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NASA GRC ICME Schema for Materials Data Management: An Executive Summary

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Abstract

Integrated Computational Materials Engineering (ICME) has received a growing emphasis in attention due its potential impact on rapid material design, reduction in cost and time to market for new applications, and the promise of 'fit-for-purpose' materials coupled with recent advances in high performance computing and material characterization tools. However, for an organization to implement ICME practices for material discovery and design, a series of both technical and cultural challenges must be overcome to foster an environment that enables efficient, traceable, and predictive multiscale simulations of material behavior to enable virtual design of materials. In 2016, NASA sponsored a 2040 Vision study to define the potential 25-year future state required for integrated multiscale modeling of materials and systems to improve both the associated time and cost for aerospace and aeronautical innovation. The study envisions a cyber-physical-social ecosystem of experimentally validated computational models, tools, and techniques, along with the associated digital tapestry, that can enable rapid, optimized, 'fit-for-purpose' design of materials, components, and systems.

A key requirement for such an ecosystem is the development of a robust information management system for materials across their full lifecycle, including material pedigree, experimental (real) and virtual (simulation) data, developed material models, and the implementation of models in engineering applications, such that process-structure-property-performance relationships can be established, thereby enabling the virtual design and optimization of materials. Such an information management system must be able to effectively capture: i) material information at each length scale; ii) test data and analysis; iii) associated material models; and iv) material and model deployment in engineering applications. These systems must also provide traceability between experimental and virtual representations of the material to ensure, when appropriate, the material digital twin is maintained. Additionally, this robust material information management system must be able to seamlessly connect with both commercial and an organization's in-house software tools, be they analysis tools, other material databases, product lifecycle management (PLM) or simulation data management (SDM) tools, etc., such that automation of the design and analysis of a material across multiple length scales is possible. In this paper, an executive summary of the NASA GRC ICME Schema for materials information management is presented. The database best practices and schema design philosophy specifically for ICME materials data management and an overview description of each element in the schema is given, along with its associated role in an ICME workflow. Additionally, auxiliary tools that interact with the database and provide judicious automation with regards to importing, exporting, and analyzing materials data are presented. Such tools are critical to an ICME ecosystem, not only for their role in enabling optimization, but also in relieving users of tedious manual tasks, thus helping to promote adoption and combat the cultural challenges organizations face in enabling ICME.

Table of Contents

1.0 Overview

With an increased focus on reducing the time and cost to market for new materials, Integrated Computational Materials Engineering (ICME) has become a fast-growing discipline that looks to address the issues associated with traditional approaches to material development. Further, top performing organizations in the aerospace and defense, automotive, chemical, electronics, and energy industries have rated new materials as one of the most important factors in meeting their innovation goals, in particular performance and cost [1]. ICME is an integrated approach to material design that links material models at multiple time and length scales (utilizing simulation-based methods to design with optimization and high performance computing) to enable rapid 'fit-for-purpose' material design for the engineering of a given application [2]. Essential to ICME is an understanding of processing-structure-property-performance relationships across the various length scales. Figure 1 illustrates how these critical relationships transverse the multiple length scales present in a material and application, and the cause/effect relationship between scales, thus signifying the importance of effectively passing information from one scale to the next in an integrated material design approach [3, 4]. Note that the evolution of elliptical line types (i.e., dotted to dashed to solid line) are purposely included to imply an increasing level of maturity/understanding of modeling at each level of scale (both temporal and geometric). Also illustrated in the figure is a distinction between the "design 'the' material" (a material scientist viewpoint) and "design 'with the' material" (a structural analyst viewpoint) as the scales are traversed, with the handshake between these two paradigms being represented by the material constitutive model, albeit deformation or damage.

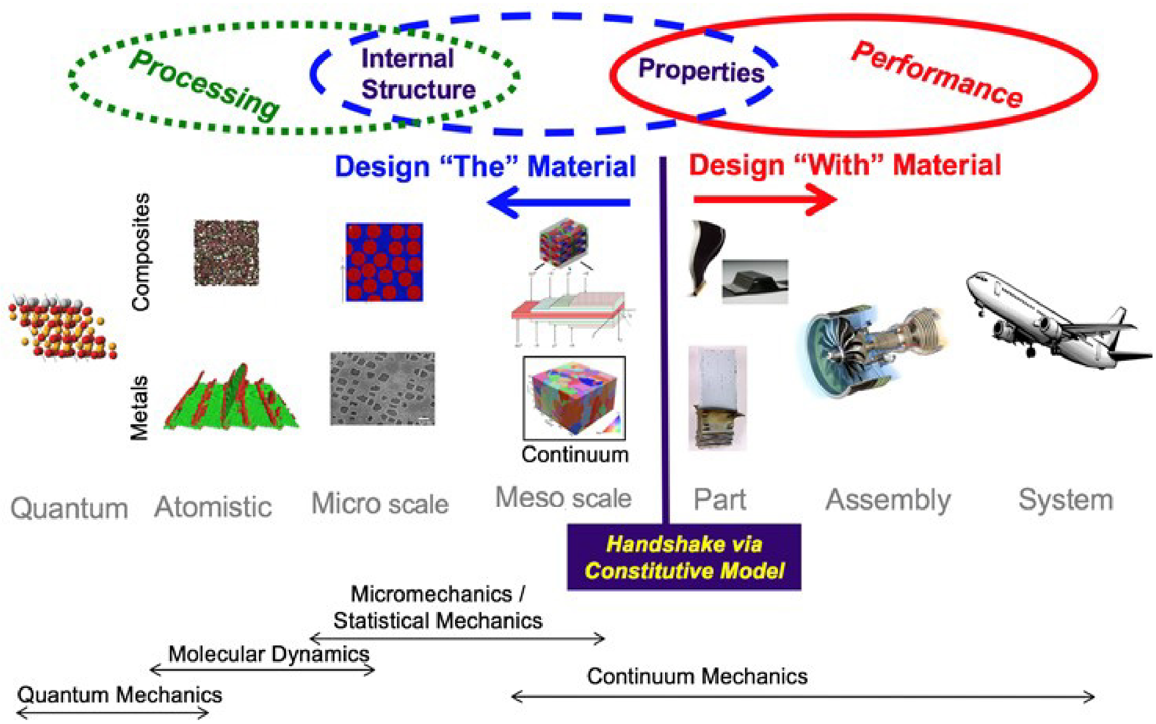

Figure 1.—Description of Associated Length Scale Dependence and Modeling Methods in the Context of ICME

In order to embrace the benefits that an ICME approach to product design can offer, a series of challenges must be overcome, both technical and cultural, as outlined by the National Research Council report on ICME by the National Materials Advisory Board (NMAB) committee [5]. First, ICME will require the development of predictive material models at the various length scales outlined in Figure 1.

These models must be compatible with multiprocessor and parallel processing capabilities to meet the high computational demands and must be able to link together with other models to perform multiscale simulations. Additionally, ICME will require a "cyberinfrastructure" in which tools, models, and databases can be integrated together to enable multidisciplinary analysis, cross-discipline collaboration, automation of workflows, and design optimization. Another key element from the NMAB committee report is the importance of linking experimental data to modeling through open-access database creation. Databases in an ICME infrastructure must be able to handle various formats of data, effectively capture multiscale material information, and provide the means for an ICME expert to find and connect important information when ICME tools are used in product design. Finally, perhaps the greatest challenge outlined relates to organizational culture changes – to realize the true benefits of ICME, the gap between the material scientist and structural engineer must be closed and the adoption of new practices and tools for ICME must be embraced by both research organizations and industry. Many of these aspects, as well as others, were substantiated in the more recent NASA 2040 Vision report, released in 2018 [6].

The NASA 2040 Vision report outlines a comprehensive study to define a potential 25-year future state for ICME, developed in collaboration with both academia and industry, which will identify the challenges and requirements needed for accelerated material design and a data-driven ecosystem for materials discovery/design. The report outlines 118 critical gaps, both technical and cultural, that face the multiscale modeling community and 180 actions to overcome those gaps across nine different Key Element areas to achieve the end goal vision by the year 2040. One of the Key Elements identified in the report focuses on 'Data, Informatics, and Visualization', including methods for capturing, analyzing, storing, and disseminating data, developing technologies for accessing and sharing data, and connecting information management systems with experiments, simulations, and manufacturing across various users and organizations. Within the 'Data, Informatics, and Visualization Key Element', 21 gaps are identified, focused on effectively storing and sharing data, developing the infrastructure for data management tools to interact with state-of-the-art data analytics platforms, establishing well-defined standardized schema, and overcoming cultural challenges and lack of organizational buy-in. To overcome these gaps, the report recommends the development of established schema standards and protocols, tools and templates for building data management plans, automation of data ingestion and storing, and creation of user-friendly tools and interfaces with simulation tools and data management that can help promote cultural adoption for materials data management. As a result, a large effort at NASA GRC has been placed on addressing these gaps in the area of data informatics to enable the overarching ICME landscape envisioned.

An ICME approach to material design is inherently dependent on material modeling and simulation-based design, with effective handoff of information across the various length and time scales to achieve optimal structural performance. It is critical that material models used in an ICME approach are experimentally validated at each scale, ensuring that the real-world performance matches that of its simulation-based counterpart, thus establishing a digital twin for the application. Additionally, the use of machine learning methods to build surrogates for such multiscale models will play a large role in the future of design of 'fit-for-purpose' materials through ICME, leveraging parallelization and high performance computing to enable the implementation of such modeling techniques for part and assembly level simulations in a realistic time frame. Combining multiple validated models (be they physics based or data driven) for a given design requires a large amount of data and meta data, and thus a **robust data management solution** that can store material pedigree information, test (experimental) and virtual (simulation) data, and link data together to establish a digital thread [7] with full traceability across the various scales is of critical importance [8]. Particularly in the case of machine learning, data management is essential to properly understanding the model intended use case, training bounds, and limitations, since the physics is purely 'simulated' by the surrogate model, resulting in improper use of the model giving entirely incorrect results. The existence of such a data management system is paramount [9, 10, 11, 12] to making ICME a reality and has prompted the design of a 21st century information management system (denoted herein as the NASA GRC ICME Schema) for capturing, analyzing, disseminating, and maintaining material information necessary to enable physics-based and data-driven modeling and determination of microstructure/property/failure relationships for various types of materials (Figure 2).

