

# Automatic construction of 3-D models in multiple scale analysis

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**Abstract** This paper discusses techniques for the automatic construction of numerical analysis models for multiple scale analyses which employ interacting models at two, or more, physical scales. Consideration is given to the methods to define the geometric representations and generate the discretizations needed by the numerical analysis procedures. The application of the techniques to multichip modules and composite structures, with interacting macromechanical and micromechanical level analyses, is demonstrated. In the multichip module analyses both heat conduction and thermomechanical analysis are performed using different numerical analysis techniques, and the two interaction of the analyses at the through levels is through a basic global/local methodology. The composite structure analysis considers crack propagation at the micromechanical level interacting with the macromechanical analysis through finite element based adaptive multiscale analysis. In both example applications the focus of the discussion is on the automatic construction of the required geometric models and their automatic discretization.

## 1

### Introduction

The need for more accurate determination of quantities of interest has led to an increased use of interrelated analyses in which the discretization processes are performed at multiple physical scales. For example, in the two applications considered in this paper, the thermomechanical analysis of multichip modules and the fracture analysis of composite structures, analyses performed at a macromechanical level are coupled to analyses performed at the micromechanical level over critical portions of the domain of interest. In addition to the development of the analysis procedures required, it is necessary to provide the appropriate modeling and discretization environment. The focus of this paper is on the development of automated techniques to support these modeling and discretization procedures.

In today's engineering environment, the amount of time and effort involved in performing an analysis using numerical analysis techniques is often dominated by the construction of the discrete representation, the mesh, of the domain of interest as needed for the analysis at hand. Since it is becoming more common for a computerized representation of the problem domain (a geometric model) to be available to the analyst, procedures to efficiently discretize these domains are being developed. The use of such geometric models provides a common basis to support multiple related analyses where different discretization methodologies can be used. Performing an engineering analysis also requires information on materials, loads, boundary conditions and initial conditions. The support of automated analysis procedures requires that this information, referred to as analysis attributes, be defined in terms of the geometric model.

The generation of a discrete representation of a given domain and its numerical analysis constitute only two of the steps in performing an engineering analysis. A critical step performed before these steps is the process of determining an idealization of the physical problem appropriate for the analysis. For example, in the case of a composite structure it is common to assume that the information of interest can be determined by replacing the microstructural detail by a homogeneous macrostructure. In the applications considered in this paper, at least two levels of idealization are used in a complete analysis process. Since the goal is to provide automated procedures to control all steps in these analyses, the procedures must include a general idealization control framework. The inclusion of such a framework has the immediate benefit of providing a feedback loop which can support adaptive idealization control processes. Section 2 discusses the techniques used to support the general definition of the problem which is used in the automatic construction of the analysis models. Section 3 discusses the idealization control framework used by the model construction processes for multiple scale analyses.

To demonstrate the application of this methodology, two multiscale analysis applications are described. Section 4 discusses a set of procedures developed to support global/local heat conduction and the thermomechanical analysis of multichip modules where the local level analysis employs the detailed microstructure in that area. Section 5 overviews the application of the methods to the multiscale adaptive analysis of the fracture of composite structures.

## 2

### Problem definition to support automated model construction

Automation of a set of engineering analyses requires that all analysis models, and their discretizations, be derived from

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a single problem definition. The two key components of this definition are the domain description (the geometric model), and the analysis and idealization attributes defined in terms of it. This single problem definition is used to support the construction of all the models employed in performing the analysis. For sake of discussion this single problem definition, from which all other models are derived, is referred to as the primary problem definition.

## 2.1

### 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 also be able to support the requirements of automated discretization construction procedures, such as automatic 3-D mesh generators which perform a large number of interrogations on a geometric representation. The primary model must be structured such that the various idealized engineering analysis models can be constructed, and the interactions between those interactions controlled. For example, at the highest level, a composite structure may be idealized geometrically as a surface, while at a second level a portion is represented as a multi-layer volume or surface, while on a third level a local region of the microstructural components are represented as volume elements.

Over the years, geometric model representations and associated software systems have been developed which can support these various forms of geometric representations. Of the various forms, only the general non-manifold geometric representations (Weiler 1988) are capable of representing the general combinations of volumes, surfaces and curves required by the various forms of analyses. Geometric modeling systems that can support the full range of geometric operations required to support engineering analysis idealization and discretization processes are highly complex, requiring a massive development effort. Since a number of commercial software packages have been developed that provide at least the base geometric modeling capabilities, the analysis idealization and discretization procedures developed in this work directly employ those functionalities. The obvious advantage of this approach is that those development efforts are not repeated. There are, in addition, important technical advantages to this approach since the geometric calculations can directly employ the tolerances employed in the geometric modeler (Shephard and Georges, 1992).

The specific requirements placed on the primary geometric model representation depend on the analysis model idealization and discretization procedures used. One approach is to assume a detailed geometric representation at the lowest physical scale is available. This is not an advantageous approach since the model sizes would be unacceptably large, the construction of the higher level models can be more complicated than the automatic construction of low level models, and the user construction of detailed lower level models can be burdensome to the design process. The approach taken here is that the representation stored has enough information so that all the required idealized geometric models can be automatically built.

As demonstrated in the two applications considered, the actual forms used can vary, however, in both cases there is sufficient information to automatically construct the complete non-manifold geometric models required for the automatic discretization generation procedures.

The most geometrically demanding processes typically 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 a macromechanical level analysis. Another example is the construction of a multi-material solid model of a representative unit cell from basic composite construction specifications. Such models are required when micromechanical models are included in the analysis process. The approach used to address these needs is to employ the geometric construction functionalities of commercial solid modelers, driven by appropriate knowledge housed in the primary model and the analysis strategy being executed. Figure 1a shows the unit cell for a composite weave automatically constructed in the Parasolid non-manifold solid modeling procedure using basic manufacturing parameters that define the weave.

