

# Automated Multiple Scale Fracture Analysis

Mark W. Beall, Vladimir Belsky, Jacob Fish, Mark S. Shephard  
Scientific Computation Research Center  
Rensselaer Polytechnic Institute  
Troy, NY 12180

**Abstract.** This paper discusses a system for automated analysis of crack propagation in heterogeneous materials. The system uses a multiscale analysis technique to account for the effect of the microstructure on the propagation of the crack. The multiscale analysis allows the microstructure of the composite to be explicitly represented in the vicinity of the crack front while using homogenized material properties elsewhere. Procedures for automatic construction and update of the models and meshes used in the analysis are described.

## 1 Introduction

The continued improvement in the price-performance of high performance workstations, and the parallel computers which build upon them, is having a dramatic impact on the ability to solve more complex physical problems. However, to take full advantage of these hardware speed improvements, advances in computational methodologies are required. One advance needed is to effectively employ the power of parallel processing. Although, this will increase the problem size possible, it does not address issues associated with (i) the need for a more detailed accounting of the physics of the problem, (ii) ensuring the reliability of the computation, or (iii) removing the labor intensive aspects of generating the numerical analysis discretizations. This paper considers the problem of discrete fracture simulation in heterogeneous three-dimensional structures and presents a set of com-

putationally efficient procedures which can automatically provide a reliable solution to these problems, while explicitly accounting for behavior at two physical scales.

To understand the failure of heterogeneous materials systems, such as reinforced concrete and structural composites, it is necessary to understand the interactions and failure of the individual constituents of the system as driven by the local stress and strain fields. The determination local fields are dictated by the behavior of the entire structure. However, it is not feasible to analyze the entire structure explicitly representing the constituents throughout the domain. This problem can be addressed by the application of multiple scale analysis methodologies which correctly combine overall models (macromechanical) for the majority of the domain with local models (micromechanical) in critical regions. The reliable application of multiple scale techniques requires mathematically sound methodologies to transfer information between the two physical scales and the ability to adaptively determine those portions of the domain where the local models are needed. Section 2 discusses the techniques used to perform and adaptively control multiple scale analyses.

Even with the ability to effectively employ multiple scale representations, the resulting discrete systems are very large and must be solved with appropriate equation solving technologies. As also indicated in Section 2, iterative equation solvers based on multigrid techniques can take direct advantage of multiple scale representations.

The failure processes considered in this paper are governed by the propagation of discrete cracks at the micromechanical level. The simulation of discrete crack growth requires criteria to indicate under what conditions a crack will propagate, in which direction it will

propagate, and how far it will propagate. Section 3 discusses the criteria used in the present work for crack propagation and discusses issues associated with the effective numerical implementation of these processes.

A final key to an effective multiple scale fracture simulation is the ability to generate and control the required models and meshes. Since any need for human intervention would introduce an expensive bottleneck, all model update and mesh generation processes must be automated. Sections 4 and 5 describe the techniques and procedures developed to support the generation of local models and meshes from a geometric model of the overall domain and a description of the microstructure. Since the geometry evolves as the crack propagates, both the models and the meshes must be updated to account for the propagation of the crack using the procedures discussed in Section 6.

It is worth noting that the entire set of procedures described in this paper employ methodologies consistent with those used in a set of parallel automated adaptive finite element procedures (Shephard et. al. 1995, de Cougny et. al. 1995) developed to take full advantage of scalable distributed memory parallel computers.

Section 7 demonstrates the application of the procedures described to crack growth in a unidirectional composite material. A comparison is made between the crack growth predicted with and without explicit consideration of the effect of the microstructure.

## **2 Adaptive Multiscale Computational Techniques for Heterogeneous Media**

In analyzing large scale structures made of heterogeneous materials it is common in practice to carry out at least three distinct levels of analysis corresponding to different length

scales: (i) macroscale (structural level), (ii) mesoscale (component level), and (iii) microscale (the level of material heterogeneity). On the structural level, structural components are treated discretely, while individual components are idealized to adequately determine their overall properties. On the component level, individual subcomponents are treated discretely, while microconstituents are treated collectively as a homogenized medium where homogenized material properties can be determined experimentally, or predicted from micromechanics. For micromechanical analysis individual phases are treated discretely, while lower scales such as material grains or atoms are treated as homogeneous.

These steps comprise a sequence of interdependent analyses in the sense that the output from one level is used as input to the next level, using constitutive laws to serve as the bridging mechanisms between the scales. It is important to note that any level of analysis is performed totally independent of the others if the required input data is available, perhaps from experiment. There is no doubt that this approach reflects a necessary compromise aimed at bridging the length scales in excess of several orders of magnitude in time and space. The obvious question arises as to the validity limits of such a step-by-step procedure. Is there a need for a coupled approach that will simultaneously consider phenomena at several different scales, and if the answer is positive, is the current status of software and hardware tools mature enough for such coupled multiscale considerations?

Let's start by addressing the first issue. Figure 1 depicts the shear stress distribution in the axial tension problem in a  $(90/0_4/90)_s$  laminate (Fish and Belsky 1994). Results are shown for one quarter of the plate cross section in the x-y plane. The lines of symmetry are at the bottom and on the right hand side of the cross section. The uniform tension load is applied normal to the x-y plane. The zoomed area of shear stress distribution in the close vicinity

to the free edge is also shown. Results of the classical step-by-step procedure based on the homogenization theory are compared to the reference solution where the size of finite elements is of the same order of magnitude as that of material heterogeneity. It can be seen that a classical step-by-step procedure predicts accurate shear stress distribution except for the close vicinity to the free edge, where it significantly underestimates maximum stress values, and along the entire interface between the two dissimilar layers. The reference solution shows oscillatory shear stresses along the entire interface, while the solution based on the classical step-by-step approach shows no such stress concentration. The magnitude of these oscillatory shear stresses is roughly  $1/3$  of the maximum shear stresses developed at the interface, but even so, these interface shear stresses may significantly affect the propagation of cracks emanating from the free edge.

Recent theoretical and numerical studies (Fish and Wagiman 1993, Fish and Markolefas 1994) have shown that in the areas of high gradients, primarily developed in the boundary layers at free edges and interfaces, the classical uncoupled step-by-step procedure may lead to poor predictions of local fields, since it assumes uniformity of macroscopic fields over the unit cell domain.

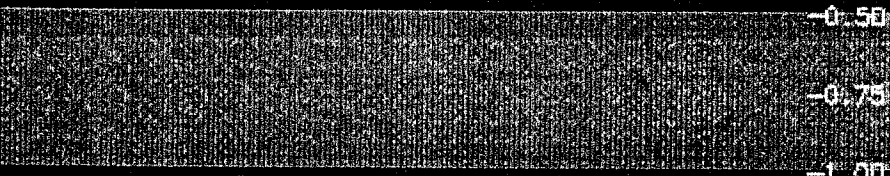
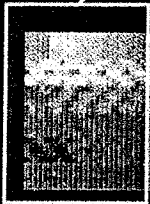
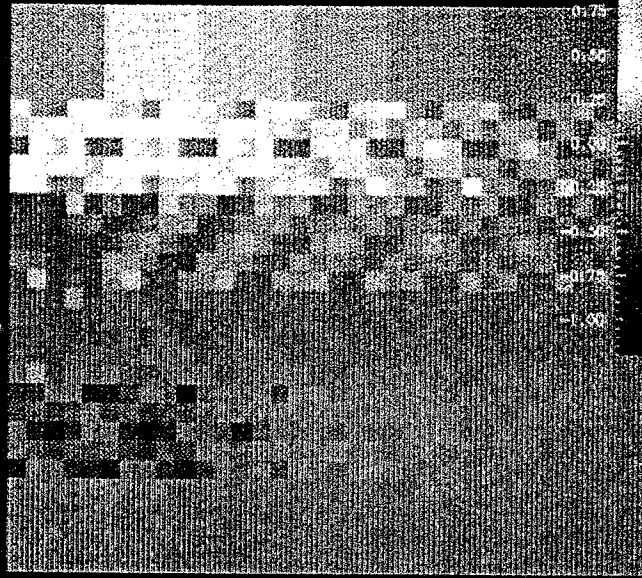
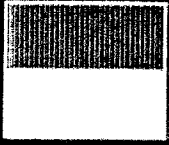
Simulation of the evolution of failure processes in heterogeneous media poses an even greater obstacle to the classical step-by-step approach. Sometimes the failure is catastrophic, and the ability to compute only the onset of failure is sufficient. Although computing the onset of failure is still a very difficult task, particularly in heterogeneous media, it is a goal that has largely been accomplished by means of a classical uncoupled step-by-step approach. However, in determining the vulnerability or survivability of a structure, a computation beyond the onset of failure is critical because there may be a considerable

# Multigrid Solution for axial tension problem

$(90/0_4/90)_S$

$\sigma_{xy}$

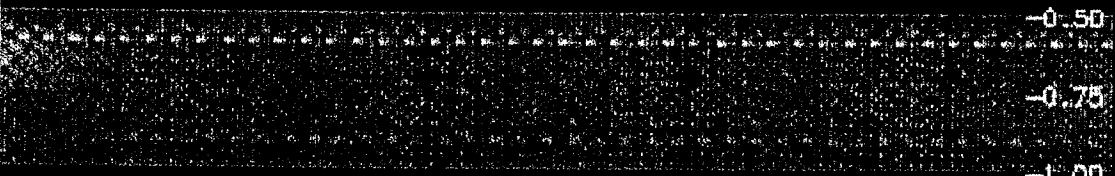
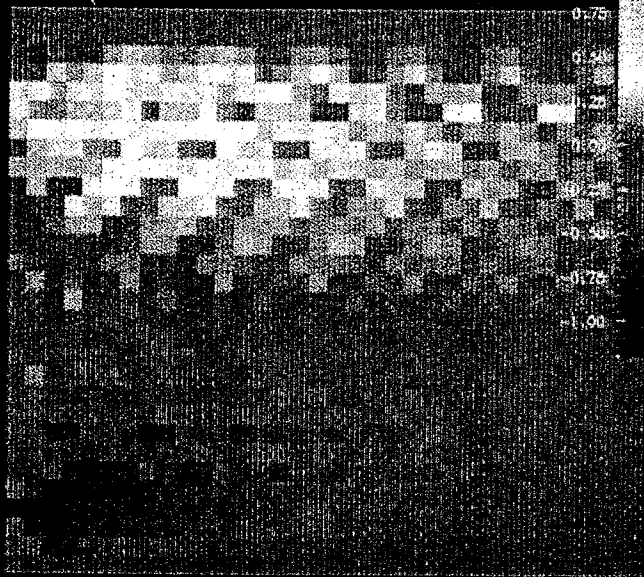
'90' layer



Homogenization Theory Solution

$\sigma_{xy}$

'0' layer



Multigrid Micro Solution

reserve strength. Reliable simulations of failure processes in heterogeneous media emanating from the smallest scale, such as microvoid nucleation and followed by their coalescence and structural failure, require revitalization of classical bridging mechanisms between various modeling levels.

