NASA/TM-20240010796

Automation of the ICME Workflow Incorporating Material Digital Twins at Different Length Scales Within a Robust Information Management System

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December 2024

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Level of Review: This material has been technically reviewed by technical management.

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Abstract

Recent successes in Integrated Computational Materials Engineering (ICME) have demonstrated the potential in designing 'fit-for-purpose' materials for a given application in a cost and time efficient manner. However, the material design process must contain a level of judicious automation in the material decision process; that is implementing some optimization algorithms to truly enable the benefits of ICME, particularly when considering materials at multiple length and time scales. Furthermore, the ability to effectively store developed material models, experimental data used for validation, and link models at multiple length and time scales must be implemented to ensure traceability across the material design process, such that the data gathered can be leveraged towards efficient material design. To enable such an optimization scheme a robust framework must exist: (1) that can capture changes made at a given length scale, (2) automatically propagate changes upstream to the highest scale, and (3) evaluate the material's performance at the structural level. In this work, a developed framework for tracking material changes, automatically running the necessary simulations to determine the properties at the next highest scale, and saving each iteration of the design process to maintain the application's digital thread is presented for polymer matrix composites (PMCs). The Automated Information Management Across Organizations and Scales (AIMAOS) program offers users an interactive graphical user interface (GUI) for defining constituent materials, building lamina and laminates, and applying effective laminate properties to finite element and composite optimization third party software. At each length scale, the necessary input files are automatically written, and subsequent analysis tools are called to solve for effective properties at the next scale, which are then read by the AIMAOS tool and displayed to the user. As changes are made to the material at lower length scales, information is automatically propagated upstream to higher length scales, and changes made are automatically tracked and versioned to maintain traceability during the design process. The AIMAOS tools serves as the first step in enabling optimized design of composites from the nano to the macroscale for a given application.

Introduction

With an increased demand in reducing the cost, effort, and time-to-market for new materials, Integrated Computational Materials Engineering (ICME) has become a fast-growing discipline that looks to address these demands with respect to material science and engineering. The potential benefits of implementing ICME practices into material design can enable faster, more cost-effective material

development and deployment, significant reduction in experimental testing, and the ability to tailor material properties to a given application, enabling the design of ‘fit-for-purpose’ materials (Refs. 1 and 2). In the context of polymer matrix composites (PMCs), which are inherently highly tailorable materials, a robust ICME approach allows designers to achieve optimal structural designs by optimizing the material properties at the various length scales present in the material’s structure. Typically, a PMCs structural performance is influenced by the resin cure kinetics and presence of nanofillers at the nanoscale (Refs. 3 to 7), the material properties of the constituents (e.g., the fiber reinforcement and matrix), volume fraction, microstructure at the microscale (Refs. 3 to 6, 8 to 19) (i.e., fiber packing, defects/voids and their arrangement, if present), the laminate stacking sequence at the mesoscale, and the part geometry and expected applied loading at the macroscale (Ref. 20).

Traditional engineering of PMCs has generally seen a clear division between the material science viewpoint and the structural viewpoint, denoted here as the ‘Design the Material’ and the ‘Design with the Material’ paradigms, respectively (Figure 1). In the ‘Design the Material’ paradigm, the effects from lower scales (i.e., the nano-, micro-, and mesoscales) are incorporated into a single anisotropic, nonlinear (if damage or inelasticity is present) material constitutive model that is then passed to geometric and structural design software (e.g., finite element analysis (FEA)) in order to participate in the ‘Design with the Material’ paradigm of a given part/component. The current ICME approach for PMC design, looks to bridge this gap between the two paradigms by allowing structural design of parts to begin at the lowest length scale selected in the material. Such an approach, however, requires material models at each scale that are experimentally validated, such that the relationships between processing, internal structure, properties, and performance are fully understood, and the inputs and outputs between each scale that meaningfully effect structural performance are known and tracked. These requirements for ICME therefore become heavily dependent on data captured and generated to define the material models, the associated metadata for each model, and the contextual linkage between length scales, such that

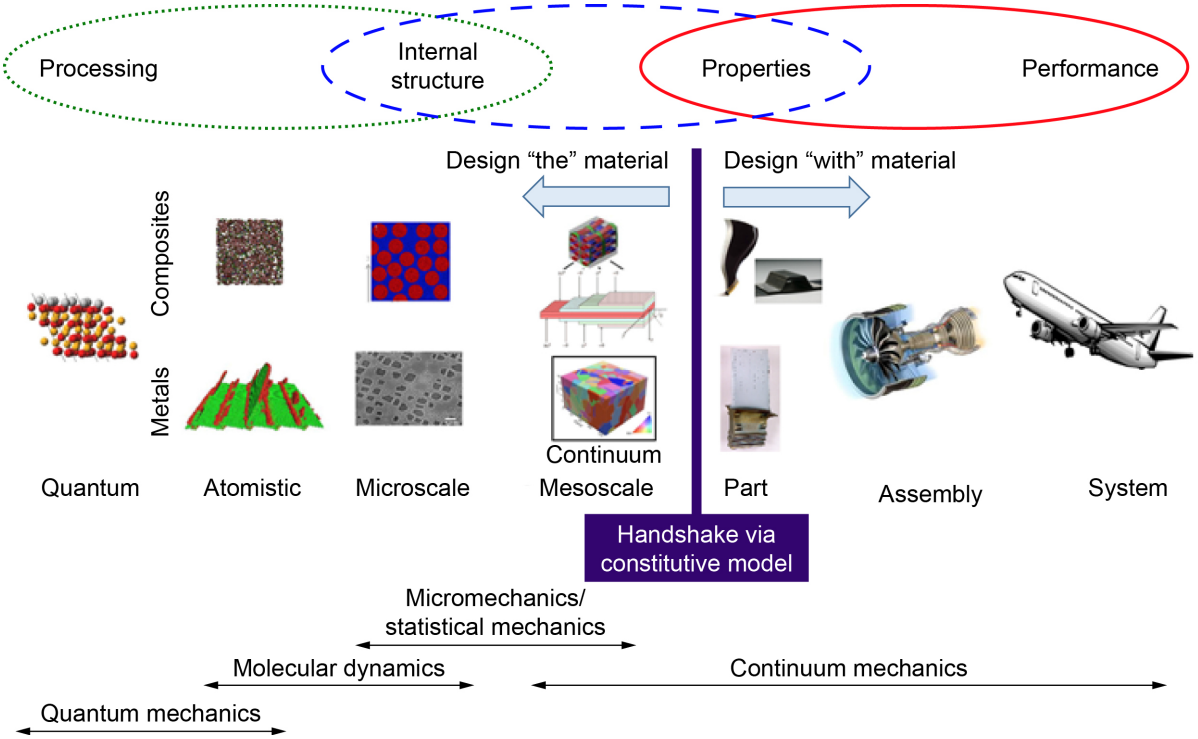


Figure 1.—Description of associated length scale dependence and modeling methods in context of ICME.

information can be effectively exchanged within and between scales to establish the necessary process-microstructure-property-performance relationships. Therefore, for any organization to implement an ICME approach to material design, a robust material information management system that can manage the digital thread (i.e., capture, analyze, link, maintain and disseminate data) is paramount to the design process.

The schema for a robust, 21st century information management system for capturing and analyzing *material* information, including material pedigree, virtual and experimental test data, and developed material models, has been shown in prior publications (Refs. 21 to 24). Figure 2 shows the ICME schema developed at NASA GRC (i.e., tables, or sets of data records stored with the same attributes, as well as the interaction, or linking, between these tables) that establish the traceability between developed models, experimental or virtual testing, and material pedigree, such that the digital thread of a material model is well-maintained. More recently, the Application table was added to the ICME schema; this table serves as the bridge from the material information management system to either product lifecycle management (PLM) or simulation data management (SDM) systems, which are typically used to store *structural* information for an application (e.g., engineering data, manufacturing processes, and associated cost from cradle to grave) (Ref. 25). The Application Table is used to store both material and application performance requirements and criteria, including spatial and temporal information on a specific part or assembly's bill of materials, microstructure, expected loading conditions, geometry, and expected failure mode. It also offers a unique location to link the material information to computer aided design (CAD) and FEA software tools, thus establishing the digital thread between a digital representation/twin at the material level and that of the application; thereby enabling maintenance of the digital thread across the various length scales associated with the application's structure. Thus, the Application Table serves as the missing link between the 'Design the Material' and 'Design with the Material' paradigms needed to conduct an ICME design process for 'fit-for-purpose' materials.