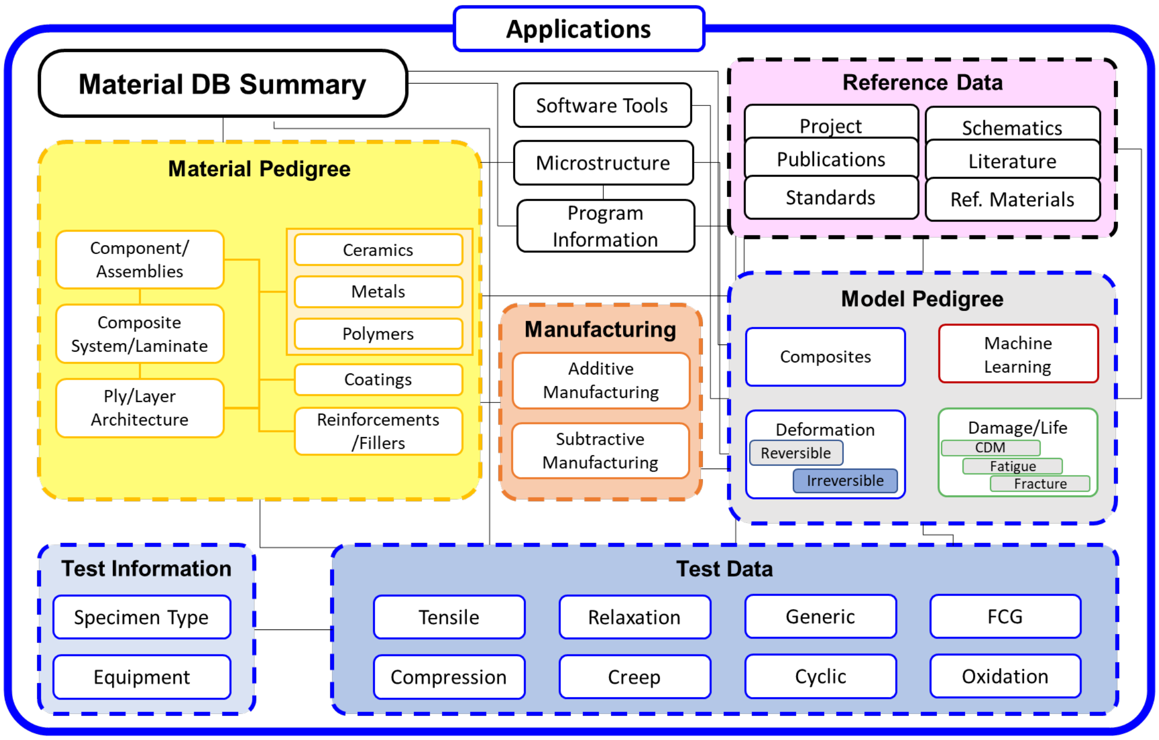

Figure 2.—NASA GRC ICME Schema

More recently, the Application table was added to the ICME schema (see the over-arching "Applications" box in Figure 2); 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) [13]. Because the Application table acts as this interface between the materials information and the structural paradigm, it contains interactions with all of the other collections (dashed boxes in Figure 2) with linkages to many tables, and is thus represented in the figure as 'encompassing' the other tables as opposed to having each individual link (black lines in Figure 2) defined. 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 finite element analysis (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, bridging the gap between the material scientist and structural engineer viewpoints.

The purpose of this executive summary is to identify the key elements, requirements, and proposed solutions for a robust information management system that can enable ICME design. Furthermore, additional tools developed that interact with the database are presented that help to build the "cyberinfrastructure" outlined in the NMAB and NASA Vision 2040 reports. In the remainder of Section 1, the database best practices and overall philosophy of the NASA GRC ICME Schema are defined, which govern the design of the schema. In Section 2, an overview of Granta MI, the commercial materials information management platform used to host the NASA GRC database, is given. In Section 3, the individual categories of the NASA GRC Schema are presented, including a description of the purpose of each category and its proposed interaction with the rest of the database. In Section 4, the auxiliary data management tools are described that both assist in the ICME process and help to promote cultural adoption. Finally, in Section 5, conclusions on the development of an ICME database schema are given.

1.1 Database Best Practices

Data for design is one very important application for materials information in today's engineering enterprises. There are many others—examples include: materials modification and new materials development, materials selection and purchasing, statistical process control, generation of 'allowable' stress levels for design, regulatory compliance, certification, and quality control and characterization and validation of models (e.g., constitutive, life, processing, etc.). The Material Data Management Consortium (MDMC)[1] has defined the material data *lifecycle* in an engineering organization as:

1. Capturing / consolidating materials data
2. Analyzing materials data
3. Managing and maintaining the information resource
4. Deploying and using materials information.

Clearly, this lifecycle can be applied similarly to other types of data associated with constitutive models, software tools in general, documentation/reference data, etc. In general, data is captured and consolidated from external sources, legacy databases, and internal (possibly proprietary) testing programs. Next, data is analyzed and integrated to create/discover useful information pertinent to the various length scales. The third and essential stage of the data lifecycle is the continual maintenance of the whole system (the data and information generated as well as the relationships, or links, between them) in an information management system that can preserve information for future use, with the last but crucial step being the deployment (dissemination) of the right information, at the right scale, to the right people, at the right time and in the right format.

To support the various activities throughout the data lifecycle, it is preferable to have a single, central source in which all relevant data is captured and consolidated from "birth" to "death" and the (preferably seamless) integration of a variety of software tools. These tools range from i) data importers/exporters; ii) reduction/analysis; iii) visualization; iv) reporting tools; v) process/microstructure/property/performance models (in the case of ICME); vi) material parameter estimation tools (of both actual and "virtual" materials); vii) statistical and other analyses to reduce the data to a form usable by designers and analysts—for example calculation of 'design allowables'; and viii) structural analysis codes that utilize a central database. Note that the models and tools listed in (v) through (viii) can operate on a variety of different length scales, thus potentially requiring scale-specific attributes [6]. If the predicted properties (i.e., virtual data) are stored in the database as well, then it is straightforward to validate such methods and models by direct comparison with actual test data. These tools should enable material and structural engineers to input, manage, and utilize information in an efficient, reliable, and user-friendly way (e.g.,

[1]A group of aerospace and energy sector organizations (both industrial and governmental) that joined forces to develop best practices and associated software tools to integrate material and structural information technology with the realities of practical product design and advanced research. https://www.grantadesign.com/industry/collaborations/consortia/mdmc/

GUI and APIs). Finally, these tools should also enable enterprise-wide (even world-wide) solution or access. In practice, such information exchanged is complicated by the fact that most organizations must deal with a federated system of data sources (be they dynamic or archived) and tools, thus making the integrity of the digital thread both challenging and critical. Consequently, to assist technologists to be good stewards of scientific and engineering data, guidelines that define what it means to make data Findable, Accessible, Interoperable, and Reusable have been established, i.e., the FAIR principles [14]. Implementing these guidelines throughout the material lifecycle has driven the development of the NASA GRC ICME Schema requirements and best practices. The schema presented herein serves as an inclusive starting point for any organization looking to implement material information management with a focus towards ICME, but can, and should, be modified based on the individual needs of each organization.

1.1.1 Capture

To maximize the impact on the material and structural discipline practitioner and/or researcher, data beyond specific, predefined (generally accepted) point-wise property values/information needs to be captured from both tests and simulations. In fact, it is essential that a best practice software infrastructure i) has the ability to capture a material's fundamental multiaxial response spectrum (under a variety of loading conditions), along with its full pedigree (e.g., chemistry, processing, heat treatment, microstructure, testing information, etc.) for subsequent analysis and modeling; ii) has the ability to capture the application potential of a given material system, be it monolithic, composite, multifunctional, etc.; and iii) enables contextual linkage and association of tacit (or hidden) knowledge (e.g., insight, intuition, skills, experience and other knowledge that has not been formally shared) within a given organization [15].

1.1.2 Analyzing Materials Data

For most organizations, a corporate materials database is a dynamic resource—they want to continually add data and analyze that data to generate new or updated information. This requires software that can process, manipulate, and perform calculations based upon the data. For example, materials experts need software to process raw materials test data and analyze it to create approved design data for wider publication. They must update and refine this information and prepare it for use in specialized applications, such as statistical process control or constitutive-life modeling. Whatever the exact nature or source of such software tools, best practice materials information management requires that these tools:

- Perform well *together,* combining to offer the range of analyses required by materials scientists and engineers—from single test results, to multiple points, to multiple curves.
- Be fully integrated with the information management system, so that data and meta data is extracted directly into the analysis tool and results are saved directly back into the correct locations in the database
- Have their results be permanently linked to raw input data and the details of the analyses performed to maintain full traceability.

1.1.3 Maintaining Materials Information

Establishing a "gold source" of materials information is not enough, as this source must also be protected, nurtured, and maintained. Several data management features are critical to this process: i) traceability, ii) access control, iii) version control, and iv) data quality control. Perhaps the most important requirement for best practice materials information management is the ability to trace relevant information on the materials beyond their property data. Knowing a "material's pedigree" or "model pedigree" information can help users understand and correctly apply the materials/models in component designs and constructions. It also provides important information (processing, microstructure, etc.) and references required for improving the materials properties or developing new materials. Design of the data schema becomes the major issue in ensuring traceability. Note that to enable both high traceability and high scalability, separating the individual data categories listed above and connecting them with adequate links becomes an essential attribute of any ‘fit-for-purpose’ information management system. For example, in NASA Glenn’s data schema (see Figure 2) the microstructure information is located in a separate table, thus enabling one to go directly to this table and quickly locate typical microstructural images, and then trace backwards through the links to the raw test results. However, for microscopy information associated with changes during (due to either mechanical or thermal loading) or subsequent (failure surface analysis) to testing, this information is typically specimen-specific and thus stored in the specific specimen record. The above comments on data traceability (i.e., the capturing of a model’s pedigree) are just as applicable to the material’s associated models, parameters, and simulation data, given all types (e.g., process-internal structure, internal structure to property, and property to performance) of models and scales. To ensure traceability exists across the different data and to reduce the overall size of the database, thus reducing maintenance efforts, it is best to, when applicable, *define* data only once in the database, and use linking to *view* that data elsewhere in the database. With this best practice, if a change needs to be made to the data, the change need only occur in one location, thus ensuring no digital threads are broken and no incorrect, outdated, or out-of-synch information exists in the database. In addition to ensuring data is well-defined and traceable, organizations must also be ensured that their data is available and well-maintained such that data is not lost and can be re-used for future projects, development, etc. Thus, organizations should have procedures in place to ensure data is regularly backed-up and, more importantly, can be easily restored from a backed-up version if data is lost or corrupted. Furthermore, an effective data management system should not only prohibit those unauthorized to see data via access control, but should also ensure that those who are authorized to view data have that capability throughout the data lifecycle.