It is now feasible to use more sophisticated mathematical models and more refined discrete models, which account for close interaction between different scales. However, it is appropriate to recall the statement made by Einstein, "The model used should be the simplest one possible, but not simpler." Adaptive multiscale modeling techniques enable the analyst to start from a simpler model and then adaptively refine both the mathematical and numerical models to permit coupled multiscale considerations, whenever and wherever needed, until the simplest possible model that provides an accurate solution is obtained.

To address the question regarding the maturity of existing hardware and software tools needed for such multiscale holistic considerations, Figure 2 demonstrates the application of this approach to analyzing a typical composite structure. The adaptive multiscale strategy starts by employing classical discretization error indicators (Zienkiewicz and Zhu 1992, Oden et. al. 1989) and adaptively refining the finite element mesh on the macromechanical (shell) level to ensure accurate macro-solutions. Subsequently, dimensional reduction error indicators (Fish et. al. 1994) identify the areas where the most critical interlaminar behavior takes place, and consequently, a more sophisticated discrete layer model is placed there. Fast iterative solvers based on the multigrid technology with special inter-scale connection operators (Fish and Belsky 1995a,b) are used to solve a coupled two-scale macro-meso model. Once the phenomena of interest on the macro-meso levels have been accurately resolved, microscale reduction error indicators (Fish et. al., 1994) are

used to identify the location of critical microprocesses and consequently, a micro-mesh is placed there. The three-scale coupled macro-meso-micro model is again solved using a three-scale multigrid process (Fish and Belsky 1995a,b). In this methodology, discretization error indicators and adaptive refinement strategy are employed simultaneously at three different scales to ensure reliable multiscale simulations.

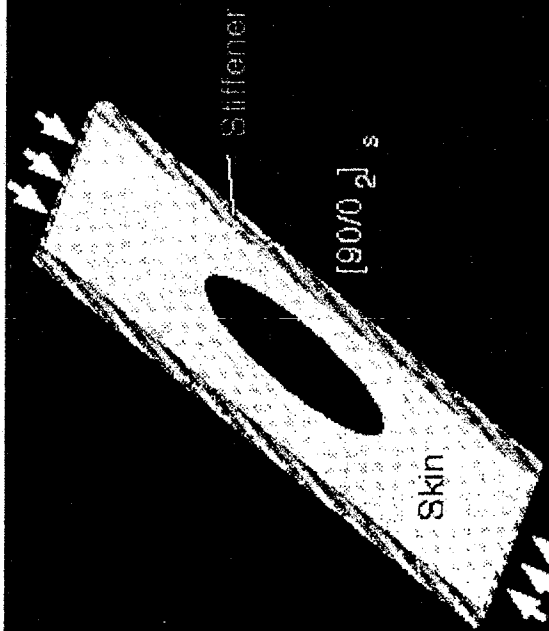
The three-scale model described in Figure 2 contains over 1,000,000 degrees-of-freedom. The estimated CPU time for solving it with a conventional direct solver based on skyline storage is over 705 hours on a single processor SPARCstation 10, which essentially makes the model intractable. With a special purpose multigrid technology for heterogeneous media, developed in (Fish and Belsky 1995a,b), the same problem has been solved in less than 16 hours on a single processor SPARCstation 10, turning it into a practical overnight job.

The derivation of the inter-scale transfer operators for the three-scale multigrid method is based on the asymptotic solution expansion, which assumes infinitesimality of the unit cell. The asymptotic forms of the prolongation and restriction operators are obtained by discretizing the corresponding asymptotic expansions. For unit cells of a finite size, the regularization function has been introduced to obtain well-behaved inter-scale transfer operators, termed as homogenization based operators. The resulting homogenization based prolongation operator is given by:

$$\tilde{Q} = Q + dQC\nabla_s N(X_g) \quad (1)$$

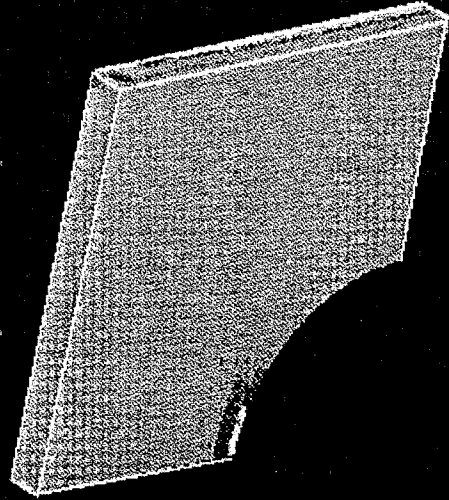
where  $Q$  is the standard multigrid linear prolongation operator,  $d$  is the unit cell solution,  $\nabla_s N(X_g)$  is the symmetric gradient of the shape functions in the auxiliary grid evaluated



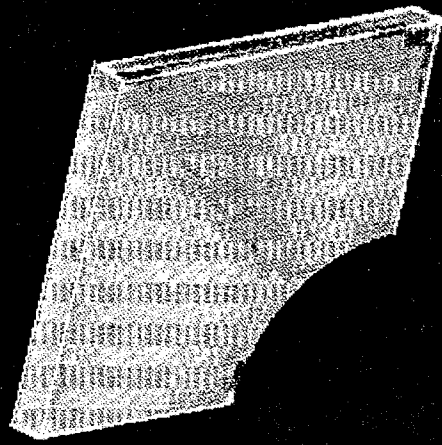


1. Composite Box with a Hole

Shell (Macro) model



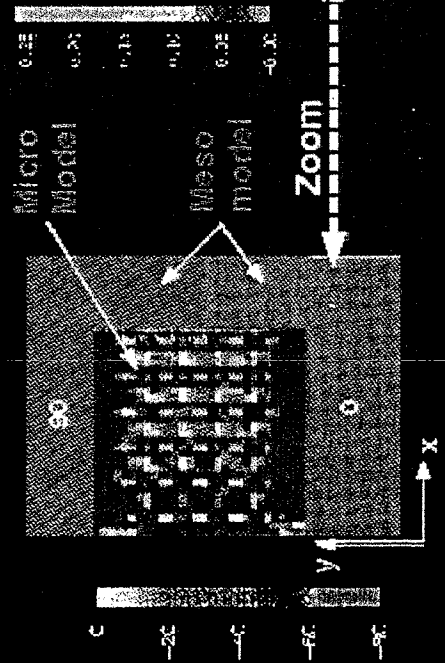
2. Strain Energy Density



3. Dimensional Reduction Errors

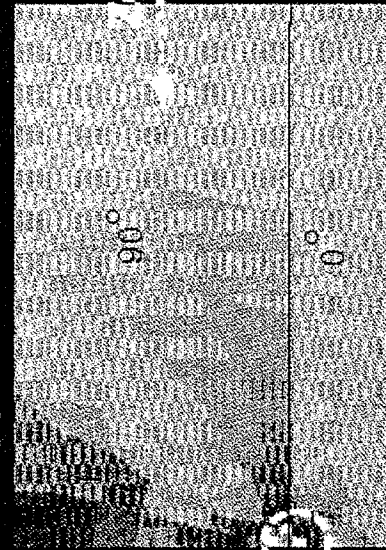
# Adaptive Multiscale Computational Technology for Composite Materials and Structures

Macro-Meso-Micro model

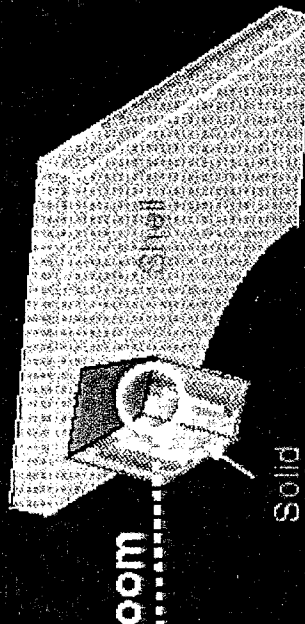


6.  $\sigma_y$  in the microstructure

Macro-Meso model



5. Microscale Reduction Errors



4. Strain Energy Density

at the Gauss points in the auxiliary mesh,  $C$  is the projection operator aimed at maintaining  $C_0$  continuity of the displacement field on the micro-scale. For a technical description of these operators see (Fish and Belsky 1995b).

The rate of convergence of the multigrid process for heterogeneous media has been studied in (Fish and Belsky 1995a,b). It has been proved that for periodic 1-D heterogeneous media problems, the rate of convergence of the two-grid method with special inter-scale transfer operators is given by:

$$\|e^{i+1}\| = \frac{q}{4-q} \|e^i\| \quad q = \frac{\sqrt{d_1 d_2}}{0.5(d_1 + d_2)} \quad (2)$$

where  $d_i$  represent the stiffnesses of microconstituents. Note that if the material is homogeneous and the mesh is uniform ( $d_1 = d_2$ ) a classical two-grid estimate is recovered:

$$\|e^{i+1}\| = \frac{1}{3} \|e^i\|. \text{ Otherwise } q < 1 \text{ resulting in } \|e^{i+1}\| < \frac{1}{3} \|e^i\|. \quad (3)$$

Note that if the stiffness of a fiber is significantly higher than that of a matrix, i.e.  $d_1 \gg d_2$ , then the multigrid method converges in a single iteration. In multidimensions, convergence of the multigrid process for periodic heterogeneous media has been studied (Fish and Belsky 1995b). It has been found that convergence trend characteristics found in the 1-D cases are closely followed in multidimensions. In practice, for fiber/matrix stiffness ratios,  $d_1/d_2$ , of approximately ten, 4 to 6 multigrid cycles are sufficient to obtain converged results.

### 3 Crack propagation procedures

There are two common approaches taken in the development of crack propagation procedures. The ‘global’ approach assumes that crack extension takes place in an idealized anisotropic homogeneous material with gross combined properties of the constituents. The ‘local’ point of view, often referred to as micromechanical approach, considers material as heterogeneous. The ‘local’ approach takes into consideration local damage patterns. In the present study we adopt a global-local approach by which ‘local’ description is used in the vicinity of the crack front while elsewhere the medium is treated as homogenized.

