MESH-OBJECTIVE MULTI-SCALE FINITE ELEMENT ANALYSIS OF UNIDIRECTIONAL FIBROUS MATERIALS USING ENERGY BASED FAILURE MECHANISM

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Abstract
In this work the commercial Finite Element software suite Abaqus is used to generate macroscopic models, e.g. components or parts. A second finite element code (IFEM) has been developed and fully integrated with the main Abaqus solver through a user material subroutine (UMAT). IFEM calculates the reaction of a microstructural model that consists of a Representative Unit Cell (RUC) which includes all constituents of the actual material, e.g. fiber, matrix, and fiber/matrix interfaces, details of packing, non-uniformities in properties etc. The energy based Crack Band Theory (CBT) is implemented within IFEMs constitutive laws to predict micro-cracking in all constituents included in the model. The communication between the micro- and macro-scale is achieved through the exchange of strain, stress and stiffness tensors. Important failure parameters, e.g. crack path, proportional limit, etc. are part of the solution and predicted with a high level of accuracy. Numerical predictions are validated against experimental results.

1. Introduction

Polymer-Matrix-Composites (PMCs) and Ceramic-Matrix-Composites (CMCs) are increasingly used in a wide range of applications. With the demand for lighter and more versatile structural components the need to understand interactive and complex failure mechanisms in these materials has grown and has become the focus of many research projects. The deformation response, subsequent damage development and failure of these multi-constituent materials is dependent on microstructural details such as variations in Fiber packing arrangement, properties at Fiber-matrix interfaces, and interactions between neighboring Fibers. Accurate numerical predictions for layered, fibrous materials are inherently dificult due to the intricate mechanisms that tie global component failure to microstructural degradation. Modeling strategies based on homogenized material properties neglect the importance of the physical behavior at the microstructural level, and thus homogenized models fail to predict critical parameters accurately that are observed experimentally, e.g. maximum load, strain to failure, crack spacing and other salient features. Often times the material direction is used as the failure direction. This might lead to erroneous crack paths for materials with similar fiber and matrix properties such as CMCs. Hence, multi-scale methods have become the focus of many research papers in recent years.

These models de-homogenize the strain and stress state for each constituent. Typically, a Representative Unit Cell (RUC) that preserves the microstructural dimensions is identified. Key et al. [1] used multicontinuum technology in a multi-scale simulation to analyze the separation of rib to skin interfaces. Multicontinuum theory decomposes the stress and strain field for each constituent using volume averages. This method is numerically fast with the cost of inaccuracy particularly for shear components. Aboudi et al. [2] introduced the generalized method of cells (GMC), a semi-analytical method, which discretised the microsctructure with rectangular subcells. Pineda et al. [3] achieved mesh objectivity with a thermodynamics based approach within GMC as well as High-Fidelity Generalized Method of Cells (HFGM). In this work the commercial Finite Element software suite Abaqus is used to generate lamina-level models. A second Integrated Finite Element code (IFEM) has been developed and fully integrated with the main Abaqus solver through a user material subroutine (UMAT). IFEM calculates the reaction of a microstructural model to an imposed displacement field. The microstructural model consists of a Representative Unit Cell (RUC) which includes all constituents of the real material, e.g. fiber, matrix, and fiber/matrix interfaces, details of packing, etc. The energy based Crack Band Theory (CBT) is implemented within IFEMs constitutive laws to predict micro-cracking in all constituents.

