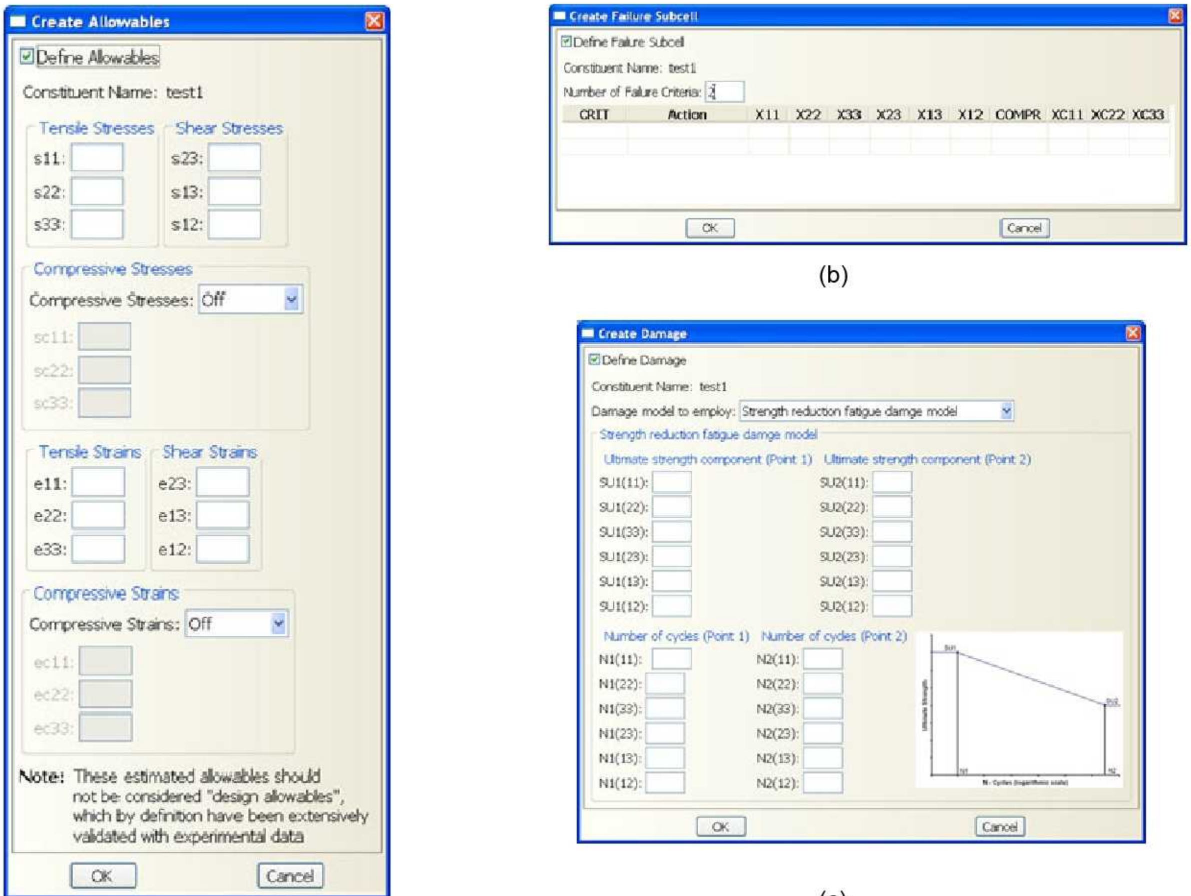


Figure 7.—Constituent Manager (a) enables the definition of either user defined (b) or predefined (c) constituent materials



(a) (b) (c)

Figure 8.—Depicts the input windows one would use to define (a) the strength allowables, (b) failure criteria, and/or (c) damage parameters for a given constituent (i.e., subcells) material.

2.2 RUC

Assuming all required constituents exist, a user now needs only to create the associated RUC for the given composite material to enable a multiscale analysis to be conducted. Again, an RUC manager has been provided to enable users to create, delete, copy, rename and edit a 2–D or 3–D RUC which can be predefined or user defined. An example of how a 2–D pre-defined material would be entered is shown in Figure 9(b). Whereas a user-defined 3–D material is constructed by slicing the 3–D RUC into a number of 2–D layers and then, for each layer, selecting the corresponding subcells (by highlighting them) for a given constituent and then assigning the constituent material by clicking on the constituent in the 'Constituent Material List' (see Fig. 9(c)). It is also possible to view the full 3–D user defined RUC by clicking the 'Show' button, which will display a new viewport with the newly created RUC (see Fig. 9(d)).