Crack growth simulations, in general, are difficult to perform because of the need for continual geometry and computational mesh updates. This process becomes even more challenging for problems in heterogeneous media where in addition to the geometry and mesh, the mathematical model has to be updated.

The crack propagation increment  $\mathbf{x}_A - \mathbf{X}_A$  is defined in terms its shape  $\{\tilde{\mathbf{S}}_A\}_{A=1}^n$  and amplitude  $\alpha$

$$\mathbf{x}_A = \mathbf{X}_A + \alpha \tilde{\mathbf{S}}_A \quad (4)$$

where  $\mathbf{X}_A, \mathbf{x}_A$  denote position of the finite element node  $A$  located at the crack front interface before and after incremental update, respectively, and  $n$  is the number of nodes on the crack front interface. Prediction of crack trajectory requires determination of  $\{\tilde{\mathbf{S}}_A\}_{A=1}^n$  and  $\alpha$ .

No generally accepted criterion exists for predicting trajectories of cracks in three-dimensional heterogeneous media. Among the popular phenomenological theories for predicting instantaneous angle of crack propagation in two-dimensional homogeneous media are

maximum tangential stress criterion, maximum energy release criterion and minimum strain energy density criterion. Two major obstacles in applying these criteria to three dimensional applications in heterogeneous media with arbitrary crack surfaces are summarized below:

1. Crack growth depends on the geometry, boundary conditions and material characteristics of microconstituents, including strength and fracture toughness.
2. Asymptotic fields are generally not known in these cases.

To overcome these difficulties we propose the following generalization of the classical crack propagation criteria:

1. The preliminary crack propagation shape  $\{\tilde{S}_A\}_{A=1}^n$  is defined on the basis of the following normalized criteria:

$$\|S_A\| = \frac{F_A}{G_A} \quad (5)$$

where  $\| \cdot \|$  denotes Euclidean norm of a vector,  $F_A$  is either maximum energy release rate, maximum tangential stress, or minimal strain energy density.  $G_A$  is either fracture toughness, strength in tension or critical energy density, respectively.

2. The unit vector  $e_A = S_A / \|S_A\|$  defining the crack propagation direction at node A points in the direction of the maximum ratio  $F_A / G_A$  (among the elements connected to node A) projected onto the plane normal to the crack tip interface at node A.
3. Deformation and stress fields are either directly extracted from the finite element analysis or by postprocessing finite element solution (Niu and Shephard 1993, Niu and Shephard 1994).

4. Smoothing is applied to the crack propagation shape as obtained from equation (5) to avoid numerically defined oscillations.

The process of finding the smoothed crack propagation shape can be viewed as constrained optimization problem, which states:

Find the smoothed crack propagation shape increment,  $\|\tilde{S}_A\|$ , such that

$$\int_L (\|S_A\| - \|\tilde{S}_A\|)^2 dL \rightarrow \min \quad (6)$$

subjected to the smoothness constraint:

$$\int_L \left( \frac{\partial}{\partial L} \|\tilde{S}_A\| \right)^2 dL < \varepsilon^2 \quad (7)$$

where  $L$  is a coordinate along the crack tip, and  $\varepsilon$  is the smoothness parameter. Solution of the constrained optimization problem yields the following differential equation:

$$\left( I - \gamma \frac{\partial^2}{\partial L^2} \right) \|\tilde{S}_A\| = \|S_A\| \quad (8)$$

subjected to periodic boundary condition. Note that the parameter  $\gamma \ll 1$  is defined by the user. Equation (8) can be solved using finite element method using bi-linear discretization of  $\|\tilde{S}_A\|$ .

Due to the history dependence of crack growth, the problem of evaluating the amplitude  $\alpha$  can be stated in terms of an ordinary delay differential equation (Fish and Nath, 1993):

$$\frac{dx_A}{d\alpha} = \tilde{S}_A(\alpha) \quad (9)$$

The special nature of ordinary delay differential equations has the effect of making the crack path smoother with evolution in ‘time’ if the evolution of the right hand side vector in (9) is smooth. For problems in heterogeneous media  $G_A$ , and thus  $\tilde{S}_A$ , are  $C^{-1}$  continuous functions in  $\alpha$  and thus the optimal integrator for such a differential equation should be based on a type of integration scheme which does not rely on the smoothness of the crack path. The simplest form of such integrator is based on a predictor-corrector scheme:

$$\begin{aligned}
 \text{Predictor} \quad \bar{x}_A &= X_A + \tilde{S}(X_A)\alpha \\
 \text{Corrector} \quad x_A &= X_A + \frac{1}{2}(\tilde{S}(X_A) + \tilde{S}(\bar{x}_A))\alpha
 \end{aligned} \tag{10}$$

The normalized local truncation error,  $\beta$ , is given as:

$$\beta = \sqrt{\frac{\sum_{A=1}^n (x_A - \bar{x}_A)^2}{\sum_{A=1}^n (x_A - X_A)^2}} = \sqrt{\frac{\sum_{A=1}^n (\tilde{S}(\bar{x}_A) - \tilde{S}(X_A))^2}{\sum_{A=1}^n (\tilde{S}(\bar{x}_A) + \tilde{S}(X_A))^2}} \tag{11}$$

The crack propagation amplitude may increase or decrease to keep the magnitude of the normalized truncation error,  $\beta$ , below the user prescribed tolerance.

## 4 Problem Definition to Support Automated Model Construction

The effective application of multiple scale analysis requires automation of the entire process. Without automation the analysis is effectively impossible due to the time and effort required to update the models and meshes needed as the analysis progresses. The automation of a set of engineering analyses requires all analysis models, and their discretizations, be derived from a single problem definition. The two key components of the problem definition are the domain description (the geometric model), and the analysis attributes

defined in terms of it. For sake of discussion, this single problem definition, from which all other models are derived, is referred to as the primary problem definition.

#### **4.1 Geometric Model**

The geometric models constructed from the primary problem definition in support of multiscale analyses vary from a representation of the middle surface of a composite structure, to one containing multiple volumes representing the micromechanical structure of a composite material. The representations used must be able to support the requirements of automated discretization construction procedures (Shephard and Finnigan 1989, Shephard and Georges 1991). The primary model must be structured such that the various idealized engineering analysis models can be automatically constructed, and the interactions between those models controlled. For example, at the highest level, a composite structure is idealized as a surface (a shell model), while at a portion is represented as a multi-layer volume, and in a local region the microstructural components are represented as volume elements. The relation of all of these models to each other must be understood by the analysis, this done by relating all of them back to the primary problem definition.

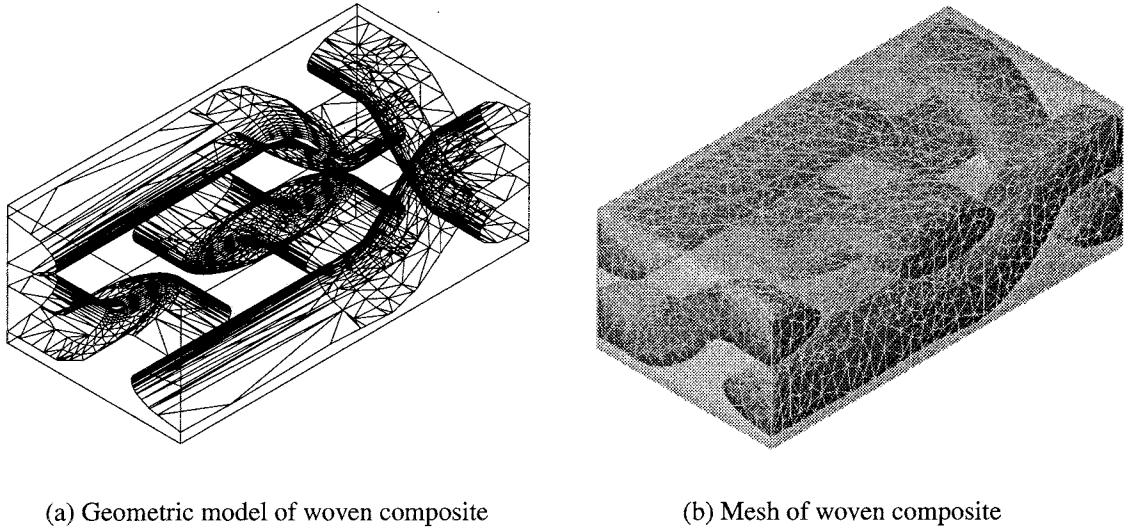
The model construction and discretization processes can be effectively supported by geometric modeling systems supporting non-manifold representations of general combinations of volumes, surfaces and curves (Weiler 1988). In addition to taking direct advantage of the massive development effort required to produce such geometric modelers, this approach can properly support all the geometry needs of automatic mesh generation (Shephard and Georges 1992).

The approach of defining the primary geometric model as a detailed geometric representation at the lowest physical scale is not advantageous for several reasons, including: (i) the model sizes would be unacceptably large, (ii) the automatic construction of the higher level models can be more complicated than the automatic construction of low level models, and (iii) user effort to construct detailed lower level models would be burdensome to the design process. The approach taken here is to store an overall geometric representation supplemented with the additional geometric feature data required to automatically construct needed idealized geometric models. Usually this means that a simple, engineering-type geometric model is used to describe the structure and attributes are used to describe the details required for the analysis, such as the material microstructure. This approach also corresponds well to the design process, where different portions of a structure will be understood to different levels of detail at various times.

The most geometrically demanding processes involve the construction of the idealized geometric models for specific analyses from the primary geometric model. One class of such operations are dimensional reductions where, for example, the middle surface of a complex three-dimensional solid, which is thin in some through-the-thickness, direction is needed for an analysis. Another example is constructing a multi-material solid model of a representative unit cell from basic composite specifications when micromechanical models are included in the analysis process. The approach used to address these needs is to employ the geometric construction functionality of commercial solid modelers, driven by appropriate knowledge housed in the primary model and the analysis strategy being executed. Figure 3a shows the a unit cell for a composite weave automatically constructed in the Parasolid non-manifold solid modeler (Parasolid 1994) using the basic manufacturing



parameters defining the weave and the procedures described in Section 5. The automatically generated mesh of this model is shown in Figure 3b.



