MECHANISM-BASED DESIGN OF COMPOSITE STRUCTURES

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ABSTRACT

The paper introduces high temperature composite software developed for mechanism-based design of composite structures. Mechanism-based design is characterized by an understanding of the critical composite behaviors at several physical scales: the fibrous (micro) scale, the ply/weave (meso) scale and the laminated part (macro) scale, and by the specification of the available design parameters to achieve functionality by those behaviors. A software framework is described which integrates material modeling and analysis codes, provides automated assistance, and links to material databases. Elastic and inelastic material modeling codes suitable for high temperature composites with complex reinforcement and weave/lay-up configurations are presented and references to their underlying theories are given. Advanced analysis techniques are outlined for numerically efficient computational plasticity based on mathematical homogenization, idealization error indicators for material scale, three dimensional crack propagation in a fibrous composite, and modeling of reactive vapor infiltration and chemical vapor deposition processes.

INTRODUCTION

Current research has been directed towards developing models of high temperature composite thermomechanical behaviors and the processes associated with their fabrication and degradation. The composite systems of interest include both metal matrix composites (MMC's) and ceramic matrix composites (CMC's), with Al_2O_3, SiC and W based reinforcements, and Al_2O_3, $MoSi_2$, NiAl, SiC, and Ti based matrices. The approach used has been motivated by current fabrication technology, which allows the material's structure to be configured for an application, and by the complexity of phenomena governing the material's behavior during fabrication and during subsequent loading cycles.

The mechanism-based approach involves modeling composite behaviors at several physical scales: e.g. the fibrous (micro), the ply/weave (meso) and the laminated part (macro) scales, and by linking the behaviors at each scale. The techniques developed can be applied to design analysis by the formulation of the appropriate idealized models at the relevant scales and the integration of those models while controlling idealization errors through multi-scale, adaptive or heuristic means. An important result of the project has been the implementation of mechanism based modeling techniques as computer codes.

The new capability can support the understanding of the relationships between a material system's meso/micro structural design parameters and its large scale functionality. For example, design changes in the reinforcement's shape and orientation can be related to the overall composite properties and hence to a part's deflection under load. In the reverse change-of-scale, a macro scale cooling hole configuration under a particular thermal-mechanical loading can be linked to the type and proximity to fiber-coating-matrix debonding. Mechanism-based models allow both alternative material and component designs to be evaluated more quickly without the expense of testing all macro scale configuration/environment permutations, and can even aid the design and sizing of test fixtures for those tests which are still needed.

The rest of the paper outlines the supporting software system, the material modeling and some of the analysis techniques required to support the design of high temperature composites structures. The system overview describes the capabilities developed, the assistance provided application of the codes by non-experts, and the material property management issues. The material modeling section briefly describes the capabilities and models developed. The analysis section describes results for computational plasticity, error control for laminates, advanced multi-scale analysis techniques needed for the coupled behaviors exhibited by HTC structures, and process modeling.

SYSTEM OVERVIEW

A set of software framework tools has been developed (Beall et al., 1994) to integrate and facilitate application of the material modeling and analysis codes to design problems. The framework accommodates a spectrum of solution cost and reliability alternatives, in order to support the different design process stages, and provides application expertise and visualization tools. The system applies existing commercial packages where possible. The framework tools integrate the material modeling and analysis techniques. Both of these codes groups can still be operated separately or combined and linked with other user codes.

The software interacts with a database housed s in the Mvision™* format and conforms to, or can be translated into ASTM and applicable PDES/STEP standards (PDA, 1993). The high temperature database contains more than 320 material systems or constituents, 18,000 values, and 180 material characteristics. Geometric modeling tools, built on the kernel of commercial geometric modelers, create micro-structures, weaves, plies and component scale models and source their data from a spreadsheet. The spreadsheet format allows users to arrange and annotate data to suit their needs, tie together design parameters for automatic updates, and to implement "back of the envelop" computations.

An analysis attribute code links material, boundary condition and other attributes with the corresponding geometric entities, for instance, associating a debond strength with a fiber/coating interface and a chemical concentration distribution with a matrix region of a model. In addition, finite element results on a mesh are mappable to the mesh of another analysis by means of their common geometric entity. Representative volumes containing the most important geometric entities are readily constructed from a library of constituents, typical flaws, etc., and these entities can be related to behavioral properties via associated attributes. Automatic meshing tools, generic mesh operations and data structures, and the interfaces to multiple finite element analysis codes complete the integration of automated modeling tools for FEA (Beall et al., 1993).