1.1.4 Dissemination of Information

For multiple reasons (e.g., competitive, legal, regulatory, and even, in some applications, national security), it is important to ensure that data is seen only by those authorized to see it. Usability is also a factor—for a massive database, many applications are easier if the user is only exposed to data that is relevant to their application. Further, in today’s global economy and international corporate environment, it is commonplace that a database is partially or conditionally shared among different divisions or partners. All this can be achieved through a feature known as access control. While simple in concept, this can be complex to implement in practice, particularly in the context of federated data sources. For maximum flexibility, access control should operate at as low a level as possible in the database, such that any single item of data (attribute) in the database can be assigned an access control status that determines whether and how it is presented (e.g., based on the user’s login information). This feature is essential when desiring to develop an ICME specific database, since typically all process related details (which directly impact microstructure) are export controlled (i.e., EAR (Export Administration Regulation) or ITAR (International Traffic in Arms Regulations)) and thus a coarser-based system (e.g., record, table, or database level security system) would make significant portions, if not all, of the database unavailable to the larger community.

Change management can be a major issue in any evolving (albeit dynamic or archival) database; consequently, a version control system is often a required feature, as it allows the database to store the history of any record, dataset, or item of data, including explanations for any changes made. In addition to adding a further level of traceability to data, it enables control of the process by which updates to the database are made and published. For example, it could be configured such that publishing new data of particular types requires specific approvals. This assures the user that they are seeing the most recent approved data, and also allows changes to be traced and analyzed in previous versions of the data, which may have been used in a design project. In NASA Glenn's current Granta MI configuration, the Data Status access control category (approved or unapproved) is utilized in place of version control, even though Granta MI supports version control.

Data users or producers typically assess data quality. Consequently, when materials property data from different sources are collected into a single database, it is desirable to either manually or automatically assign a "quality score" to the data. This enables users or software applications to determine the degree of confidence they may have in the information as well as its suitability for various applications. Further, when conducting ICME projects wherein multiple software packages/models at varying levels of scale will be used to predict specific outcomes (e.g., material properties) for use by tools at the current or higher scales, the concept of a 'P-basis'[2] or 'P-index' to indicate when a given parameter or "property" is calculated (or predicted—thus the P designation) is particularly important to consider, as is the uncertainty associated with that predication. This way, one can trace the percolation (through various scales) of the various data (be it real or virtual) and its potential impact (e.g., downgrading of quality, epistemic uncertainty) on higher scale calculations. Further, as more data is captured and assessed the quality index associated with P-basis may or may not change. Such a concept should also facilitate the specification/utilization of needed verification experiments or readiness levels (e.g., Technology, Manufacturability, Integration). Consequently, when establishing a quality rating, either manually or through an automated system, the quality of a set of data should be viewed as a function of the end use. The concept of a quality index attached to a given model's performance can also be used in a workflow algorithm to initiate a "re-characterization" of the model when its simulation capability (albeit correlative or predictive) exceeds a specified acceptance level. Unfortunately, often "quality" is a subjective thing and therefore can be very difficult for an organization to implement without significant controversy, though quantitative measures can be devised for automation purposes in some cases.

1.2 NASA GRC ICME Schema Philosophy

In the context of materials discovery or design through ICME, different organizations have different roles and desired outcomes for what should be accomplished through data-driven materials science. As a result, the design of the materials information management system deployed by an organization should match those objectives. Typically, academia and research institutions are more focused on actual material discovery (science), pushing the limits for new materials through various, often unique, research and development efforts. Industry, on the other hand, looks to leverage material data digitization and advances in research and development efforts to maximize return on investment, through material design (engineering) while still ensuring the materials they use are certified, consistent, and cost-effective [12]. Although NASA GRC is a research institution, and thus has many aligned goals with regards to effective data management as academia and other research labs, NASA is still interested in leveraging material informatics in actual part and assembly design for space and aeronautic research, including developing the infrastructure and traceability to effectively use data-driven materials science in its missions. Thus, NASA has a unique perspective, and consequently a unique information management schema design, that can be used by and bridge the gap between research and industry.

The NASA GRC ICME Schema outlined in Figure 2 is specifically designed to enable the development of processing-structure-property-performance relationships while following the best practices defined in Section 1.1. The schema is divided into a series of collections, denoted by the colored

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[2] As distinct from 'A-Basis' and 'B-Basis' properties as used in (for example) the MMPDS handbook to define 'allowable' material strength values at 95% confidence levels.

boxes in Figure 2, which group similar data that contribute to the establishment of these relationships. Within each collection, individual tables, represented by the white boxes within each collection, define a set of attributes (see Section 2.1) that applies to all records contained within (Figure 3). In general, a new table is created and added to a collection if a large number of attributes need to be added to an existing table to effectively capture data and the purpose of the data stored does not coincide with the purpose of an existing table, as outlined below in Section 3. Additionally. if data is repeated in multiple records, it is generally best to create a new table and link information to the existing tables so as to minimize duplication and human error, following the above defined best practices.

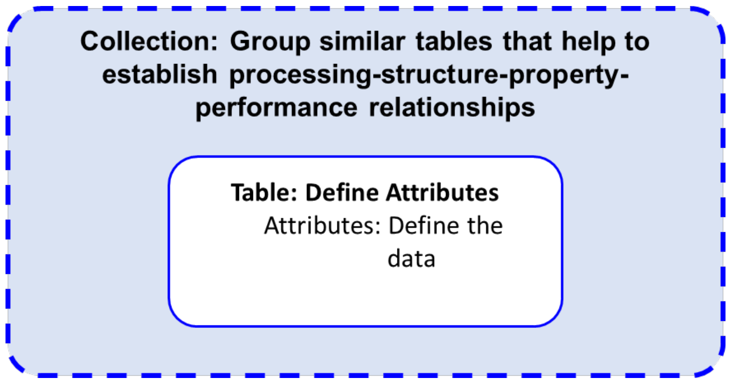


Figure 3.—Visual representation of Collections, Tables, and Attributes in the NASA GRC ICME Schema

In addition to the definition of the collections, tables, and attributes that comprise the NASA GRC ICME schema, the tree structure for viewing records in each table plays a pivotal role in ensuring data is findable, and thus deserves careful consideration during schema design. Note both schema and tree structure implicitly contain/communicate significant corporate knowledge relative to material information. In general, record and folder naming conventions should help direct the user to data and should be organized hierarchically by what is most important to a consumer of the data. Therefore, at each level in the tree structure, similar useful information is easily found by the user to reduce search time and improve efficiency when finding material information. For example, when finding Tensile Test Data in the NASA GRC ICME Schema, records are organized by material class, material name, test temperature, test strain rate, and finally the individual test. At each level in the tree structure, the user is then presented with all tests that meet the same criteria, which is further refined as the number of subfolders increases.

When designing a database schema for ICME, a major barrier that must be accounted for is cultural adoption, and a large deterrent to adoption of such a database can be the intimidation factor due to the complexity of the schema and various interconnection between tables. Thus, there is an existing tension between this intimidation and oversimplification, as well as attribute complexity vs database speed. In general, the best practice implemented in the NASA GRC ICME schema is to have the minimum number of attributes in a table that still fully define the data and its associated pedigree in order to reduce this intimidation factor and improve database performance. Profiles for different users can also be used to hide certain tables, records, or attributes from specific users to further reduce the perceived database complexity and only present relevant information to the user, allowing for some tailorability to each specific end-user. Additionally, the development of intuitive import and export tools should be developed for each table in the database, facilitating the process of capturing, maintaining, and disseminating data while simultaneously reducing the burden of the user, further promoting cultural adoption.

One major concern for any database solution revolves around data security. It is essential that any data management system has security measures in place that ensure data is only accessed by those authorized to see it. In general, security can be implemented in two different ways within the Ansys Granta MI system: record-based security, in which users are given access to an entire record and all of its attributes based on their credentials, and attribute-based security, in which security controls are assigned to each individual attribute and are hidden from the user if they do not meet the security requirement. The NASA GRC ICME Schema uses the attribute-based security control. Although this security measure is more complex and requires a larger effort by the database administrators who design the schema, it maximizes the information in a given record that any one person can see as opposed to hiding an entire record if only one attribute is restricted, thus improving the findability of data within the organization. In addition to restricting access via security controls, data should also be easily accessible by those who are authorized to view it, and should be easily restored from a previous version if data is lost or corrupted. At NASA GRC, backups of the database are performed every night and are archived daily (over the course of one week), weekly (over the course of one month), and monthly (archived indefinitely), such that data a previous instance of the database can be restored from any one of the archived instances. Additionally, the database platform chosen to host the NASA GRC offers a license in perpetuity, such that NASA GRC will always have access to their current instance of the database. As an additional measure for data security, the backups are written in a database neutral file format, such that data could be restored and transferred to another database platform if necessary.

When designing an information management system, for various reasons (security, separation of programs, etc.) organizations may choose to have multiple databases as opposed to one holistic database. Multiple databases are simpler to implement due to their specialized nature, but often need more sophisticated tools to maintain, synchronize, and update to ensure data maintenance. A single database is much more complex, due the additional tables, additional attributes, and complicated linking behavior, but can allow for better and more straightforward connectivity, comparison of different types of data, and schema synchronization. Issues surrounding database complexity are best mitigated by having clear, accessible documentation of the schema, including table purposes, expected linking behavior, and record organization, as well as well-developed training and instructions for users. The benefits of a single database are particularly applicable to an ICME framework, in which material design optimization may want to explore a large design space of different materials and processes, and the established linking between materials and their associated models is readily defined. Thus, a single database for materials information management is implemented in the NASA GRC ICME Schema.

The final decision an organization must make when creating an information management solution for ICME is to use either a commercial 3rd party database platform or develop one in-house. At NASA GRC, a commercial system is used due to its robust infrastructure, ability to connect to other commercial tools and in-house codes to enable automation, and its built-in security controls. Although the license fees of a commercial system may appear to be a large cost, the actual full cost (including the infrastructural development of the database, maintenance, updating of importers, exporters, and communication with other tools as each tool updates its software, and cost associated with having dedicated employees for database administration) of in-house development can far outweigh the cost of licenses for a commercial tool. Using a commercial database solution can further enable organizations to focus on development of ICME tools and technologies that they know best for database integration and automation of multiscale analyses and workflows to fully benefit from the potential of ICME. At NASA Glenn, the commercial tool Granta MI is used to host the ICME information management system.