**FIGURE 3. Automatically constructed and meshed unit cell model**

#### **4.2 Analysis and Idealization Attributes**

Analysis attributes consist of the information past the geometric model needed to specify an analysis model. Analysis attributes include material property, boundary condition, load, and initial condition information. Idealization attributes define the information needed to convert a primary model to the idealized model used in an analysis process. Examples of idealization information are specification of the use of the middle surface for an overall deformation analysis, and the information defining the microstructure of a unit cell. To support an automated environment, the analysis and idealization attributes must be defined directly in terms of the physical parameters and associated directly with the geometric representation of the primary geometric model (Shephard 1988, Wong 1994). When defined in this manner they can be properly transferred to the idealized analysis models and their discretizations.

The physical description of all analysis attributes are in terms of tensorial quantities. The components of the structure used to define the attributes' physical information include (i) the order of the tensor, (ii) an indication of the coordinate system the tensor is defined in, (iii) the symmetries possessed by the tensor, and (iv) the distribution information defining each component of the tensor in the given coordinate system.

Since a number of basic attributes, such as material parameters, are likely to be used in multiple analyses, it is advantageous to allow the single specification of an attribute and to collect the attributes appropriate for an analysis into the specific analysis case desired. A hierarchical organization structure that allows the convenient collection of attributes, including the application of multipliers has been put into place.

Finally, attributes must be associated with the entities in the geometric description of the domain. Complications are introduced in the case of multiple scale analyses since it is necessary properly transfer the appropriate attribute information from the primary attribute definition to the idealized analysis models. The transfer of the attributes must correctly deal with such processes as dimensional reductions and replacement of a set of heterogeneous constituents with a homogeneous continuum.

## **5 Automatic Generation of Models and Meshes for Multiscale Analysis**

The multiscale analysis used here treats the problem being solved as a three level problem. The top level is the component (macro) level, where all the material properties are considered to be homogenized. The bottom level is the microstructural level where all the details of the microstructure, and damage that is occurring to the microstructure, are represented.

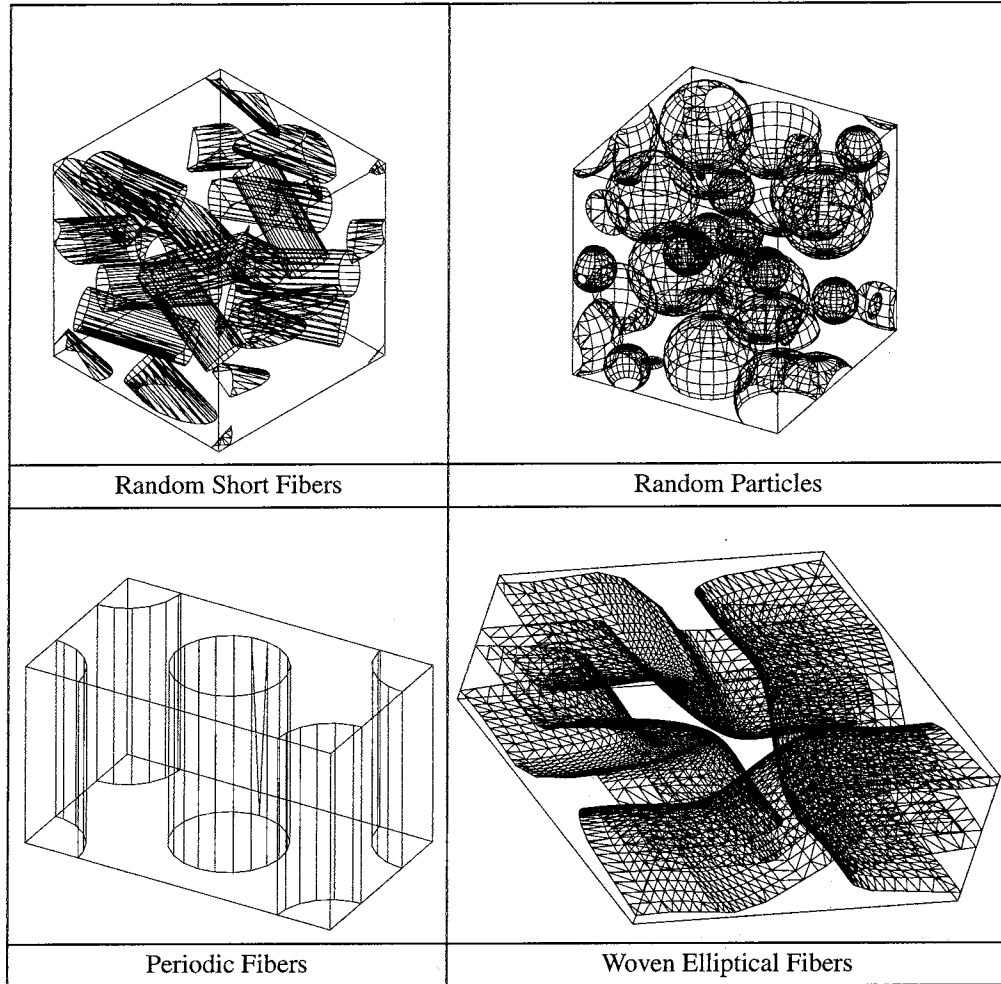
The middle level serves as a transition between these two level and incorporates any macro level damage.

For the discrete crack propagation problem discussed here primary problem definition consists of a solid geometric model of the physical structure being analyzed (the macro model) with appropriate analysis attributes and idealization attributes that describe the layup and microstructure of the composite. These attributes include the type of microstructure, the parameters needed to build a unit cell, the material properties of the constituents and the orientation of the unit cell with respect to the macro model. The models that represent the lower levels of the analysis are constructed using the information in this problem definition. The initial crack geometry is also specified in the primary problem definition.

## **5.1 Unit Cell Construction**

The primary model definition includes a definition of the unit cell that describes the microstructure. This definition is in terms of the parameters that define the unit cell (such as volume fraction and fiber diameter for a continuous fiber composite). The geometric model of the unit cell is created by the system when needed.

Currently, the microstructure geometry is assumed to be periodic which allows it to be represented by the repetition of a single unit cell. This unit cell is used for the calculation of homogenized material properties using standard homogenization procedures (Bakvalov and Panasenko 1989, Guedes and Kikuchi 1991) and for construction of the microscale model of the composite. Both the model and the mesh of the unit cell must be periodic.

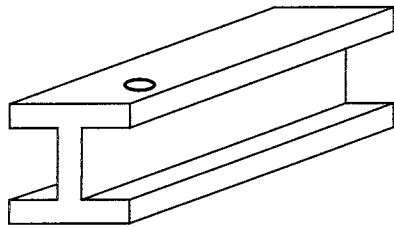


**FIGURE 4. A sample of the various types of unit cells that can be created.**

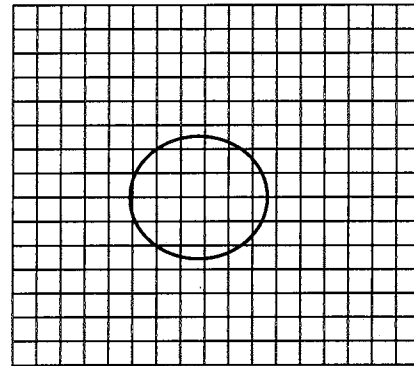
Common composite unit cells are: aligned fibers, random chopped fibers, random particles, and woven fibers (Figure 4). The unit cells fall into two categories: those with prescribed structure and those with random structure. The unit cells with prescribed structure, such as the aligned fiber and the woven fiber cells in Figure 4, are created from a parametric model of the unit cell. The parameters in the model include fiber size, volume fraction, and other geometric properties of the unit cell. The unit cells with random structure, such as chopped fibers and particles, are generated using a stochastic procedure that randomly inserts appropriate reinforcements into the unit cell while enforcing the periodicity requirement (Shephard et. al. 1995b).

## 5.2 Microscale Model

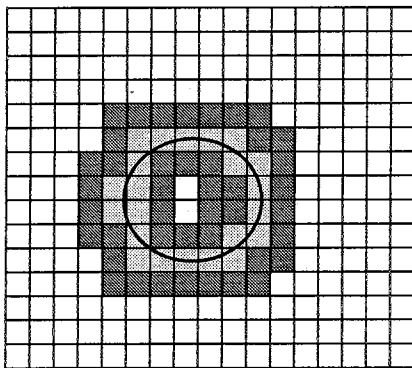
The domain of the micro model is the set of unit cells that encompass the critical areas of the model where it is necessary to resolve local fields. For the crack propagation problem this area is the unit cells that enclose the crack front. The steps to find this domain for the crack propagation problem are:



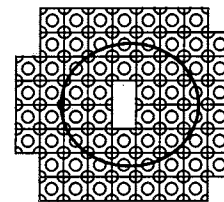
(a) Macro model with crack location indicated



(b) unit cell grid overlaid on model



(c) domain of micro model found



(d) micro model created

**FIGURE 5. Defining the domain of the micro model.**

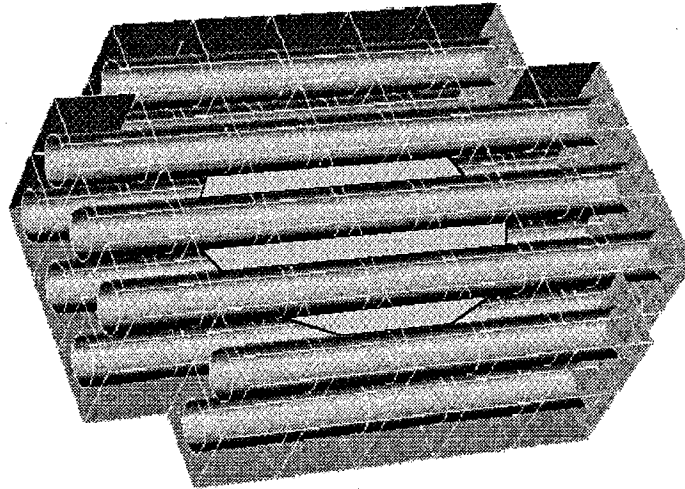
1. Given the overall model (Figure 5a) a regular grid is defined over the portion of the macro model that encompasses the required microscale domain. Each grid cell is one unit cell in size (illustrated in Figure 5b with the third dimension removed for clarity).

This grid must be defined to be aligned with the microstructure such that when the unit cells are inserted in the grid cells, the correct microstructure is created. The grid is only “defined”, it is not actually created in the geometric modeler.