User application and assistance

Expertise in several areas, including material and process modeling, analysis techniques and detailed software operation need to be applied simultaneously for reliable HTC analysis. High temperature composite material technology is evolving rapidly, requiring flexible application of mechanism based design tools rather than execution of prescriptive or handbook design procedures. This means that the software must support a process of i) definition of the required functionality, e.g. control heat flow in a given direction, resist a set of loading conditions within prescribed deflections, self-heal when damaged, etc. ii) development of the material behaviors and geometric features to support those functions, and iii) specification of the type of analysis results, cost (time) and reliability needed to confirm the governing behaviors or define unknown design parameters. The resulting description of the design and the analysis characteristics constitutes an "analysis goal", and is the starting point for automatically selecting and assembling material modeling and analysis codes to achieve it. The goal description is converted into

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* M/VISION is a registered trademark of MSC/PDA Engineering.

a plan, represented in part by a data flow model, and the plan is refined into a sequence of code executions. The result is a "strategy", the execution of which provides the desired results to the user.

The approach requires translation of concepts and nomenclature for the user and the management of information on code capabilities and operation. Code capabilities may be controlled by the underlying theory or the current implementation of the theory and are modeled in terms of their required/optional inputs and outputs, restrictions on values, cost, reliability, and a classification of the behavioral assumptions used. These code attributes determine its "applicability" for strategy creation and require hierarchal and relational data structures. The information can be used to translates between the concepts and nomenclature of the mechanism based designer and the appropriate composite theory, and to automatically assemble strategies based on compatible data flow and underlying modeling assumptions. The implementation of the approach requires the framework tools described earlier to facilitate material modeling and analysis, and a standardized exchange of data between codes developed from multiple sources.

A data flow schematic of a basic composite property strategy is diagramed in Figure 1. The arcs indicate the type of information shared by the boxed computational functions. The goal is to estimate linear elastic laminate properties in seconds from given constituent properties, micro-structural and ply lay-up. The method used can depend on the shape of the reinforcement, and this aspect of the applicability would need to be refined based on the user input before any code would be executed.

From the user's perspective, the execution of the analysis goal is no more involved than using any other spreadsheet function, requiring no expertise or involvement in software development. The current design parameters are recovered from the spreadsheet, and transferred to the goal processor. If data is missing or out of the applicability range of available strategies, then the user is informed of the specific problem, otherwise the results are automatically computed and returned to the spreadsheet, used as input for other analysis (as shown), or displayed by visualization code, e.g. such as the plots of Figure 2 and 3.

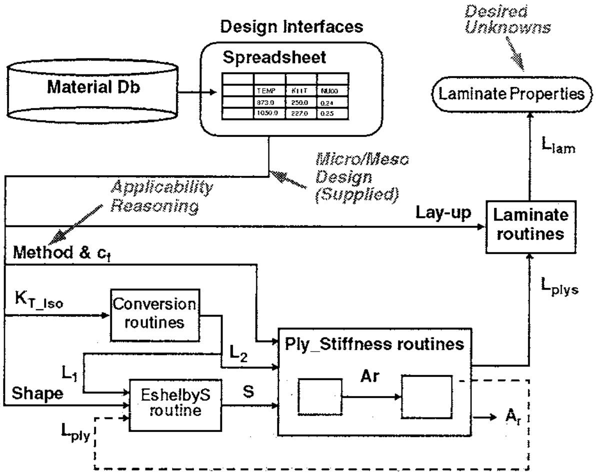


Figure 1: Data Flow for Laminate Properties

Material Property Management

Several database related features are available which either directly support the conceptual design process in material selection, or support analysis strategies. Material data requires the structuring of data so as to define not only the value to be used in an analysis, but also the scale, specimen characteristics, source of data and the environmental parameters of the test - the "pedigree". Reliable analysis requires that the pedigree be consistent with the underlying analysis models, so the extraction of relevant data is related to the creation of strategies from modeling codes. For example, the modulus of a SiC/SiC CMC will not only vary with temperature, but also with time depending on the degree of micro mechanical damage before the measurement and the presence of water and oxygen. The material database is not only a source of material parameters, but also a source of known behaviors caused by the environment. Translation between the standard procedures and nomenclature of the testing community and the material parameter needs of analysis and design functions is also required in order to obtain meaningful data.

Sources include published papers, industry data sheets, handbooks, and test data generated at Rensselaer. Constituent properties (matrix and reinforcements), data for dog-bone and tubular test specimens, and durability of tested parts in oxidizing and corrosive environments are stored. Manufacturing size, porosity or volume fraction limitation data are available where supplied by vendors, and background documentation and SEM images of material systems are also accessible. The database facilities can be configured for automated search and merit indicy plotting (Ashby, 1992).