2.0 Granta MI: Overview

Granta MI Enterprise is a material data management software system offered by Ansys that allows users to capture, manage, and share material information in an integrated relational database platform

[16]. The software package gives users access to both a variety of reference databases with vetted material properties for use in simulation and design, as well as the ability to create organization-specific databases for in-house material information. It offers a series of commercially available and maintained features and services that allows the tool to be an ideal candidate for managing data throughout the material lifecycle for both government and industry use.

The primary benefit of using Granta MI for material data management, particularly with the goal of achieving ICME design processes, is the ability to link data records to one another in the database, ensuring traceability of data created and maintenance of the digital thread across the material's various length scales. Furthermore, Granta MI enables data security through a fully customizable built-in access control system, in which designations for ITAR, EAR, Government Only, etc. as well as organization-defined user groups for reading and writing privileges for both entire data records or individual attributes within a given data record can be imposed (Figure 4). This security feature maximizes the data that can be consumed by each user while ensuring that for restricted or sensitive data, only the right people have access to view it. Granta MI also offers the ability to automatically generate material comparison charts/plots through selective user-defined criteria (Figure 5), enabling faster material selection and comparison of materials for design.

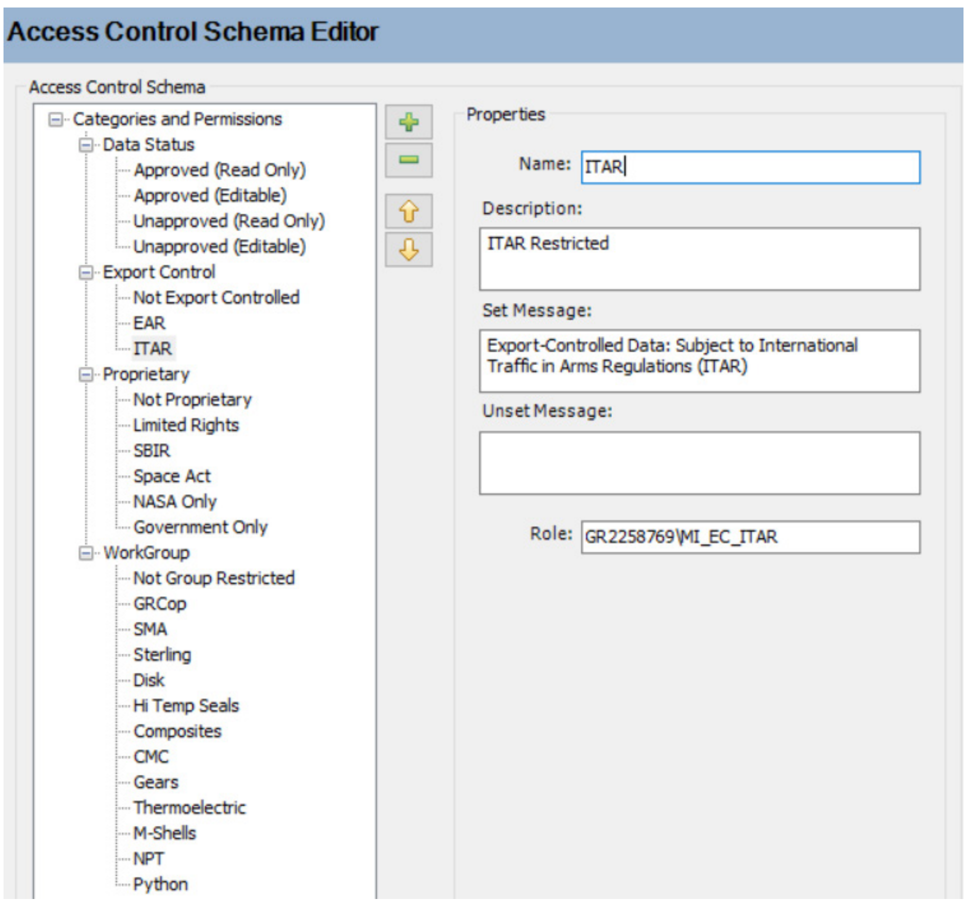


Figure 4.—NASA GRC Security Control Groups

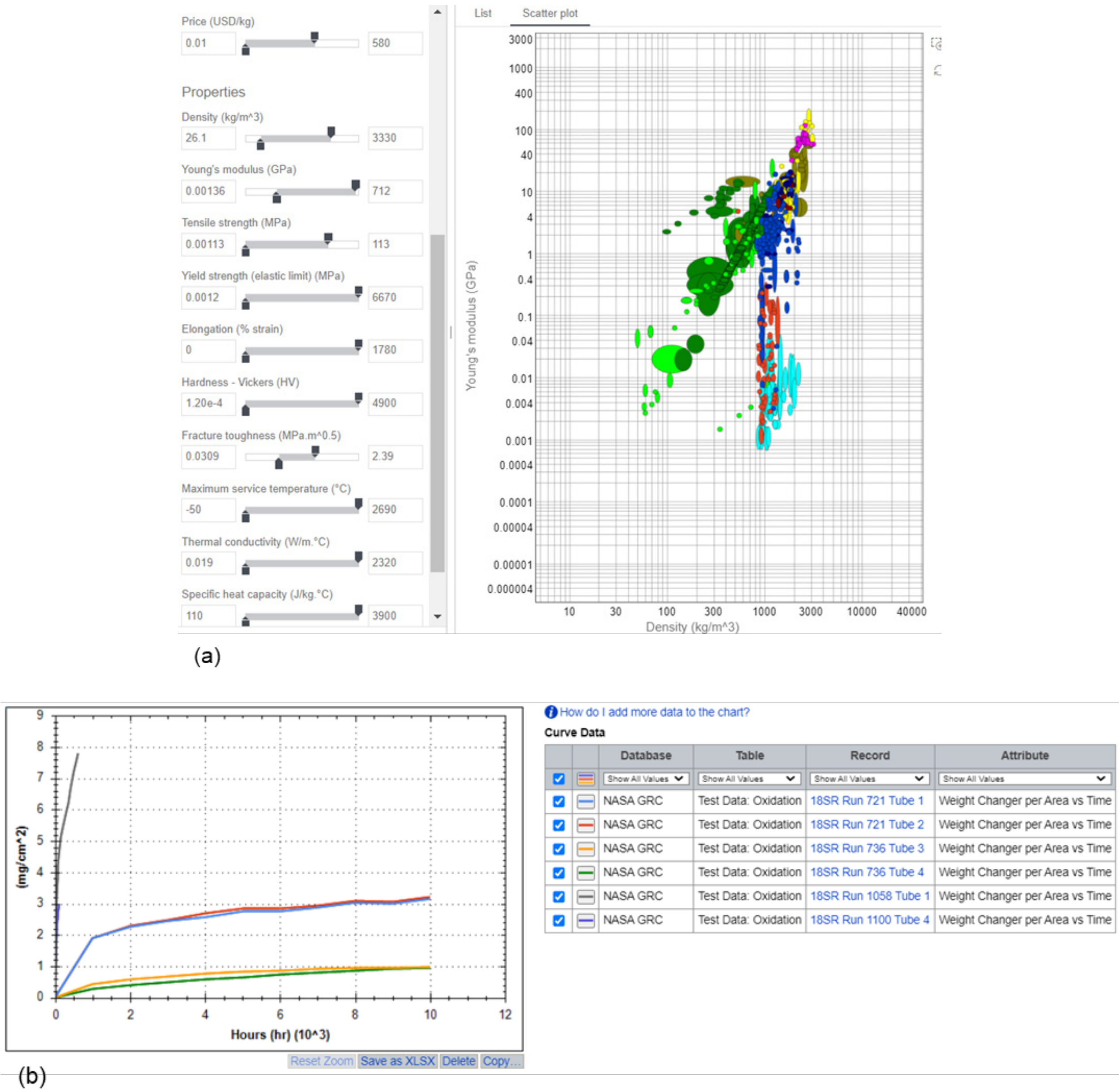


Figure 5.—Granta Enables Users to Easily Produce (a) Comparison Charts and (b) Comparison Plots

Granta MI also offers users connections (through the MI: Gateway application) to supported 3rd party software, including Computer Aided Design (CAD) tools (such as Creo), Finite Element Analysis (FEA) tools (such as Abaqus and Ansys Workbench), and Product Lifecycle Management (PLM) tools (such as Windchill), for automatic material definition from the database. Furthermore, these Gateway connections are maintained by Granta MI for each tool's version releases, ensuring data can be efficiently extracted from the database and used in simulation and design tools. For unsupported 3rd party software, such as in-house tools, and for general expediting of importing and exporting, Granta MI also offers the ability to connect to the database via custom scripting through a Python SDK. This capability enables users to efficiently upload data to the database and minimize potential human error through judicious automation, as well as disseminate data to the right people in the correct format for further use in simulation and design tools.

2.1 Granta MI Definitions

The Granta MI Enterprise platform was selected to host NASA GRC data due to its customization capability and the many advantages it offers in effective material data management, such as its ability to capture the full response spectrum (as well as pointwise properties) along with full pedigree information throughout the material life cycle (capture, analyze, maintain, deploy). Because the data will be stored within the Granta MI platform, the following definitions, within the context of Granta, will be used in the description of the NASA GRC ICME schema:

Schema – How data is organized in a relational database, including table names, attributes names, data types, meta data, record organization and naming conventions, and the relationships between these elements.

Server – A computer which manages access to a centralized resource or service in a network; herein, it is a system than can host multiple databases for an organization, as well as data import, export, and analysis tools.

Database – An organized collection of structured information, or data, that can be related and is typically stored electronically in a computer system.

Table – Database element used to organize and group data (e.g., folders, records) in the database by common characteristics or properties. All records within the same table will have the same set of attributes to define.

Table Collections – This is a grouping of individual tables that have a similar function, see dashed boxes in Figure 2. For example, Test Data (see Fig. 2) is a collection of tables containing different types of test data that are related to the applied loading, i.e., monotonic loading (tensile), constant load (creep), constant strain (relaxation), constant loading and unloading sequence (cyclic).

Folder – Container used to organize records within a given table, like a computer directory, see Figure 6a.