Again, after a RUC is created the user can add one or more advanced features to the RUC like "Failure Cell" criteria as seen in Figure 10(a), "Debond" criteria at specific faces as in Figure 10(b) and "Curtin" fiber breakage parameters to the subcells to account for the stochastic nature of ceramic fibers, see Figure 10(c), [Bednarcyk and Arnold (2002)].

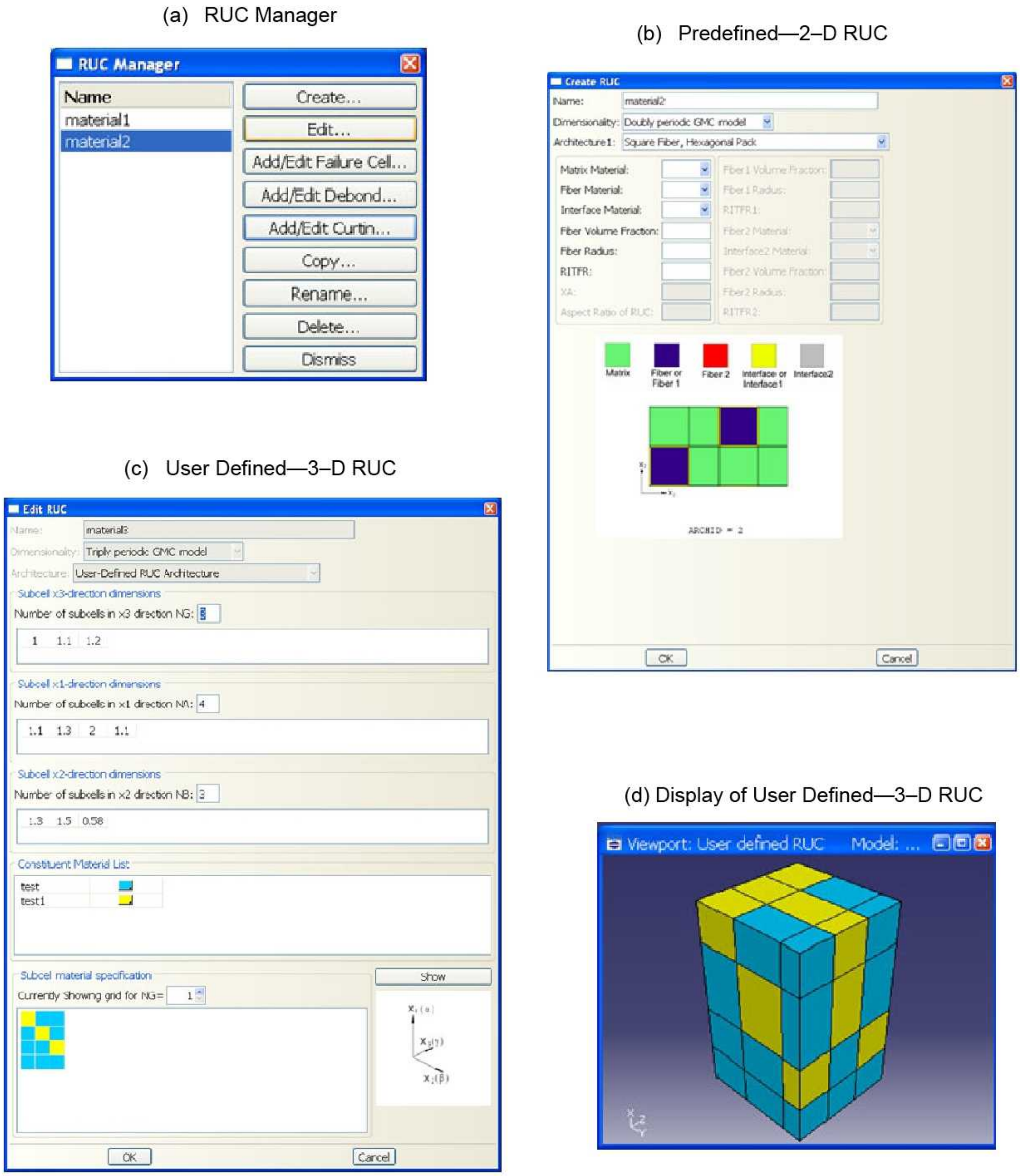
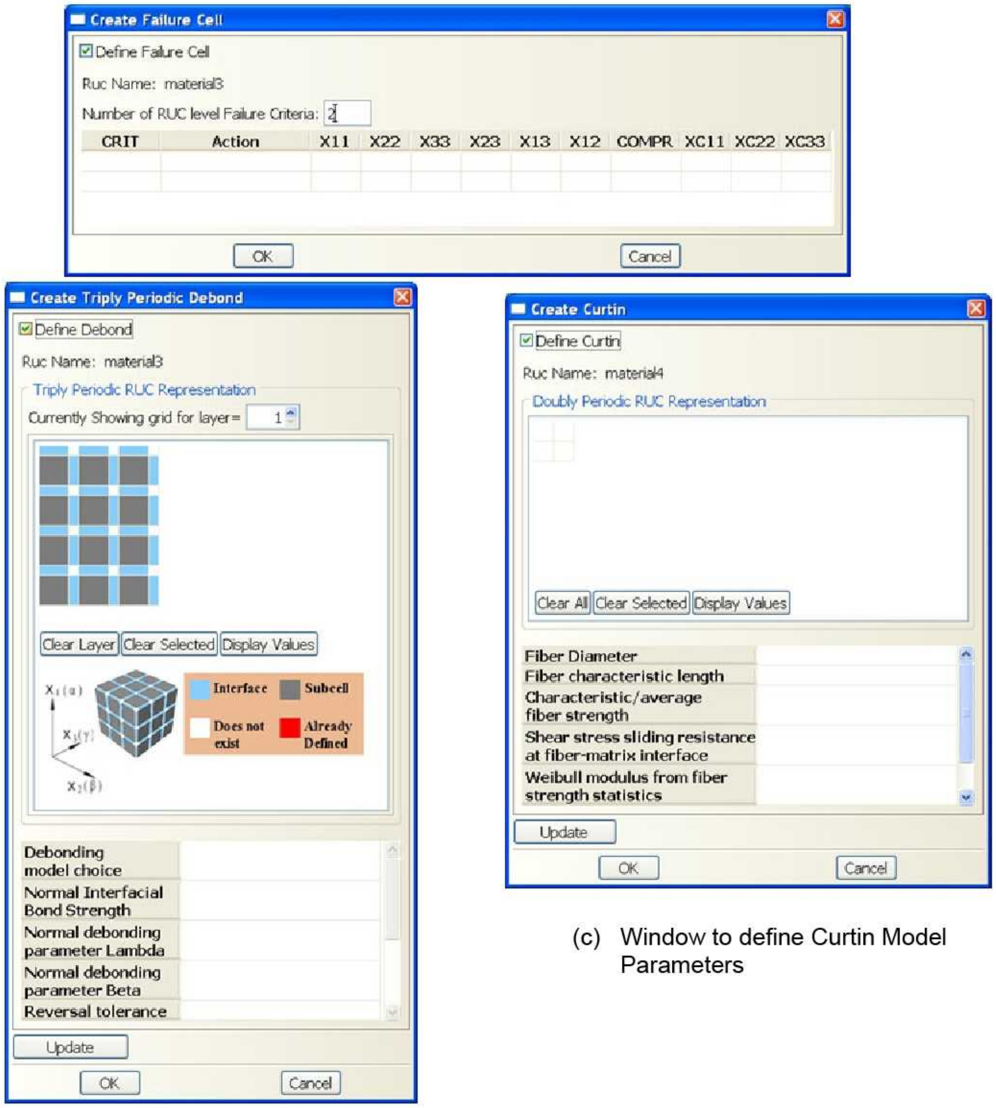