Automatic discretization procedures, such as automatic finite element mesh generators, must also interact with the geometric model, interrogating it to determine information not

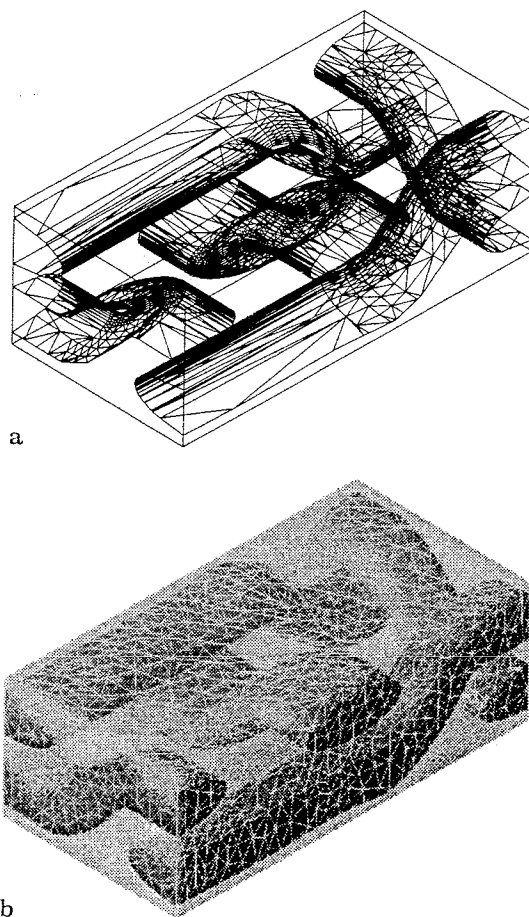


Fig. 1a, b. Automatically constructed and meshed unit cell model

directly stored in the data structures of the geometric model. Since most commercial geometric modelers provide libraries of basic geometric interrogations, it is possible to develop the automatic discretization generation procedures employing operators built on those libraries. An example of one such mesh generator is Finite Octree (Shephard and Georges, 1991) which interacts with the geometric modeling system through a specific set of 21 geometric operators. The integration of Finite Octree with a new geometric modeling system only requires the creation of those geometric operators with respect to that modeler. This requires no knowledge of the operation of the mesh generator, or the data structures internal to the geometric modeling system. What is required is a knowledge of the basic interrogation operators available from the geometric modeling system which can be used to build the specific Finite Octree geometric operators. Using this approach Finite Octree has been integrated with four geometric modeling systems including Parasolid, ACIS, SHAPES and an in-house modeler. Figure 1b shows an automatically generated Finite Octree mesh of the unit cell in Fig. 1a.

One complexity in the use of commercial solid systems modeling to support multiple scale analysis is that they have historically been limited to 2-manifold geometric models, which, put simply, limited the objects represented to faces which have solid material on one side, and edges with only two faces coming into them. However, a careful examination of the detailed functionalities of commercial 2-manifold geometric modelers indicates that although they cannot properly represent non-manifold geometric models, they can often perform the basic geometric operations required to define the entities needed for specific classes of non-manifold models. For example, there are operators to support modified union operations needed to combine individual material assemblies. These operations create sets of coincident faces, edges, and vertices at each of the contact faces. Such redundant topology represents inconsistencies which will cause the automatic mesh generator to fail. By maintaining an understanding of the redundant relationships, the model's topological representation is postprocessed to eliminate the redundant entities and construct the correct topological use needed by a proper non-manifold representation. One method to store this information is the radial-edge, non-manifold, topological structure (Weiler 1988). Seeing the need for non-manifold representations, commercial solid modeling systems are altering their internal data representations so they can properly represent non-manifold objects.

## 2.2

### Analysis and idealization attributes

Analysis attributes are the information past the geometric model needed to specify an analysis model. Analysis attributes include material, 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.

The specification of attributes is typically done employing ad-hoc processes specific to the analysis procedure. Such approaches do not properly support an automated environment

when a number of different analysis techniques may be applied. 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. When defined in this manner they can be properly transferred to the idealized analysis models and their discretizations. An attribute manager, following the basic approach outlined in Shephard (1988), has been developed to support these requirements (Wong 1994).

Since the physical description of all analysis attributes are in terms of tensorial quantities, their effective specification must be in terms of various order tensors and their distribution. The most convenient means to score a tensor is in terms of its components defined in a particular coordinate system. Since many of the tensors used to define physical quantities possess various forms of symmetry, it is advantageous to account for these symmetries to minimize the amount of information required to specify an attribute. Based on this, the components of the structure used to define the attributes' physical information are (i) the order of the tensor, (ii) an indication of the coordinate system the attribute is defined in, (iii) the symmetries possessed by the attribute, and (iv) the distribution information defining each component of the tensor in the given coordinate system.

The specification of a particular analysis requires the proper grouping of a number of individual attributes. 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.

The third major component of the attribute manager is the association of the attributes with the geometric description of the domain. At the primary model level, this is the association of the attributes with entities in the primary geometric model. When the primary model is defined in a solid modeling system, a scheme of associating the attributes with the correct topological entities in the geometric model, including basic augmentation functions to support when an attribute is defined over a portion of an entity, is sufficient (Shephard and Finnigan, 1989). Additional complications are introduced in the case of multiple scale analyses because it is necessary to properly transfer the appropriate attribute information from the primary attribute definition to the idealized modes used in the analysis process. 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. The case of dimensional reduction is complicated by the geometric operations required. Determining average material properties is complicated by the fact that it is, in itself, an analysis process and consideration of the range of procedures available to determine them with their relative cost versus accuracy trade-offs. In a properly controlled multiple scale analysis structure, this process must be adaptively controlled in the same manner as all the analysis steps.

A specific set of procedures within the attribute manager have been developed to support the definition of attributes, their

grouping into analysis cases and their association with both the primary geometric model and the various idealized geometric models (Wong 1994). These procedures are used in conjunction with the analysis idealization control procedures described in the next section to support the multiple scale analysis applications described in this paper.

### 3

#### Control of analysis idealizations processes

Given a primary problem definition and the modeling tools required to convert the information into the input required for the various analysis processes, an overall structure is needed to control the execution of each of the idealization and discretization steps performed. Since the range of analysis idealization and discretization processes vary widely, this overall structure must be quite general.