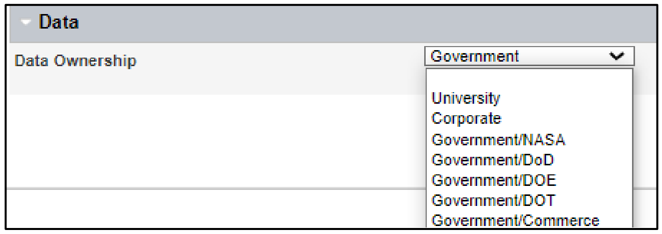
Record: Location in the database where individual data is stored (i.e., where attributes are populated) (Figure 6b).

Generic Record – Combination of a record and a folder. Generic records can have one or more child records and may also contain its own attributes that may be populated to store data (Figure 6c). Herein Generic Records will typically contain summary information about the children records contained within it, e.g., summarize temperature dependent data.

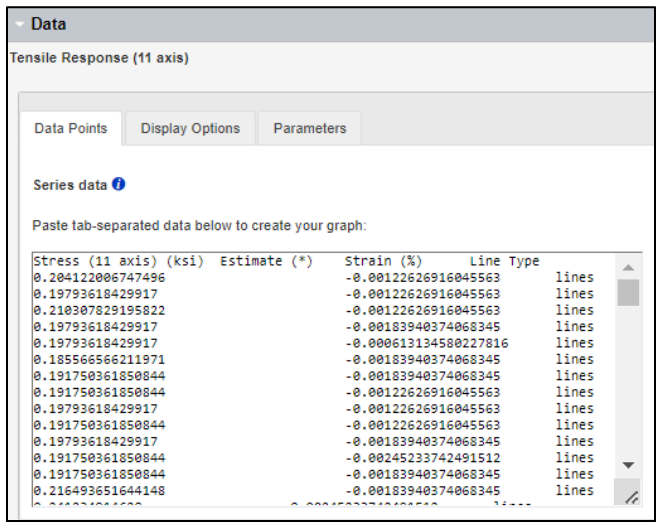
Figure 6. —Granta MI Symbols for (a) Folder, (b) Record, and (c) Generic Record

Attribute – Table-level objects that store data in a record. The various data types that attributes can take are summarized below in Table 1. In the table, the attribute abbreviation, description, and an example of each is given. In the example column, both the 'Invoke' (i.e., how the user enters the data in Granta MI) and 'Display' (i.e., how the data is viewed in the database) are given. Specific attribute types like PNT, FDA, and TABL need to have a consistent unit system associated with them as well.

TABLE 1.—ATTRIBUTE TYPES IN GRANTA MI

<table>
<tr><th>Type</th><th>Type Description</th><th>Example</th></tr>
<tr><td>DCT</td><td>Discrete Text (specified choices from a drop down list)</td><td>Invoke:


Display:

</td></tr>
<tr><td>FDA</td><td>Functional attribute (series data, plots)</td><td>Invoke:


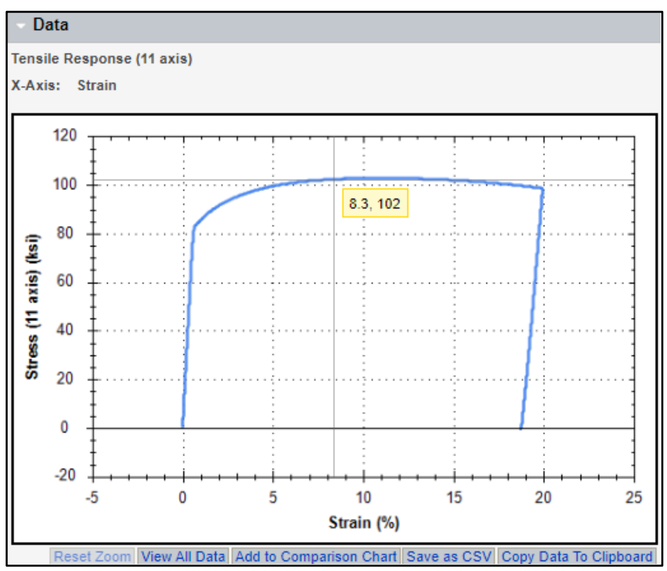
Display:

</td></tr>
</table>

TABLE 1 (CONTINUED)

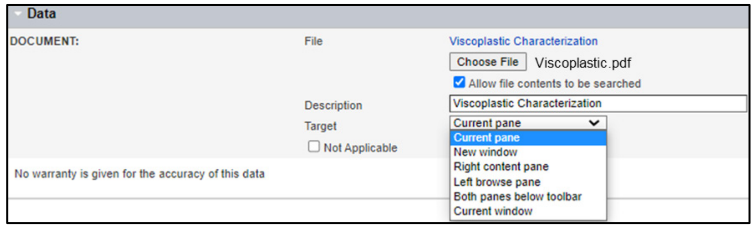
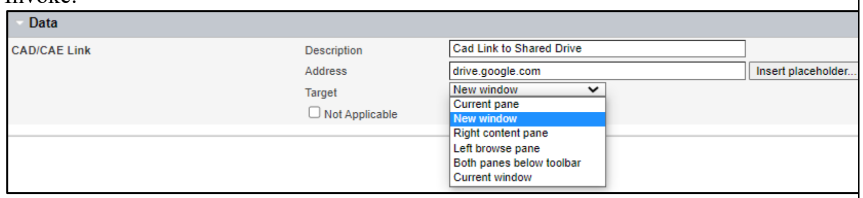
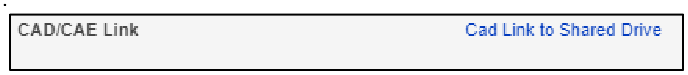
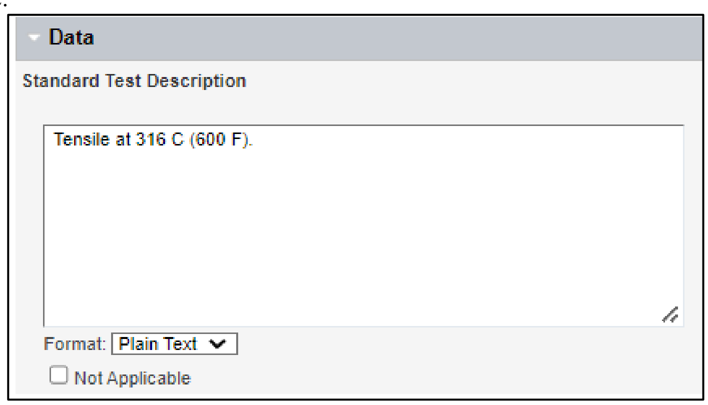
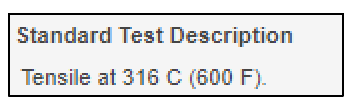
Type	Type Description	Example
FILE	Allows the association of any file type to a given attribute	Invoke:  Display: 
HYP	Hyperlink to a web-based address	Invoke:  Display: 
LTXT	Long Text Field (1,000,000 character maximum)	Invoke:  Display: 

TABLE 1 (CONTINUED)

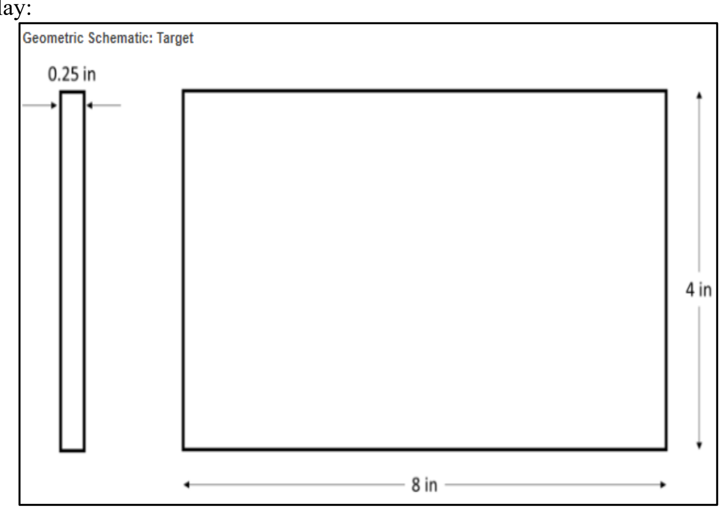
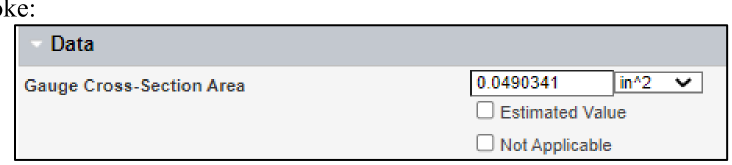
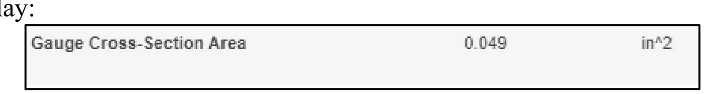
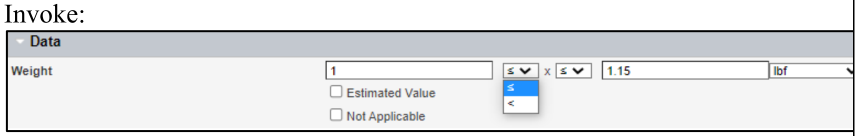
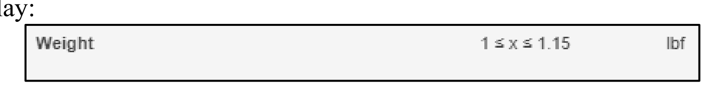
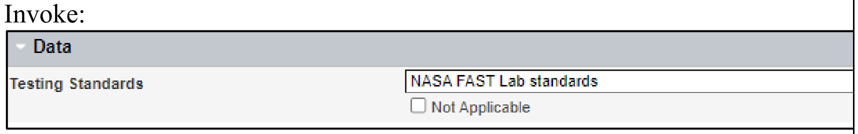
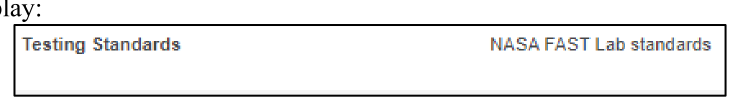
Type	Type Description	Example
IMG	Allows association of any image file (*.png, *jpg, etc.) to a given attribute	Invoke:  Display: 
PNT	Point (numeric) value	Invoke:  Display: 
RNG	Range of point values	Invoke:  Display: 
STXT	Short Text Field (255 character maximum)	Invoke:  Display: 

