SOFTWARE FRAMEWORK FOR MECHANISM-BASED DESIGN OF COMPOSITE STRUCTURES

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ABSTRACT

A software framework supporting mechanism-based design of high temperature composite structures is described. The framework extends material property databases by allowing the investigation and simulation of small scale behaviors which cause full scale effects. The framework integrates a full range of modeling processes, including automated model generation tools, numerically efficient analysis codes, post-processing and visualization, so as to minimize the effort required to develop mechanism-based models for new behaviors and materials.

INTRODUCTION

The need for advanced software capabilities are 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. Current research has developed mechanism-based models of thermomechanical behaviors for high temperature composites and the associated fabrication and degradation processes. From the standpoint of design, the new capability provides insight of the relationships between a material system's meso/micro structural design parameters and its overall behaviors.

The mechanism-based approach links behaviors at three physical scales: e.g. the fibrous (micro), the ply/weave (meso) and the part (macro) scales. For example, design changes in the reinforcement's shape and orientation can be translated into overall composite properties and hence to a part's deflection under load. Alternatively, a macro-scale cooling hole configuration under thermal-mechanical loading can be linked to the type and proximity of fiber-coating-matrix debonding. Mechanism-based models allow both current and alternative material and component designs to be evaluated more quickly without the expense of testing all macro scale configuration/ environment permutations, and can also aid the design and sizing of test fixtures for those tests which are required.

The balance of the paper outlines some unique features of the software system, and is organized by the functional role of the framework tools in the overall modeling process [1]. The aim is to present a range of software tools which can be assembled to support specific design problems. Specific application examples are referenced where needed. Covered are the engineering modeling tools for geometry, material test data management, applications for modeling material behavior on multiple scales, tools for creating and manipulating numerical models, fast and efficient analysis codes required for large linear or non-linear problems, post-processing and visualization, and techniques by which the framework integrates the composite analysis tools.

GEOMETRY AND ATTRIBUTE DEFINITION

The framework provides tools for the definition of engineering design geometry and the engineering attributes to be associated with engineering features on the model. Tools are provided which can construct standard geometric features from given design parameters, and assemble these into non-manifold geometric models. Example features on a small scale are cross sections of bundles, bundle paths, repetitive woven patterns, such as satin or plain weaves, standard reinforcement shapes such as fibers, cracked matrix layers and voids left as a result of vapor deposition type operations. Figure 1 illustrates the process where a) the cross-sectional shape and path parameters are defined to create a bundle, b) the bundle interlacing is defined by a schematic to form a weave, and c) the bundles and matrix are assembled into a unit cell for subsequent meshing and analysis. Not all geometry must come from parameters: micro-graphs can be scanned to define bundle paths. The geometric modeling is performed in stages, where the features to be combined are selected, defined in terms of their size and position parameters, translated into a sequence of basic construction operations, and the operations are executed in terms of their equivalent commercial geometric modeling function calls. Features can be tagged for later identification of their topological entities after construction operations have been executed. Features can also be linked across multiple models, allowing a 1D idealization of a weave (its path) to be associated with the appropriate region in a solid model of a unit cell. Visualization tools are available to display 3D models in real time as both shaded and semi-transparent images. The same facilities have been used to create and modify macro scale models. Special tools are also available for matching topological entities for complex unit cells.