By combining specific methodologies developed for controlling engineering decision processes, with the feedback loop structure of adaptive procedures, an analysis idealization control mechanism, called an analysis strategist, has been developed (Shephard, et al. 1990; Wentorf and Shephard, 1993). The analysis strategist considers an engineering analysis as a stepwise process of reducing the physical description and behaviors of the system into a set of solvable algebraic equations representing one or more of the behaviors of interest of a design, object or process. At each step decisions must be made as to what specific idealizations to employ. The selection of a specific idealization must consider the goal of the analysis and the interaction of this idealization step with others. The analysis goal specifies the domain of interest, the type of result desired, the limiting time (cost) and the desired reliability of the results. The reliability and accuracy of an analysis is a function of the approximation errors created by each idealization step. Since it is often possible to obtain better estimates of the error introduced by a particular idealization based on a posteriori evaluation, the analysis strategist employs a feedback loop where the influence of idealization steps can be examined and the idealization improved in a re-analysis loop until the desired level of accuracy is obtained.

The strategy is an abstract plan or template which is selected from a library and then refined into a detailed sequence of software operations. The strategy is represented by a network of frames (Minsky 1981), where each frame represents a computational component which performs a function. A frame groups information about the entity which it represents using slots, where each slot has a label, one or more values, and data which characterizes the type of the value and its source called "facets". The values may also be linked with other frames, called "relationships". The relationships connecting the computational components represent the characteristics of the information which is input and output by the component. Naturally, the characteristics of the output of one component must match with the input characteristics of the next. Each component of the strategy can be refined, in a recursive manner, into a sub-network of more specific components, where the total inputs and outputs of the refined network are inherited from the less refined "parent" component. The refinement stops when the plan is sufficiently detailed to be implemented by a modeling operation, database query, execution of an analysis package, etc. As a last resort, if no

source for information critical to the analysis can be found, the user is queried. In essence, the refined strategy is a functional model of an analysis "machine" which takes the given domain as input and creates the desired results of the analysis goal. Reasoning based solely on this information flow net is only one aspect of refining and implementing an analysis strategy.

The physics of the design must also be used to create suitable models for achieving the desired analyzed results. This is done by using a functional model of the artifact being analyzed, which specifies the required physical phenomenon, the geometry and attributes used to implement each functional component and the physical relationship between functional components (Wentorf, Shephard and Korngold, 1989). For example, if the purpose or function is to transfer load as part of a load path, and the refinement of that function is specified in terms of flanges, holes, bolts, pre-tensioning torques, etc. (functional components, geometric forms and attributes), then the basic modeling ingredients for idealizing the connection between domains in the analysis model are available. The functional model is represented using frames and has additional relationship slots which link the corresponding geometric and attribute entities with each component. The network is processed with rules, some of which traverse the physical relationship slots of the network, performing graph based operations, while other rules match with specific component slot values. An example of the former rules are that which establish "load paths" in a functional network by using "structurally connected" type relationships. The rules produce a network of idealized components, also with additional relationships pointing to the corresponding idealized geometric and attribute entities. The processes used to create the idealized model are complex and involve interactions between the three modelers. For example, the proximity or extent of a geometric feature may need to be evaluated in order to determine whether it should be included in the idealized model. If a component has a slot value used for idealization and it is modeled explicitly in the primary model, e.g. geometric proximity, then the value is filled by an external procedure call to the geometric modeler automatically when the component is created.

As a minimum, the idealization control process must consider the physics envisioned for the design. Extra intelligence is added if the system can automatically deduce physical phenomenon beyond the original design intent. For example, a structural connection can also imply a thermal connection relevant to heat transfer analysis.

A third category of knowledge used to refine and implement an idealization control strategy is analysis expertise. They may be based upon knowledge of the theory used to formulate the computational component (e.g. a linear elastic model) or may be based upon experience matching modeling technique with empirical results. This knowledge is used to estimate and evaluate the time (cost) and reliability of the results, and can determine the next best computational component or idealized model constituent to use for feedback strategies. Mathematical modeling and applicability description slots in each computational component, combined with access to cost/error estimation procedures provides the representations needed for reasoning.

The mechanism for control of idealization processes must be able to reason about what must be recomputed if the problem

definition parameters change. For example, when examining ceramic composite material failure by cracking, using a linear elastic theory, a change in material processing temperature does not require reanalysis for determining the applied stresses. This can be deduced from the detailed strategy network and increases the apparent performance of the strategy in this case.

#### 4

### Application to global/local analysis of multichip modules

#### 4.1

#### Global/local analysis procedures

A multichip module (MCM) is characterized by having a number of layers containing wires and vias in various configurations, in conjunction with a general chip and cooling structure layout. The prediction of a mechanical failure, such as a wire fracture due to thermomechanical loading, is critical to ensuring the ability of a multichip interconnect to perform its intended electrical functions. The accurate prediction of these failures must involve the local microstructural details of the MCM at a potential failure site, in an analysis accounting for nonlinear behavior. However, analyzing a finite element discretization of the entire MCM microstructure would produce a set of equations with orders of magnitude and more unknowns than can be realistically solved on today's computers.

An alternative methodology to analyze MCMs is to employ global/local procedures, in which cost effective global analyses are performed to provide the boundary condition information needed for an accurate local analysis of the critical regions where the wires, vias, etc. are fully represented. Both the global and local analyses employ continuum models to provide a mathematical description of the heat conduction and thermomechanical behavior. In addition, it is assumed that the heat conduction and thermomechanical problems are uncoupled.

To be computationally efficient, the global analyses procedures employ a more extensive set of idealizations on both the physical scale of the analysis and the behavior of the governing continuum equations. To limit the size of the systems required, the detailed geometry of the interconnect is eliminated by employing averaging techniques to convert each layer in the MCM into an equivalent homogeneous medium. In the global analysis problems it is sufficient to employ linear constitutive relationships.

The global analysis procedures are based on a variational technique in which the differential equations and certain interface and boundary conditions are satisfied exactly. Therefore, the numerical solution process must only perform area integrals, as opposed to full volume integrals and the number of unknowns in the procedure does not increase as the number of interconnect layers increases. See Sham, et al. (1993) and Tiersten, et al. (1993) for a description of the specific procedures developed for the global heat conduction and thermomechanical analysis of MCMs.

Because the interconnect is idealized in a layerwise fashion for the global analyses, the based domain information needed includes the "in-plane" dimensions, the thickness and volume fractions for each layer. In addition, knowledge of the chip arrangements on the upper surface is required. Because

it does not need any information from other analyses, the global heat conduction analysis is the first analysis performed. It provides the global thermomechanical analysis with the global temperature field.