One of the major challenges with implementing an ICME approach is proper maintenance of the digital twins/digital representations (which exist whenever the physical entity no longer matches the virtual entity) at each length scale, and the established traceability between each twin to maintain the application's digital thread. Though the established ICME schema for storing data does provide the means

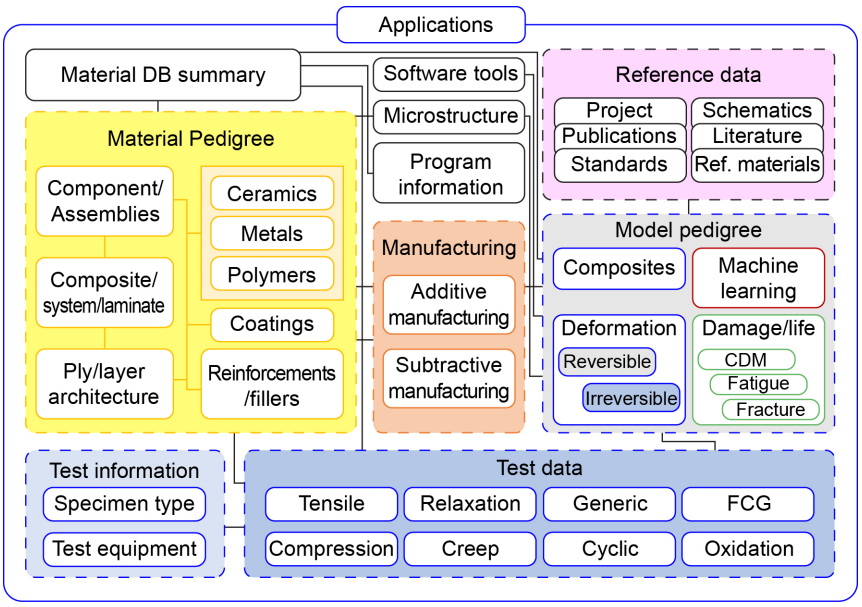


Figure 2.—NASA Glenn's ICME schema for storing material information.

to establish such connections between scales, it still relies on the user to place data in the correct location in the database and establish the appropriate linkage between pedigree, test data, models, and application, and is thus prone to human error that can break the digital thread. Furthermore, an efficient ICME approach will generally require some level of iteration or optimization at each length scale since the influence on structural performance from the properties at each scale is relatively complex. This iteration will further hinder the ICME design process, since users will have to run the necessary analyses at each scale through the appropriate simulation tools and populate the database with the relevant outputs before the analyses at the next scale can be completed for each iteration of the design.

Consequently, the objective of this work is to address the challenges associated with leveraging the developed ICME schema for the design of 'fit-for-purpose' materials by developing a framework for automating the flow of information and creation/maintenance of digital twins across each length scale, denoted herein as AIMAOS (Automatic Information Management Across Organizations and Scales). The developed Python tool allows users to define constituent materials, laminas, and laminates that can then be applied to structural models for geometric optimization and material evaluation. The tool interacts with various material simulation tools, judiciously automating the process of writing and reading input and output files across the various length scales, significantly reducing both execution time for analysis and the potential for human error. Furthermore, it also tracks how the digital thread evolves as changes are made at each individual length scale, providing both version control history needed for proper data management and relevant metadata that can be leveraged for future material optimization. The framework presented is the necessary backbone for any iteration or optimization scheme for the design of 'fit-for-purpose' materials and can be utilized in various applications for ICME design.

Use Case: ICME Optimization of Advanced Composite Components of the Aurora D8 Aircraft

To demonstrate the features and benefits of the developed framework for automation of the ICME workflow, the developed Automated Information Management Across Organizations and Scales (AIMAOS) tool will be used for the use case of optimizing the composite Y-joint of the Aurora D8 aircraft through an integrated, multiscale approach (Figure 3). This work was first presented as a

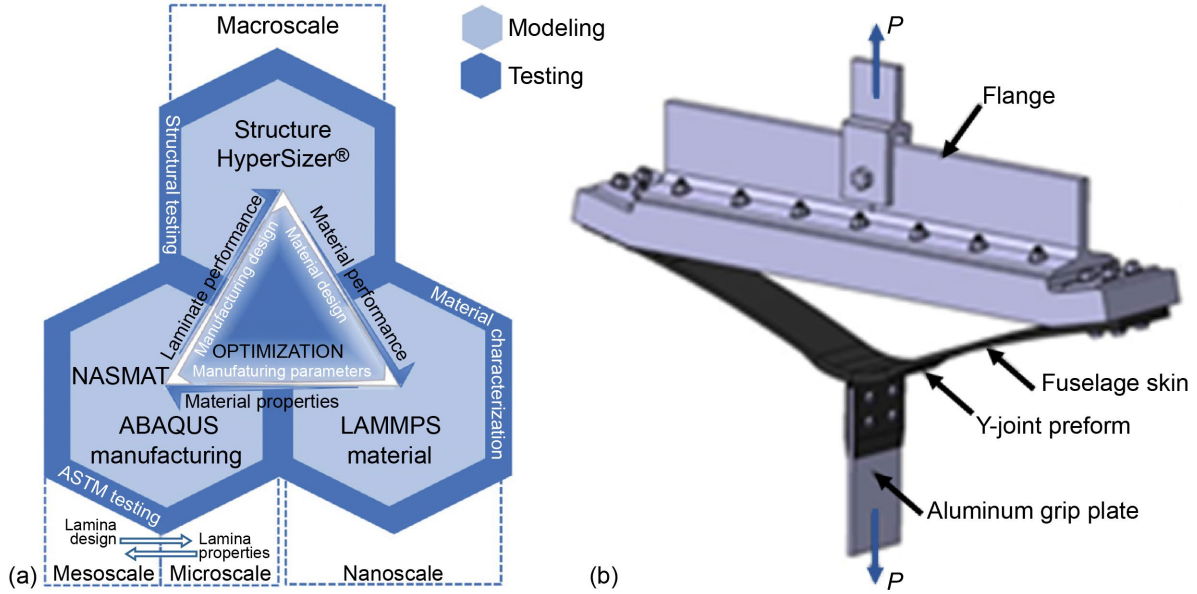
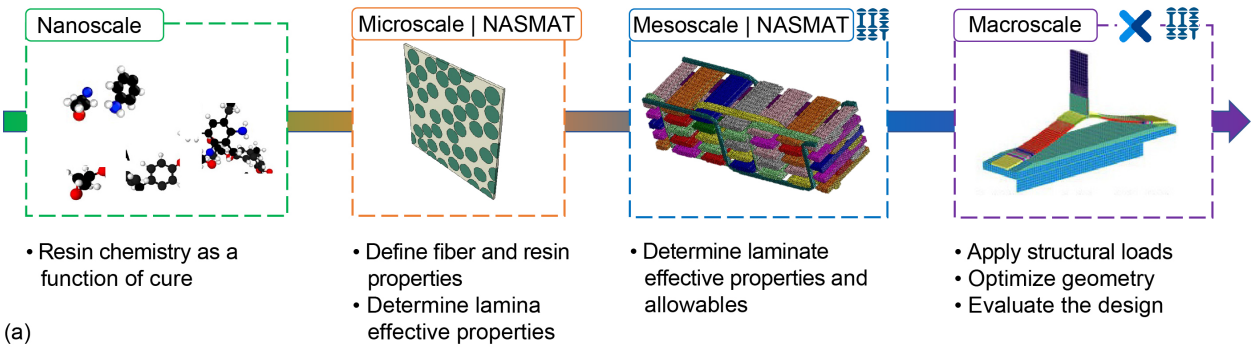


Figure 3.—(a) ICME approach for optimal structural design. (b) Schematic of composite Y-joint.

collaboration between University of Massachusetts Lowell, Michigan Technical University, NASA, Aurora, and Collier R&D in Reference 26. The purpose of the study was to develop and utilize an ICME approach to optimize the Y-joint in an effort to demonstrate the benefits of using an ICME approach to design as opposed to traditional engineering practices. The ICME modeling of the composite component included integration of four levels of scale—nano-, micro-, meso-, and macro—wherein molecular dynamics (MD) simulations of the cure kinetics of the resin, addition of nanoparticle reinforcements to the resin, developing effective properties at the microscale given the resin and fiber properties, volume fraction, microstructure of a given lamina, and the finite element analysis and geometric optimization of the laminate stacking sequence to meet the structural requirements of the Y-joint.