2. The grid cells containing the crack front, the minimal domain for the micro model, are determined as follows: Pick a point on the curve defining the crack front and determine which cell the point is in. Add this cell to the list of cells that the crack front passes through. Find which cell face, edge or vertex the curve passes through as it exits the cell by intersecting the curve with the planes defined by each cell face of the current cell. Add the cell on the opposite side of the face to the list of cells that the crack front passes through. If the crack front passes through an edge or vertex then add all the cells touching that edge or vertex. Continue this procedure, tracking the curve as it passes from one cell to another until the entire curve has been traversed. This is illustrated by the light grey filled cells in Figure 5c.
3. This minimal domain is extended by adding  $n$  layers of cells surrounding the minimal cells to the model (Figure 5c shows one layer of these cells added, shaded dark grey) giving the domain of the micro model. The number of additional layers depends on how far the crack will be allowed to advance in a single analysis step. The crack front must always remain within the micro model.

Once the domain of the micro model has been determined, the actual model can be constructed. For each cell in the grid that has been determined to be in the domain of the micro model, the model of the unit cell is duplicated, translated and rotated so that it corresponds to the position and orientation of that grid cell. The boundaries of adjacent unit cell are then sewn together to make a single model. This model, when unioned with the portion

of the crack model that is interior to the unit cells, makes up the microscale model. Material property attributes are then associated with the entities in the micro model by copying them from the corresponding entities in the unit cell model. The result of this process for a delamination problem is shown in Figure 6.

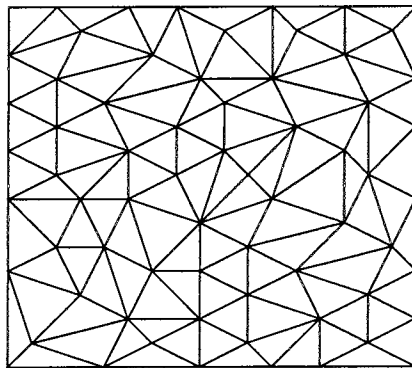


**FIGURE 6. Microscale model of delamination crack**

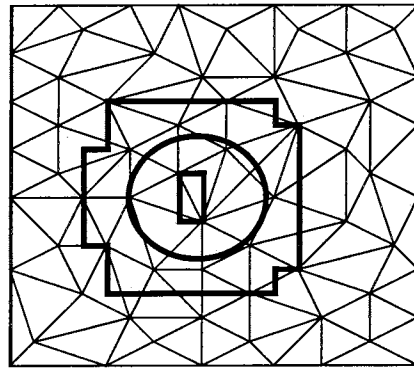
To support the analysis procedures, the mesh on the micro model boundary must be identical to that which is on the boundary of the unit cell that was used to calculate the homogenized material properties. The mesh on the interior of the model has no restrictions. This requirement is enforced by copying the mesh from the boundary of the unit cell to all the faces on the boundary of the model, then meshing the other (interior) faces of the model using the Finite Octree mesh generator (Shephard and Georges 1991). Finally the interior of the model is meshed using an element removal procedure that works from the given boundary mesh.

### 5.3 Transition Model

The transition model is used to connect the macro model, with its coarse mesh and homogenized material properties, and the micro model, with its fine mesh and explicit microstructure. The outer boundary of the transition model is the boundary of the union of all the elements in the macro mesh that the micro model is interior to (Figure 7). (In addition some elements that the micro model is very close to may be added). Imbedded in the interior of the transition model are a set of non-manifold faces (faces with model regions on both sides) that represent the outer boundary of the micro model and the portion of the crack face that is external to the micro model (Figure 7c). The portion of the crack internal to the micro model does not need to be represented, but it can be, and is in the examples shown here (whether or not this part of the crack is represented is irrelevant since the micro model represents the correct geometry in that portion of the domain). The transition model created for the delamination crack in Figure 6 is shown in Figure 8.



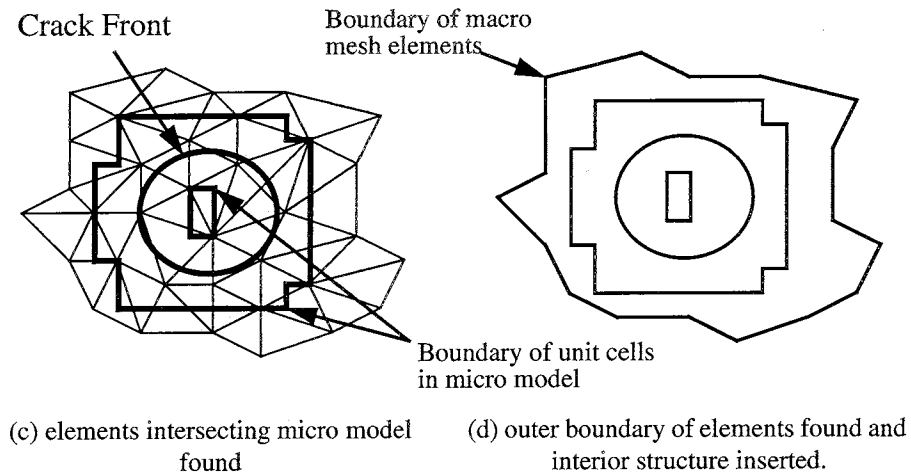
(a) Macro-mesh



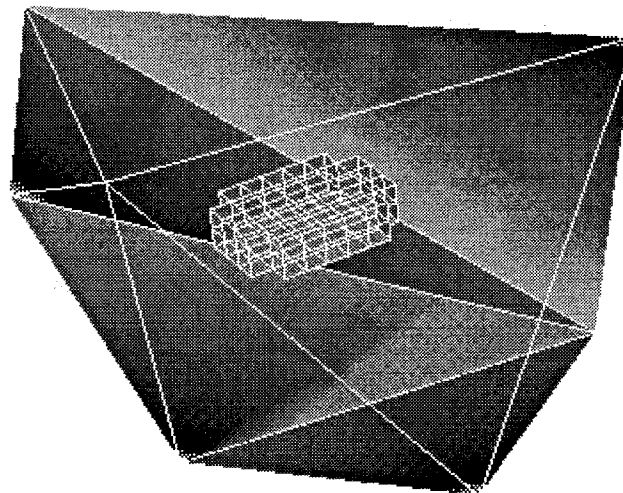
(b) micro-boundary superimposed over macro-mesh

**FIGURE 7. Construction of the transition model**





**FIGURE 7. Construction of the transition model**



**FIGURE 8. Transition model**

The mesh for the transition model does not need to be compatible with the mesh of the macro model, however there should be no elements on the boundary of the transition mesh that are in more than one macro mesh element face. This is ensured by constructing the transition model so that the edges of the macro mesh are retained on the boundary (i.e. coplanar faces on the boundary are not unioned to make a single face so the edges that define the original faces are retained). Although compatibility of the mesh is not required, it is

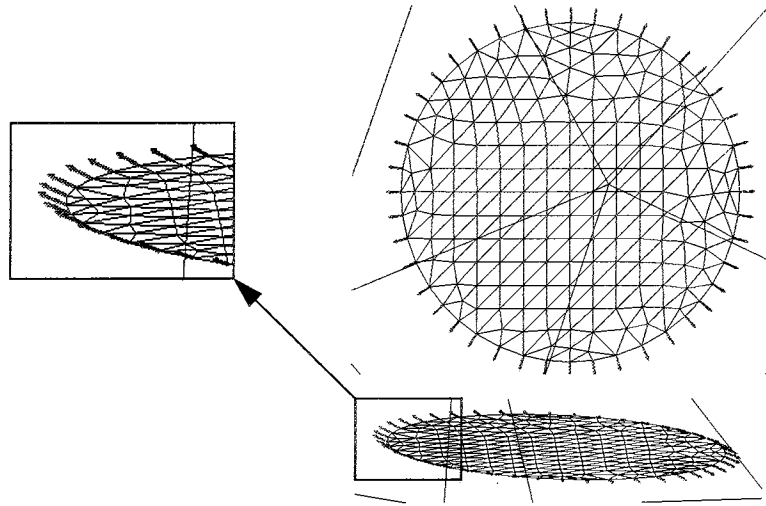
desirable, from a convergence standpoint, to have the size of the elements in the transition mesh roughly (within a factor of 3 to 5) the same size as the elements in the macro mesh on its outer boundary and roughly the size of the elements in the micro mesh on that interior boundary.

## **6 Model and Mesh Updates for Crack Propagation**

To simulate the growth of the crack for a step, the analysis must update the representation of the crack to account for the growth predicted at the last step. This process can be made efficient by performing local modifications to the models and meshes to reflect the growth of the crack. This works well since the majority of the updates only change the representation at the micro level. As the crack grows, it eventually approaches the boundary of the micro model, requiring the micro model domain and, thus, the transition model and mesh to be updated. The updates of the higher level models only happen occasionally. An outline of the steps in the model update are as follows:

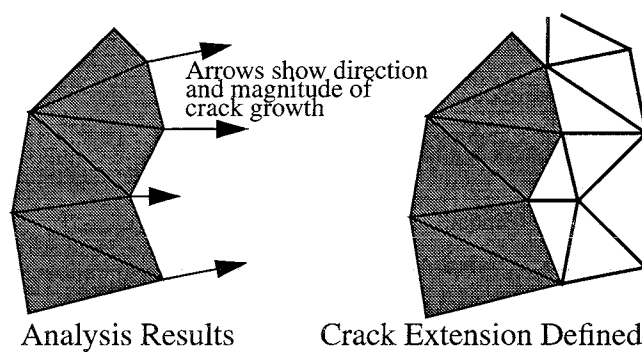
1. From the results of the analysis determine the updated geometry of the crack.
2. Update the crack representation in micro model and mesh to reflect the crack growth.
3. If the crack front nears the boundary of a unit cell, the micro and transition models are updated as follows:
  - a. Add unit cells ahead of crack and remove them behind, to ensure that the micro-model exists for the desired distance ahead of the crack front.
  - b. Update the transition model to reflect the new micro model domain.

## 6.1 Crack Update



**FIGURE 9. Analysis results showing predicted crack growth.**

As shown in Figure 9, the analysis provides the direction and magnitude of the crack growth at each vertex on the crack front. This information is used to define the “crack extension” which is the geometric representation of the new crack surface. To avoid placing unnecessary constraints on the growth of the crack the crack extension is defined independently of the mesh. It is defined as a set of triangular faces extending from the current crack front to new locations for the vertices on the crack front given by the analysis (Figure 10).