Figure 9.—Illustrates (a) the RUC Manager and the input schema for both (b) predefined RUCs, (c) User Defined RUCs and (d) the display window for the RUC.

(b) Window to define Failure Cell



(c) Window to define Curtin Model Parameters

(a) Window to define debond surfaces within RUC

Figure 10.—Input windows one would use to define (a) failure cells and criteria, (b) debond surfaces and (c) Curtin fiber breakage model.

2.3 FEAMAC Module

Upon completion of the RUC definition, an Abaqus User material will be created for use within the Abaqus FEA as shown in Figure 11. This material definition is then used in a section definition and thus enables assignment of material properties within the current Abaqus/CAE paradigm for setting up an FE model. When a user writes an input file (or submits a job), the ASCII input file associated with the MAC/GMC material is created along with the Abaqus input file in the same directory. This ASCII input file is identified by using the RUC material name followed with a .mac extension. Therefore a user need only run the Abaqus job with the FEAMAC user subroutines to be able to make use of the MAC/GMC material in this analysis.

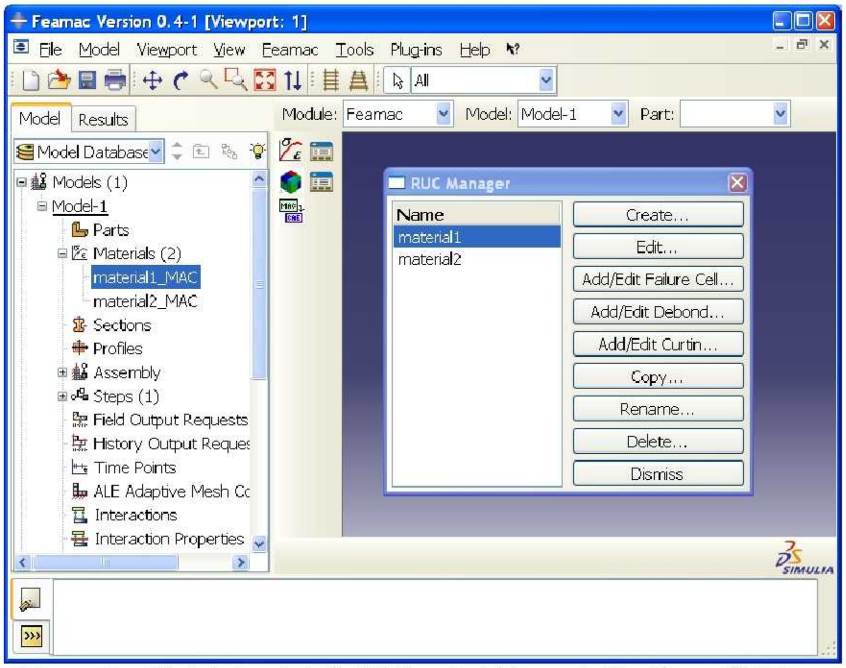


Figure 11.—Material material1_MAC material is created in Abaqus/CAE when an RUC material named material1 is created.

3.0 FEAMAC-Post

Subsequent to executing an analysis run using User Subroutines, the Output Database (.odb file) is converted into a format which FEAMAC-Post can run on due to the influence of the environment file. This process essentially consists of copying the existing odb file, generating new elements in it to create a subcell representation for every integration point of the MAC/GMC material, and transferring Solution Dependent State Variable (SDV) results to the subcells in tensor format so that invariant computations can be automated. A new file called a .set file is also created to provide a faster lookup between the analysis's element section point integration point data and its subcell representation.

When results from such an analysis are opened within FEAMAC-Post, it will automatically display all the different RUC materials used in the analysis, as shown in Figure 12. Component and Subcell level viewports are present while displaying results. When the Subcell Viewport is made current, the Component Viewport highlights (by color coding) the element whose subcell information is being displayed in the Subcell Viewport.

Two types of tools are available at this point: tools to manipulate and display subcell level information (e.g., Show Subcell, Show Subcell Results, Show XY-Plot, Show Combined XY-Plot; see the Tools dialog box shown in Fig. 12) and tools to manage the display of other information (e.g., Remove Subcells from Component Viewport, Show Material Viewport, Cascade Material Viewports, and Remove Material Viewports; see the icons in red circle, Fig. 12). To display Subcell results, the user has to first display the subcell by clicking on the "Show Subcell" tool. This tool prompts the user to pick an element, and prescribe the section point and integration point for that element. FEAMAC Post displays the RUC representation for the selected element, section point, integration point in a new viewport and puts this information in its title to create a display as shown in Figure 12. Then the user has option of displaying subcell results on this RUC by clicking on the "Show Results" tool and by selecting the variable to display using dialog box shown in Figure 13(a) to create a display of type shown in Figure 13(b).

To create XY-Plots against time, the user has to display the results as a contour plot in the RUC representation, and then click the "Show XY-Plot" button. This prompts the user to select the subcell for which this plot will be created to generate a plot as shown in Figure 13(c). To create combined XY-Plots, the user has to select a subcell from the RUC viewport (Fig. 13(b)) and describe the X and Y axis variables (see Fig. 13(d)) to be used for creating a combined plot as shown in Figure 13(e).

