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

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Abstract

To truly enable the benefits of Integrated Computational Materials Engineering, particularly when considering materials at multiple length scales, a framework that enables seamless communication between simulation tools is necessary for material optimization and design of 'fit-for-purpose' materials. The Automated Information Management Across Organizations and Scales (AIMAOS) program developed at NASA GRC offers users an interactive graphical user interface for connecting material information management systems with both commercial and in-house simulation tools at various length scales to enable judicious automation in the handoff across scales and maintenance of material digital twins and the digital thread. As changes are made during material optimization at a given length scale, information is automatically propagated upstream to higher scales, and changes made are automatically tracked to maintain traceability and transparency during design. The AIMAOS tool serves as the first step in enabling optimized design of composites from the nano to the macroscale for a given application.

Introduction

Integrated Computational Materials Engineering (ICME) has received growing emphasis due to its potential benefits with regards to reducing material testing, product design and development cost, and time-to-market for new materials and applications. By relying heavily on simulations that are able to capture material behavior at multiple length scales and replace expensive physical testing, ICME design practices offer the ability to produce 'fit-for-purpose' materials, thereby rapidly accelerating the design process for structural applications [1, 2]. Consequently, ICME is heavily predicated on having experimentally validated multiscale models and methodologies that embody processing-structure-property-performance (PSPP) relationships across multiple length and time scales and firmly establish the integrated connection between structural engineering (denoted as 'designing with the material') and material science (denoted as 'designing the material') (Figure 1). Because it is infeasible to have one simulation toolset that can capture mechanics that occur at each individual length scale, ICME design practices will have to rely on the interaction of multiple, specialized simulation tools. Thus, it is critical that an organization not only have the simulation capabilities at each appropriate scale, but also an integrated framework that can easily connect simulation tools, and the subject matter experts that can operate each toolset, together to facilitate the ICME process. Such a framework will need to be able to generate the required input for a given tool, run the analysis, and parse the output at the current scale for information needed at the next scale and associated simulation tool(s). Further, to enable material optimization and design of 'fit-for-purpose' materials, an ICME toolset framework must be able to seamlessly automate the handoff between scales and evaluate the performance of the material and structure at each scale.

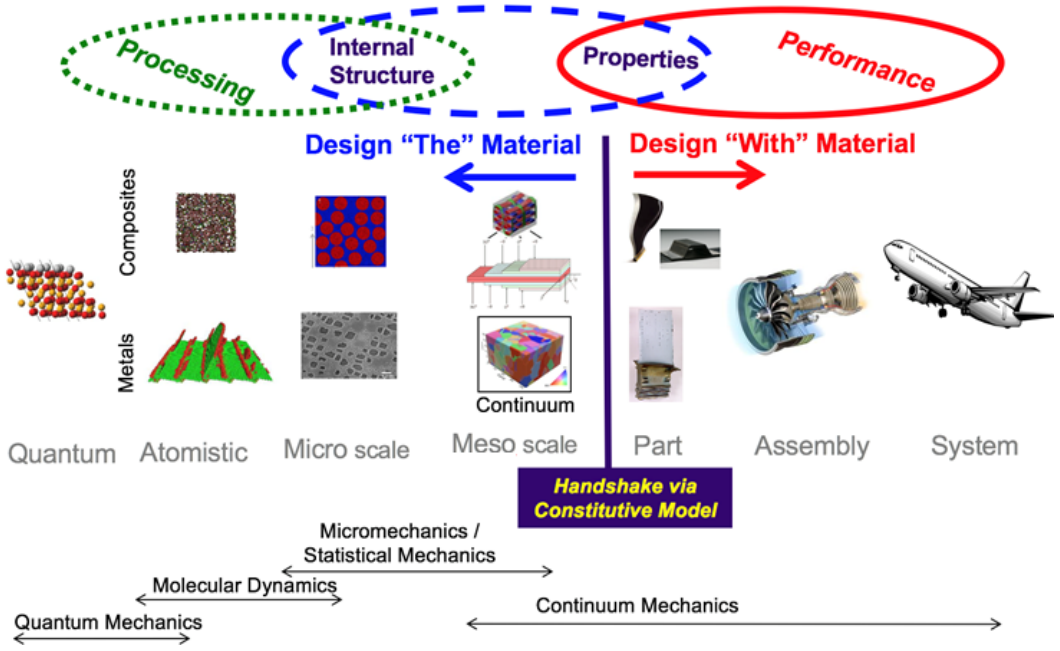


Figure 1.—Description of associated length scale dependence and modeling methods in the context of ICME