The work presented relative to the ICME design of the composite Y-joint successfully demonstrated the potential benefits of such an ICME approach and was awarded the 2022 AIAA ICME Prize. Through their ICME approach, the multiorganizational team was able to demonstrate a 17 percent savings in manufacturing costs, a 30 percent reduction in weight for the part compared to the traditionally designed part made by Aurora, resulting in an in-service fuel cost savings of $1204 per aircraft per year. The ratio of manufacturing cost savings to the investment of additional material cost produced a return on investment of 200:1, thus demonstrating the business case for organizations to implement an ICME design approach, particularly for PMCs. Though the work was successful in benchmarking the benefits of ICME, the process relied on each team member *manually* (1) creating input files for the analysis at each scale, (2) running the analysis, and (3) passing the necessary outputs to the next team member; thereby opening the design process to potential errors and inefficiencies, further exacerbated by the fact that team members were in different organizations. Thus, the ICME optimization of the composite Y-joint serves as an excellent use case for demonstrating the utility of the AIMAOS toolset (i.e., to automate passing information across scales) with an eye toward establishing an iteration scheme for ICME design.

The integrated approach used for the material and geometric optimization of the composite Y-joint requires engagement with multiple experimentally validated material models at various length scales, and thus requires the seamless interfacing of various engineering tools (Figure 4). For example, at the nanoscale, the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) (Ref. 27) was used to determine the resin properties as a function of the cure kinetics. LAMMPS is a molecular dynamics (MD) simulation tool used to simulate the crosslinking that occurs during curing which in turn impacts the prediction of mechanical and thermal properties at the nanoscale level. These LAMMPS output results are then used as the constituent input properties for the microscale analysis. At the microscale, NASA's Multiscale Analysis Tool (NASMAT) (Refs. 28 and 29) is used to determine lamina (ply) level properties. NASMAT uses the Generalized Method of Cell (GMC) (Ref. 30) along with a given repeating unit cell (RUC) analysis to produce homogenized properties for a lamina (ply) given constituent material properties (i.e., the fiber and matrix) and the lamina microstructure. Similarly, laminate level homogenized material properties at the mesoscale can be found using NASMAT lamina properties and classical lamination theory (CLT), FEA or HyperX (Ref. 31). The strength allowables used in the structural analysis of the Y-joint are found through performing monotonically loaded NASMAT laminate simulations, or by pairing NASMAT (through a user-defined material routine) with the commercial FEA code Abaqus (Ref. 32) for out of plane or complex loading. Laminate level response results are computed using Hyper X, a composite analysis tool for weight reduction and geometry optimization, which pairs with multiple FEA software (herein Abaqus) to determine the optimal stacking sequence for a structural component given the computed lamina material properties.



(a)

LAMMPS

Large-scale Atomic/Molecular Massively Parallel Simulator
- Molecular Dynamics (MD) code for materials modeling
- Simulate curing of the resin to establish thermodynamic properties as a function of the processing
- Characterize resin properties as a function of cure for higher scales

NASMAT

NASA Multiscale Analysis Tool
- Determine homogenized lamina and laminate propertiesgiven constituents and microstructure
- Determine macroscale strength allowables by performingvarious monotonically loaded simulations

Abaqus
- Finite Element Analysis (FEA) software used to analyze the Y-joint at the structural level
- Inherent connections to NASMAT (UMAT) and HyperX (post-processing/optimization)

HyperX
- Composite analysis tool for weight reduction/geometry optimization, stacking sequence determination and material selection
- Interfaces with Abaqus to evaluate the Y-joint and determine the optimal weight given the macroscale material properties

(b)

Figure 4.—(a) Overview of length scales and associated modeling tools used. (b) Descriptions of each modeling tool.

The input and output files along with associated metadata, for each of the above-described tools, constitute the digital twins at each lower length scale associated with the composite Y-joint. The Y-joint digital representation itself being a digital twin when appropriately paired with its physical counterpart. The purpose of the developed automated framework (AIMAOS) presented herein is to facilitate the creation of the scale specific digital twins, automate the flow of information from one tool to the next (i.e., upscale and downscale the required information), and provide the necessary traceability and storage of the twins to maintain the digital thread of the structural component. The tool must therefore be able to store model outputs, automatically generate input files, read output files, and link material models at each scale to be an effective tool for driving an ICME design process.

Automated Information Management Across Organizations and Scales (AIMAOS)

To facilitate the judicious automation of establishing's the digital twins at the various length scales (i.e., creating the required input decks) and executing the associated analyses, a Python-based graphical user interface (GUI) was developed using the tkinter Python package (Ref. 33). The program allows users to define constituent materials, laminas, and laminates, run multiscale analyses, and connect to HyperX

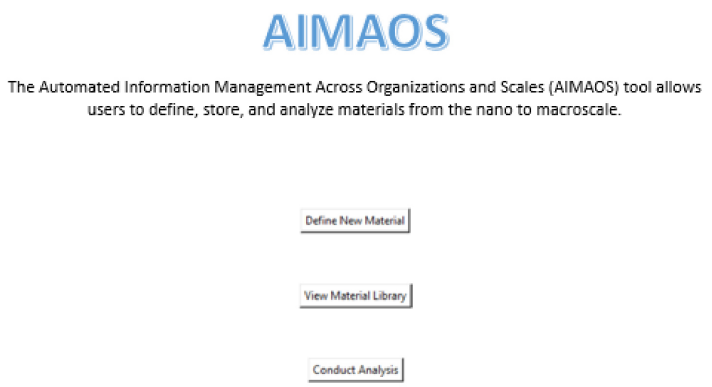


Figure 5.—AIMAOS home page.

for structural analysis and geometric optimization of the Y-joint for the defined material in a user-friendly, easily applied executable environment. The home page for AIMAOS (Figure 5) gives users three separate options, each of which will be described in further detail, to choose from:

1. Define New Material
2. View Material Library
3. Conduct Analysis

Define New Material

The ‘Define New Material’ page in AIMAOS allows users to define multiscale materials at each of the considered scales. When selected, the user is presented with the option to define a constituent, lamina, or laminate (Figure 6(a)). For defining a fiber or matrix, the user is prompted to enter either transversely isotropic material properties or isotropic material properties, respectively, as well as a material name and any additional information associated with the source of the information (Figure 6(b)). Adding a material to the library stores it for future use within the GUI either at the same or higher length scales, and stores the information entered in a local database with an associated global unique identifier (GUID) generated for the material, which is used to link information across scales.

When defining a lamina, users are asked to define a unique lamina name, the constituents, degree of cure, fiber volume fraction, ply thickness, and the RUC geometry that represents the lamina microstructure (Figure 7). When defining the constituents in a lamina, users must select a fiber and matrix that already exist in the database, which can be defined on the previous page (Figure 6(a)). If the matrix properties are defined as a function of cure from MD simulations, the slider (see Figure 7) will adjust the properties correspondingly. The ‘Select the RUC’ drop down menu currently offers three options for the lamina microstructure: a 2x2 RUC, a 7x7 RUC, and a 26x26 RUC, all of which are contained within the internal NASMAT library (Figure 8). Additional canned RUCs from the NASMAT library can be added to the GUI, as well as an additional subroutine to allow users to define a custom microstructure, which is supported in NASMAT. When a lamina is added to the library, first the resin characterization code is called to obtain microscale properties for the resin as a function of the defined cure percentage. A NASMAT ASCII input file is automatically created for the lamina, and the NASMAT program is called to predict the associated lamina properties for a given RUC. The output file generated by NASMAT is then read and parsed by the program to extract the lamina effective properties and effective stiffness matrix, which is then written to the local database in a record with an associated new lamina GUID. The generated input and output files are also written to the database within the created record for the lamina,

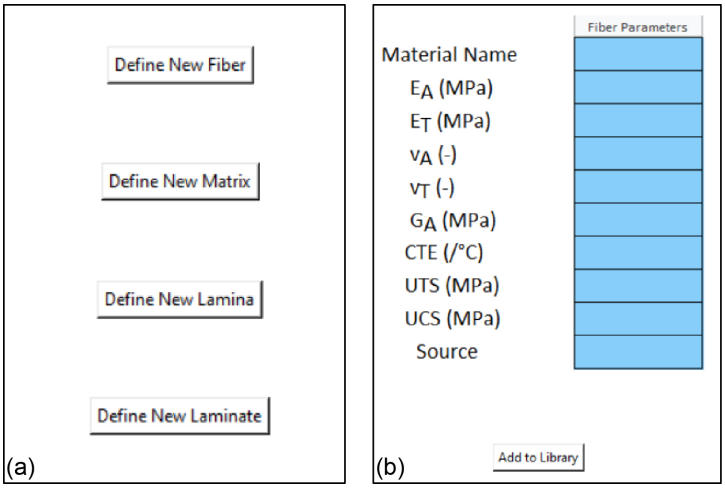


Figure 6.—(a) Options for defining new materials. (b) Defining a new fiber.