MATERIAL MODELING

Software tools described here include linear elastic property estimation codes, initial failure maps of the constituents and their interfaces, and mathematical homogenization of unit cells with complex geometries. Their capabilities are presented and some example results are shown.

Linear Elastic Properties and Limits

Routines are available to predict overall material properties for linear elastic analysis in terms of constituent thermo-elastic properties, volume fractions, and micro-structural geometry. Those related to ply properties are the Hashin-Strikman Bounds (Hashin and Rosen, 1964) for the overall elastic moduli of two-phase composites, the Mori-Tanaka (Mori and Tanaka, 1973) and the self-consistent methods (Teply and Dvorak, 1988), providing estimates for several reinforcement shapes in either aligned or random configurations. Figure 2 compares the methods for the overall transverse modulus of a fibrous ply as a function of volume fraction and Figure 3 visualizes trends in overall elastic axial shear properties as a function of volume fraction and temperature. Additional codes evaluate linear coefficients of thermal expansion (CTE) of two-phase or multi-phase composite materials in terms of overall and phase elastic moduli, phase CTE's and volume fractions.

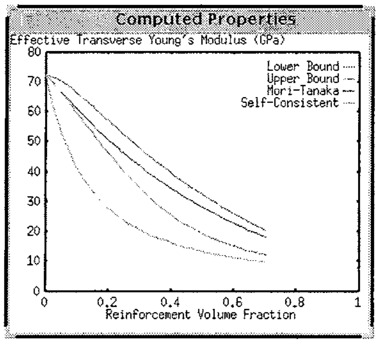


Figure 2: Method Comparison

Other codes evaluate mechanical, thermal, and transformation concentration factors, which are useful for estimating phase stress and/or strain averages in two-phase and multi-phase composites subjected to uniform overall stress or strain, a uniform change in temperature, and uniform eigenstrains in the phases (Dvorak and Benveniste, 1992). If properties for a constituent are not available from tests, they can be computed "in-situ" by the Mori-Tanaka or self-consistent methods from known overall moduli, phase volume fraction, and the known properties of the other constituent. Figure 4 shows the results of a strategy to study the effects of variations in reinforcement aspect ratio and volume fraction on the effective axial shear modulus of a single ply. The designer can easily see the effects of changes in both application temperature and volume fraction.

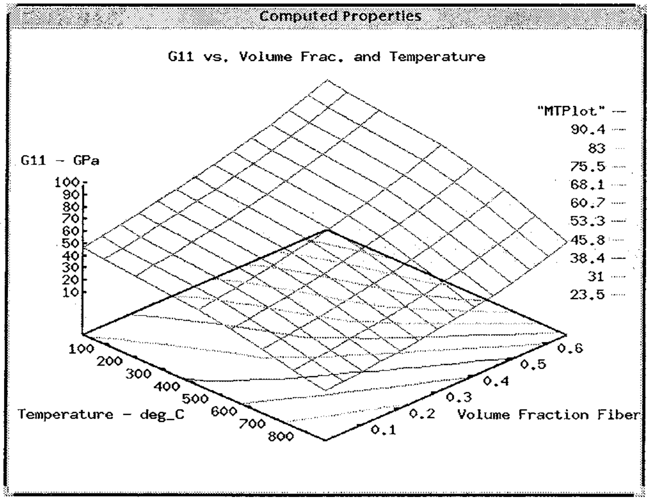


Figure 3: Ply Property Trends

At the next larger scale, the plane stress stiffness, the compliance of asymmetric laminated plates under uniform in-plane loads, and the transversely isotropic coefficients of thermal expansion of a symmetric laminated plate under a uniform temperature can be estimated. Codes evaluate the mechanical, thermal, and transformation distribution factors, leading to average stresses in plies of a symmetric laminated plate under uniform in-plane loads, temperature change, and ply eigenstrains. Other supporting routines evaluate the Eshelby tensor for transformed homogeneous inclusions of an ellipsoidal shape in an anisotropic solid, compute the P-tensor for an ellipsoidal inclusion in an anisotropic solid, perform numerical operations with tensors or mathematical expressions, and convert between elastic constants, stiffness and compliance matrix forms.

Initial brittle and plastic material failure of fibrous composites due to thermal-mechanical loading can also be predicted by the software. Debonding at the interfaces between the fiber, coating and matrix, and fracture of the fiber, coating or matrix materials are predicted for symmetric laminated plate configurations. The software implements the theory found in (Dvorak, 1992), (Dvorak and Benviniste, 1992), (Dvorak et al., 1992), by mapping macro scale FEA temperatures and stress distributions onto the micro-mechanical failure map model. The model accounts for residual stress effects due to a difference between a stress free state, e.g. the processing temperature, and operating temperature. The models uses the linear elastic constituent properties, composite configuration and known allowable stresses in or between phases: fibers, coatings, or matrix.