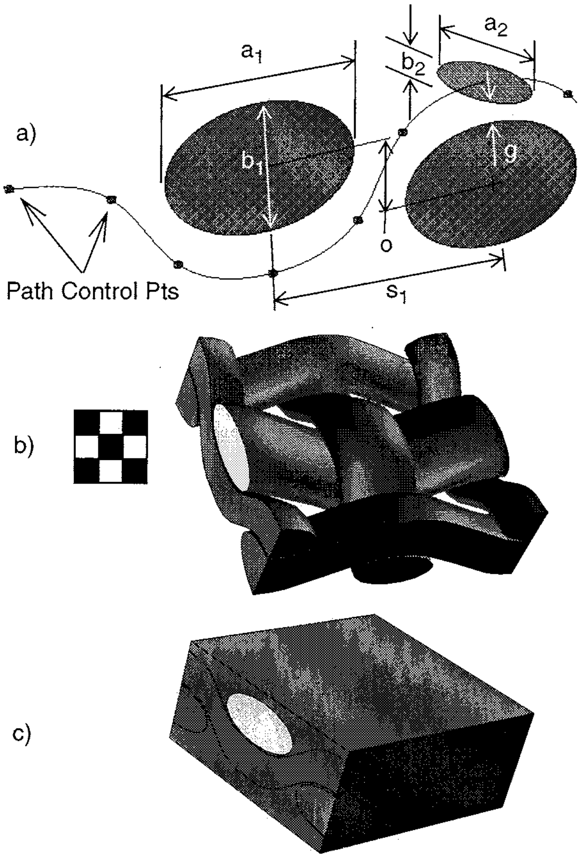


Figure 1: Parametric geometry definition

Attributes such as the constituent materials, periodic boundary conditions or prescribed displacements are defined with respect to the features and properties translated into analysis attributes. The SCOREC analysis attribute manager (SAM) manages the attribute information by defining distribution of its tensorial components, links to topological model entities, and how it fits into an organizational hierarchy. Example of a tensorial distribution is a parabolic loading produced by a pin or bolt normal to the surface of the hole, the state of residual stress in a fiber, or the temperature distribution on the surface of a part. Examples of links with topological entities are the association of an elastic modulus with a solid model region representing a fiber, or the association of an interface strength with the common surface (topological face) between a 3D fiber and matrix.

The task of collecting together all undamaged material properties which are related to the bundles of a weave would be accomplished by the organizational hierarchy.

TEST DATA STORAGE AND PROCESSING

The framework makes use of a material database which uses the commercial MSC M/VISION™ format and which conforms to, or can be translated into ASTM and applicable PDES/STEP standards [2]. The high temperature database developed for the project contains more than 320 material systems or constituents, 18,000 values, and 180 material characteristics. Database 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 managed.

Several database related features are available which either directly support the conceptual design process in material selection, or support analysis strategies. The database application can be configured for automated merit indicy plotting [3], or for retrieval of material systems which have performed in similar environments. Supporting reliable analysis requires data structuring so as to define not only the analysis properties, but also the scale, specimen characteristics, source of data and the environmental parameters of the test - the "pedigree". Reliable analysis requires a pedigree consistent with the underlying analysis models. Translation between the standard procedures and nomenclature of the testing community and the material parameter needs of analysis and design is required in order to obtain meaningful data, e.g. a standard full scale "creep" test may quantify a behavior caused by mechanisms in a CMC which are effected by different conditions from those in metals. The material database is also a source of known behaviors caused by the environment. For example, the modulus of a CMC may vary with both temperature and time, depending on the degree of micro mechanical damage before the measurement, and the presence of water, oxygen and corrosive compounds [4, 5].

The commercial database package also provides a spreadsheet, by which design parameters are edited, organized and annotated, automatically flagged when in need of update, and connected with "back of the envelop" computations. The framework augments the spreadsheet with the means to execute analysis strategies with these design parameters. Additionally, image processing tools were developed to analyze images for composite modeling parameters, such as volume fractions, aspect ratios, spacing and relative positions of constituents.

COMPUTED THERMOMECHANICAL PROPERTIES

Design analyses require material properties not available directly from test data. The framework provides tools to compute missing properties from what is known. The tools are categorized as either for standard geometries and constitutive behaviors, which have fast execution times, or for complex geometries and behaviors, which employ more complex analysis procedures.

For standard geometries, which include plies of parallel fibers, random or aligned whiskers, or particulate reinforcement, tools are available to predict overall elastic and thermal expansion properties in terms of constituent thermo-elastic properties and volume fractions. The codes related to ply properties implement the Hashin-Strikman Bounds [6], the Mori-Tanaka [7] or the self-consistent methods [8]. The resulting properties computed from the methods can be compared graphically or plotted as a function of application temperature or reinforcement volume fraction. If tested properties for a constituent are not available, they can be computed "in-situ" by the Mori-

Tanaka or self-consistent methods if overall properties, phase volume fraction, and the properties of the other constituent are known.

Software tools also compute mechanical, thermal, and transformation concentration factors. These 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 [9]. Such capabilities are used as part of post-processing for thermal-mechanical analysis at larger scales. Additional tools provide the plane stress stiffness, the compliance of asymmetric laminated plates under uniform in-plane loads, and the transversely isotropic coefficients of thermal expansion for symmetric laminated plate structures under a uniform temperature. The mechanical, thermal, and transformation distribution factors are estimated, leading to average stresses in plies of a symmetric laminated plate under uniform in-plane loads, temperature change, and ply eigenstrains. Other routines for standard geometries 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. For non-linear behavior of fibrous MMCs, the periodic hexagonal array and bimodal plasticity models [10] are available as ABAQUS™ routines.