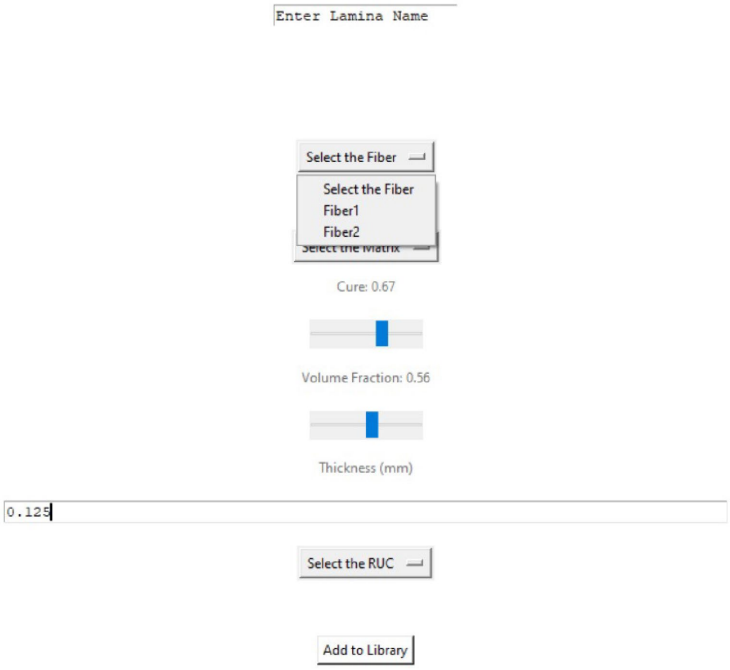


Figure 7.—Defining a new lamina.

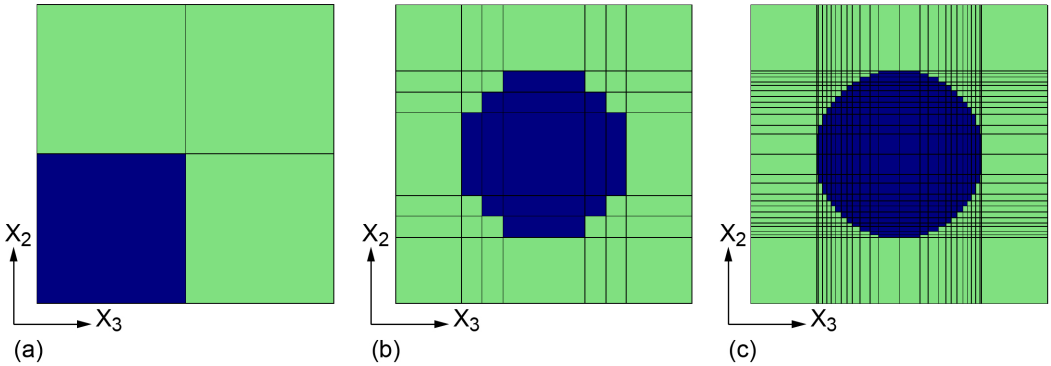


Figure 8.—NASMAT RUCs. (a) 2x2. (b) 7x7. (c) 26x26.

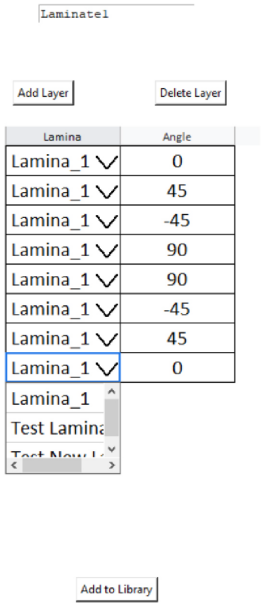


Figure 9.—Defining a new laminate.

thus storing the digital twin (e.g., RUC) of the material and providing full traceability between the microscale properties and homogenized mesoscale properties through each record's GUID (i.e., the fiber record, matrix record, and new lamina record).

When defining a laminate, users are asked to define a unique name for the material and the stacking sequence. The stacking sequence is presented to the user as a table, with the left column defining the lamina name, the right column defining the ply orientation (from –90 to 90), and each row representing an individual ply (Figure 9). Lamina in the left column must be selected from the existing material library; therefore, no additional information is needed to define the laminate, since each lamina has associated constituents, volume fraction, and microstructure. Similar to the lamina, when a laminate is added to the library, the program uses the associated GUID's for each lamina, and subsequently the associated GUID's for each constituent, to retrieve the material properties, volume fraction, and microstructure for each ply, automatically write a NASMAT input file for homogenization, and automatically execute the NASMAT program. Furthermore, additional NASMAT input decks are created and executed (with applied loading in the 11 and 22 (both tension and compression) and 12 (shear) directions) so as to determine the macroscale strength allowables needed for conducting the structural analysis. The effective laminate properties (e.g., ABD matrix) and strength allowables are extracted from the output files by the AIMAOS program and written to the local database with an associated laminate GUID.

View Material Library

The 'View Material Library' page allows users to both view what materials, at each scale, currently exist in the local database and edit the properties that are defined in 'Define New Material' pages. When changes are made to any material, a new GUID for that material is created with the updated change, and a version controlled history of the previous material properties and GUID are stored in the database to that material record. Furthermore, when a change is made to a material, all effected materials upstream (i.e., at higher length scales) that are affected by the change are automatically updated by creating new input decks and re-running the relevant analyses to ensure the digital thread for each material system remains intact.

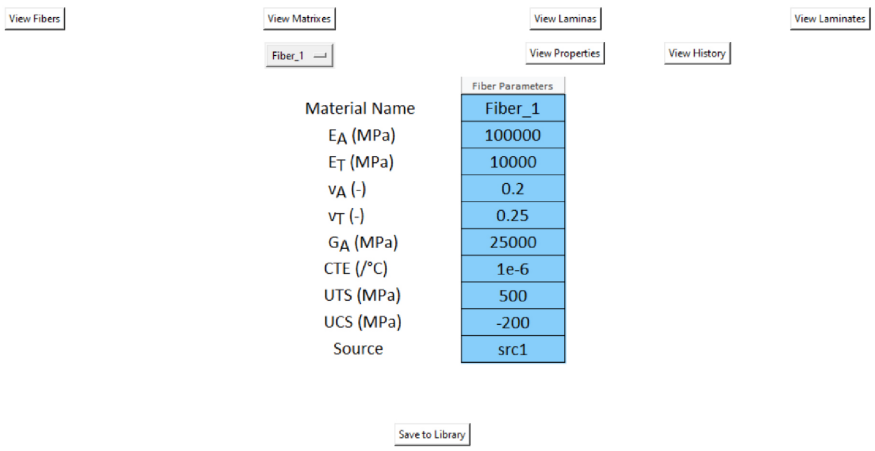


Figure 10.—Viewing and editing a material.

When the ‘View Material Library’ page is selected, users can view any material previously created, be it a fiber, matrix, lamina, or laminate (Figure 10). When a material is selected via the drop down menu and the material properties are displayed via the ‘View Properties’ button on the GUI, a table with the material properties *defined only in the GUI* are presented to the user, all of which can be edited. For example, when viewing a fiber, the Elastic (Young’s) moduli, Poisson’s ratios, coefficient of thermal expansion, and strengths can all be edited by user. For a lamina, the fiber material, matrix material, cure, volume fraction, thickness, and microstructure can be edited, but the effective properties of the matrix, solved for by AIMAOS as a function of cure, cannot be changed, which helps to ensure that all results are program controlled, thus maintaining the integrity of the digital thread.