**FIGURE 10. Definition of crack extension from analysis results**

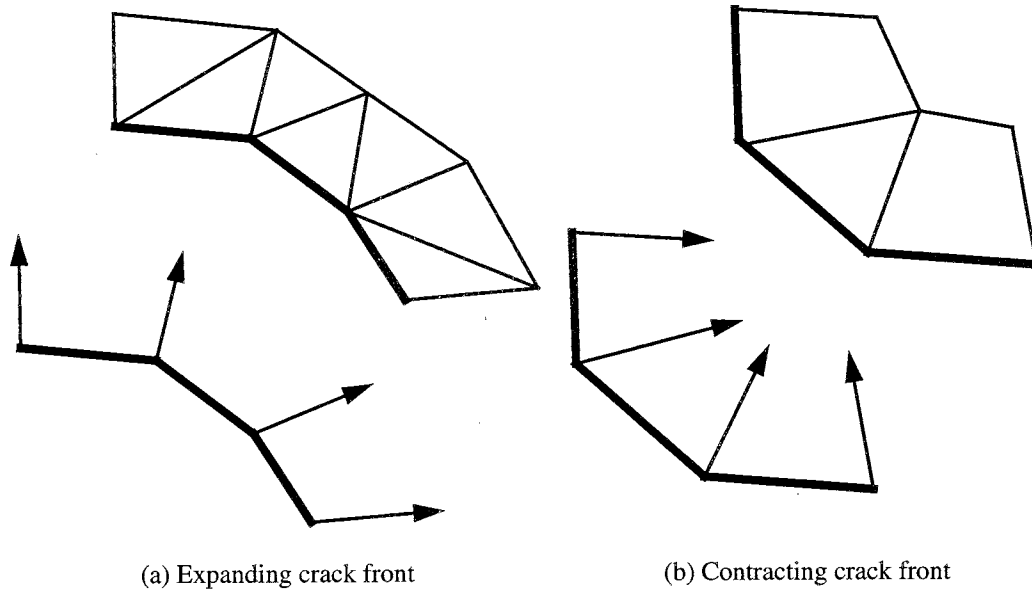
To construct the crack extension, the direction and magnitude of growth from each node on the crack front is added to the nodes current location and a new position is found. A triangular mesh is then constructed that extends from the old crack front to these new locations. The triangulation procedure must account for crack front expansion or contraction as illustrated in Figure 11, using the following procedure:

Let  $d_{ij}$  be the distance between two adjacent vertices,  $i$  and  $j$  that will form the new crack front.  $l_{max}$  is the maximum desired edge length on the crack front.  $\alpha$  ( $\alpha > 1$ ) and  $\beta$  ( $\beta < 1$ ) are two constants that define a criteria to guide the triangulation process to account for expansion and contraction.

If  $d_{ij} > \alpha l_{max}$ , then crack front is expansion must be accounted for by the introduction of new vertices on the front. A new vertex is introduced midway between those two vertices and the mesh is created accordingly as shown in Figure 11a.

If  $d_{ij} < \beta l_{max}$ , then the crack front contraction must be accounted for by coalescing the two adjacent vertices into a single vertex as shown in Figure 11b. This procedure helps prevent the crack from locally self intersecting as the crack front contracts.

For the examples shown later in this paper,  $l_{max}$  was selected to be equal to the maximum amount of propagation of the crack for a given step. This was done to ensure well shaped elements could be created around the propagating crack since the mesh currently created around the new crack will use these faces as faces in the mesh (as described in the next section). The other two parameters were selected as:  $\alpha = 1.2$  and  $\beta = 0.3$ , which can be shown to maintain control of the element shapes.



(a) Expanding crack front

(b) Contracting crack front

**FIGURE 11. Special cases for creating crack extension**

## 6.2 Micro mesh update

The crack extension is taken as the geometric representation of the growth of the crack. Since the crack extension intersects elements in the current mesh at places other than their boundaries, a method is needed to update the mesh to make it conform to the crack extension. Two approaches have been developed to allow this arbitrary crack growth: local remeshing and mesh modification. Local remeshing deletes the portions of the mesh that are intersected by the crack extension, and then creates a new mesh that reflects the presence of the new crack growth in this local area. Mesh modification uses the geometry defined by the crack extension to split mesh entities in the existing mesh to reflect the crack growth. Only the local remeshing procedure will be discussed in this paper, the mesh modification will be described in detail in a later paper.

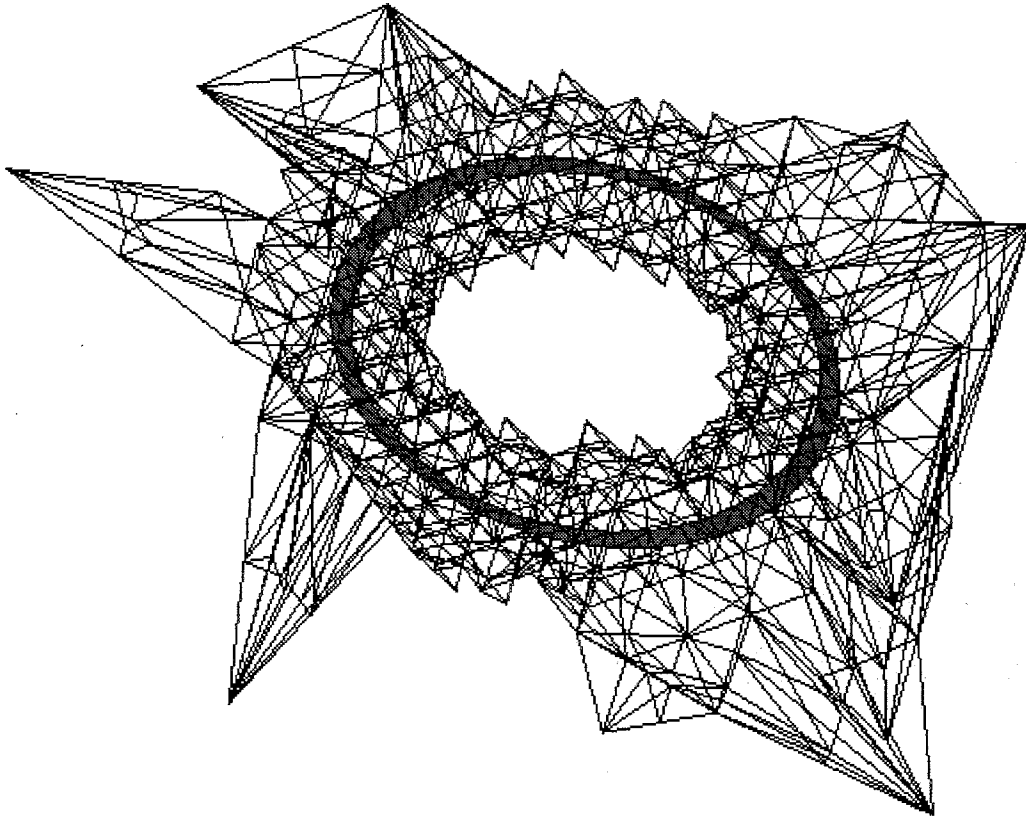
The first step in growing the crack is to determine the interaction of the crack extension with the existing mesh. For each face in the crack extension, the mesh regions it interacts with are found as follows:

1. Get the mesh regions surrounding any mesh vertices on original crack front.
2. Intersect edges of extension face with faces of the regions, if intersection is found add the region on the other side of the intersected face to the list regions to be checked.
3. Intersect the extension face with edges of the regions found in step 2, add any new regions of the intersected edges and vertices to the list of regions to be checked.
4. Repeat 2 and 3 until no more regions are found.

This step is repeated for each face in the crack extension, resulting in a list of mesh regions in the original mesh that the crack extension touches or passes through.

The next step is to delete all of the mesh regions that were found to interact with the crack extension, creating a hole in the mesh into which the crack extension mesh is inserted. One additional layer of mesh regions surrounding this hole in the mesh is then also deleted, for two reasons. First, the mesh in front of the crack needs to be refined to allow a good solution to be obtained. By removing this additional layer of mesh regions and refining the mesh on the boundary of the hole (by splitting mesh edges which are longer than a certain length) this is easily accomplished. Second, the original hole in the mesh can be extremely close to the crack extension, which can result in a poor mesh being created when the hole is remeshed. By moving this boundary away from the crack extension a much better mesh is obtained.

After the hole has been cleared out in the existing mesh, the crack extension mesh is inserted as shown in Figure 12. The hole is then meshed using a face-removal meshing procedure.



**FIGURE 12. Boundary of hole in mesh created for local remeshing procedure. Grey surface is the crack extension**

There are issues that arise in the local remeshing procedure when the growing crack intersects a material boundary in the model (such as growing from the matrix into a fiber). One consideration is whether or not such a situation can be detected. In the procedures described here the situation can be easily detected while the interaction of the crack extension with the micro mesh is found. This is done by checking the classification (relation of the mesh entities to the model entities they are discretizations of) of the mesh regions that are found to interact with the crack extension. This classification information is stored as

part of the data structure describing the mesh (Beall and Shephard 1995). Given the list of the mesh regions that a crack extension face interacts with, if the classification of any mesh region in the list differs from the others, then the crack extension face interacts with a model boundary. Once this situation has been detected there are issues involving both the analysis procedure and the mesh update procedure. Since the analysis does not take into consideration that the crack may propagate from one material to another it may not be correct to update the model to reflect this occurrence. The local remeshing mesh update procedure described here requires does not handle the situation of propagating the crack across material boundaries without modification. A more general mesh update procedure has been developed that does handle this situation without having to consider special cases. Both of these issues will be addressed further in a subsequent paper.