During manipulations of display, if in the Component Viewport, all subcell information is also displayed, then subcells can be removed using a single button click of “Remove subcells from component viewport”. The “Show material viewport” tool is used to display the RUC representation of any element. This is similar to the “Show Subcell” tool except that the title of Viewport created shows the MAC/GMC material name for that element. If the analysis consists of many MAC materials, then the “Cascade Material Viewports” cascades all the materials, and to simultaneously remove all the material viewports the “Remove Material Viewports” tool can be used.

4.0 Application

The above described seamless coupling of the Finite Element Analysis—Micromechanics Analysis Code (FEAMAC) with the recently developed pre- and post-processing capability, named FEAMAC—CAE, enables full nonlinear multiscale composite structural analysis; wherein the composite material response (deformation and failure) at each integration point is computed on the fly at each loading increment and iteration by MAC/GMC. This consistent multiscale framework circumvents the need for complex, multiaxial, anisotropic damage and constitutive models that are required to operate on the macroscale for nonlinear composite structural analyses. Furthermore utilization of the Abaqus material grouping allows very efficient execution of large structures (see for example a payload shroud for the Ares V rocket, Fig. 14) since a majority of elements can be analyzed using anisotropic continuum properties (see the blue regions in Fig. 14) while only elements in regions of high stress (interest) need be computed using a micromechanics-based analysis (see orange and red regions in Fig. 14).

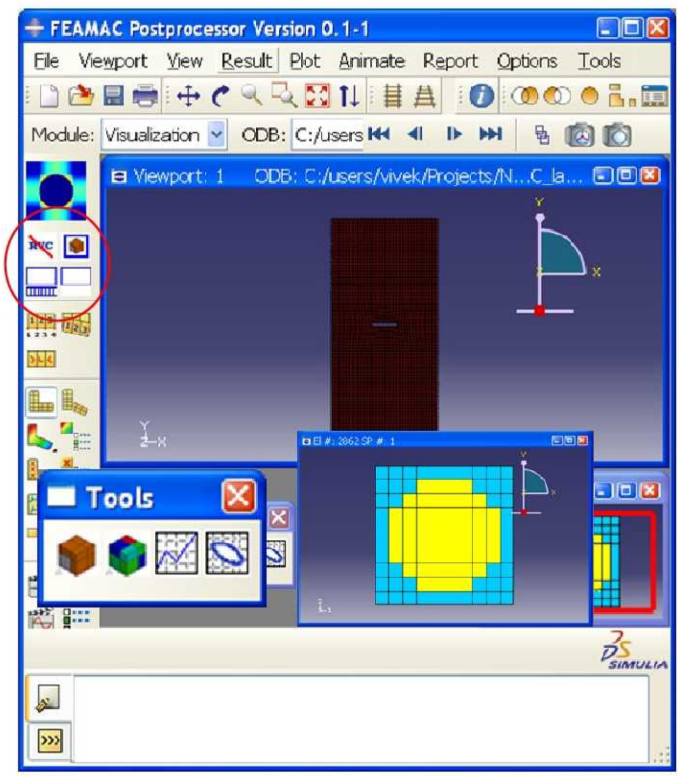


Figure 12.—Shows the CAE environment and the various viewports available when FEAMAC-Post is running, e.g., global level viewport and RUC viewport. Four utility subcell display tools are also shown.