TABLE 1 (CONTINUED)

<table>
<tr><th>Type</th><th>Type Description</th><th>Example</th></tr>
<tr><td>TABL</td><td>Tabular attribute (each column can be PNT, RNG, STXT, LTXT, DCT, IMG, or LINK)</td><td>
Invoke:
Cycle Stage Summary
<table>
<tr><th>Block Number</th><th>Cycle Index</th><th>No. of Cycles</th><th>Stage Number</th><th>Cumulative Stage Number</th><th>Stage Type</th></tr>
<tr><td></td><td>1</td><td>1</td><td>1</td><td>1</td><td>Tensile Loading</td></tr>
<tr><td></td><td>1</td><td>1</td><td>2</td><td>2</td><td>Compression Loading</td></tr>
<tr><td></td><td>1</td><td>1</td><td>3</td><td>3</td><td>Compression Unloading</td></tr>
<tr><td></td><td>2</td><td>2</td><td>1</td><td>4</td><td>Tensile Loading</td></tr>
<tr><td></td><td>2</td><td>2</td><td>2</td><td>5</td><td>Compression Loading</td></tr>
<tr><td></td><td>2</td><td>2</td><td>3</td><td>6</td><td>Compression Unloading</td></tr>
<tr><td></td><td>3</td><td>3</td><td>1</td><td>7</td><td>Tensile Loading</td></tr>
<tr><td></td><td>3</td><td>3</td><td>2</td><td>8</td><td>Compression Loading</td></tr>
<tr><td></td><td>3</td><td>3</td><td>3</td><td>9</td><td>Compression Unloading</td></tr>
<tr><td></td><td>4</td><td>4</td><td>1</td><td>10</td><td>Tensile Loading</td></tr>
<tr><td></td><td>4</td><td>4</td><td>2</td><td>11</td><td>Compression Loading</td></tr>
<tr><td></td><td>4</td><td>4</td><td>3</td><td>12</td><td>Compression Unloading</td></tr>
<tr><td></td><td>5</td><td>5</td><td>1</td><td>13</td><td>Tensile Loading</td></tr>
<tr><td></td><td>5</td><td>5</td><td>2</td><td>14</td><td>Compression Loading</td></tr>
<tr><td></td><td>5</td><td>5</td><td>3</td><td>15</td><td>Compression Unloading</td></tr>
</table>
Add a blank row

Display:
Cycle Stage Summary Hide table
Save as CSV Copy To Clipboard
<table>
<tr><th>Cycle Index</th><th>No. of Cycles</th><th>Stage Number</th><th>Cumulative Stage Number</th><th>Stage Type</th></tr>
<tr><td>1</td><td>1</td><td>1</td><td>1</td><td>Tensile Loading</td></tr>
<tr><td>1</td><td>1</td><td>2</td><td>2</td><td>Compression Loading</td></tr>
<tr><td>1</td><td>1</td><td>3</td><td>3</td><td>Compression Unloading</td></tr>
<tr><td>2</td><td>2</td><td>1</td><td>4</td><td>Tensile Loading</td></tr>
<tr><td>2</td><td>2</td><td>2</td><td>5</td><td>Compression Loading</td></tr>
<tr><td>2</td><td>2</td><td>3</td><td>6</td><td>Compression Unloading</td></tr>
<tr><td>3</td><td>3</td><td>1</td><td>7</td><td>Tensile Loading</td></tr>
<tr><td>3</td><td>3</td><td>2</td><td>8</td><td>Compression Loading</td></tr>
<tr><td>3</td><td>3</td><td>3</td><td>9</td><td>Compression Unloading</td></tr>
<tr><td>4</td><td>4</td><td>1</td><td>10</td><td>Tensile Loading</td></tr>
<tr><td>4</td><td>4</td><td>2</td><td>11</td><td>Compression Loading</td></tr>
<tr><td>4</td><td>4</td><td>3</td><td>12</td><td>Compression Unloading</td></tr>
<tr><td>5</td><td>5</td><td>1</td><td>13</td><td>Tensile Loading</td></tr>
<tr><td>5</td><td>5</td><td>2</td><td>14</td><td>Compression Loading</td></tr>
<tr><td>5</td><td>5</td><td>3</td><td>15</td><td>Compression Unloading</td></tr>
</table>
Save as CSV Copy To Clipboard
</td></tr>
</table>

Layout – Organization of the headers and placement of each attribute within each header

Subset – Allows customization of an associated layout for a given table which can be used to reduce/restrict access to specific attributes, simplify data by only showing relevant records or attributes, or provide a different perspective on the data within the table.

Profile – A means of grouping together individual databases and tables for a set of people. Profiles determine which databases and tables are available for viewing, editing, and searching for each user group.

Tree Structure – This is the naming convention adopted for Tables, Folders, and Records which dictates their order of appearance in the left pane within GRANTA MI. A consistent naming practice within a given Table is essential to enable the user to have an effective and repeatable experience. In the NASA GRC database within the test data collection typically the highest level of the tree contains the name of the material, followed by a breakdown by temperature, then significant loading feature (which is test dependent, e.g., strain rate for tensile, stress for creep, etc.), see Figure 7. Examples of tree structures for each of the tables within the ICME Schema are given in Appendix A. It should be noted that in Granta MI, the order of tables in the tree structure is set by the user, but folders and records are listed in alphabetical order.

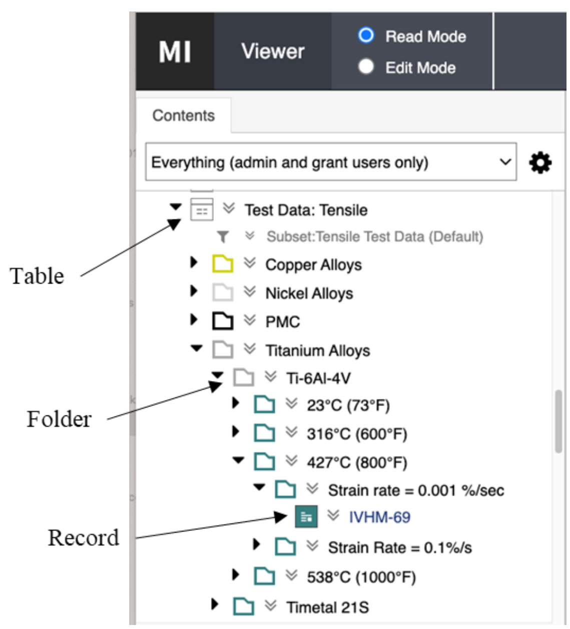


Figure 7.—Example Tree Structure for Tensile Test

2.2 Linking Behavior in Granta MI

Granta MI is a relational database platform, and therefore information can be linked across different records and databases to enable traceability across a material's lifecycle, enabling consistency management of material digital twins [8] and maintenance of the digital thread [7] . Links from one record to another can be either static links or smart links. Static links allow the user to manually link two records together by searching through the database, whereas smart links will automatically link two records together based on user-defined rules and the value of specific attributes within the record. Granta MI also allows data within a record to be linked to other records within the same database via the tabular attribute. As a result, data can be *defined* in one record and *viewed* in other records, thereby eliminating both duplication of data following the previously outlined best practices and the need to navigate through multiple records to view relevant data. However, as implemented within Granta MI, a single tabular attribute cannot be both defined in one record and viewed in another within the same table. To work around this limitation at GRC, Define Tabular and View Tabular attributes have been created for those attributes that need to be accessed within the same table (e.g., Model table). When implementing the viewed linking capability, records are linked via a linking value, or the value of a user-defined attribute, to populate the tabular attribute automatically and dynamically with viewed data. For example, a material's composition should only be defined once in the database, but it may be useful to see that composition with each associated test performed on that material. In Figure 8, the composition is *defined* in a Pedigree record. For each associated test record, the composition can be *viewed* by *invoking* the linking value (i.e., the batch number attribute in this example) in each test record.

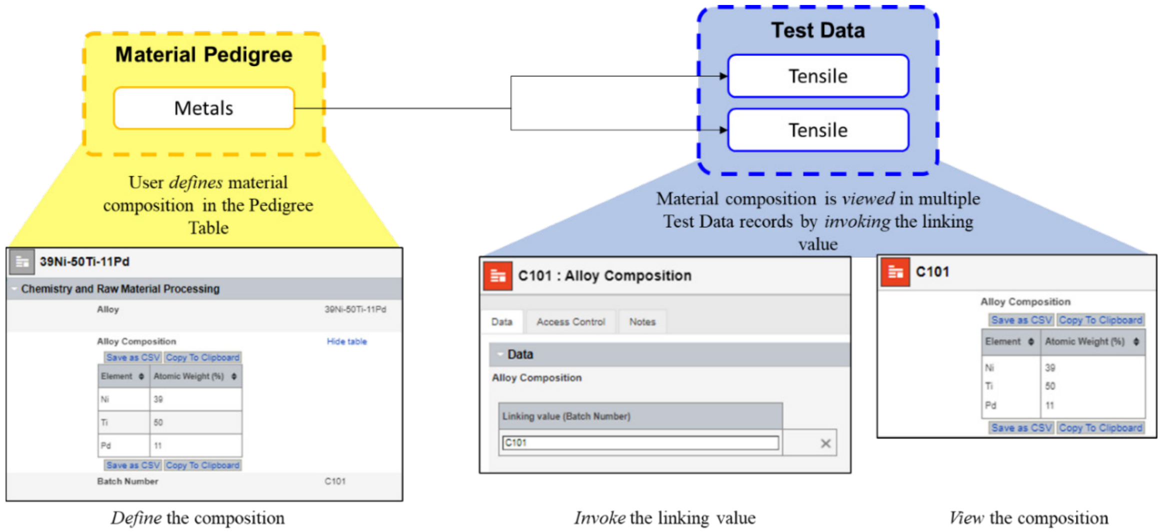


Figure 8.—Viewing Linked Data in Granta MI

3.0 NASA GRC Schema Elements

The NASA GRC ICME Database is divided into a series of *collections* of tables (see Figure 2) that share similar schema, attributes, and data types, but differ enough to justify separation into distinct tables. The different collections (see dashed lined boxes in Figure 2) in the NASA GRC ICME Schema, listed alphabetically, are:

1. Manufacturing
2. Materials Pedigree
3. Model Pedigree
4. Reference Data
5. Test Data
6. Test Information

The remainder of Section 3 provides a brief description of each collection and the tables contained within these collections along with a linking diagram of the specific tables involved in each collection and how they interact with other tables from other collections.