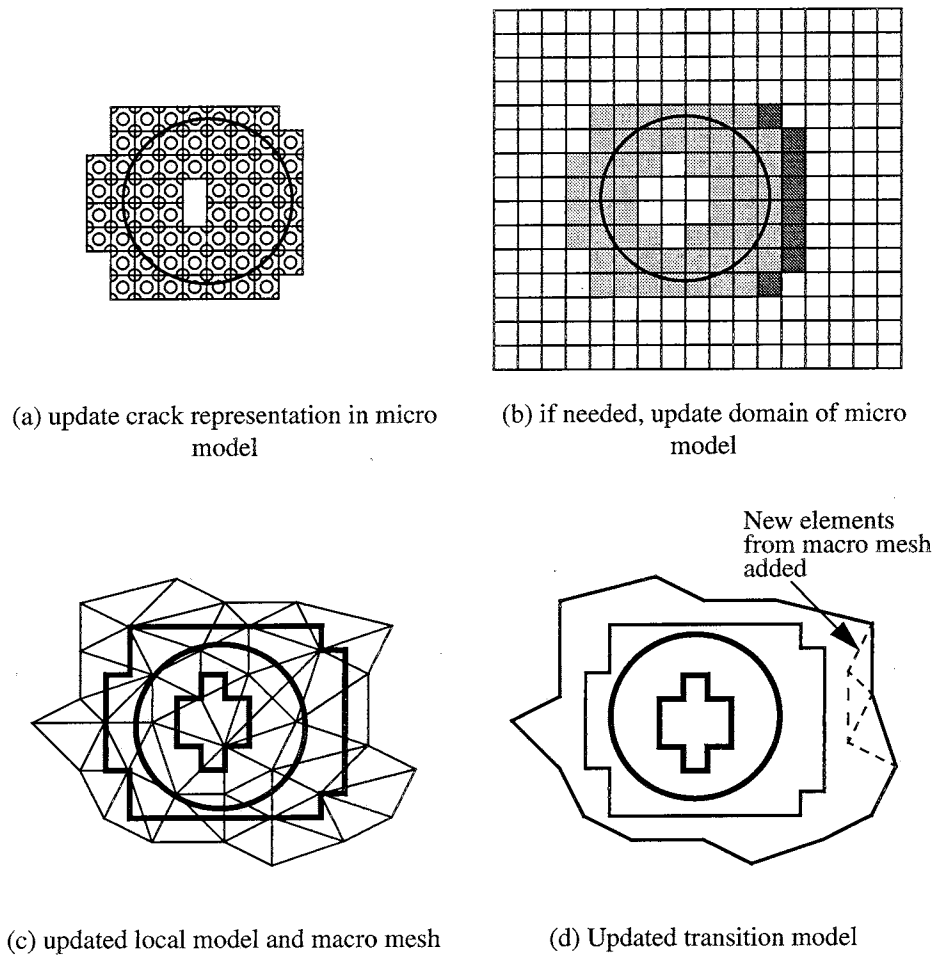
### **6.3 Micro and transition model update**

Eventually, as the crack front moves through the micro model, the original selection of the domain for the micro model will no longer be optimal for the analysis for one of two reasons. First, the crack front needs to be sufficiently far away from the boundary of the micro model for the analysis to be accurate. When the crack approaches the boundary the micro model will need to be extended. Second, there will be unit cells in the micro model that are no longer close to the crack front. This makes the micro model larger than it needs to be, reducing the efficiency of the analysis. These unit cells should be removed from the micro model.

Modification of the domain of the micro model requires updating the transition model. This is due to the change in the boundary of the micro model and also, possibly due to the



need to expand the transition model, by adding more elements from the macro mesh, due to the changes of the micro model. The process of updating the transition model is illustrated in Figure 13.

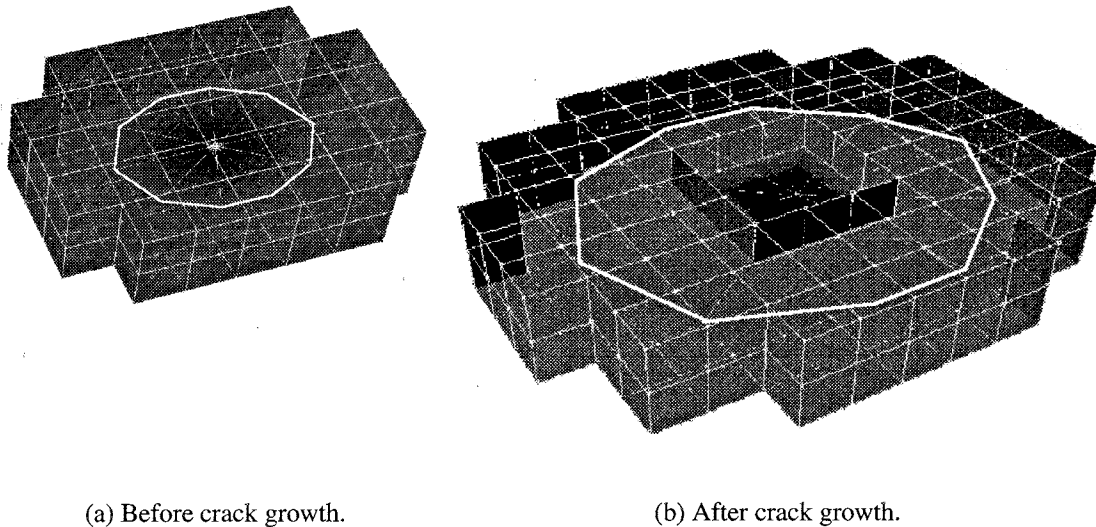


**FIGURE 13. Construction of the transition model.**

When new unit cells are added to the micro model, they can be meshed using the mesh that was created on the unit cell when the homogenization procedure was done. This is a simple procedure since the mesh on the boundary of the micro-mesh is identical to the mesh on the boundary of the unit cell.

When unit cells are removed from the micro model, the domain of the transition model cannot be reduced since all of the geometry of the crack must still be contained interior to transition model. For these analyses this is done by only adding macro-mesh elements to the domain of the transition model and never removing them as the crack grows. Thus, although the micro model domain only surrounds the area immediately around the crack tip, the transition model encompasses the entire crack.

Figure 14 shows the boundary of the micro model, before and after the crack grows. It can be seen that after the crack growth there is a portion of the model near the center of the crack where unit cells have been removed from the micro model since they are far from the current crack front.



**FIGURE 14. Boundary of micro model.**

## 7 Results

The procedures described in the previous sections have been put together into a system for analyzing the propagation of discrete cracks in heterogeneous media. The following two analyses are an example of the difference in crack growth that is found comparing an anal-

ysis using homogenized material properties to one using explicitly represented microstructure.

In both cases the problem being analyzed is an initially circular crack. The macro model is a cube loaded in off axis tension at an angle of 45 degrees to the crack surface (Figure 15). The material used is a unidirectional fiber reinforced composite. Both the fiber and matrix are taken as isotropic with the fiber properties:  $E_f = 50000$ ,  $\nu_f = 0.25$  and the matrix properties:  $E_m = 10000$ ,  $\nu_m = 0.25$ .

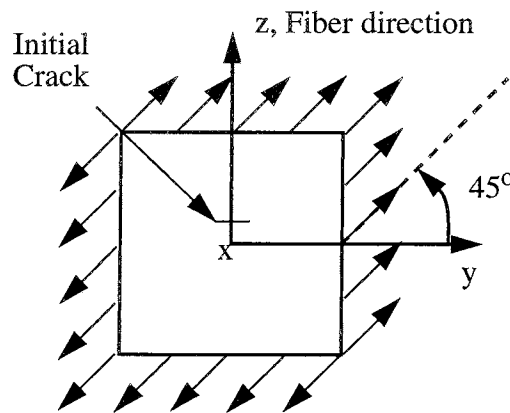
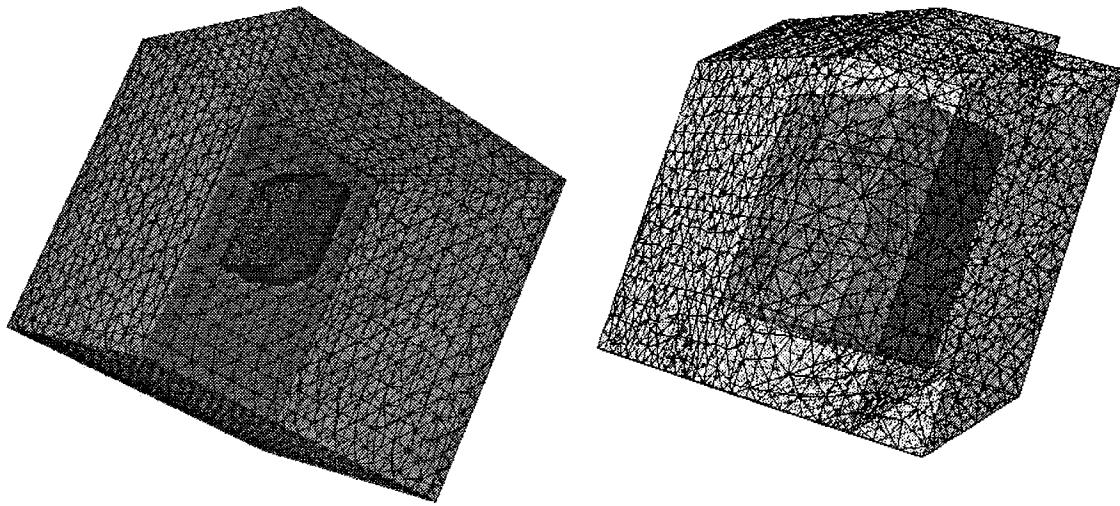


FIGURE 15. Test problem.

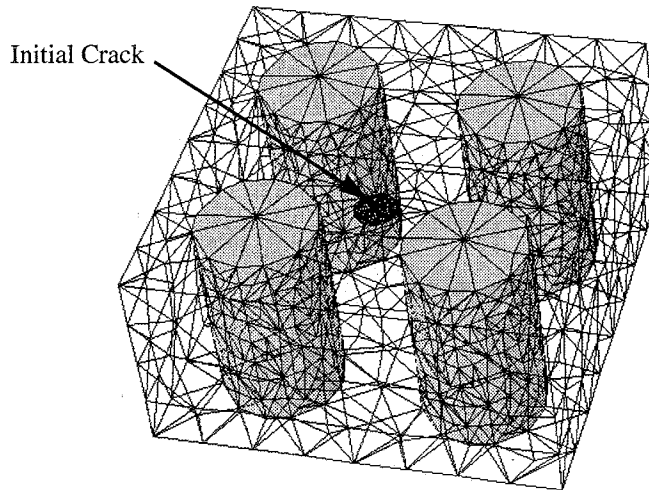
The first analysis was run using homogenized material properties, calculated from the unit cell of the composite, throughout the problem domain. The second analysis uses explicit microstructure in the vicinity of the crack front. The current capabilities of the system do not allow the crack to propagate through the fibers so only the initial growth of the crack can be analyzed (A new local mesh modification procedure, which is just nearing completion, will allow this. Results of that capability will be given in a future paper).