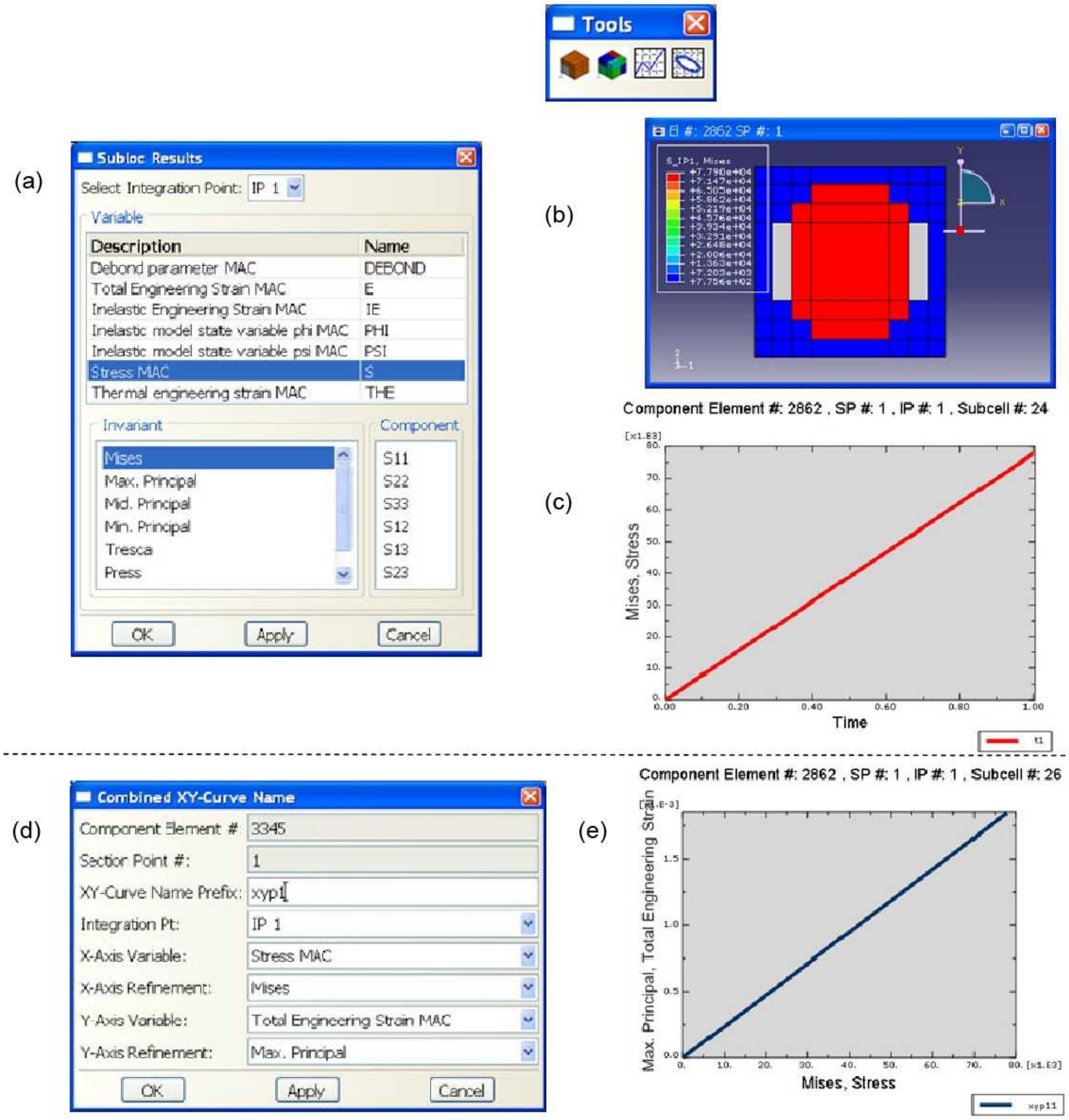


Figure 13.—Shows the input windows when one invokes the options for contour plotting as well as X-Y plotting of local fields within the RUC.

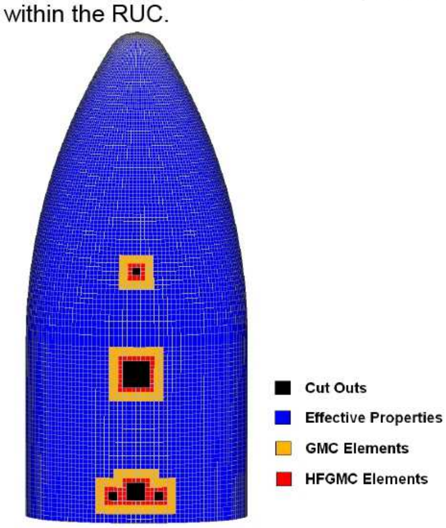


Figure 14.—Abaqus FE mesh for an Ares V shroud structure.

To illustrate the power and utility of the framework a 25 percent fiber volume fraction SiC/Ti titanium matrix composite (TMC) test specimen (i.e., structure) was modeled with a one-eighth symmetry FE mesh with symmetry boundary conditions applied to the three faces (see center insert Fig. 5). The specimen was modeled with a total of 300 C3D8 elements, each containing eight integration points per element. A thermomechanical loading cycle was imposed consisting of a 16 hour cool-down to a room temperature of 23 °C from a uniform 900 °C heat treatment; a temperature rise to 650 °C over 5 minutes; and then a monotonic uniaxial tensile loading applied at a displacement rate of $3*10^{-4}$ in/s until complete fiber failure (i.e., structural failure) is obtained at 650 °C.