There are five additional tables that do not belong to any one collection but perform very important roles within the ICME Schema. The tables included are:

1. **Microstructure** – This table is used to store microstructure images and analysis of images, regardless of whether the imaging was performed in-house or taken from the literature.
2. **Software Tools** – This table is used to establish traceability between generated simulation data and the software tools used in the data creation. Further, it is used as a reference for the organization on what software tools are available for future simulations.
3. **Materials Summary** – This table provides a summary of the in-house testing that has been performed and the material availability for potential use in applications. Records in the Materials Summary table are sorted by materials and then test program, and thus offer experimentalists and program managers a unique location to store a test program matrix and monitor the progress of the testing program over time.
4. **Applications** – This table serves as the bridge between the materials paradigm and the structural paradigm, providing a unique place in the database to link material pedigree, properties, and models to designed parts and assemblies, and the necessary information, pedigree, and traceability to establish a digital twin for the application. Records in the Application table contain information on the applications geometry/manufacturing requirements, performance requirements, analysis results, failure information, material requirements/selection, inspection, and readiness levels. A detailed explanation of the Application table can be found in Ref. [13].
5. **Program Information** – This table stores program or project information associated with the funding and initial use case for the data stored in the database. Data stored includes program names, funding sources, project descriptions, testing organizations, and restrictions on who the data can be shared with (as an additional measure to the built-in security controls). Records in the Program Information table can be linked to those in the Microstructure table, Test Data collection, Model Pedigree collection, and Application table via viewed tabular attributes to eliminate repetition of data and follow the database best practices.

Each of these tables have linkage out to other tables within the various collections as shown generically in Figure 9. For more detailed information on each table the reader is referred to Appendix A.1.

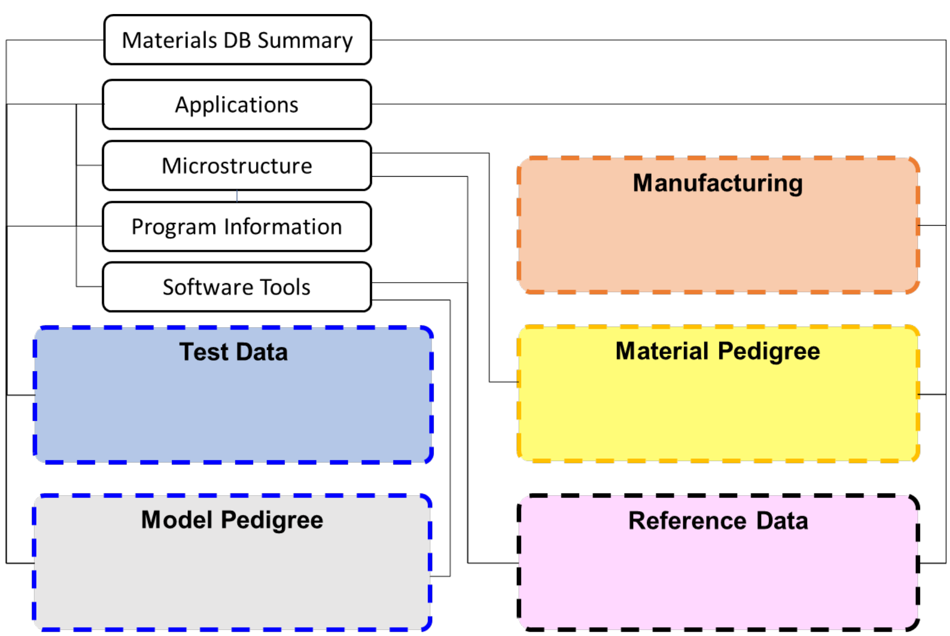


Figure 9.—Additional Tables and Associated Linkage with Other Collections

3.1 Manufacturing

The tables within the Manufacturing collection store the various manufacturing and processing methods used on either batch materials (albeit monolithic or composite) or individual test specimens within the database. Records in this collection contain information describing the process, a list of approved materials for the process, typical ranges of parameters that must be defined for a given material, and associated schematics and references. Manufacturing records are used to define a general description of a given method, rather than specific information related to an individual material's processing. Within the Manufacturing collection, there are currently two tables:

1. **Subtractive Manufacturing** – This table stores general information on the various traditional/subtractive manufacturing processes/methods that can be applied to a material that change the expected behavior to external loading. This includes both subtractive methods for part production (e.g., milling, drilling, turning, cutting, grinding, etc.) as well as traditional methods for processing materials (e.g., casting, extrusion, forming, forging, hot isostatic pressing, etc.) Such records contain a detailed description of the process, associated schematics outlining the process, physical attributes, attributes related to the economics and cost modeling of the process, and geometric descriptors, and any additional characteristics.
2. **Additive Manufacturing –** This table stores general information on the various manufacturing, preprocessing, and postprocessing methods for additively manufactured materials. Records contain a description of the process, geometric parameters relating to the build size, information on the feedstock, a list of the parameters used to define the build with typical ranges for each parameter, associated pre- and post-processing methods typically employed for that process, and list of compatible materials, linked to the pedigree tables.

The processing method(s) applied should then be linked to the corresponding Material Pedigree collection as well as the Test Information collection so that any machines or tools used for the given processing method can be established. For example, records within the Additive Manufacturing table are also linked to the build machine, stored in the Equipment table, such that the relationship between the method and the actual build, as well as pedigree information on the machine calibration, maximum build geometry, and machine location, is identified. For more detailed information on each table the reader is referred to Appendix A.2.

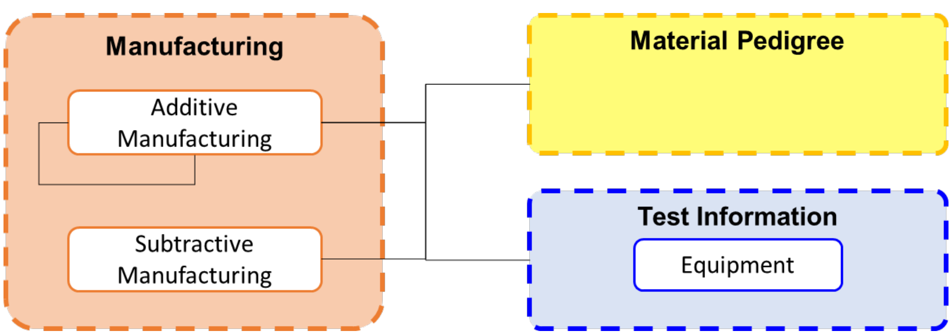


Figure 10.—Manufacturing Collection and Associated Linkage with Other Collections

3.2 Materials Pedigree

The Materials Pedigree collection is used to store pedigree information for metal, ceramic, polymer, composite, reinforcement, and coating materials used in subsequent experimental testing. Records within the Materials Pedigree collection represent specific batch productions of material characterized, associated chemistry and processing of the material, cutout diagrams for individual specimens used for experimental testing, and performed inspection data on the material. Record links are used to provide traceability between records within the Material Pedigree collection and associated experimental testing, published literature data, and the Materials Summary table. Within the Materials Pedigree collection, there are currently eight tables:

1. **Ceramics –** This table stores material pedigree information for ceramic materials.
2. **Coatings –** This table stores material pedigree information for coatings.
3. **Metals** – This table stores metallic material information, including the alloy chemistry, raw material processing, intermediate processing, final processing, heat treatment, and material properties.
4. **Polymers** – This table stores material information for polymer matrix materials, including the polymer chemistry, constituent (i.e., the resin and hardener) information, mixing ratios, and vendor material properties.
5. **Reinforcements** – This table stores material information for reinforcement materials used in composites, including weaves, fibers, and particulates.
6. **Composite Ply Architecture –** This table stores material information for single ply laminas, made from a reinforcement, coating, and matrix material (albeit ceramic, metallic or polymer) also stored in the database.
7. **Composite System-Laminate –** This table stores material information for a laminate system, where laminates are made from single laminas (or plies) defined in the Composite Ply Architecture table. The Composite System Laminate table contains information on the laminate architecture, dimensions, properties, and defects, the ply stacking sequence, the matrix material and reinforcement pedigree, the laminate processing/cure cycle, applied coating, and vendor supplied properties.
8. **Component/Assemblies –** This table stores pedigree information on typical components or assemblies used in manufacturing, such as sandwich or stiffened panels. Records contain information on the material system used and the component geometry. The records are organized by the type of component (e.g., Panel Structure, Stiffened Structure), then the shape or configuration of the structure (e.g., hat stiffener, I-Stiffened panel, T-Stiffened panel), and then the actual component.

Records in any of the first five tables can be linked to the Composite Ply Architecture table, Composite System Laminate table, and Component/Assemblies table if the material is used in a composite, as well as to records in the Manufacturing collection for any information related to the processing of the material. Records can also be linked to any of the Test Data tables in the database for any corresponding tests that were conducted from that specific batch of the material. Similarly, for any microstructure images or characterization records can also be linked to the Microstructure table (Figure 11). For more detailed information on each table the reader is referred to Appendix A.3.