UNIT CELL

With the unit cell approach, the material designer can create custom material configurations with complex features or behaviors at micro or meso scales. This need arises when manufacturing processes or component loading/environments produce material defects or exercise internal mechanisms not represented by the theory underlying the standard configuration codes. The effects of including an additional geometric feature of a constituent or altering the size parameters of a constituent can be studied [11]. The main disadvantages have been the complex modeling process and the computational expenses of a general numerical approach. To overcome these, the software framework provides both automated modeling tools and efficient solvers.

The method requires that a representative geometry of the composite configuration be defined. In the framework this begins by user defined combinations of constituent features such as fibrous shapes, weaving patterns, crack or void patterns. The features are sized with dimensional parameters defined from processed images or as specified by the designer. Constituent material properties are either retrieved test data or computed from analysis on a smaller scale. Properties are assigned to the material regions of the geometric model, and orientation geometry, such as bundle center lines, are automatically created and linked with the solid constituents. Other geometric modeling tools automatically match corresponding geometric entities to ensure model periodicity. Automatic meshing works directly from the geometric model, and the analysis interface tools automatically assign the material properties and periodic boundary conditions. This method of constructing geometric and attribute models before meshing gives the framework considerable representative flexibility. Highly efficient solvers compute both homogenized properties (the equivalent properties of the material at a larger scale) and stress concentration factors for later post-processing. The classical mathematical homogenization theory for heterogeneous medium has been generalized [12] for this application to account for eigenstrains.

Unit cell modeling has been used in the multi-scale computational technique and for non-linear analysis with a plasticity model. Given a 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, e.g. for process modeling. Parameterized unit cells for oriented fibers, periodic "random" fibers, "random" particles, and 2D woven fabrics with cracks and voids have already been developed.

NUMERICAL MODEL DEVELOPMENT

Conversion of the engineering geometry to a finite element mesh is supported by automatic mesh generation, mesh modification and facilities for structuring and storing mesh data. SCOREC developed tools for automatic meshing of either 3D surfaces or volumes can be used [13]. The automatic meshing tools have features which automatically control the numerical solution around critical features or through the thickness of parts where the manufacturing or degradation processes will cause layered variations in behaviors or micro structures. The automatic meshing works for models on all scales, and are used for building periodic meshes of unit cells. Mesh modification tools can be used to remove the effects of undesired small features created unintentionally by geometric modelers, and were used for the crack propagation analysis [14]. Special mesh modification capability was developed which adjusts the volume of a material region. This capability is useful with unit cell models of meso scale weaves or micro scale reinforcements, allowing the volume fraction to be adjusted directly through the mesh. In addition, this provided an efficient means to study the sensitivity of overall properties to changes in volume fractions.

ANALYSIS

The framework automatically constructs the input for analysis packages such as ABAQUS™ or specialized solvers by extracting the mesh data from the generic mesh database and the associated material properties, loads and boundary conditions from the attribute structures. The specialized solvers include an iterative solver with multiple right-hand-sides, which is both time and disk space efficient. The analysis efficiency is very useful for mechanism-based simulations, where complex micro-structures such as weaves and/or non-linear behaviors require large numerical models and/or many solution increments [15]. Efficient solutions for materials with nonlinear history dependent behaviors have been addressed in [12] and [16].

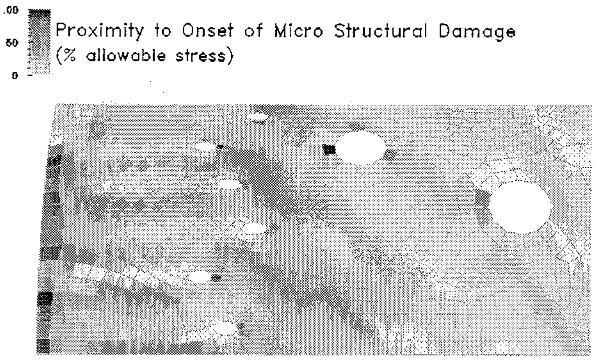
The design and performance of a HTC component is often governed by the mechanical behavior near highly stressed features, such as attachments. The seemingly straight forward approach of explicitly modeling the composite microstructure throughout the component would require computational resources far greater than available or needed. Unit cell or representative volume approaches make the computations feasible but are based upon assumptions of periodicity and uniformity of macroscopic fields, which are often not valid near critical features. To solve these problems, special analysis tools and techniques were developed which automatically locate critical areas and then coordinate and adapt the numerical models on multiple scales, so as to capture failure processes down to the micro scale [17, 18].