The local heat conduction analysis is performed using a stochastic for solving Laplace's equation based on the floating random-walk method, (Le Coz and Iverson, 1992). The local heat conduction analysis employs the temperature defined by the global heat conduction analysis on the boundary of the local window.

Since the details of the local stress fields are critical to the prediction of failure quantities, the local thermomechanical analysis procedure must accurately represent the local geometric detail in an analysis, including nonlinear material behavior. The most effective means to meet these goals is to employ an automated adaptive finite element methodology (Shephard, et al. 1993). The local thermomechanical analysis obtains displacement boundary conditions from the global thermomechanical analysis and a temperature field from the local heat conduction analysis.

#### 4.2

#### Construction of idealized geometric models and their discretization

The four analysis procedures employ three different idealized geometric and discrete representations which must be generated from the available primary definition. The most appropriate unique geometric representation, from which to generate the numerical analysis discretizations, is a non-manifold solid model. However, consideration of the design and manufacturing representations employed for MCMs indicates a more commonly used domain description is a CIF file (Mead and Conway, 1980). Although convenient, a CIF file is not a complete and unique geometric representation of the non-manifold geometry of an MCM. Therefore, the approach taken in this work is to use the CIF file, attributed with a limited amount of additional needed information, as the basis of the MCMs primary definition, and to develop the procedures required to interpret the CIF files to construct the idealized geometric model needed by the automated discretization generation procedures.

The current assumptions and associated limitations on the CIF file are: (i) entities are defined on a layer-by-layer basis with all layers being explicitly represented, (ii) entities within a layer are rectangular parallelepipeds with edges aligned with the edges of the interconnect, (iii) all entities defined in the CIF file are associated with a specific layer, and (iv) neighboring material regions must share one or more faces. These assumptions and limitations can be altered by the application of new CIF file interpretation rules, combined with the appropriate construction procedures.

The global heat connection and thermoelastic analyses employ a layerwise discrete representation of the overall interconnect configuration, where each layer is assigned the appropriate averaged material properties. The procedure to determine this information employs the attributed CIF file to construct models of each layer from which the calculation of layerwise volume fractions can be determined for use in the material property averaging procedure. The size and position of the chips on the top surface of the MCM is also obtained from the information in the CIF file.

The idealized geometric representation for the local thermal analysis must represent the microstructure in the local window as a set of materially homogeneous rectangular parallelepipeds with all edges in one of the three perpendicular directions. The current restrictions on the primary model match this requirement. Given the set of parallelepipeds, the discretization for the local heat conduction analysis is simply the diagonal endpoints and thermal conductivity of the parallelepipeds. Geometric and material data for the local heat conduction analysis are directly extracted from the CIF format, and extended to three-dimensions. Layer thicknesses, wire thicknesses, and corresponding thermal conductivities are extracted from the analysis attribute information.

The goal of local thermomechanical analysis is to be able to predict the initiation of local failures such as a wire fracture. Since failure phenomena are strongly influenced by the local geometric details of the numerical analysis, model generation and discretization generation procedures must be able to deal with these details. Although current CIF file restrictions limit the amount of geometric detail in the primary geometric model, the procedures developed for the local thermal mechanical analyses do not suffer from such limitations. Simple methods to avoid these restrictions are demonstrated below.

The finite element discretizations for the local thermomechanical analyses are automatically constructed using the Finite Octree mesh generator (Shephard and Georges, 1991) which is capable of creating graded meshes of general 3-D non-manifold domains (Weiler 1988). However, to operate Finite Octree requires the domain to be meshed to be defined within a solid modeling system which supports the required geometric interrogations. Since the CIF file maintains only basic geometric parameters, it is incapable of supporting the required geometric interrogations. Therefore, it was necessary to develop a procedure to build, from the information in the CIF file, the non-manifold solid model in a geometric modeling system that can support the mesh generator's geometric interrogations. In the current efforts both Parasolid and ACIS solid modeling systems, with the proper non-manifold extensions for multiple material domains, have been developed.

The procedure used to generate the multiple material solid model in an extended solid modeling system starts with a CIF file containing a 2-D description of the MCM layers in terms of rectangles, polygons, circles, and paths. When attributed with a thickness parameter, each such CIF entity can be formed into an appropriate solid primitive in the solid modeling system. The primitives of a single material type are intersected against a box defining the local window of the analysis and then unioned to form the collection of solid bodies of that material type referred to as a material assembly. To make this process computationally efficient, CIF file entities which do not interact with the selected parallelepiped are not included in the Boolean operation processes. For example, layers with z-values that do not overlap the parallelepiped need not be considered, while entities in layers of interest which do not overlap the  $xy$ -rectangle of the parallelepiped need not be considered. Pairs of material assemblies are examined and their interactions defined by performing appropriate modified Boolean operations. If there is no interaction, proceed to the next pair of material assemblies. If their interaction is only at common boundaries, it is resolved by the elimination of the appropriate pairs of duplicate entities.

If their interactions include domain overlap, rules as to how to handle the overlay region are invoked and the new common boundary interactions are recorded.

Figure 2 shows non-manifold solid models built using three different local windows defined in the vicinity of a specific chip in a seven layer MCM. The largest window shows the entire area under the chip, while the other two windows show close-ups of a specific critical junction area.

Figure 3 shows a simple three-dimensional test example, the automatically generated initial mesh, and the adaptively refined mesh of a highly local region. As expected the elemental error estimators predicted refinement at the juncture of the via and wire.