2. Representative Unit Cell Modeling in a Multi-Scale Framework

Most commercially available finite element suites offer the user to implement custom constitutive material laws. In this work Abaqus has been chosen to solve the largest scale (e.g. lamina level) finite element problem. User material subroutines, called UMAT (*Abaqus User Manual* [4]), are readily accessible through the computer language Fortran. The UMAT subroutine is called at each integration point of the Abaqus model for each element within an element set that has been defined with a user material. In a multi-scale scheme information are exchanged between multiple length and/or time scales. Here the focus lies on a concurrent technique that exchanges essential stiffness information between a lamina-level simulation and a microstructure level simulation. This technique employs FEM at both the Fiber/Matrix scale and the macroscopic, e.g. lamina level scale. It is often referred to as FEM^2. The constitutive response at the coarse scale is purely dictated by the Fiber/Matrix level model. Localization techniques, as discussed below and referenced in Eqn. **??** are employed for transforming displacement fields from a global state to a local state. Back-transformation is achieved through a homogenization step according to Eqn.1. The concurrent information exchange between the scales is shown Fig. 1. A strain field is passed to the user defined material definition. Stress and stiffness tensors are calculated and passed back to Abaqus. In this work a Integrated Finite Element Method (IFEM) has been developed and implemented in Fortran to predict the behavior of a representative unit cell on the micro-scale. Interactions of fibers, interfaces, and matrices are captured without loosing computational efficiency. IFEM is entirely embedded in Abaqus' user subroutine UMAT. IFEM is being called at each material integration point of the macroscopic model. Volume averaged stresses, Eq. 1, are calculated and passed back to Abaqus in order to update the stress state of the element in the macroscopic model.

$$\sigma_{ij}^{V} = \frac{1}{V} \int \sigma_{ij}^{e} \, \mathrm{d}V \tag{1}$$

A two dimensional generalized plane strain finite element code, denoted as 2D-IFEM, has been developed to reduce the required simulation time while maintaining a good level of accuracy.

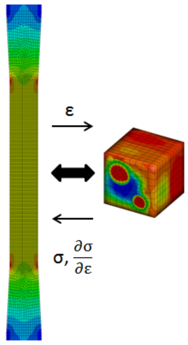

Figure 1. Multi-Scale Information Exchange between the Scales

This version is based on a linear 4-noded element formulation. Implementing an FEM code in Fortran was essential for a highly efficient multi-scale framework. It allows the macroscopic model to be run in a cluster environment and hence solving multiple material integration points simultaneously. During the localization step the load has to be transferred at each material point in the coarse scale model to the microscopic subscale. In this paper Periodic Boundary Conditions (PBCs) are used to apply the homogenized strain state at each integration point of the macroscale model on the RUC. PBCs enforce displacement continuity on all outer surface nodes of the RUC (*Heinrich et al.* [5]) with the assumption that the RUC is part of a infinite continuum. The PBC constraints are implemented within IFEM using the Penalty Approach.

3. RUC Characteristics

The objective of multi-scale analyses is to decompose a general homogenized stress- and strain field of a lamina-level model into constituent stress- and strain states. Post-peak softening is purely based on these decomposed stresses and strains and therefore failure is dependent on geometrical features withing the RUC. In this work the maximum number of fibers per RUC was limited to five. Furthermore, the discretization size should be selected to arrive at a minimum number of degrees of freedom within the RUC. Often overlooked is the importance of microstructural details on the failure mechanisms in numerical models. Detailed views of microstructures of composite materials reveal a random organization of fibers. Perfectly hexagonal packed RUCs, as they are often used in numerical models due to the simple architecture, can merely be an approximation. Multi-scale methods are a perfectly suited to implement a random microstructure by using several RUCs with varying architectures randomly distributed throughout the macroscopic model. Hence, each element within the macroscopic model will use a RUC that slightly differs from the neighboring RUCs. Fig. 2 shows examples of four geometrically different two and three dimensional three phase (Fiber,Matrix,Interface) RUCs. In this paper

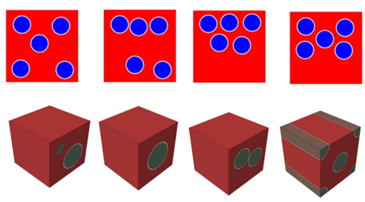

Figure 2. Selection of two- and three-dimensional RUCs

two and three phase Representative Unit Cells (RUCs), including Fiber,Interface and, Matrix, have been created to represent the microstructure of Polymer Matrix Composites (PMC) and Ceramic Matrix Composites (CMCs), respectively. However, the code is not limited to these types of material. One phase material RUCs for example are possible and can be used to model the matrix rich layers in unidirectional CMC composites.