Figure 5 (left) shows the application of the failure surface codes to the inside "hot" layer of a thermally loaded ceramic combustor geometry with cooling and other hardware holes. Elements are shaded based on their proximity to the given debond strength limit, indicating potential problem areas on the part. Similar distributions are available for other material failure modes. An animated stepping "through the thickness" helps visualize interior-exterior trends. Figure 5 (right) applies the model in an alternative format, plotting the required matrix cracking strength for each element in the combustor above as a function of temperature. Other codes are available to predict the onset of material plasticity (Dvorak and Bahei-El-Din, 1987).

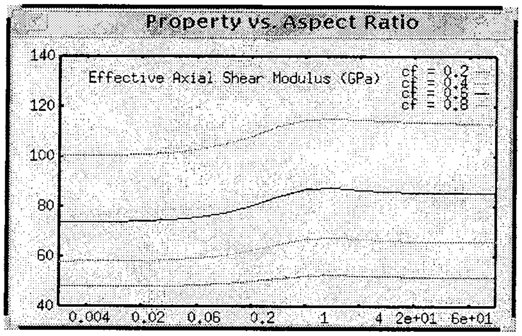
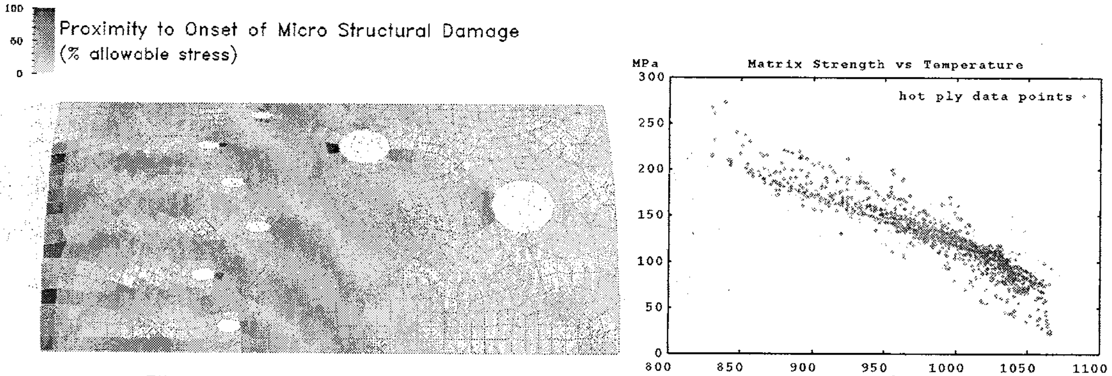


Figure 4: Aspect Ratio Variations



Fiber—matrix debonding — Level 1

Figure 5: Failure Map Applications

Unit Cells

The classical mathematical homogenization theory for heterogeneous medium has been generalized (Fish et al., 1996a) to account for eigenstrains. The resulting method first defines a three dimensional geometric model of a unit cell, assigns constituent material properties, automatically meshes the geometry, and then analyzes the model for homogenized properties. The software framework provides facilities to automatically create the unit cell geometric models from size parameters of the constituent features. Though it is computationally more expensive than other methods, it is useful for geometrically complex microstructures where a representative geometry can be defined. Unit cell modeling has been used in the multi-scale computational technique and for non-linear analysis with a plasticity model (Shephard et al., 1995). Given an appropriate representative geometry, it can also predict linear elastic properties for woven composites for use directly with conventional macro-scale analysis tools and can be readily adapted for thermal conductivity and chemical diffusion problems. Unit cells for oriented fibers, periodic "random" fibers, periodic "random" particles, and plain weave fabrics are available, see Figure 6 below. Unit cells for other woven fabrics, defects and more complex three dimensional fiber architectures are under development.