An examination of the results of the adaptive analysis indicate a overly high stress concentration at the intersections of the vertical and horizontal components of the wires caused by using a shape corner to represent this region. To obtain more realistic stress values, a geometry closer to that which is actually manufactured is required in the local thermomechanical analysis. Figure 4 shows the original CIF level idealization and a more realistic geometry for the intersection of two wires and the area under a solder connection. This more realistic geometry is automatically constructed using the same basic process as above, except additional

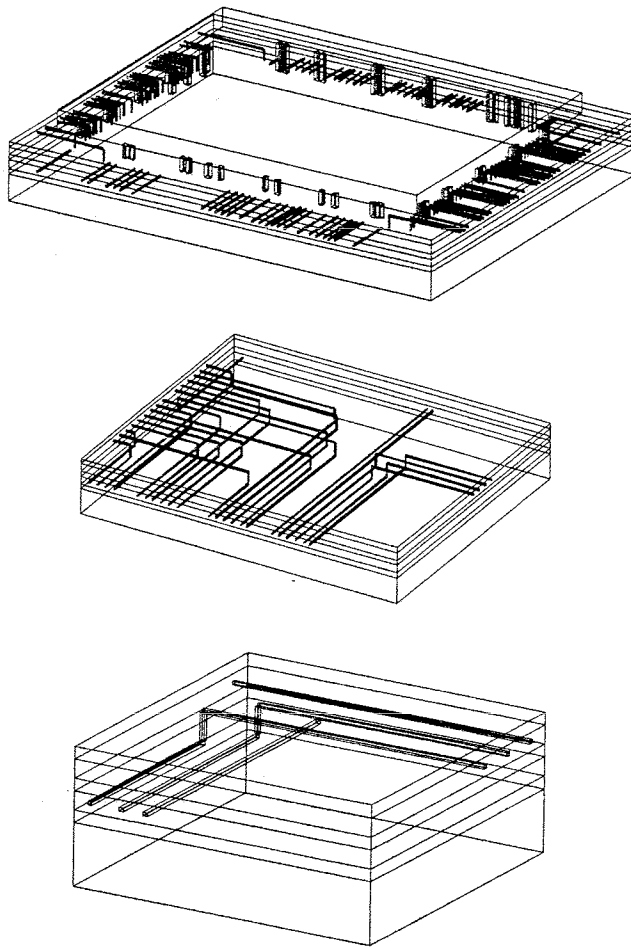


Fig. 2. Views of a Parasolid model of a simple one chip interconnect created from a CIF file

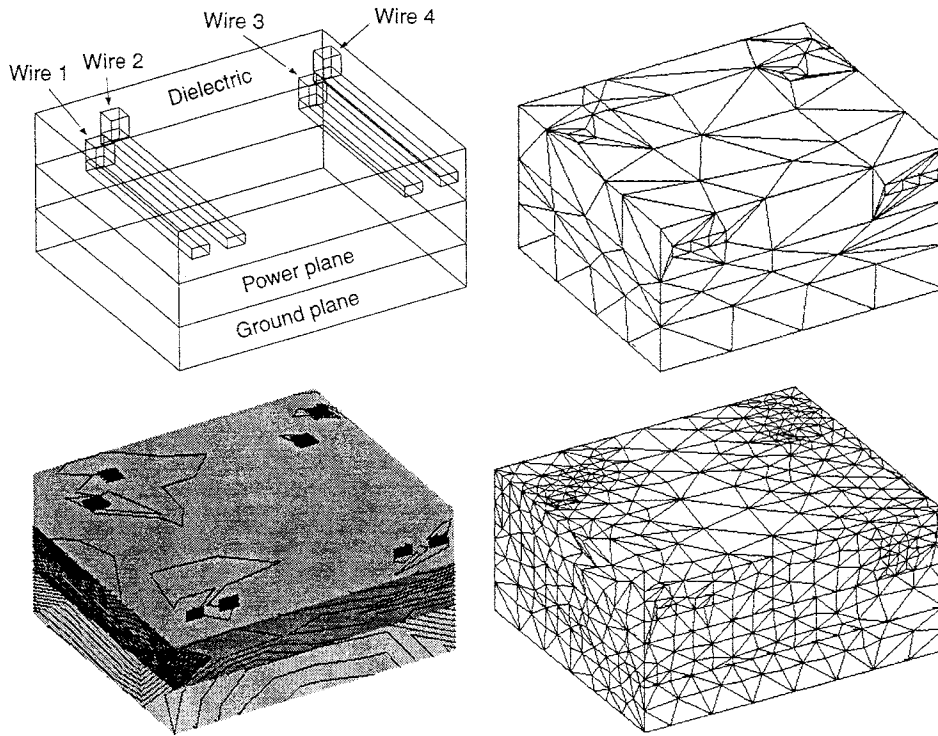


Fig. 3. Three-dimensional test example with initial and adaptively refined finite element mesh. Meshes show only the element faces on material boundaries

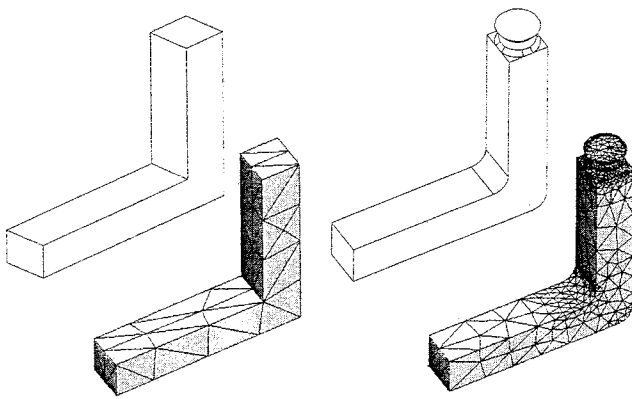


Fig. 4. Models and meshes of wires, vias and solders in local window with sharp corners blended

attribute information on how the component geometries would actually blend during manufacture has been added and the solid model construction procedures extended to account for that information.

## 5 Application to adaptive multiscale analysis of composite structures

Composite structures are a natural area for multiscale modeling. Good estimates of overall behavior can be obtained by analyses using homogenized microstructures. However, the failure processes that must be taken into account typically initiate at the scale of the microstructural constituents. Modeling an

entire component at the scale of the microstructural constituents is not a practical approach due to the extreme size of the resulting problem. However in areas where failure is likely to initiate, it is necessary to perform analyses on the microstructural scale to model the initiation of the failure and its effects on the rest of the structure.

As the microscale damage evolves, it affects the behavior of the composite at the macroscale. Therefore, it is necessary to perform the analysis in such a manner that this coupling between the scales is represented. One technique that shows much promise for this type of analysis is the multiscale analysis of Fish and Belsky (1995a, b).

### 5.1 Multiscale composite analysis

The multiscale analysis being used for composites is a three level analysis. 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 is represented. The middle level serves as a transition between these two levels and incorporates any macro level damage. During an analysis the top level remains unchanged while the second and third level are automatically created and updated throughout the analysis.