4. Crack-Band Failure Model

In this paper the energy based crack band failure approach similar to the one by *Z. P. Bažant [6]* has been implemented for the 2D-IFEM version. It is assumed that a crack can grow upon satisfaction of the failure criterion. Furthermore, it is assumed that the crack grows perpendicular to the maximum principle strain direction (local 2-direction) as can be seen in Fig. 3. The crack-band failure method falls into the category of smeared failure approaches. Cracks

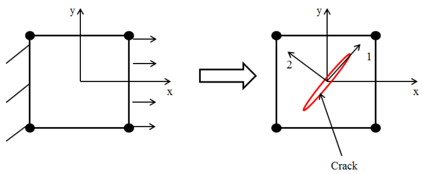

Figure 3. Idealized Crack Growth in 4-noded Element

are not explicitly modeled inside an element but rather incorporated in the element constitutive law. After crack growth has been initiated the stiffness perpendicular to the crack, e.g. in maximum principle strain direction, is reduced according to a traction separation law. The stiffness in crack direction is assumed to be unaffected. As a result a previously isotropic element becomes orthotropic after damage initiation. In most numerical applications, the secant

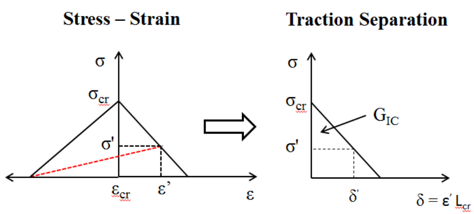

Figure 4. Crack Band Traction Separation Law

stiffness in maximum principle direction is chosen such that the tractions will follow the curve of the traction separation law shown in Fig. 4. In this work a triangular traction-separation law is employed. The area under the curve corresponds to the mode I fracture toughness (G_{IC}) of the material. Objectivity with respect to the discretization size of the microscale model is achieved through introduction of a characteristic element length. Here the largest dimension of the element perpendicular to the crack normal is used. The current separation δ' is calculated as follows

$$\delta' = (\epsilon' - \epsilon_{cr})L_{char} \tag{2}$$

where ϵ' is the current maximum principle strain, ϵ_{cr} is the critical strain and L_{char} is the characteristic element length. Subsequently the current stress can be calculated by

$$\sigma' = \sigma_{cr}(1 - \frac{\delta'\sigma_{cr}}{2G_{IC}}) \tag{3}$$

where σ_{cr} is the critical stress of the material and G_{IC} is the fracture toughness. Using the current strain and stress the new secant stiffness can be calculated as

$$E_{new} = \frac{\sigma'}{\epsilon'} \tag{4}$$

In addition, healing can not be permitted which leads to the necessary constraint

$$\dot{E}_{new} \leq 0 \tag{5}$$

This constraint is achieved by storing the secant stiffness from the previous converged increment in Abaqus' state variable space. In case of a relaxation of the element, meaning a smaller ϵ', the secant stiffness of the previous converged increment is used. Now, the new orthotropic stiffness matrix in the local principal 1-2-coordinate system can be calculated as

$$[C] = \begin{bmatrix} \frac{(1-\nu)E_{old}}{(1+\nu)(1-2\nu)} & \frac{\nu E_{old}}{(1+\nu)(1-2\nu)} & 0 \\ \frac{\nu E_{old}}{(1+\nu)(1-2\nu)} & \frac{(1-\nu)E_{new}}{(1+\nu)(1-2\nu)} & 0 \\ 0 & 0 & G\frac{E_{new}}{E_{old}} \end{bmatrix} \tag{6}$$