As organizations move to a simulation and data driven approach to integrated material and structural design, the amount of data generated at each scale and the need to link data across each scale to establish material and structural digital twins and maintain the associated digital thread(s) will require a robust information management system. Such a system will not only need to capture the entire material lifecycle (i.e., capture, analysis, maintenance, and dissemination, see Ref [3]), but will also have to interact with the multiscale simulation and analysis tools for automatic tracking of material and structural information for digital thread maintenance. At NASA GRC, an ICME schema for robust information material information has been previously established utilizing the Anays Granta MI platform, demonstrating the ability to store and link material pedigree information, virtual and experimental test data, developed material models, manufacturing information, and application information (Figure 2) [3, 4, 5, 6, 7]. Though each element of the schema shown in Figure 2 is important in establishing material digital twins, the Application table is the critical component to ICME design of parts and assemblies, as it serves as the link between the 'design the material' and 'design with the material' paradigms by linking all relevant material information for an application in a single location that can connect to relevant structural analysis tools (e.g., Product Lifecycle Management (PLM), Simulation Data Management (SDM), Computer Aided Engineering (CAE), etc.). The Application table also stores relevant analyses from structural tools, geometric information for the application, requirements for performance, material compatibility, manufacturing, and environmental considerations, and failure information. Thus, when properly integrated with a framework that can run simulations at given length scale, propagate information across scales (and/or organizations), and evaluate the defined requirements and criteria, the Application table serves as the "brains" behind an optimized ICME design of a structural component.

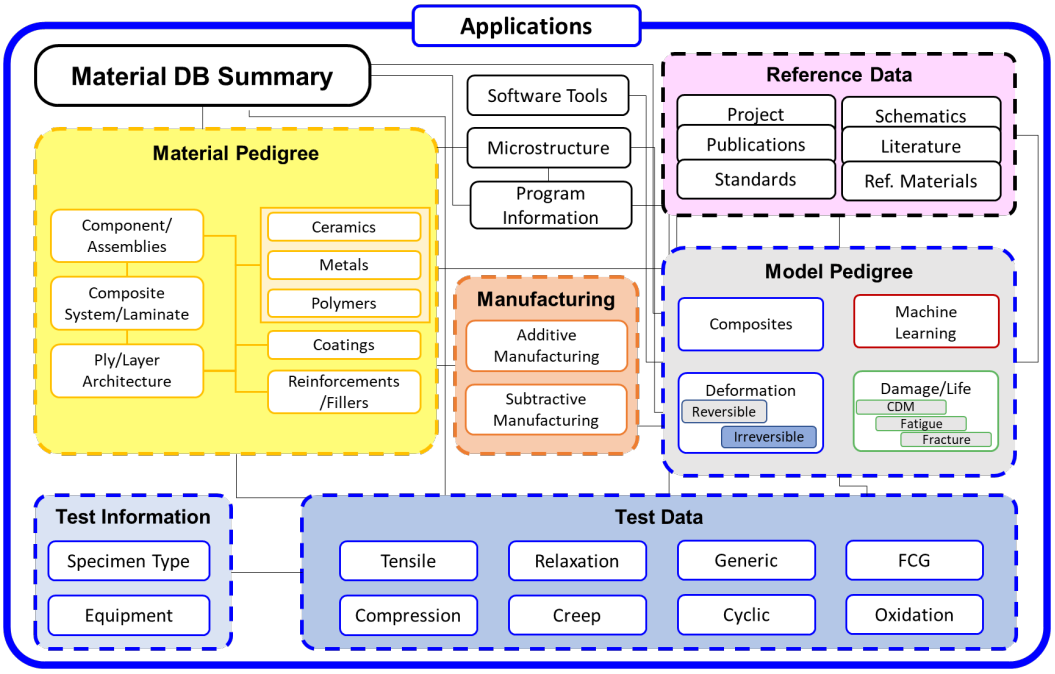


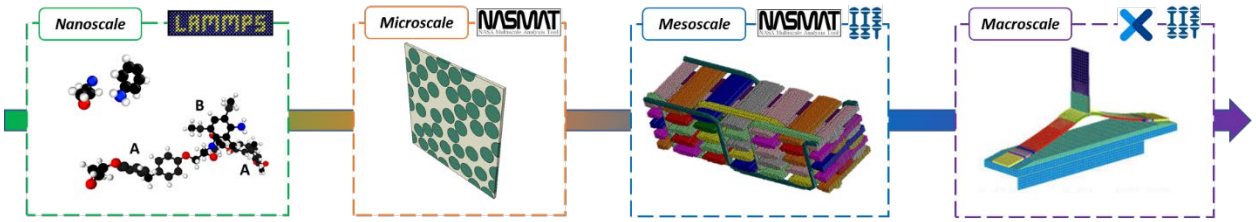
Figure 2.—NASA Glenn's ICME Schema for storing material information.