The analysis uses an iterative multigrid procedure to solve the problem. A homogenization based prolongation operator (Fish and Belsky, 1995a, b) is used to couple the solution between the transition mesh (with homogeneous material properties) and the micro-mesh (with heterogeneous material properties). Further information regarding the details of the analysis can be found in the references.

## 5.2

### Example-Crack propagation

The example used to demonstrate the model building procedures necessary for multiscale composite analysis is the propagation of a crack through the microstructure of a composite plate. To predict the growth of the crack it is necessary to have a detailed representation of the microstructure near the crack front. However in other areas of the model, such as far ahead of the crack or sufficiently behind it, such detail is unnecessary and a homogenized representation of the microstructure can be used. Thus for this analysis the micro-model will be needed only in a small area around the crack tip.

The 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 layout and microstructure of the composite. These attributes include the type of microstructure, the parameters needed to build a unit cell as described below, the material properties of the constituents and the orientation of the unit cell with respect to the macro-model.

In addition, the primary problem definition also includes the initial geometry of the crack. It is assumed at this point, for the sake of simplicity, that the initial crack geometry is a convex, planar polygon. As the crack grows it is allowed to become non-convex and non-planar. The crack is assumed to remain a single face throughout the analysis, although it may develop interior holes. The crack front is the set of edges that bound this face including any edges bounding interior holes.

### 5.2.1

#### Unit cell construction

Before any analysis can be done, a model of the microstructure of the composite must be created. Currently the microstructure geometry is assumed to be periodic and, thus, can 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 (Bakhvalov 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.

Common composite unit cells are: aligned fibers, random chopped fibers, random particles, and woven fibers. Samples of unit cells of each of these types are shown in Fig. 5. 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 Fig. 5, 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 cell is constructed by first creating a cuboid of the correct size of its boundary and then creating each reinforcement as specified by the parameter values (e.g. for the aligned fiber unit cell, the diameter of the fibers is calculated from the fiber volume fraction), then the reinforcements are unioned with the boundary to create the finished model.

The unit cells with random structure, such as the chopped fibers and particles in Fig. 5, are generated using a stochastic procedure as follows. For each piece of microstructure in the

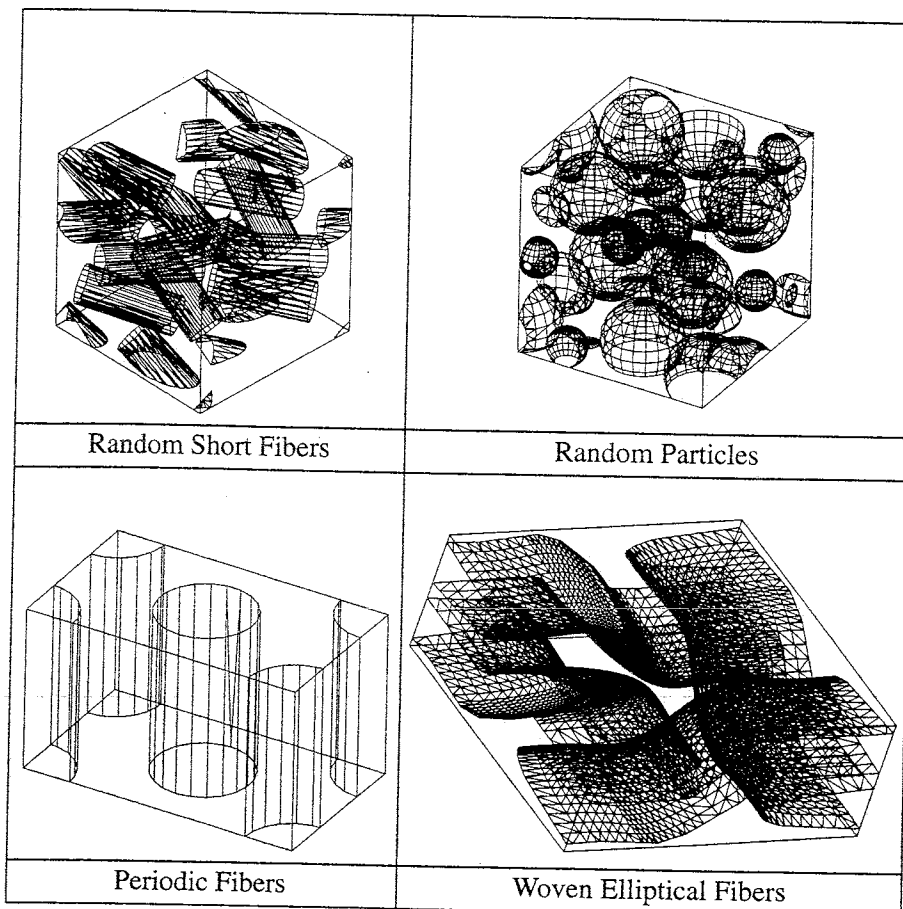


Fig. 5. A sample of the various types of unit cells that can be created



unit cell a random location, and orientation, if needed, is selected. A check is then made to determine if the "periodic extension", described below, of this piece of microstructure will interfere with any already in the unit cell. If it does not then it is inserted into the unit cell and the process is repeated until the correct volume fraction is reached.

Before each piece of microstructure can be checked for interference with others it must be determined if it intersects any of the boundaries of the unit cell. If it does intersect any boundary of the unit cell then, to enforce periodicity of the model, that piece of microstructure must be duplicated so that it enters the unit cell from the opposite side. This duplication must be done for each boundary of the unit cell that the piece of microstructure intersects. The union of the original piece of microstructure and all of its periodic duplicates is called its "periodic extension". It is this periodic extension that must be checked for interference with existing microstructure and, if there is no interference, unioned with the model. This procedure works well as long as the volume fraction of the reinforcement is not too high. When the volume fraction of the reinforcement is too high (the volume of which depends on the shape of reinforcement, but is typically 30–40%) it becomes difficult to insert the needed amount of reinforcement into the model due to interference with previous inserted reinforcements.