If a change is detected between the originally presented version and the current table when the user presses ‘Save to Library’, the automatic updating of information upstream is initiated. For example, the user can edit a fiber constituent property in the library. A new version of the fiber record would be written to the database and would trigger a search for all lamina that contain the original fiber GUID. The process outlined in Figure 11(a) would be conducted for each found lamina, in which the fiber material properties would be updated, and a simulation tool would be executed to establish new effective properties at the mesoscale. Consequently, because the lamina properties have now changed (and each have a new associated GUID), all affected laminates must also be updated. The process outlined in Figure 11(b) would be conducted for each effected laminate (macroscale) with the correct associated lamina properties, ensuring data stored in the database is always consistent and up to date. The version history for any material can be found in the ‘View Material Library’ page by selecting the ‘View History’ button. For the example of changing the fiber axial Poisson’s ratio, the program will display the original material properties under the header ‘Revision_0’ and the new material properties under the header ‘Revision_1’ (Figure 12(a)). In the ‘Notes’ row, a standardized description of what changed between adjacent columns is automatically generated and populated to the material library. Additional changes to the material would result in the creation of additional GUIDs for the material, and thus additional columns would be displayed to the user when viewing the material history. When viewing an effected lamina (Figure 12(b)), again two columns will appear, even though the user did not explicitly change the lamina, since the properties are automatically propagated to higher length scales. The previous versions input and output files are renamed to match the revision number, such that the current version always has the same input and output filename, and again a standardized description of the change between revisions is automatically populated in the ‘Notes’ row.

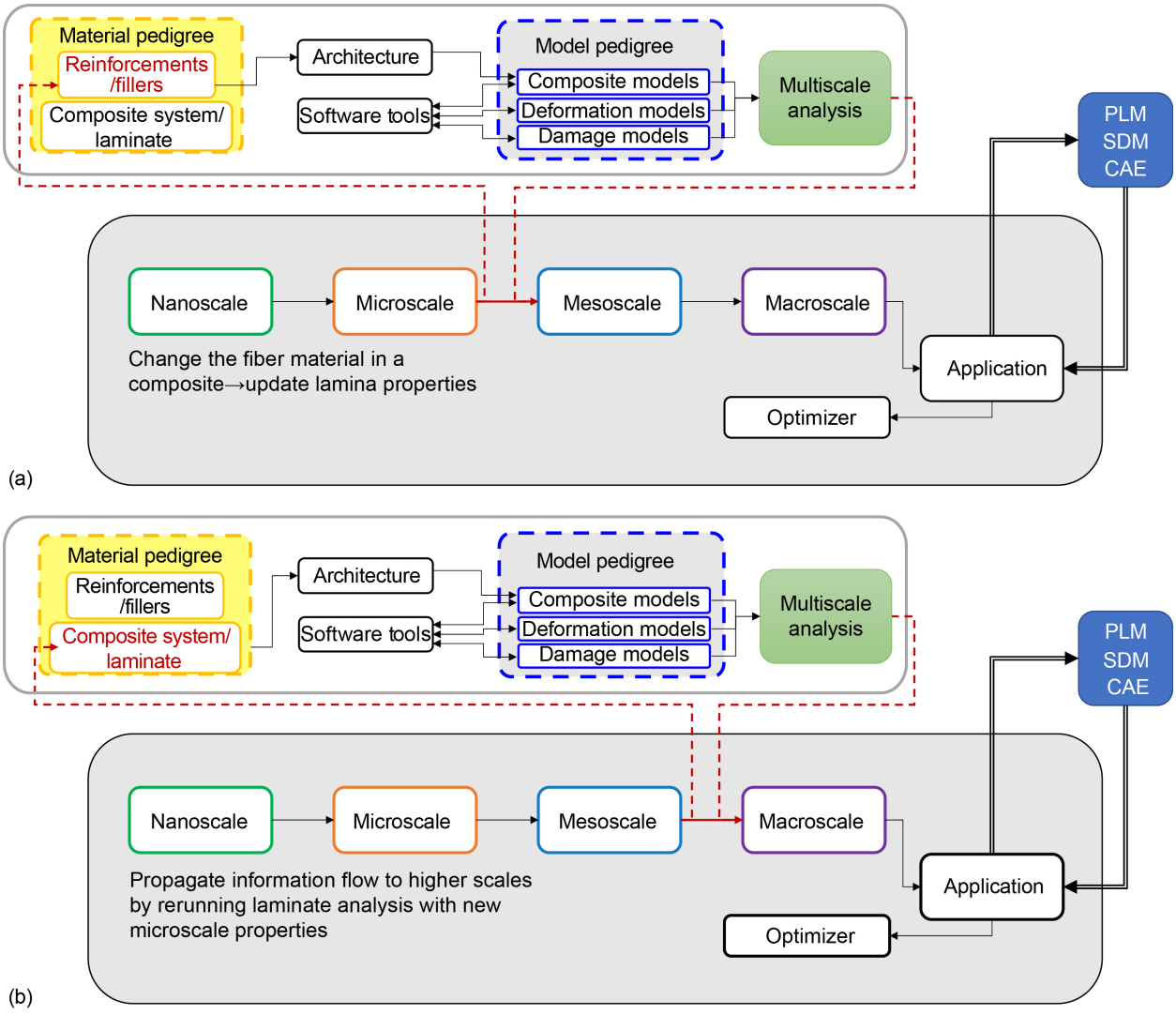


Figure 11.—Example AIMAOS workflow and information management system interaction for changing material properties at microscale. (a) Updating of mesoscale properties based on user input. (b) Automatic propagation of information at macroscale.