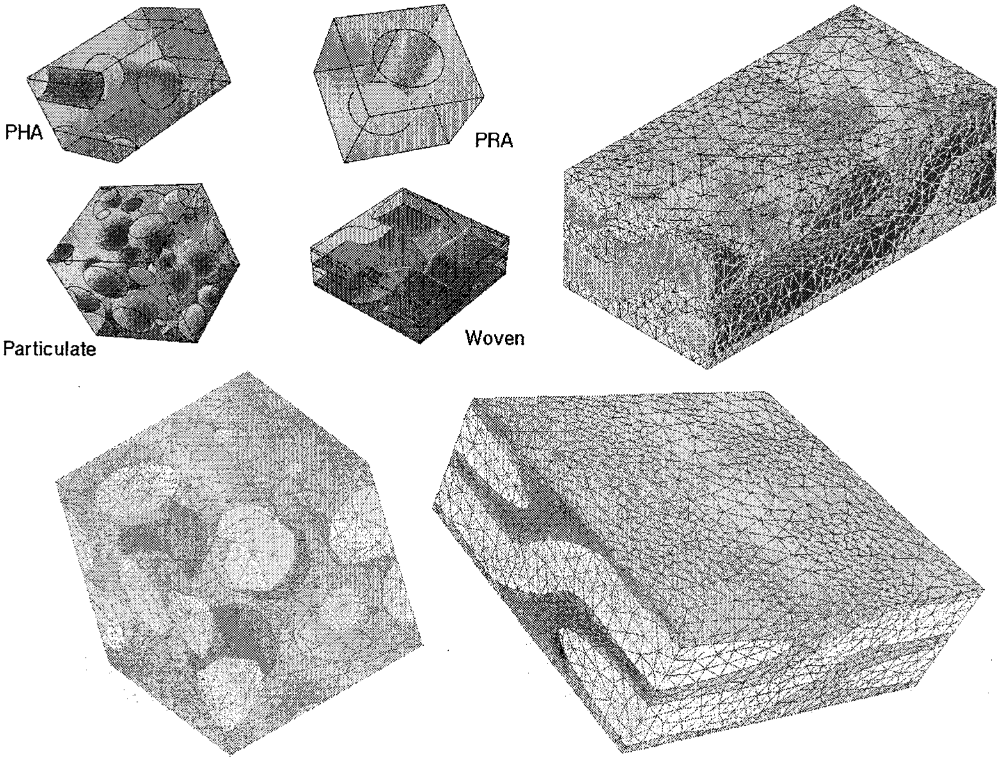
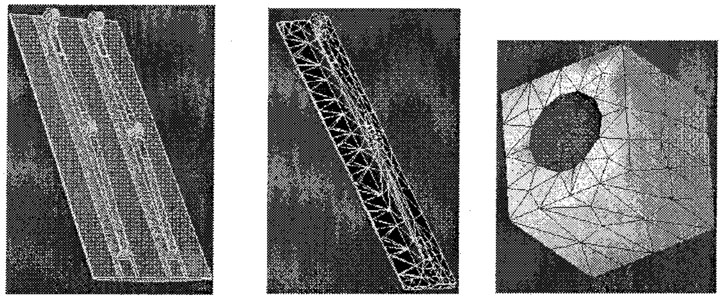


Figure 6: Unit Cell Geometry and Mesh Examples

ANALYSIS OF COMPOSITE STRUCTURES

Computational Plasticity for Composite Structures Based on Mathematical Homogenization



Exhaust Nozzle Flap FE Mesh Unit Cell Mesh

Figure 7: Engine Flap Example

The computational challenge of solving nonlinear heterogeneous systems is enormous. While for linear problems a unit cell or a representative volume problem has to be solved only once, for nonlinear history dependent systems it has to be solved at every increment and for each integration point. Moreover, history data has to be updated at a number of integration points equal to the product of integration points at all modeling scales considered. To illustrate the computational complexity involved we consider elasto-plastic analysis of the two-scale composite flap problem shown in Figure 7. The macrostructure is discretized with 788 tetrahedral elements (993 unknowns), whereas the microstructure is discretized with 98 elements for the fibers and 253 elements for the matrix. The CPU time on a SPARC 10/51™ for this problem was 8 hours, as opposed to 10 seconds if metal plasticity was used instead, which means that 99.7% of CPU time is spent on constitutive evaluation in the unit cells.

The application of a novel modeling scheme based on mathematical homogenization theory with eigenstrains (Fish et al., 1996a) and transformation field analysis (Dvorak, 1992) enables the solution of these large scale structural systems in heterogeneous media at a cost comparable to problems in homogeneous media without significantly compromising on solution accuracy. The approach represents a breakthrough compared to, existing modeling schemes which are either too inaccurate to provide reliable solutions for difficult problems, or too expensive due to the computational complexity involved.

The heart of this new technique is the generalization of the classical mathematical homogenization theory for heterogeneous medium to account for eigenstrains (Fish et al., 1996a). Starting from the double scale asymptotic expansion for displacements and eigenstrains we derive a close form expression relating arbitrary eigenstrains to the mechanical fields in the phases. Subsequently, the overall structural response is computed using an averaging scheme by which phase concentration factors are computed in the average sense for each phase, i.e. history data is updated only at two/three points (fiber and matrix/ interphase) in the microstructure, one for each phase. Macroscopic history data is stored in the data base and then subjected in the post-processing stage onto the unit cell in the critical location identified by microscale reduction error indicators.