5. Results and Discussion

5.1. Notched CMC Tension Simulation

Laminated ceramic matrix composites are of increasing interest especially in the aerospace and energy sector. In contrast to other materials they experience small degradation of stiffness at very high temperatures. Due to proprietary regulations exact material properties can not be given here. It should be noted that with matrix and fiber elastic properties being similar the failure mechanisms are vastly different compared to polymer matrix composites. However, 2D-IFEM is well suited to predict damage, e.g. crack paths at the macroscopic level. This will be shown for a cross-ply single notch tension simulation. The notch radius is chosen to be large compared to the fiber diameters. The lay-up is $[0/90]_{2S}$ and model details are given in Fig. 5. The gauge section width is 10.16mm, grip section width is 12.7mm, and the overall length is 152.4mm. It further shows the boundary conditions and loading on the model. The edges X_0 and X_1 are subjected to a displacement in negative and positive x-direction, respectively. The corner A at X_0 is prevented from moving in y- and z-direction to avoid rigid body movements. The model is meshed with 22237 two dimensional reduced integration point elements (S4R and S3R in Abaqus v6.11 (*Abaqus user manual* [4]). Important to note here is that like any real specimen no strict symmetry in geometry with respect to the center line of the notch exists which leads to unsymmetric failure as described below. In order to break symmetry in the model nine geometrically different RUCs were randomly distributed throughout the model. The RUCs consisted of five fibers each. Three RUCs were modeled with touching fibers. Although comparable in elastic properties, e.g. pre-peak behavior, differences exist for the post-peak regime. RUCs with clustering fibers exhibit higher stress concentrations and tend to initiate

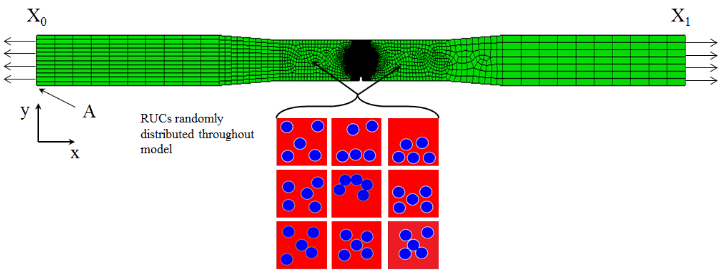

Figure 5. Cross-Ply Laminate Model Details

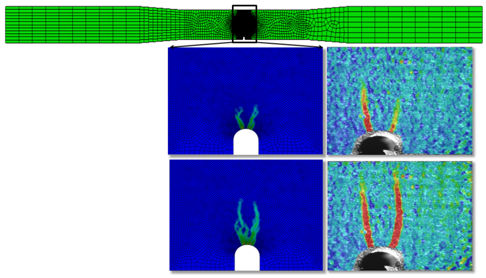

Figure 6. Comparison of Crack Paths of 2D-IFEM and DIC

failure earlier compared to other RUCs. Damage was predicted with the crack-band method on the RUC scale. However, the coupon level failure matches with crack growth observed with Digital Image Correlation (DIC) as can be seen from Fig. 6. Two cracks initiate at the notch tip and progress outward. Initially the cracks grow under an angle particular for the each lay-up before turning perpendicular to the loading direction. The initial angle appears to be determined by the maximum principle strain directions. Eventually one crack path will grow faster which then determines the catastrophic failure path of the specimen. This type of crack path would not be captured with a symmetric model, e.g. symmetric mesh and no geometric randomness, since there is no numerical preference for one crack to advance more quickly. Next, results from a uni-directional zero-degree single layer laminate simulation are compared to experimental results. The sample was 21.65 mm long, 6.35 mm wide and 0.38mm thick with the notch dimensions given in Fig. 7. The model consisted of 47564 degrees of freedom. Three

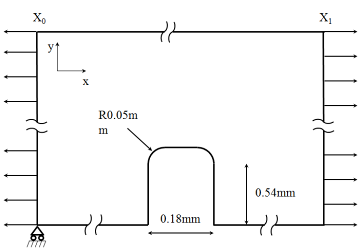

Figure 7. Sketch of Unidirectional Notched Model

dimensional elements with reduced integration points were used (C3D8R) with one element through the thickness. The edges X_0 and X_1 are subjected to a displacement in negative and positive x-direction, respectively. Similar to the results from a cross-ply laminate two cracks initiate at the notch. However, the angle spanned between the cracks is larger. These predictions are very consistent with experimental observations shown in Fig. 8. Comparable to the cross-ply laminate the cracks turn perpendicular to the loading direction further away from the notch. Eventually, one crack propagates faster which defines the final crack path. For both laminates