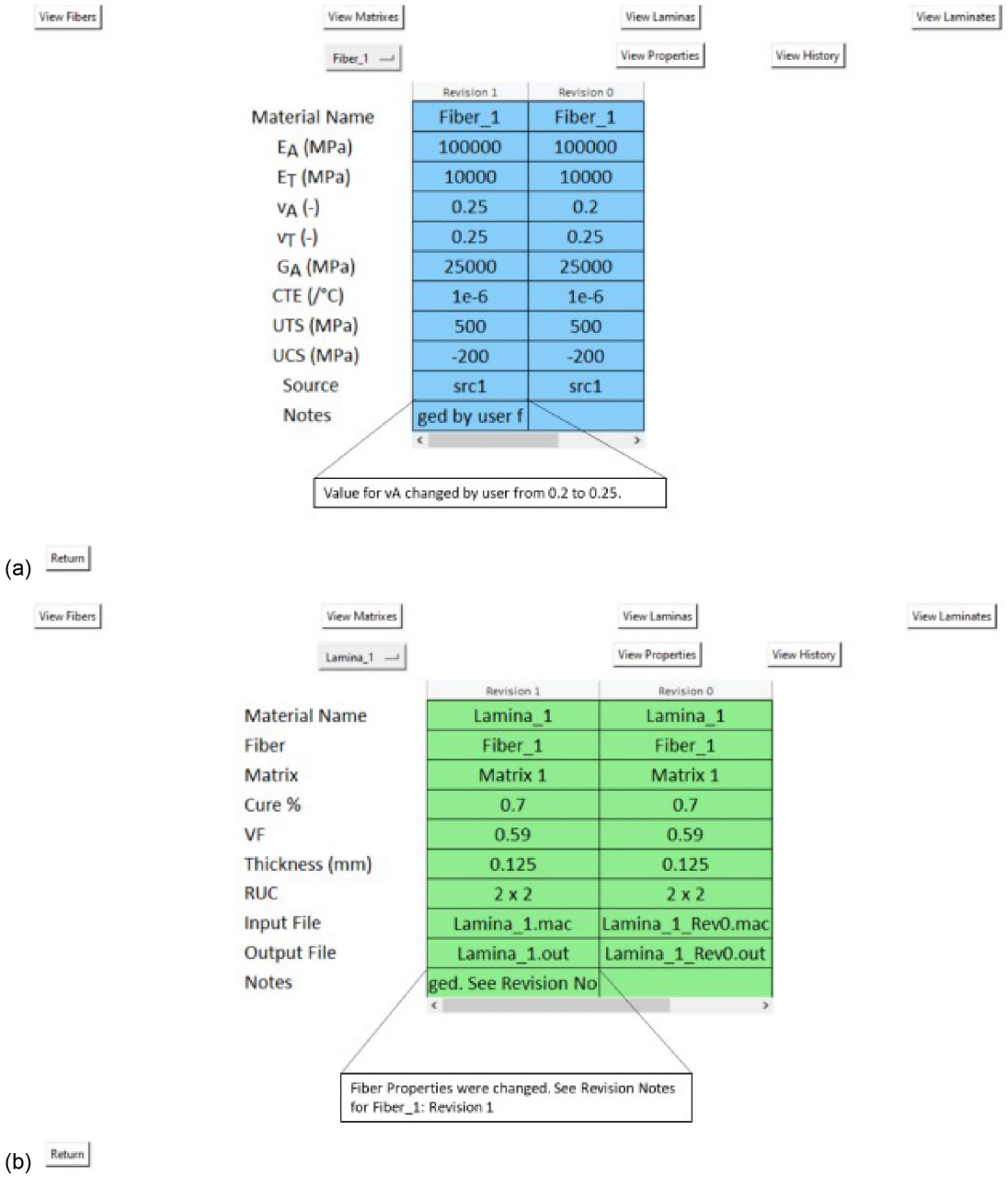


Figure 12.—Viewing Material Version History. (a) Change made to fiber. (b) Automatic propagation of information upstream.

The ability to both automatically propagate information upstream by calling the associated multiscale analysis tools used and generate standardized notes that track what changes occurred not only provides the traceability required for robust material information management, but also reduces the potential for human error during the design process. Because the hand-off between scales is automated once any change occurs, there is no opportunity for scales to become ‘out-of-sync’ from varying material properties, helping to prevent the transfer of incorrect information from one scale to another. Furthermore, the potential for human error is reduced by limiting the number of inputs a user must enter. In a non-automated ICME process where multiple iterations occur at each length scale, the design process relies heavily on users entering material information from the correct iteration into each input deck, which

can be highly susceptible to mistakes. This error is further exacerbated when multiple organizations are contributing to the analysis, in which communication between organizations isn't highly effective due to geographical and institutional barriers. By eliminating this source of error, designers can be more confident that the properties given to the macroscale are correct and that the digital thread for the component has been maintained, with a standardized method for viewing the changes that have occurred at each iteration. An additional benefit of the automatically generated notes for material changes is that it provides metadata on the design process itself. As a design either improves or worsens, the program automatically stores the change that occurred at each scale that resulted in a change in performance. This information can be leveraged in an iteration or optimization scheme to determine what parameters influenced the performance of the design, which can in turn be used to improve the optimization or iteration scheme for future 'fit-for-purpose' material development.

Conduct Analysis

The 'Conduct Analysis' page of the developed GUI allows users to bridge the material and structural paradigms by defining multiscale materials, or selecting existing materials from the database, and applying the homogenized material properties to a structural FEA model to perform geometric optimization. Users have the option to start from any scale (i.e., nano-, micro-, or meso-), and must choose materials at lower length scales and define materials at higher length scales to conduct the analysis. For example, Figure 13 shows the option of conducting analysis from the microscale to the macroscale, where the fiber and matrix are selected from the library, but the lamina and laminate must be defined, along with optional additional parameters for the composite that are not needed for the NASMAT simulations. The blue 'Conduct Analysis' button repeats any of the steps defined in the 'Define New Materials' section for any new materials (e.g., run microscale analysis for the lamina from the defined constituents and mesoscale analysis for the laminate), and then writes all relevant composite information to a JSON material library.

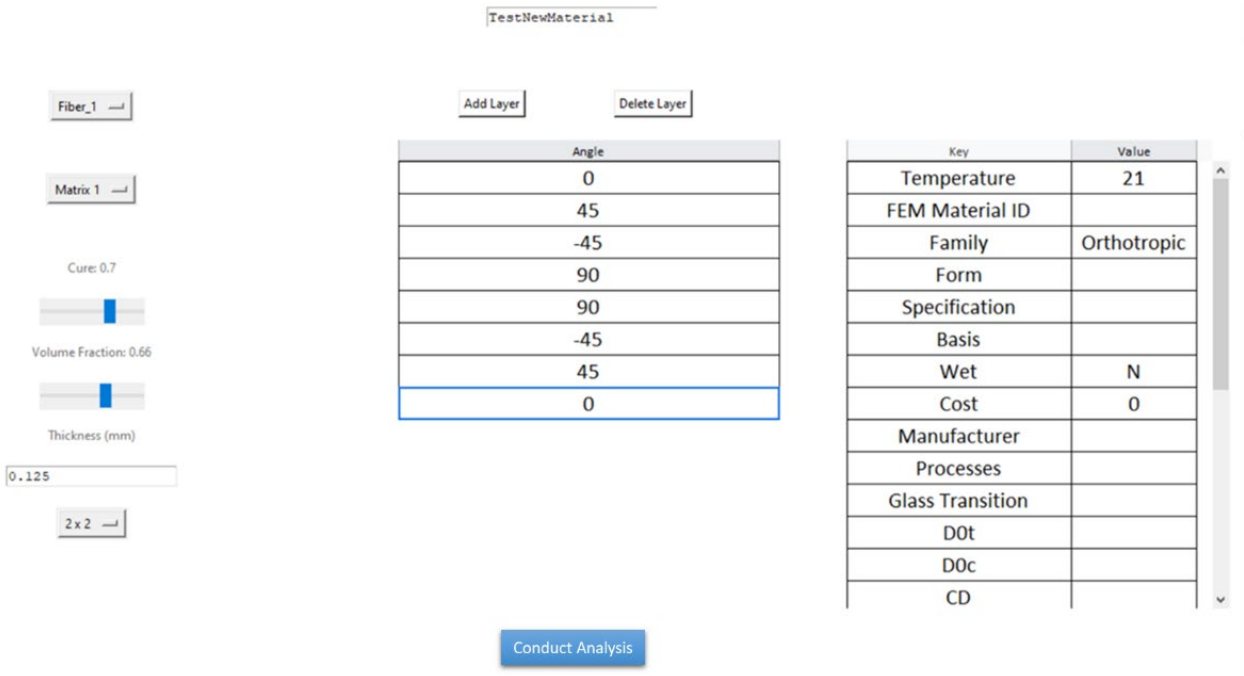


Figure 13.—Conduct analysis from microscale to macroscale.

Macroscale structural analysis of the Y-joint for geometrical optimization is carried out with a rapid design tool, HyperX (Ref. 20). The macroscale analysis procedure is automated through Python scripts which heavily utilize the HyperX scripting API to communicate with the rapid design tool. In its current state, the JSON material library database is read by the preprocessing Python script along with other relevant variables which serve as an input to HyperX (**user_material** in Figure 14). The associated Y-joint constituent material properties for the skin, preform and adhesive are assigned to the corresponding components of an existing FE structural model of the bonded Y-joint. The Macroscale optimization code is then called to access the material in the JSON library, load the structural model of the part, select the bonded joint, and apply boundary conditions and applied loading. The HyperX software is then utilized to determine optimized macroscale geometry and analyze the resultant stresses in the joint in the optimal configuration. The script then postprocesses the HyperX output to read back the stresses and margin of safety, which can ultimately be used in an optimization scheme to optimize the material at each length scale.

It is important to note here that HyperX offers a predefined set of standard bonded joint designs. The Y-joint, considered in this study, is a modified configuration of the standard Pi-joint included in the HyperX design library. To account for the curvature of the Y-joint relative to the standard Pi-joint, the boundary conditions are modified automatically by updating the appropriate forces and moments in the preprocessing step. Furthermore, the boundary conditions are updated to reflect in-service loading conditions. In addition to the material properties and boundary conditions, the laminate stacking sequence and orientation information (for the skin and preform) is also parsed from the material library to define the joint design and configuration. HyperX also offers an array of failure modes to choose from for bonded joints. After selecting the appropriate failure modes for the Y-joint, the joint is analyzed for critical failure mode, and peel and shear stress distribution along the bondline. Furthermore, a margin of safety is also computed to provide valuable feedback for weight reduction/geometry optimization. By iterating over several important parameters such as the skin thickness, laminate stacking sequence, joint curvature and joint material, an optimized joint design configuration can be established.