The multi-scale technology has also been used to simulate the growth of a crack in a fibrous composite [14], and the dominant factors affecting crack growth on the micromechanical level have been investigated. Automatic tools were developed that explicitly represent the microstructure of the composite at the crack front while using homogenized material properties elsewhere. A significant difference in the crack growth pattern was found when the microstructure model was incorporated into the analysis. Crack propagation criteria in the microstructure was based on the energy release rates, fracture toughnesses of the microconstituents and their interface.

The process modeling codes included in the framework simulate the time varying production, or degradation, of composite materials. The analysis codes find the solution for models involving the reaction and transport of chemical species and material flows. In the most basic applications, designers can alter process parameters to improve production rates and/or minimize manufacturing defects. Since the analysis code is interfaced with the framework tools, the opportunity exists for designers to couple themomechanical and chemical process simulations to estimate processing residual stresses or to 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 [19-21]. Inputs for the general analysis 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

POST PROCESSING

Post processing and visualization tools provided by the framework map analysis results into behaviors and graphics to aid interpretation and understanding for design of mechanism-based models. For linear elastic analysis, initial brittle and plastic material failure of fibrous composites due to thermal-mechanical loading can be graphically depicted 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 framework tools provide the designer with an animated "through the thickness" sequencing of these micro scale failures at each lamination, allowing interior-exterior trends to be visualized. The software implements the theory found in [16, 9, 22], 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 the operating temperature. The codes have been applied to SiC/Ti MMCs and to a SiC/Al_2O_3 woven CMC combustor housing with cooling holes and other hardware features, and loaded by large thermal gradients. Overall thermal stresses mapped to the fibrous scale result in the macro scale distribution shown in Figure 2 (top), where shading indicates proximity to fiber/matrix debonding failure on the inner ply.



Fiber–matrix debonding – Level 1

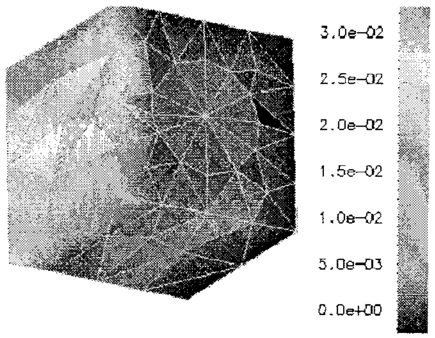


Figure 2: Post processing of macro scale stress

Post processing tools are also used to recover the critical micro scale behaviors in unit cell models. The computational plasticity analysis tools described earlier rely on post-processing of the strain histories stored for each critical macro scale element (Gauss point). In an example problem using a SiC/Ti fibrous composite, the recovered strain history was mapped to the micro scale, showing fiber and matrix stresses and areas of permanent deformation around the linkage connections [12]. The distribution of micro scale stresses are shown at the bottom of Figure 2.

INTEGRATION OF SOFTWARE TOOLS

Several features of the framework allow it to ultilize the software tools described earlier [1]. In order to communicate with commercial packages, such as geometric modelers, framework tools make queries and edit operations through a layer of generic operators. Each commercial code is then interfaced to the rest of the system by a set of functions which translate the generic instruction into the specific functions supported by the package. This avoids the need to customize a version of each framework tool for each commercial package, or version of a package. Relational database queries are specified in terms the SQL language, which performs a similar function. In order to write generic operators and support multiple, possibly specialized tool capabilities, the essential computational functions are abstracted, and the abstractions organized into type hierarchies.

Expertise in several areas, including material and process modeling, analysis techniques and detailed software operation are needed for reliable HTC mechanism-based analysis and design. For a given analysis goal desired by the user, the framework facilitates the sequencing of tools into analysis strategies, the execution of which provides the desired results. 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, 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, or displayed.

CONCLUSION

High temperature composites have required progressively more complex micro-structures and behavioral understanding. Supporting design requires analytical tools which can yield insight into the underlying behaviors at multiple scales, are efficient to use, and which can be adapted to new material configurations. Application of these tools has shown their usefulness in design.

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