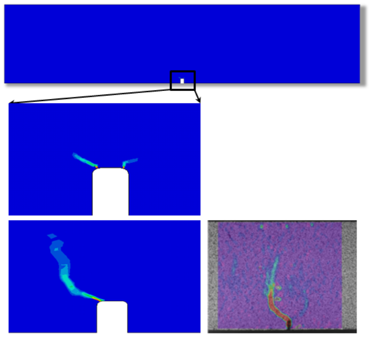

Figure 8. Damage of Zero Layer Laminate

crack initiation and propagation were predicted accurately. No change to the input of the IFEM model was required. This demonstrates the strength of the IFEM multi-scale code and shows that the physical behavior is precisely modeled.

5.2. Smooth Bar CMC Tension Simulation

In this section 2D-IFEM will be used to analyze the failure of an eight layer ($[0/90]_{2S}$) cross-ply smooth bar ceramic matrix composite specimen. The specimen was 152.4mm long, 10.16mm wide at the gage section, and 12.7mm wide at the grip section. Boundary Conditions were equal to the ones of the notched tensile simulations. As before nine randomly distributed RUCs containing five fibers each were used in order to more accurately represent the real microstructure. Three of these RUCs contained touching fibers which is often observed in this type of CMCs. The stress-strain responses for both the numerical prediction and experimental result is shown in Fig. 9. The stress and strain axes are normalized due to proprietary restrictions. However, exact numbers are not of importance here since merely a comparison between the two curves is of interest. The strain corresponds to the accumulated strain over the gage section and was measured using an extensometer. It can be seen that the onset of non-linearity in the simulation appears to be more abrupt. This might be a result of small residual stresses still present in the real specimen. In an effort to minimize the effects of residual stresses in the experiment specimens were heat treated before testing. The overall response predicted with 2D-IFEM is in good agreement with the experimental results. No distinctive cracks are observed at the lamina level probably due to the lack of geometric stress concentrations. More realistic results may be achieved by introducing a Weibull distribution of the matrix strength or fracture toughness on the macro-scale level. Future work will include the property based randomization.

6. Conclusions

In this work a finite element code has been developed and fully integrated within Abaqus' user material subroutine. This enables a computational efficient tie between a lamina level model to a fiber/matrix level model. It could be shown that information exchange between these two

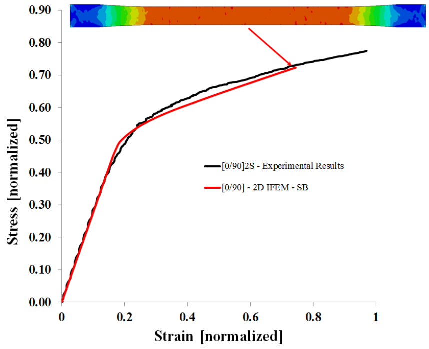

Figure 9. Normalized Stress-Strain Response of a CMC Smooth Bar Tension Test and 2D-IFEM Calculations

scales through stiffness can capture damage on the lamina level model with failure methods implemented on the fiber/matrix level model. A crack-band model for the 2D-IFEM method has been developed. Results were verified against experimental results. Excellent agreement was achieved for notched tensile specimens and smooth bar fibrous ceramic matrix composites. The predicted failure modes obtained with 2D-IFEM matched well with physical failure modes observed from experiment. It was shown that the proposed failure scheme is well suited in a Multi-Scale framework to model progressive failure. Mesh objectivity on the RUC scale was achieved through introduction of a characteristic element length. Effects of anomalies of the fiber packing were captured by resolving stress and strain fields for each constituent and using randomly distributed RUCs throughout the lamina-level model. Non-symmetric failure modes as shown for the notched specimen were predicted accurately with this technique. However, future work should more rigorously study the effect of property based "randomness", e.g. varying matrix strength and fracture toughness within a RUC. This effect could be most important for CMC specimens which lack a geometric stress concentration. Future work should also include a study on the effects of the amount of detail included in a RUC.

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