### 5.2.2

#### Microscale model

The microscale model fully represents the geometry of the microstructure of the composite. It is only created for regions of the macro-model that are a small distance (on the order of several unit cells) from the crack front. The first step in creating the microscale model is to determine its domain. The basic idea to determine this is to follow the crack front through a three dimensional regular grid where each cell in the grid represents the boundary of a unit cell. Each grid cell that the front intersects must be included in the microscale model. In addition several layers of unit cells around those that the front passes through need to be modeled to ensure the accuracy of the analysis process. This procedure is described in more detail below and is illustrated for a simple 2-D problem in Fig. 6:

1. Define a regular grid over the macroscale model where each cell in the grid is one unit cell in size (Fig. 6b). This grid must be defined so that when the unit cells are inserted in the grid locations the correct microstructure is created. Thus, it is necessary for the grid to be aligned with the fiber direction for composites with continuous aligned fibers. The grid is only defined not actually created in the geometric modeler.
2. Determine which grid cells the curve that defines the crack front passes through, this is the minimal domain for the micro-model. This is illustrated by the grey filled cell in Fig. 6c. In the 2-D example shown, the crack front is simply the two ends of the crack, however for a 3-D problem the front is a closed curve.

For the 3-D problem determining the grid cells that the crack passes through is done as follows: Pick a point on the curve 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

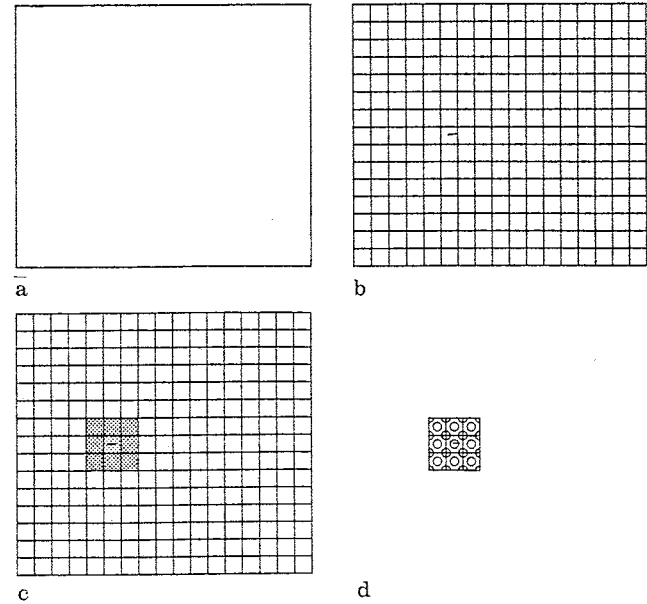


Fig. 6a-d. Defining the domain of the micro model

passes through as it exits the cell by intersecting the curve with the planes defined by each cell face. 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 have been traversed.

3. Extend this minimal model by adding  $n$  layers of cells surrounding the minimal cells to the model (Fig. 6c shows one layer of these cells added, shaded dark grey). This defines the domain of the micro-model.

Once the domain of the micro-model has been determined the actual model can be constructed. The construction is done by duplicating the model for a single unit cell and translating and rotating it so that it aligns with the grid. This is done for each cell in the grid that has been determined to be needed in the micro model. The boundaries of adjacent unit cells 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.

The results of this process in 3-D are shown in Figs. 7 and 8. The 3-D problem being modeled is a flat plate with a delamination as shown in Fig. 7a. Also shown near the middle of the plate is the delamination crack. The simple unit cell for an aligned fiber microstructure, as shown in Fig. 7b, is being used. The microscale model of the area around the delamination is shown in Fig. 8. This model includes the explicit representation of both the microstructure and the crack.

The mesh that is created for the micro-model has the restriction that, for the exterior faces of the model, the mesh must be identical to that which is on the boundary of the unit cell that was used to calculate the homogenized material properties. This requirement on the boundary mesh is imposed by the analysis. The mesh on the interior of the model has no restrictions. To create the mesh for this model the faces on

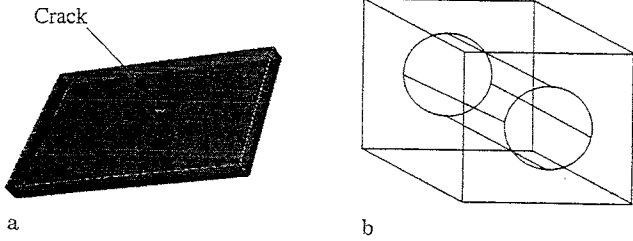
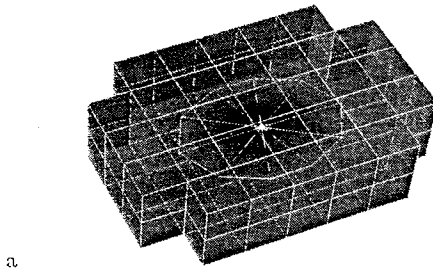


Fig. 7a, b. Macro-model and unit cell



a

b

Fig. 9a, b. Boundary of micro-model

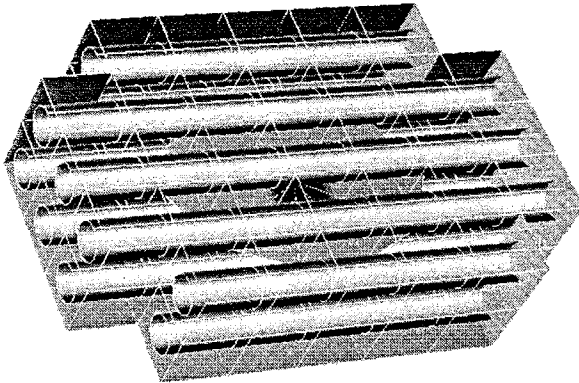


Fig. 8. Microscale model of delamination crack

the boundary of the model are first meshed using the mesh from the boundary of the unit cell. Then the other (interior) faces of the model are meshed using the Finite Octree mesh generator (Shephard and Georges). Finally the interior of the model is meshed using an element removal procedure that works from the given boundary mesh.

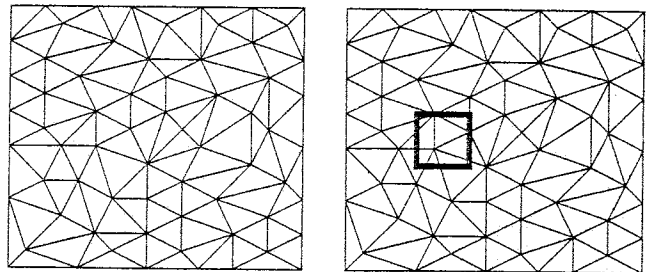
**5.2.3**

**Transition model**

The transition model is defined to tie the microscale model to the mesh of the macroscale model. To create the transition model, the outer boundary of the unit cells in the micro-model must be found. This is done in the same manner as the creation of the micro-model, except a cuboid of the size of the boundary of the unit cell is used instead of the model of the unit cell. The result of this procedure on the 3-D model is shown in Fig. 9a, note that all of the internal structure of the model, as compared to Fig. 8, has been eliminated, except for the crack.