The objective of this work is to develop such a framework that can connect various multiscale analysis and simulation tools with the NASA GRC ICME Information Management System to enable optimized ICME design of 'fit-for-purpose' materials. Specifically, AIMAOS (Automatic Information Management Across Organizations and Scales), a Python tool developed at NASA GRC, is presented, which automatically conducts multiscale simulation of polymer matrix composites (PMCs), including nanoscale resin characterization, micro and mesoscale modeling of the lamina/laminate, and macroscale analysis of a structural component. The developed framework enables judicious automation of the composite analysis process by automatically writing and reading input and output files across the various length scales and conducting the appropriate analyses with current, propagated information, reducing both execution time and the potential for human error across all scales. Furthermore, the tool is able to track how the digital thread evolves as changes are made at each scale, providing both version control history critical for information management best practices and providing relevant metadata that can be leveraged for future material design. Thus, the presented framework acts as a necessary first step in development of an ICME optimization scheme for 'fit-for-purpose' materials and application design.

Methodology and Use Case

To demonstrate the features and benefits of AIMAOS, the use case of optimizing the composite Y-joint of the Aurora D8 aircraft through an integrated, multiscale material and structural modeling approach is shown. This work was first presented as a collaborative effort between University of Massachusetts Lowell, Michigan Technical University, NASA, Aurora, and Collier R&D in Ref [8]. The purpose of this effort was to demonstrate the potential benefits of implementing an ICME approach to design as opposed to traditional engineering practices, considering molecular dynamics simulations of the cure kinetics of the resin, micromechanics simulation of lamina with representative microstructure, effective property determination of the laminate at the mesoscale, and geometric optimization of the laminate stacking sequence at the macroscale (Figure 3). The program was successful in demonstrating the benefits of an ICME approach, finding a 17% savings in manufacturing costs and a 30% weight reduction 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 and a ratio of manufacturing cost savings to the investment of additional material cost produced a return on investment of 200:1 (see Ref. [8]). The ICME process utilized in Ref. [8], however, relied on team members across various organizations to *manually* 1) create input files for the analysis at each scale, 2) run the analysis, and 3) extract and pass the necessary outputs to the next team member (at higher length scale) for input. Thus, the design process was open to potential human errors and inefficiencies, and a true optimization of the material and structural design could not be accomplished. Consequently, 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.



(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

NASA Multiscale Analysis Tool

- Determine homogenized lamina and laminate properties given constituents and microstructure
- Determine macroscale strength allowables by performing various monotonically loaded simulations

ABAQUS

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

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

The AIMAOS software looks to address these inefficiencies and potential sources for error by replacing the manual processes described above. The AIMAOS Graphical User Interface (GUI) gives users three options: defining a new material, viewing the material library, and conducting an analysis. Defining a new material allows the user to define a multiscale material, wherein at each of the considered

scales a material digital representation (possibly a twin[1]) is defined. Users can define constituent properties used in microscale analysis (i.e., fiber and matrix with molecular dynamics results for cure kinetic characterization), laminas (i.e., a fiber, matrix, and associated microstructure that exist in the library), and laminates (i.e., stacking sequences of defined lamina in the library). In AIMAOS, each scale and subsequent material is configured to the NASA GRC ICME Schema (see Figure 2) to create a unique record with an associated global unique identifier (GUID). GUIDs are then linked across each scale to establish the digital thread for the multiscale material. For defined lamina (Figure 4a) and laminates (Figure 4b), the NASMAT multiscale analysis tool is called with the appropriate material properties from the next lowest length scale. The AIMAOS software is able to read the information from the database, automatically write the appropriate input deck, call the NASMAT executable, parse the output from NASMAT, and write the new record to the database. The input and output files from NASMAT serve as digital representations/twins for the material at that length scale (thus constituting part of the digital thread for the application) and are subsequently stored within each material record.