The MAC/GMC micromechanics model is called as a user material (UMAT) subroutine 2400 times per time step. This procedure emphasizes the necessity of a computationally-efficient means of relating both the properties and the local stress/strain fields of the constituent phases of the composite to the effective properties and deformation response of its homogenized continuum representation. Within the context of the MAC material, the TMC's SiC (SCS-6) fiber was modeled with a linear elastic, isotropic constitutive model and a maximum stress failure criteria, while the titanium matrix (Ti-21S) was modeled as a rate/temperature dependant isotropic material using the Generalized Viscoplasticity with Potential Structure (GVIPS) constitutive model, Arnold et al. (1996), that is available as one of the internal constitutive models within the MAC/GMC code. Furthermore the statistical nature of the fiber strength is accounted for both globally throughout the tensile specimen (structure), see Figure 5 and locally within the RUC that contain 25 fibers, see insert in Figure 15, using a simple maximum stress criterion.

The analysis results in Figure 15 indicate that the multiscale framework is able to capture quite nicely the progressive failure behavior and characteristics of the experimental data, wherein results are shown using a vendor-supplied fiber strength distribution (modeled as a Weibull distribution with a length scale parameter, lambda ($=L/L_0$), which accounts for differences between the fiber length (1 in.) tested by the vendor and the applicable effective fiber length within the structure. Clearly, the effective length scale representing that associated with effective load transfer distance of a given fiber (i.e., the shear lag length) agrees most closely with experiments. Consequently, in Figure 16 we further illustrate how FEAMAC—CAE enables one to peer down into the material's local fields to discover that the bulk of the nonlinearity of the stress stain curve of Figure 15 is due to fiber breakage followed by significant matrix inelasticity, see Figure 16.

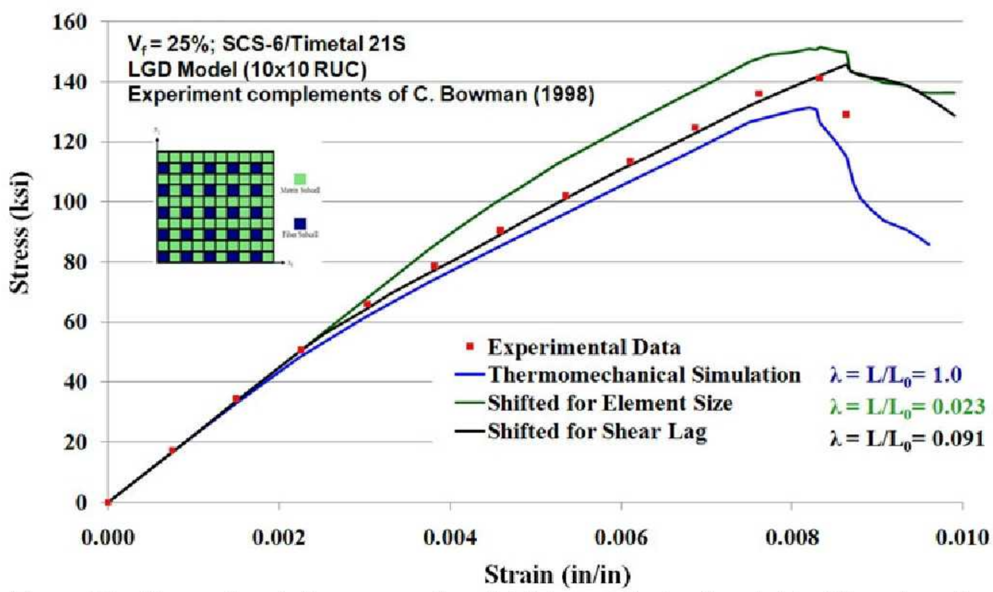


Figure 15.—Comparison between experimental data and the local and global fiber strength distribution model prediction for a uniaxial longitudinal tension experiment of SiC/Ti (SCS-6/Ti-21S) at 650 °C wherein the residual stresses developed during heat treatment are accounted for.