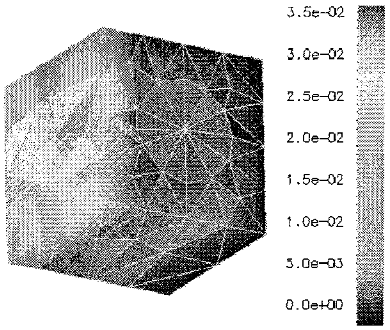


Figure 8: Unit Cell Relative Error

For the flap problem considered in Figure 7 the CPU time for the averaging scheme with variational micro-history recovery is only 30 seconds on SPARC 10/51™ as opposed to 8 hours using classical mathematical homogenization theory. Figure 8 shows that the maximum error in the micro-stress in the unit cell located in the critical region is only 3% in comparison to the classic homogenization theory.

Idealization Error Estimators

Idealization error estimators for laminated composite shell structures developed in Fish et al. (1994a), Fish et al., (1994b) are aimed to quantify three sources of errors and to address the following issues:

i. What are the regions within the problem domain where the macromechanical description (shell model), which is the most inexpensive modeling capability, is insufficient, i.e., where the shell model introduces unacceptable errors with respect to a more comprehensive ply-by-ply (mesomechanical) model. Idealization error estimators should be able to identify not only the precise location within the plane of the shell, but also the layers within the laminate where the use of mesomechanical description may result in unacceptable errors of interlaminar stresses.

The Dimensional Reduction Error estimator (DRE) developed in Fish et al. (1994a) builds on a combination of mechanistic insight and a rigorous mathematical approach. By this technique the dimensional reduction error is approximated by a linear combination of some basis functions in the auxiliary mesomechanical finite element mesh that accurately represent the kinematics of individual plies (Fish et al., 1994a).

ii. Enriching the fundamental kinematics of the equivalent single-layer (macro) model with a discrete-layer (meso) model in the vicinity of the most critical layers enables to model various failure modes on the lamina level such as delamination. Unfortunately, in many cases the mechanism that causes failure is at a smaller scale - the scale of microconstituents. A common computational rationale today is to investigate various microprocesses that may lead to a progressive failure by considering a unit cell or a representative volume problem. The mechanisms that allow us to do so are the classical assumptions of periodicity and uniformity of macroscopic fields. However, in the areas of high stress concentration, which are of critical interest to the analyst, periodicity assumptions are not valid, and thus the application of conventional homogenization techniques in the "hot spots" may lead to poor predictions of local fields.

The adequacy (or lack of it) of the homogenization theory has been studied in Fish et al. (1994b) on the basis of assessing the uniform validity of the double scale asymptotic expansion, which serves as a basis of mathematical homogenization theory. The quality of the homogenization has been assessed on the basis of the relative magnitude of the first term neglected by the classic homogenization theory to those taken into account.

A closed form expression for an idealization error estimator associated with the microscale reduction has been derived in Fish et al. (1994b). The Microscale Reduction Error (MRE) estimator relates the homogenization (or scale reduction) error to macroscopic fields (strain and strain gradients) and to the details of microstructure (compliances of phases, volume fraction and the size of the unit cell). It has been found that there are four factors affecting the homogenization error: (i) the size of the unit cell in the physical domain Y, (ii) the mismatch parameter, (iii) the volume fraction, (iv) the strain gradients on the macro-scale.

Besides the discretization error indicators there are other sources of idealization errors, such as microstructure randomness, material and geometric nonlinearities, which so far have not been considered.

Fast adaptive Iterative Solvers for a Heterogeneous Medium

The multigrid technology with special inter-scale connection operators has been developed in Fish and Belsky (1995a), Fish and Belsky (1995b), Fish et al. (1996a). The multigrid procedure starts by performing several smoothing iterations on the micro-scale in the regions identified by MRE indicators. Consequently, the higher frequency modes of error are damped out immediately. The remaining part of the solution error is smooth, and hence, can be effectively eliminated on the auxiliary coarse mesh. It has been shown (Fish and Belsky, 1995a), (Fish and Belsky, 1995b), (Fish et al., 1996a) that the finite element mesh on the meso-scale (ply level) serves as a perfect mechanism for capturing the lower frequency response on the micro-scale. Therefore, the residual in the finite element mesh on the micro-scale is restricted to the meso-scale, while the smooth part of the solution is captured in the finite element mesh on the meso-scale. The oscillatory part of the solution on the meso-scale is again damped out by a smoothing procedure. The lower frequency response on the meso-scale is resolved on the macro-mesh (shell level). The resulting solution on the meso-scale is obtained by prolongating displacements from the macro-mesh back to the finite element mesh on the meso-scale and by adding the oscillatory part of the solution previously captured on the meso-scale. Likewise, the solution on the micro-scale is obtained by prolongating the smooth part of the solution from the meso-scale and by adding the oscillatory part that has been obtained by smoothing. This process is repeated until satisfactory accuracy is obtained.