Viewing the material library in the GUI allows users to view what materials at each scale have already been defined, and to make changes if desired. If a change is made to a material at a given scale, a new version of that material (i.e., a new record in the database with a new GUID) is created. Additionally, any records in the database that have the original material GUID linked are also automatically updated without user intervention to ensure the digital thread of the material is maintained. 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 4a 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 4b 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 AIMAOS software additionally tracks what change has occurred, and why it has occurred, for a given material between subsequent versions, such that users can quickly determine what prompted a new analysis to be run. This information can be further leveraged when AIMAOS is paired with an optimization scheme for material design to determine what changes yielded optimal material design.

[1] A digital representation becomes a twin (and vice versa) when the real entity (herein material at current length scale) matches a set of requirements (i.e., chemically, mechanistically, geometrically, etc.) within a given tolerance, see Ref [9].

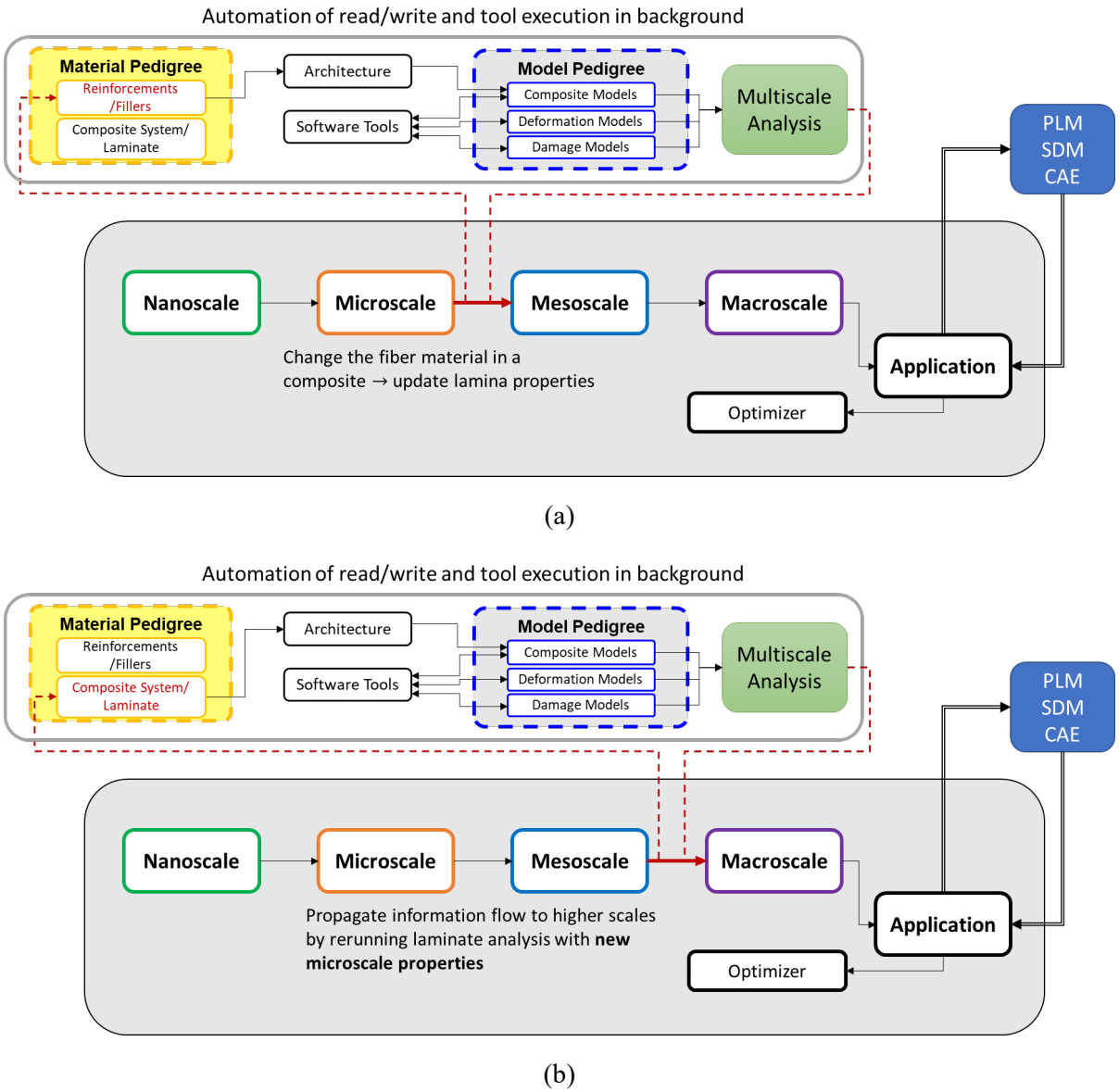


Figure 4.—Example AIMAOS Workflow and Information Management System Interaction for Changing Material Properties at the Microscale: (a) Updating of mesoscale properties based on the user input and (b) Automatic propagation of information at the macroscale