Figures 16 and 17 show the models that were automatically created by the analysis. Figure 16a shows the transition model in relation to the macro model. Figure 16b shows



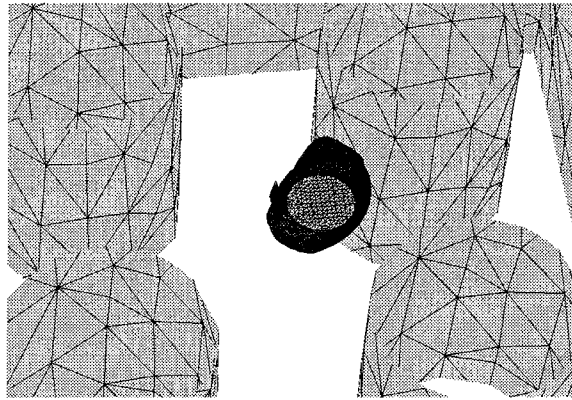
(a) Macro model with embedded transition model      (b) Transition model with embedded micro model

**FIGURE 16. Models created by the analysis**



**FIGURE 17. Micro scale model with crack location indicated**

the micro model in relation to the transition model. The micro model consists of four unit cells. The initial crack is circular and located approximately a quarter of a fiber diameter away from the nearest fiber as shown in Figure 18. The same micro model was used throughout the analysis since the amount of crack growth was small.



**FIGURE 18. Crack growth shown in relation to composite microstructure**

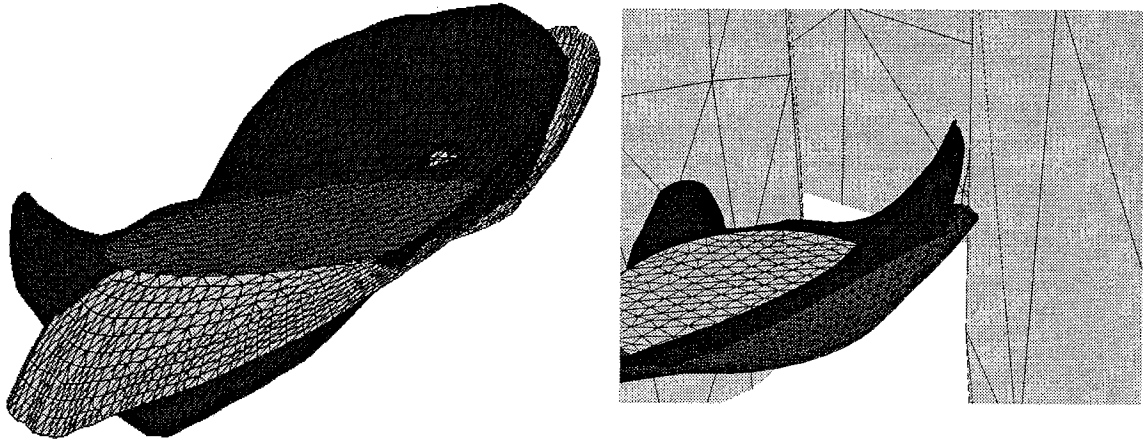
Figure 19 shows the crack growth predicted from the two analyses. The crack in the homogeneous material is shown in the lighter grey and the crack for the heterogeneous material is shown in dark grey. The closest fiber is on the right side of the view.

The analysis with the homogeneous material exhibits the expected behavior in this situation. The crack is growing so that it becomes perpendicular to the direction of the loading. The final step shown in the results is right after the crack would have come in contact with the fibers.

In the inhomogeneous case the crack exhibits more complicated behavior. It can be clearly seen that the presence of the fibers is affecting the growth of the crack. As the crack is approaching the fiber on the right side it bends away from the fiber and becomes more parallel to it.

## **8 Closing Remarks**

The analysis system described in this paper builds on several important technologies. First, a multigrid, multiscale solution technique that correctly accounts for the coupling



**FIGURE 19.** Analysis results showing the difference in crack growth when accounting for the microstructure. The light grey crack grew in a homogeneous material, the dark grey crack grew with the microstructure explicitly represented.

between overall models with homogenized material properties and local models with explicitly represented microstructure.

Second, automatic model and mesh generation procedures required to automate the complex analysis process involving several evolving models and meshes. These procedures operate from a common description of the analysis problem defined in terms of geometric model and attributes.

All of the procedures described in this paper have been implemented in a manner consistent with those used for parallel automated adaptive finite element analysis. Although the current simulations are being run on single processor workstations, larger problems will be able to take advantage of parallel processing.

Further development of the system is underway which will allow a microscopic flaw to be propagated until it grows to the point where macroscale failure of the component occurs. At this point analyses can be run to investigate the ultimate failure strength of components in the presence of various types of initial flaws.

## 9 Acknowledgments

This research was supported by ARPA/ONR under grant N00014-92J-1779.

## 10 References

Bakhvalov, N. S.; Panasenko, G. P. (1989). "Homogenization: averaging processes in periodic media." *Mathematical Problems in the Mechanics of Composite Materials*, Kluwer Academic Publishers.

Beall, M. W. and Shephard, M. S. (1995). "Mesh data structures for advanced finite element computations." Technical Report 19-1995, Scientific Computation Research Center, Rensselaer Polytechnic Institute, Troy, NY 12180-3590. submitted to *Int. J. Num. Meth. Engng.*

de Cougny, H. L., Devine, K. D., Flaherty, J. E., Loy, R. M., Ozturan, C., and Shephard, M. S. (1995). "Load balancing for the parallel solution of partial differential equations." *Applied Numerical Mathematics*, 16, p. 157-182.

Fish, J. and Wagiman, A (1993). "Multiscale finite element method for heterogeneous medium." *Computational Mechanics: The International Journal*, 12, 1-17.

Fish, J. and Markolefas, S., Guttal, R. and Nayak, P. (1994). "On adaptive multilevel superposition of finite element meshes," *Applied Numerical Mathematics*, Vol 14., 135-164.

Fish, J., Nayak, P. and Holmes, M.H. (1994). "Microscale reduction error indicators and estimators for a periodic heterogeneous medium." *Computational Mechanics: The International Journal*, 14, 323-338.

Fish, J. and Belsky, V. (1995a). "Multigrid method for a periodic heterogeneous medium. Part I: Convergence studies in 1-D case." *Comp. Meth. Appl. Mech. Engng.*, 126, 1-16.

Fish, J. and Belsky, V. (1995b). "Multigrid method for a periodic heterogeneous medium. Part 2: multidimensions," *Comp. Meth. Appl. Mech. Engng.*, 126, 17-38.

Fish, J. and Nath, A. (1993). "Adaptive and hierarchical modeling of fatigue crack propagation", *Int. J. Num. Meth. Eng.*, 36, 2825-2836.

Guedes, J. M.; Kikuchi, N. (1991). "Premat/postmat. A computer software for computational mechanics of composite materials." *Proceedings of the International Conference and Exhibition on Computer Applications to Materials Science and Engineering*, Elsevier Science Publishers.

Niu, Q. and Shephard, M. S. (1993). "Superconvergent extraction techniques for finite element analysis." *Int. J. Num. Meth. Eng.*, 36, 811-836.

Niu, Q. and Shephard, M. S. (1994). "Superconvergent boundary stress extraction and some experiments with adaptive pointwise error control." *Int. J. Num. Meth. Eng.* 36(5), 877-891.

Oden, J. T., Demkowicz, L., Rachowicz, W. and Westermann, T. A. (1989). "Toward a universal h-p adaptive finite element strategy, Part 2. A posteriori error estimation", *Computer Methods in Applied Mechanics and Engineering*", 77, 113-180.



Parasolid Version 6 KI Programming Reference Manual (1994). Electronic Data Systems Corporation, Parker's House, 46 Regent Street, Cambridge CB2 1DB England.

Shephard, M.S. (1988). "The specification of physical attribute information for engineering analysis." *Engineering with Computers*, 4, 145-155

Shephard, M.S.; Finnigan, P.M. (1989). "Toward automatic model generation. State-of-the-Art Surveys on Computational Mechanics, A.K. Noor and J.T. Oden, editors, NY, ASME, 355-366.

Shephard, M.S.; Baehmann, P.L.; Georges, M.K.; Korngold, E.V. (1990). "Framework for the reliable generation and control of analysis idealizations." *Comp. Meth. Appl. Mech. Engng.*, 82, 257-280.

Shephard, M.S.; Georges, M.K. (1991). "Automatic three-dimensional mesh generation by the finite octree technique." *Int. J. Numer. Meth. Engng.* 32(4), 709-749

Shephard, M.S.; Georges, M.K. (1992). "Reliability of automatic 3-D mesh generation." *Comp. Meth. Applied Mechanics and Engng.* 101, 443-462.

Shephard, M. S., Flaherty, J. E., de Cougny, H. L., Ozturan, C., Bottasso, C. L. and Beall, M. W. (1995a). "Parallel automated adaptive procedures for unstructured meshes", *Parallel Computing in CFD*, AGARD, Neuilly-Sur-Seine, France, R-807, 6.1-6.49.

Shephard, M. S., Beall, M. W., Garimella, R., Wentorf, R. (1995b). "Automatic construction of 3-D models in multiscale analysis." *Computational Mechanics*, 17(3), 196-207.

Weiler, K.J. (1988). "The radial-edge structure: A topological representation for non-manifold geometric boundary representations." *Geometric Modeling for CAD Applications*, M.J. Wozny, H.W. McLaughlin and J. Encarnacao, editors., North Holland, 3-36

Wentorf, R.; Shephard, M. S.; Korngold, E. V. (1989). "The use of functional models to control engineering idealizations." *Proceedings of the 1989 ASME International Computers in Engineering Conference and Exposition*, Anaheim, California, July, 63-70.

Wentorf, R.; Shephard, M. S. (1993). "Automated analysis idealization control." *Concurrent Engineering: Automation, Tools, and Techniques*, Andrew Kusiak Eds., John Wiley, New York, 41-73,

Wong, V.S. (1994). "Qualification and management of analysis attributes with application to multi-procedural analysis of multi-chip modules", TR23-1994, Scientific Computation Research Center, Troy, NY

Zienkiewicz, O. C. and Zhu, J. Z. (1992). "Superconvergent derivative recovery techniques and a posteriori error estimation in the finite element method - part 2: The Zienkiewicz-Zhu a posteriori error estimator." *Int. J. Numer. Meth. Engng.*, 33, 1365-1382.