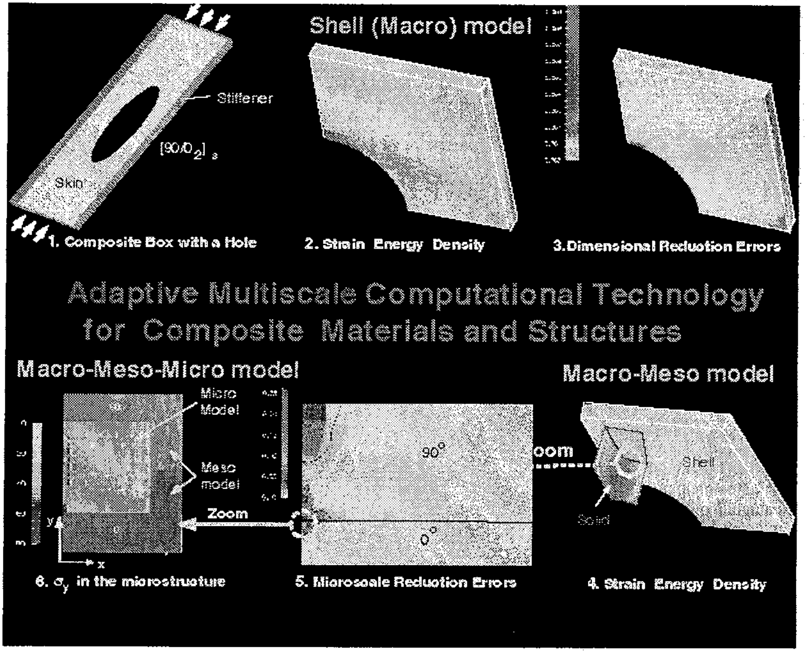


Figure 9: Multi-scale Example

The adaptive strategy, illustrated by example in Figure 9, starts by employing Discretization Error indicators and adaptively refining the finite element mesh on the macromechanical (shell) level to ensure accurate Macro-solutions. Subsequently, Dimensional Reduction Error (Fish et al., 1994a) indicators 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), (Fish and Belsky, 1995b), (Fish et al., 1996a) 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 (Fish et al., 1994b) indicators 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), (Fish and Belsky, 1995b), (Fish et al., 1996a). Finally, 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 9 contains over 1,000,000 degrees-of-freedom. The estimated CPU time for solving it with conventional solvers based on skyline storage is over 700 hours on a single processor SPARCstation 10/51™, which essentially makes the model unusable from the practical point of view. Using a special purpose multigrid technology for heterogeneous media developed in (Fish and Belsky, 1995a), (Fish and Belsky, 1995b), (Fish et al., 1996a) the same problem has been solved in less than 16 hours on a single processor SPARCstation 10/51™, turning it into an overnight job

The derivation of the inter-scale transfer operators is based on the asymptotic solution expansion. The asymptotic forms of the prolongation and restriction operators were obtained by discretizing the corresponding asymptotic expansions. For unit cells of finite size the regularization functions were introduced (Fish and Belsky, 1995b) in order to obtain well-posed inter-scale transfer operators, termed homogenization based operators.

The rate of convergence of the multigrid process has been studied in Fish and Belsky (1995a). It has been proved that if the stiffness of a fiber is significantly higher than that of a matrix, then the multigrid method converges in a single iteration. This behavior of the multigrid method for heterogeneous media together with its linear dependence on the number of degrees-of-freedom, makes it possible to solve large scale coupled global-local problems with the same amount of computational effort, or faster, than would be required to solve the corresponding uncoupled problem using direct solvers.