The Conduct Analysis option in the 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. If materials at the micro and mesoscale aren't already present in the database, the tool allows users to defined them in this window and perform the same functions outlined in defining new materials. Macroscale structural analysis of the Y-joint for geometrical optimization is carried out with the rapid design tool HyperX [10]. 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, which is populated via connection and material selection with the NASA GRC ICME material information

management system, is read by the preprocessing Python script along with other relevant variables which serve as an input to HyperX (user_material in Figure 5). 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.

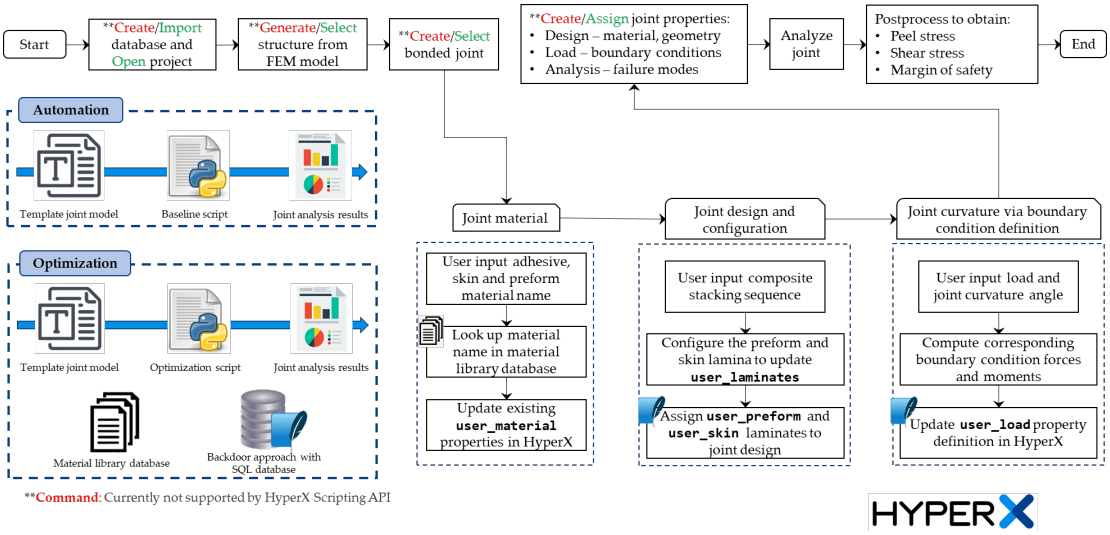


Figure 5.—Macroscale Optimization Framework

AIMAOS for ICME Material and Structural Design and Optimization

AIMAOS currently enables automatic tracking and propagation of information across multiple length scales as a composite design evolves, but relies on the user to make each material change after viewing and evaluating the macroscale solution. To obtain a true 'fit-for-purpose' material, an ICME design process should rely on optimization techniques to make the appropriate material decision(s), thus kicking off the next iteration of information propagation automated by AIMAOS (Figure 6) in an efficient manner to minimize a single or multi objective function (weighted combination of cost, weight, manufacturability, etc.). The "Evaluate" portion of Figure 6 should be able to make inverse design decisions, indicating what aspects of lower length scale parameters need to be changed in order to meet the requirements at the macroscale, then rely on the AIMAOS software to propagate the lower length scale changes for evaluation and iteration in the optimization scheme. 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 hierarchical manner and enabling both an optimized material and geometric design for an application.