The outer boundary of the transition model is the boundary of the union of all elements in the mesh of the macro-model that the micro-model is interior or close to. The procedure for finding these elements is as follows (illustrated for the 2-D case in Fig. 10.)

Given the domain of the micro-model as found above and the macro-mesh as illustrated in Figs. 10a, b, first find the elements which have a non-null intersection with the micro-model domain. In addition any elements which are considered very close to the micro-model domain is added to those that intersect it. The definition of 'close' in this case depends on the relative size of the elements in the macro-mesh



a

b

c

d

Fig. 10a-d. Construction of the transition model

to the size of the unit cells. The goal is to ensure that the transition mesh is a smooth change in element sizes from those in the macro-mesh to those in the micro-mesh. Once the elements of interest have been found, a model is constructed that is the boundary of the union of all of these elements and the inner structure of the transition model (the outer boundary of the micro-model) is inserted.

This same process carried out on the 3-D models shown previously results in the geometry shown in Fig. 11.

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. co-planar faces on the boundary are not unioned to make

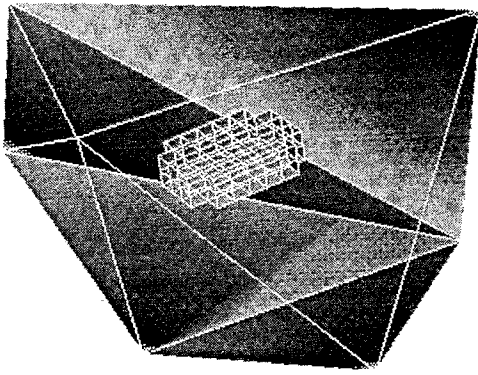


Fig. 11. Transition model

a single face, the edges that define the original faces are retained).

### 5.3

#### Model updates

One of the results of the analysis is the direction and distance that the crack front moves at each step. For the next analysis step to take place the models and meshes must be updated to reflect this growth of the crack. The steps in the model update are as follows:

1. Update crack representation in micro model to reflect the growth of the crack (Fig. 12a)
2. If the crack front exits a unit cell, the micro and transition models are updated as follows:
  - a. Update the micro model domain (add unit cells ahead of crack and remove them behind (Fig. 12b)) to ensure that the micromodel exists for the desired distance ahead of the crack front.
  - b. Update the transition model, including adding the domain of more elements from the macro mesh if micro model grows into them as shown in Figs. 12c, d.

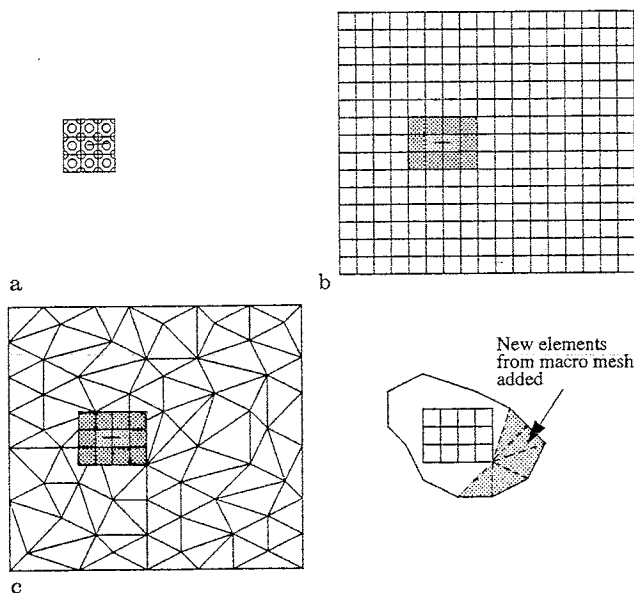


Fig. 12a-d. Micro and transition model updates

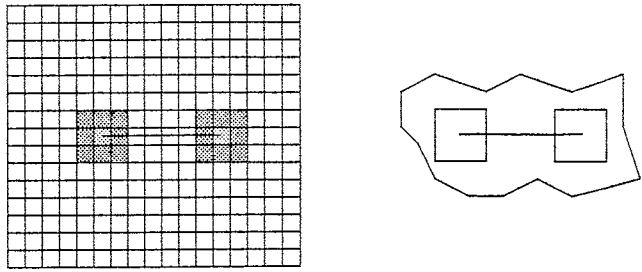


Fig. 13. Further update of micro and transition models

One goal is to keep the updates as local as possible to minimize the amount of geometric manipulation that must be done and to minimize the amount of the model that must be remeshed at each step. This step in the 3-D example is shown in Fig. 9 which shows the inner boundary of the transition model after the update.

As the crack grows there will be a portion of the crack that is far enough away from the front to not need to be modeled at the micro-scale as shown in Fig. 13. In this case all of the geometry of the crack must still be contained interior to the transition model. For these analyses this is done by only adding macro-mesh elements to 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.

In 3-D the elimination of the unnecessary areas behind the crack front from the micro-model keeps the problem size reasonable as the crack front grows. Without this the problem size would quickly grow to be much too large to solve. Figure 9b shows the 3-D example after the crack has grown.

Meshing the update models needs to be done as locally as possible. If the only change is that the crack has grown a small amount (i.e. no new unit cells have been added to the micro-model) the mesh is only updated locally around the crack front. 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.

### 6

#### Closing remarks

The successful application of advanced multiple scale procedures requires the ability to effectively develop the required analysis models. This paper has presented a framework and associated procedures for the automatic construction of models and meshes as required for multiple scale analyses. Specific sets of model construction procedures have been demonstrated for two multiple scale analysis procedures which employ different modeling and analysis procedures. Key ingredients in these example applications include the geometric modeler, automatic mesh generator, attribute manager, and the model building and discretization strategies used to ensure the correct idealized analysis models are constructed and discretized.

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