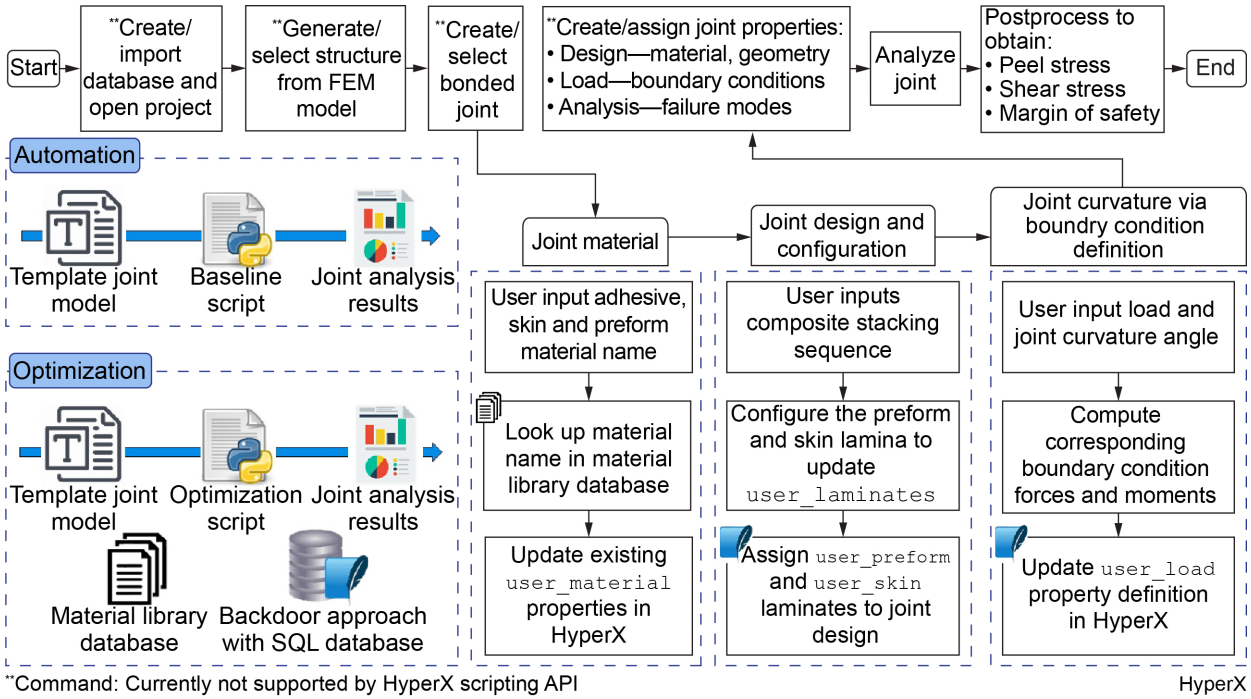


Figure 14.—Macroscale optimization framework.

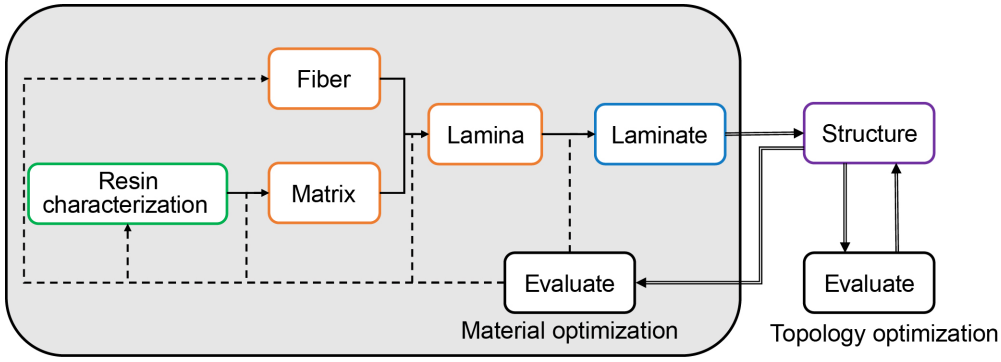


Figure 15.—Schematic of iteration/optimization scheme required for composite ICME design.

AIMAOS for ICME Material and Structural Design Optimization

In its current state, AIMAOS is a useful tool for the automatic propagation of information across length scales as a design evolves, but it relies on the user to take the output generated from the macroscale solution and make a material decision at any one of the lower length scales to change the design. Ideally, for efficient design of 'fit-for-purpose' materials, the decision process would be replaced with an iteration or optimization scheme that can evaluate the macroscale response and make a material decision (thus kicking off the next iteration of information propagation automated by AIMAOS (Figure 15) in an efficient manner to minimize some objective function that is likely a function of weight, cost, manufacturability, etc. The 'Evaluate' portion of Figure 15 for material optimization should be able to make inverse design decision, indicating what aspects of lower length scale parameters need to be changed in order to meet the requirements of the macroscale. Similarly, the 'Evaluate' portion of Figure 15 for topology optimization should *periodically* perform structural optimization for the given material. This methodology not only enables concurrent material and structural 'fit-for-purpose' design, but also allows for interaction between the 'Design the Material' and 'Design with the Material' paradigms that can capture any "lurking failure modes" and thus minimize resource utilization. The determination of the optimization algorithm for the composite Y-joint is outside of the scope of this work, but the benefit that such a scheme would enable in ICME design outlines the necessity for a robust framework that can connect to an optimization module, apply the changes made at any length scale, and automatically propagate information upstream, thus allowing iteration in an efficient manner and enabling both an optimized material and geometric design for an application.

Conclusions

ICME has received widespread growth in recent years due to its promise in reducing the cost, time, and effort associated with engineering design and the prospect of developing 'fit-for-purpose' materials. Previous work has shown the potential benefits that an ICME approach can have on component design, but has also highlighted the potential for inefficiencies and introduction of human error as information is manually passed between length scales. Furthermore, a true, highly efficient ICME approach requires rapid iteration on material and geometric design at each length scale with an informed decision process for the changes that occur at each iteration, thus demonstrating the need for an information management tool that can automatically create digital twins of the material and structure at each length scale, propagate information from one scale to the next, maintain the traceability between length scales to ensure the integrity of the digital thread, and track the changes that occur at each iteration to leverage for future material design and optimization scheme improvement. The Automated Information Management Across

Organizations and Scales (AIMAOS) tool developed addresses these needs by providing the necessary framework to be used in such an iteration scheme. Users can create material digital twins at various length scales without directly interfacing with the multiscale analysis tools that perform the analysis from one scale to the next and can leverage the automatic propagation of information upstream to minimize the potential for human error to effect design decisions. They can also view the automatically generated revision notes as the material design evolves to inform the next material decision, allowing for smarter, faster material iteration in an attempt to design a 'fit-for-purpose' material. The AIMAOS program will serve as the backbone for an advanced ICME optimization scheme, enabling the potential for a robust, efficient, and cost effective method for an integrated approach to material and structural design.