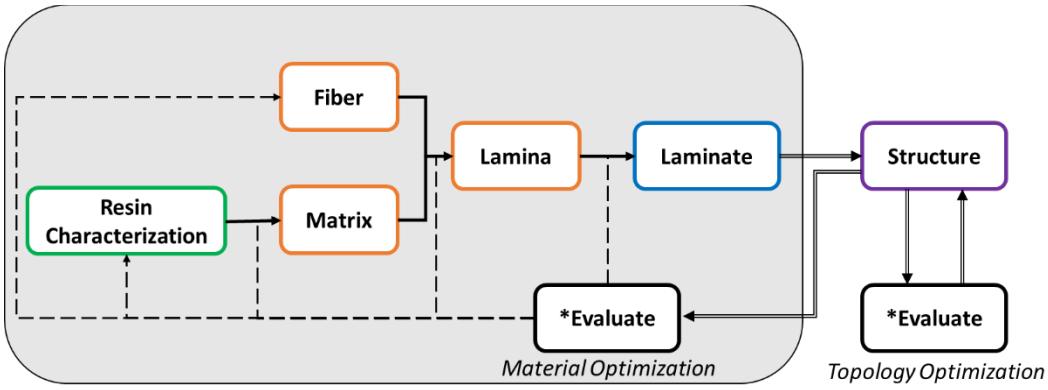


Figure 6.—Schematic of the Iteration/Optimization Scheme Required for Composite ICME Design

To successfully implement an optimization scheme and achieve an optimal material and structural design, it will be necessary for the application to have well defined metrics and requirements that can be used to develop an objective function, as well as the means to evaluate those requirements and objectives from the provided solution. Thus, it is critical that AIMAOS be paired with an information management system that not only stores material information, but also captures structural information, as is done in the Application Table in NASA GRC's ICME schema. As stated in Section 2, the Application table serves as the brains behind an ICME design process by bridging the gap between the material science and structural engineering paradigms, offering a connection point between the two sides of application design. With a robust data management schema for storing application requirements, an effective framework for multiscale material optimization, and a framework for structural/topology optimization of applications given a set of material properties, a concurrent material and structural ICME design of specific applications can be achieved. The AIMAOS framework is employed to optimize the material for a given application geometry, which periodically (condition based) will connect with the structural optimization scheme via the Application table to update part geometries, given the current material(s). This interaction between the material design and structural design will capture any "lurking failure modes" and thus minimize resource utilization. Such an integrated schema should enable true ICME design, significantly reducing material and manufacturing cost.

Conclusions

ICME has received a large increase in attention in recent years due to its ability to reduce cost, time, and effort associated with engineering design and offering tailorable, 'fit-for-purpose' materials for a given application. Recent work has demonstrated and benchmarked the potential benefits ICME can offer, but also identified current shortcomings revolving around human inefficiencies when dealing with various multiscale toolsets for simulation and organizations. To help alleviate these shortcomings, manage material digital representations/twins at each length scale along with the associated digital thread, and develop the necessary framework for material optimization, the AIAMOS software was developed at NASA GRC. AIMAOS allows users to create digital representations/twins of materials at each length scale, connected with a robust information management system, and chain together toolsets to automatically traverse length scales for a given application. Further, the software is able to automatically propagate information across scales by connecting with each multiscale analysis tool when material changes are made at lower length scales and track the changes made with effective version control and history tracking, allowing for smarter, faster material iteration. The AIMAOS program (although currently limited to composite materials) 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 general material and structural design.

References

[1] X. Liu, D. Furrer, J. Koster and J. Holmes, "Vision 2040: A Roadmap for Integraded Mulitscale Modeling and Simulaiton of Materials and Systems," *NASA/CR-2018-219771.*

[2] J. Llorca and e. al., "Multiscale Modeling of Composite Materials: a Roadmap Towards Virtual Testing," *Adv. Mater.,* vol. 23, no. 44, pp. 5130-5147, 2011.

[3] B. Hearley and M. Arnold, "NASA GRC ICME Schema for Materials Data Management: An Executive Summary," *NASA TM-20230018337,* 2023.

[4] S. Arnold, F. Holland, T. Gabb, M. Nathal and T. Wing, "The Coming ICME Data Tsunami and What Can Be Done," in *54th AIAA/ASME/ASCE/AHS/ACS Structures, Structural Dynamics, Materials Conference*, Boston, MA, 23-27 April 2013.

[5] S. Arnold, F. Holland Jr. and B. Bednarcyk, "Robust Informatics Infrastructure Required for ICME: Combining Virtual and Experimental Data," in *AIAA SciTech Forum*, National Harbor, MD, 13-17 January 2014.

[6] B. Hearley, S. Arnold and J. Stuckner, "A Robust Machine Learning Schema for Developing, Maintaining, and Disseminating Machine Learning Models," *NASA Technical Memorandum 20220017137,* 2022.

[7] 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.

[8] 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.

[9] AIAA Digital Engineering Integration Committee, “Digital Thread: Definition, Value, and Reference Model.” American Institute of Aeronautics and Astronautics (AIAA), June 2023

[10] *HyperX,* Available from: https://hypersizer.com/hyperx/.