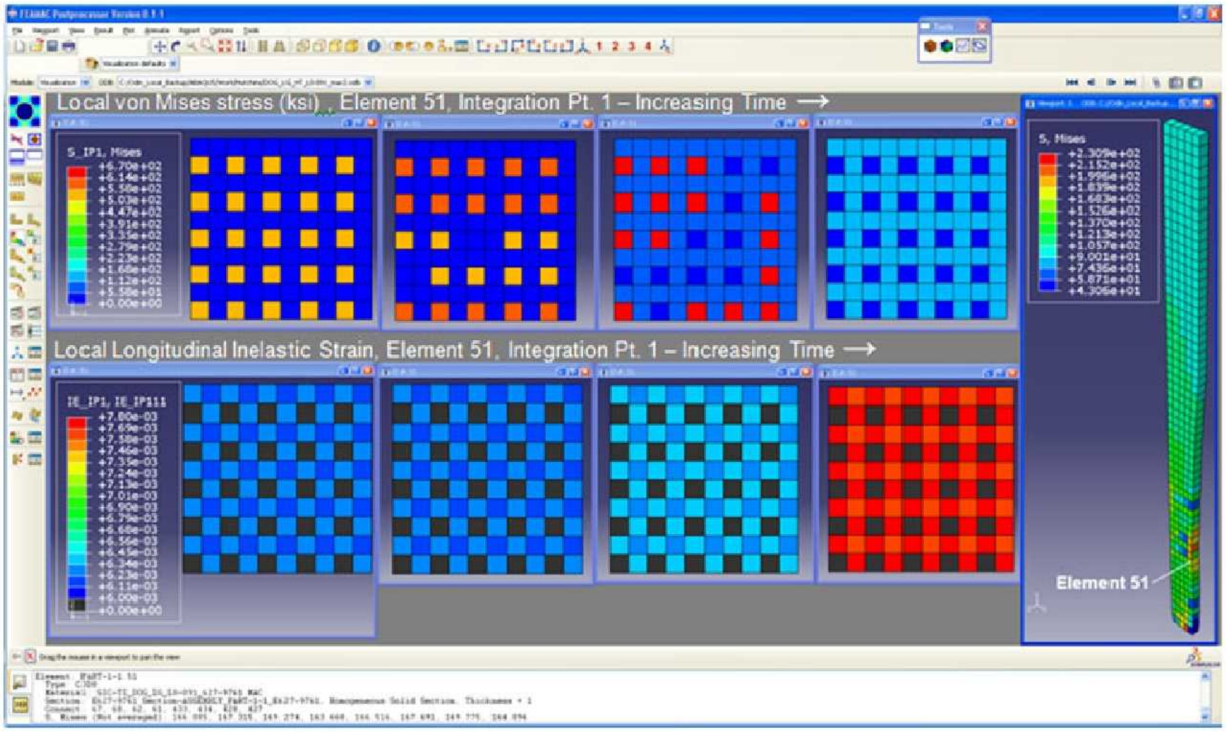


Figure 16.—Shows the local von Mises stress and Inelastic strain within the RUC associated with integration point 1 of element 51 within the dogbone specimen. Global stress-strain response is that shown in Figure 15 for the shear lag effective length case.

5.0 Conclusions

Herein we have introduced the seamless, multiscale, micromechanics-based, finite element modeling framework for composite structures known as FEAMAC and FEAMAC-CAE. This framework offers both accuracy and efficiency, at not only the global level of a composite structural analysis but also at the constituent level where micro-scale stresses and strains throughout the fiber/matrix constituents can be extracted and visualized at any desired point within the analysis. This publicly-available, user-friendly software includes a wide range of capabilities, including libraries of deformation and damage models that operate on the scale of the fiber/matrix constituents, architectures of reinforcements (discontinuous, continuous, laminate and woven) and failure criteria.

This extremely efficient multiscale method was demonstrated by simulating the stochastic failure nature within a TMC tensile specimen subjected to a thermomechanical analysis that incorporated manufacturing residual stresses and progressive failure via FEAMAC at each integration point within the finite element mesh.

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14. ABSTRACT
A unified framework is presented that enables coupled multiscale analysis of composite structures and associated graphical pre- and post-processing within the Abaqus/CAE environment. The recently developed, free, Finite Element Analysis--Micromechanics Analysis Code (FEAMAC) software couples NASA's Micromechanics Analysis Code with Generalized Method of Cells (MAC/GMC) with Abaqus/Standard and Abaqus/Explicit to perform micromechanics based FEA such that the nonlinear composite material response at each integration point is modeled at each increment by MAC/GMC. The Graphical User Interfaces (FEAMAC-Pre and FEAMAC-Post), developed through collaboration between SIMULIA Erie and the NASA Glenn Research Center, enable users to employ a new FEAMAC module within Abaqus/CAE that provides access to the composite microscale. FEAMAC-Pre is used to define and store constituent material properties, set-up and store composite repeating unit cells, and assign composite materials as sections with all data being stored within the CAE database. Likewise FEAMAC-Post enables multiscale field quantity visualization (contour plots, X-Y plots), with point and click access to the microscale (i.e., fiber and matrix fields).

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