References

1. X. Liu, D. Furrer, J. Kosters, and H. Holmes, "Vision 2040: A Roadmap for Integrated, Multiscale Modeling and Simulation of Materials and Systems," NASA, Mar. 2018. Accessed: Mar. 03, 2020. [Online]. Available: https://ntrs.nasa.gov/search.jsp?R=20180002010
2. J. Llorca, González C., Molina-Aldareguía J.M., Segurado J., Seltzer R., Sket F., Rodríguez M., Sádaba S., Muñoz R., Canal L.P., "Multiscale Modeling of Composite Materials: a Roadmap Towards Virtual Testing," Adv. Mater., vol. 23, no. 44, pp. 5130–5147, 2011, doi: 10.1002/adma.201101683.
3. G. M. Odegard, Sagar U. Patil, Prathamesh P. Deshpande, Krishan Kanhaiya, Jordan J. Winetrout, Hendrik Heinz, Sagar P. Shah, and Marianna Maiaru., "Molecular Dynamics Modeling of Epoxy Resins Using the Reactive Interface Force Field," Macromolecules, vol. 54, no. 21, pp. 9815–9824, Nov. 2021, doi: 10.1021/acs.macromol.1c01813.
4. S. U. Patil, S. P. Shah, M. Olaya, P. P. Deshpande, M. Maiaru, and G. M. Odegard, "Reactive Molecular Dynamics Simulation of Epoxy for the Full Cross-Linking Process," ACS Appl. Polym. Mater., Oct. 2021, doi: 10.1021/acsapm.1c01024.
5. S. P. Shah and M. Maiarù, "Effect of Manufacturing on the Transverse Response of Polymer Matrix Composites," Polymers, vol. 13, no. 15, Art. no. 15, Jan. 2021, doi: 10.3390/polym13152491.
6. S. P. Shah, S. U. Patil, C. J. Hansen, G. M. Odegard, and M. Maiarù, "Process modeling and characterization of thermoset composites for residual stress prediction," Mech. Adv. Mater. Struct., pp. 1–12, Dec. 2021, doi: 10.1080/15376494.2021.2017527.
7. P. Deshpande, S. Shah, S. Patil, M. Olaya, G. Odegard, and M. Maiarù, "Process Modeling of Cure in Epoxy based Polymer Matrix Composites using ICME," in World Congress on Integrated Computational Materials Engineering 2022, Apr. 2022.
8. S. Patil, S. Shah, P. Deshpande, K. Kashmari, G. Odegard, and M. Maiarù, "Prediction of Residual Stress Build-up in Polymer Matrix Composite During Cure using a Two-scale Approach," in Proceedings of the American Society for Composites—Thirty-fourth Technical Conference, Sep. 2019. doi: 10.12783/asc34/31378.
9. S. Patil et al., "Multiscale Approach to Predict Cure-Induced Residual Stresses in an Epoxy System," in Proceedings of the American Society of Composites 35th Technical (Virtual) Conference, American Society of Composites, Sep. 2020.
10. S. Patil, S. Shah, P. Deshpande, M. Olaya, G. M. Odegard, and M. Maiaru, "Multiscale Approach to Predict Cure-Induced Residual Stresses in Bis-F/DETDA Epoxy System," in Society of Engineering Science Virtual Conference, Society of Engineering Science, Sep. 2020.
11. S. Shah and M. Maiaru, "Microscale Analysis of Virtually Cured Polymer Matrix Composites Accounting for Uncertainty in Matrix Properties During Manufacturing," in Proceedings of the

American Society for Composites—Thirty-third Technical Conference, Sep. 2018. doi: 10.12783/asc33/25958.
12. S. Shah and M. Maiarù, “Process Modeling of Virtually Reconstructed Composites with ICME,” in World Congress on Integrated Computational Materials Engineering 2022, Apr. 2022.
13. S. P. Shah and M. Maiaru, “A Novel Closed-form Solution for Transverse Tensile Strength of Polymer Composites based on Virtual Testing,” in AIAA SCITECH 2022 Forum, in AIAA SciTech Forum. American Institute of Aeronautics and Astronautics, Dec. 2021. doi: 10.2514/6.2022-1241.
14. S. Shah, S. Patil, P. Deshpande, K. Kashmari, G. M. Odegard, and M. Maiaru, “Multiscale Modeling of Thermoset Composites to Predict Process-Induced Residual Stresses,” in International Conference on Composite Materials, Melbourne, Australia: International Conference on Composite Materials, Jan. 2019.
15. S. Shah et al., “Multiscale Modeling for Virtual Manufacturing of Thermoset Composites,” in AIAA Scitech 2020 Forum, in AIAA SciTech Forum. American Institute of Aeronautics and Astronautics, Jan. 2020. doi: 10.2514/6.2020-0882.
16. S. Shah et al., “In-Situ Characterization of Polymer Matrix Composites and Progressive Damage Analysis of Virtually Reconstructed Microstructures,” in Proceedings of the American Society for Composites—Thirty-fifth Technical Conference, Sep. 2020. doi: 10.12783/asc35/34906.
17. S. Shah et al., “Quantification of Thermoset Composite Microstructures for Process Modeling,” in AIAA Scitech 2021 Forum, in AIAA SciTech Forum. American Institute of Aeronautics and Astronautics, Jan. 2021. doi: 10.2514/6.2021-1774.
18. S. Shah, M. S. Radue, G. M. Odegard, and M. Maiaru, “Novel Multiscale Approach for the Virtual Manufacturing of Thermoset Composites within ICME,” in AIAA Scitech 2019 Forum, American Institute of Aeronautics and Astronautics, Jan. 2019. doi: 10.2514/6.2019-1202.
19. S. P. Shah and M. Maiaru, “Analytical Model for Composite Transverse Strength based on Computational Micromechanics,” Int. J. Multiscale Comput. Eng., vol. 21, no. 6, pp. 77–97, Apr. 2023, doi: 10.1615/IntJMultCompEng.2023048428.
20. E. Plaka, S. P. Jones, B. A. Bednarcyk, E. J. Pineda, R. Li, and M. Maiarù, “Verification And Validation Of A Rapid Design Tool For The Analysis Of The Composite Y-Joint Of The D8 Double-Bubble Aircraft,” Int. J. Multiscale Comput. Eng., vol. 21, no. 6, 2023, doi: 10.1615/IntJMultCompEng.2023047801.
21. S. Arnold, F. Holland, T. Gabb, M. Nathal and T. Wong, “The Coming ICME Data Tsunami and What Can be Done,” in 54th AIAA/ASME/ASCE/AHS/ACS Structures, Structural Dynamics, Materials Conference, Boston, MA, April 23–27, 2013.
22. S. Arnold, F. Holland, and B. Bednarcyk, “Robust Informatics Infrastructure Required for ICME: Combining Virtual and Experimental Data,” in 55th AIAA/ASME/ASCE/AHS/ACS Structures, Structural Dynamics, Materials Conference, National Harbor, MD, January 13–17, 2014.
23. S. Arnold, F. Holland, B. Bednarcyk, and E. Pineda, “Combining material and model pedigree is foundational to making ICME a reality,” Integrating Materials and Manufacturing Innovation, vol. 4, pp. 37–62, 2015.
24. B. L. Hearley, S. M. Arnold, and J. Stuckner, “A Robust Machine Learning Schema for Developing, Maintaining, and Disseminating Machine Learning Models,” NASA Technical Memorandum, vols. NASA/TM-20220017137, pp. 1–41, 2022.
25. S. M. Arnold, B. L. Hearley, and D. Cebon, “Application Table: A Bridge Connecting the Designing “With-The-Material” and “The-Material” Paradigms,” NASA Technical Memorandum, vols. NASA/TM-202200184033, pp. 1–48, 2023.

26. M. Olaya, H. A. Mahmud, E. Plaka, K. Bukenya, S. Patil, S. Shah, P. Desphande, M. Nagaraj, A. Krief, E. J. Pineda, B. A. Bednarcyk, R. Li, J. Chambers, S. Jones, C. Collier, G. M. Oegard, and M. Maiaru, "ICME Optimization of Advanced Composite Components of the Aurora D8 Aircraft," AIAA 2022 ICME Prize, 2022.
27. M. Olaya, H. A. Mahmud, E. Plaka, K. Bukenya, S. Patil, S. Shah, P. Desphande, M. Nagaraj, A. Krief, E. J. Pineda, B. A. Bednarcyk, R. Li, J. Chambers, S. Jones, C. Collier, G. M. Oegard and M. Maiaru, "ICME Optimization of Advanced Composite Components of the Aurora D8 Aircraft," AIAA 2022 ICME Prize, 2022.
28. E. J. Pineda, B. A. Bednarcyk, T. M. Ricks, S. M. Arnold, and G. Henson, "Efficient Multiscale Recursive Micromechanics of Composites for Engineering Applications," International Journal for Multiscale Computational Engineering, vol. 19, pp. 77–105, 2021.
29. E. J. Pineda, T. M. Ricks, B. A. Bednarcyk, and S. M. Arnold, "Benchmarking and Performance of the NASA Multiscale Analysis Tool," in AIAA SciTech Forum, Virtual Event, 2021.
30. J. Aboudi, "Micromechanical Analysis of Thermo-Inelastic Multiphase short-Fiber Composites," Composites Engineering, vol. 5, no. 7, pp. 839–850, 1995.
31. HyperX, Available from: https://hypersizer.com/hyperx/
32. ABAQUS Unified FEA, Available from: https://www.3ds.com/products-services/simulia/products/abaqus/.
33. Graphical User Interfaces with Tk, Python Software Foundation, Available from: https://docs.python.org/3/library/tk.html.