Crack Growth Simulation

In Beall et al. (1996) the crack growth analysis methodology that accounts for the dominant influence factors affecting crack growth on the micromechanical level has been investigated. An automated system has been developed that explicitly represents the microstructure of the composite at the crack front while using homogenized material properties elsewhere. Procedures for automatic construction and update of the models and meshes used in the analysis have been developed in order to avoid any time consuming human intervention. Figure 10 shows the


Macro Scale Specimen

Macro to Micro Scale Transition Mesh

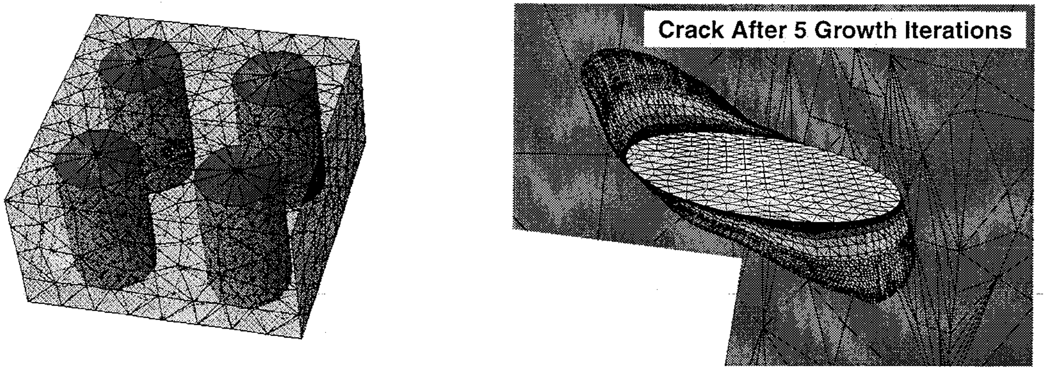

Four Fibrous Unit Cells

Figure 10: Crack Propagation Models

evolution of the micro-crack growth in the turbine blade. It has been found (Beall et al, 1996) that there is a significant difference in the crack growth pattern when accounting for the microstructure. Crack propagation criteria in the microstructure is based on the energy release rates, fracture toughnesses of the microconstituents and their interface (He and Hutchinson, 1989)

Process Modeling

The process modeling codes simulate the time varying production, or degradation, of composite materials. The models include the reaction and transport of chemical species and material flows. Altering process parameters can improve production rates and/or minimize defects. Product designers can estimate processing residual stresses or simulate oxidation/hot corrosion for life prediction. Codes have been applied to the reactive vapor infiltration process for forming $MoSi_2$ from Mo powder, CVD fiber coating with βAl_2O_3, and for oxidation simulations of SiC composites (Adjerid et al., 1995), (Adjerid et al. 1996). Inputs for the general code are the initial geometry and mesh, process attributes per phase, and boundary condition distributions as a function of time. Models input to the code are categorized as chemical reaction models, expansion, mechanical models for solid phases, diffusion models of gaseous phases, and surface models for phase interfaces. Error control parameters are given for the adaptive refinement techniques. Outputs are the time varying volume change, shape, velocity, temperature, concentration and pressure fields.

Figure 11 shows one frame of a result for the βAl_2O_3 coating simulation. The image is a cross section of a tubular reaction chamber, through the center of which moves the fiber to be coated (left). Reactants, concentrations of which can be shown in color, are injected at the bottom of this design, and the flow field of the gaseous phase is indicated by the vectors. The code is currently used to both optimize and control the actual production hardware. Results can be animated to show the dynamic behaviors resulting from the initial design geometry and boundary conditions.

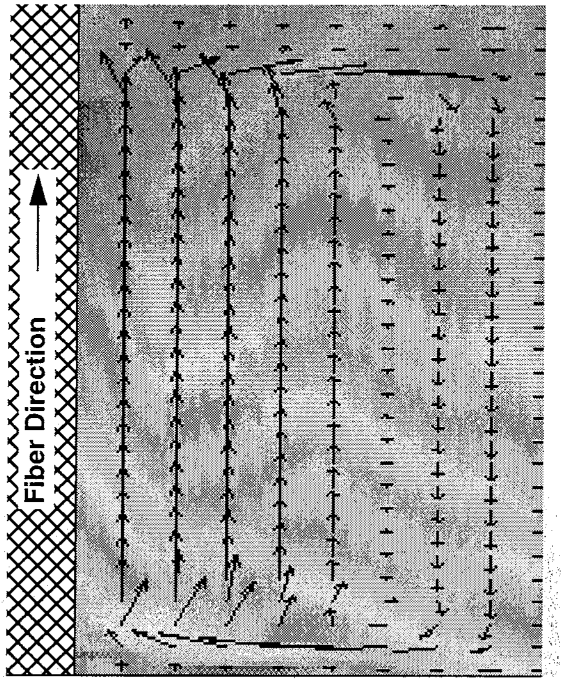


Figure 11: Fiber Coating Simulation

CONCLUSION

Success with high temperature composites has required progressively more complex micro-structures and behavioral understanding. Design requires support by mechanism based analytical tools to take full advantage of HTC properties and to avoid material failures. The models and tools developed, integrated with their supporting framework, are capable of simulating key composite behaviors and processes at multiple scales

ACKNOWLEDGMENT

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