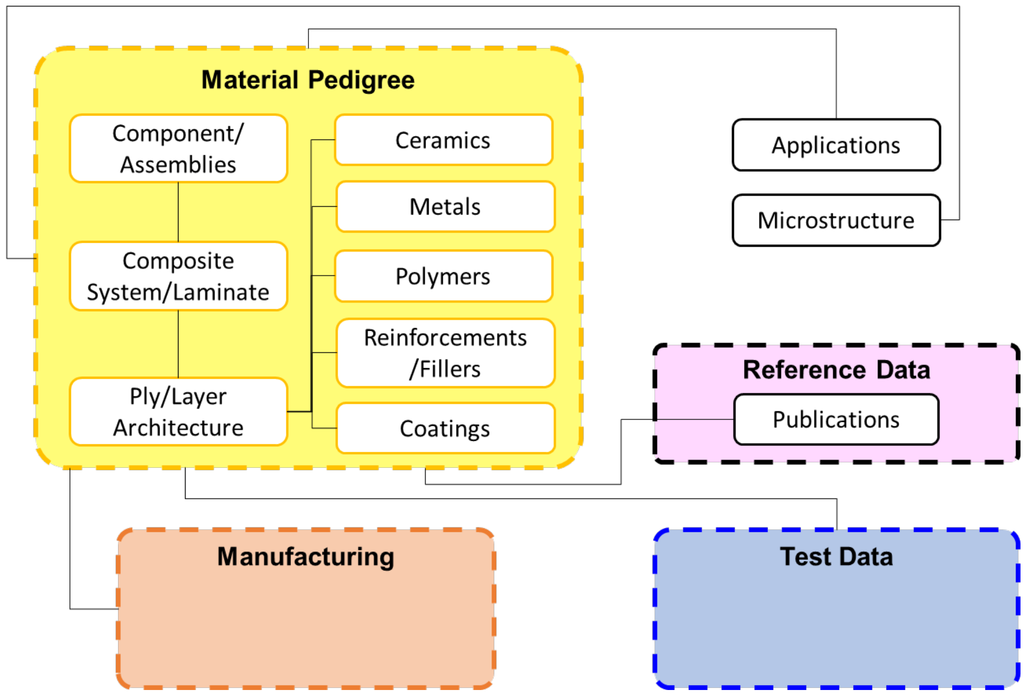


Figure 11.—Material Pedigree Collection and Associated Linkage with Other Collections

3.3 Model Pedigree

The Model Pedigree collection stores all information related to simulations performed at various length scales of a material. Records in the Model Pedigree collection are used to store model parameters and simulation results that correspond to both characterization and validation test results. As such, records in this collection typically contain some description of the material, a description of the model implemented, the methodology for material characterization and parameter estimation within the context of the employed model, the material/model parameters, the simulation results, and associated references and links to establish traceability between the material pedigree, testing, and any resultant publications. Within the Model Pedigree collection, there are currently four tables:

1. **Composite** – This table is used to store multiscale material models for composite materials at various length scales. At the microscale, records contain simulations of a single ply or lamina (i.e., the material response of the constituents within a given microstructure (RUC) to applied loading). At the mesoscale, simulations of laminate behavior and homogenized properties are stored.
2. **Deformation –** This table is used to store physics-based material models and associated model parameters for simulating linear and nonlinear deformation under applied thermomechanical loading.
3. **Damage/Life –** This table is used to store physics-based material models and associated model parameters for simulating damage and property degradation due to uniaxial and multiaxial loading profiles (e.g., monotonic, fatigue loading).
4. **Machine Learning –** This table is used to store data-driven (e.g., machine learning) models developed for material simulation. Records in this table contain model information, model architecture, data definition, validation information, and further pedigree information.

Records in the Model Pedigree collection typically link to the tables in the Test Data collection to establish the traceability between experimental tests performed to enable determination of model parameters and model validation. They can also link to records in the Model Pedigree collection if multiple models (physics-based or data-driven) were used during the simulation. Further, records can also be linked to the Software Tools table to reference any software used to conduct the simulation at any length scale and/or the Application table to relate any material models used in the design and analysis of parts or assemblies, thus ensuring maintenance of that application's digital twin. For machine learning models, records can be linked to the Reference Data: Machine Learning Data table to establish traceability between the model and any virtual data created for model training, validation, and testing (see Ref. [17] for additional details). Finally, records in the Model Pedigree collection can be linked to the Reference Data: Publications table for any associated publications. This linkage is illustrated in Figure 12. For more detailed information on each table the reader is referred to Appendix A.4.

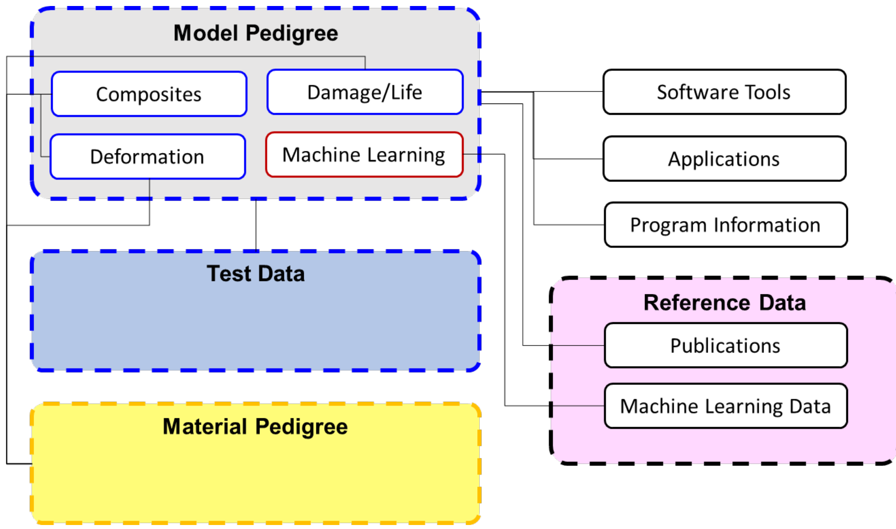


Figure 12.—Model Pedigree Collection and Associated Linkage with Other Collections

3.4 Reference Data

The Reference Data collection contains various types of reference data tables in the database, including literature data, virtual data, access to other databases and resources, and different standards. Within the Reference Data collection, there are currently six tables:

1. **Materials** – This table is used to store material information from the literature, including various material composition, material properties, functional data curves for properties that vary with temperature, physical characteristics of the material, and manufacturing/commercial availability of the material.
2. **Machine Learning Data** – This table is used to store virtual (simulation) data created solely for the purpose of training a machine learning model. Records include information on the Data Series information, the data itself, and links to associated records.
3. **Publications** – This table stores published papers and reports, along with associated publication metadata, related to all information in the database produced in-house. Records contain direct links to the publication (i.e., the pdf file), point of contact information, project/funding information, and links to associated data throughout the database.

4. **Schematics** – This table is used to store general schematics that are not specific to any given application. Rather, schematics stored in this table can be used as a reference for general applications (e.g., typical rolling bearings vs. a specific rolling bearing for an engine).
5. **Information/Resources** – This table is used to store reference information on other available databases, research organizations, laboratories, societies, and conferences, publishing information (i.e., materials journals and publishers), material suppliers, and other reports that are not published for the public.
6. **Standards** – This table is used to store various standards for material and application testing, manufacturing, and evaluation. Records contain the individual elements of a given standard such that they can be individually viewed and evaluated for a given material or application via the viewed tabular attribute.

Records in the References collection can be linked to the various tables in other collections, such as Material Pedigree tables, Test Data tables, Manufacturing tables, and the Application table to associate any resource with existing data in the database, see Figure 13. For more detailed information on each table the reader is referred to Appendix A.5.

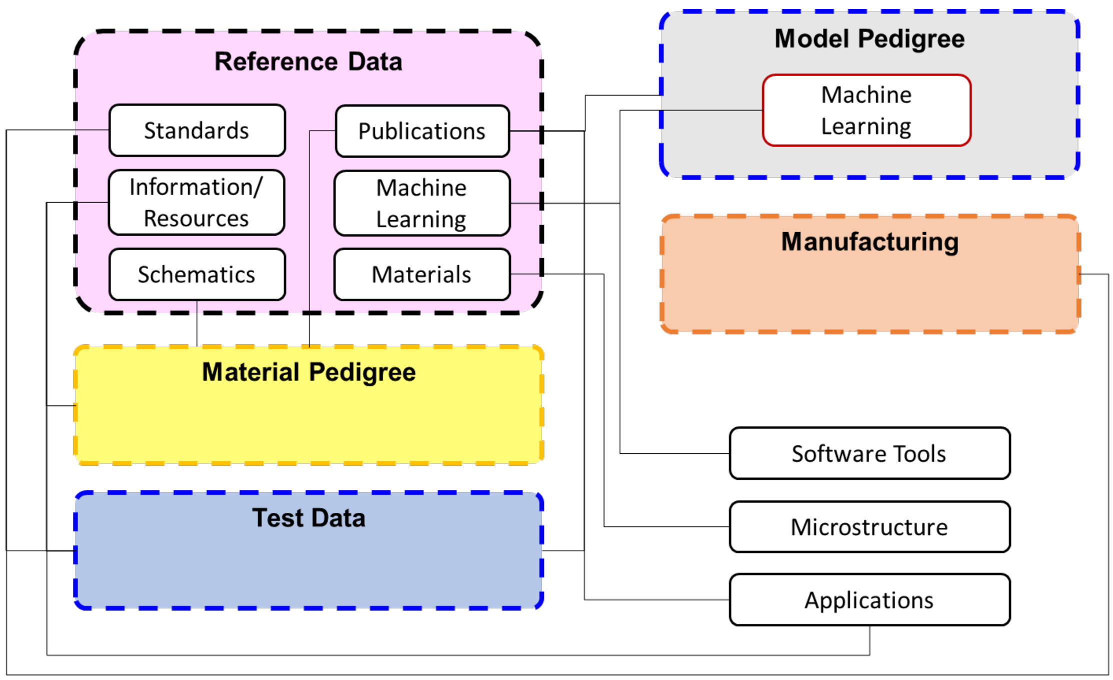


Figure 13.—Reference Collection and Associated Linkage with Other Collections

3.5 Test Data

The Test Data collection is used to store in-house test data and associated test pedigree information. In general, records within the Test Data collection contain data pertaining to the test information, material/processing information, specimen information, test conditions, test response, test results, and data collection. Within the Test Data collection, there are currently eight tables:

1. **Tensile** – This table stores in-house test data for uniaxial tensile tests.
2. **Compression** – This table stores in-house test data for uniaxial compression tests.
3. **Creep** – This table stores in-house test data for single stage uniaxial creep tests.
4. **Relaxation** – This table stores in-house test data for single stage uniaxial relaxation tests.

5. **Generic** – This table stores in-house test data for single or multistage complex, thermomechanical uniaxial or multiaxial tests. For a generic test, stages can include tensile loading/unloading, compressive loading/unloading, creep (i.e., constant stress), relaxation (i.e., constant strain), and applied thermal changes. Records in the Generic table contain information on each individual stage, as well as analyzed point values for stages that coincide with the Tensile, Compression, Creep, and Relaxation tables if there is no prior load history to provide additional statistical data for model parameter determination.
6. **Cyclic** – This table stores in-house test data for uniaxial cyclic/fatigue tests, albeit stress or strain controlled.
7. **Fatigue Crack Growth** – This table stores in-house test data for uniaxial fatigue crack growth tests.
8. **Oxidation** – This table stores in-house test data for oxidation of different metals.

Records in the Test Data collection can be linked to the various tables in other collections (such as the Material Pedigree collection, Test Information collection, Reference collection, etc., see Figure 14). For more detailed information on each table the reader is referred to Appendix A.6.

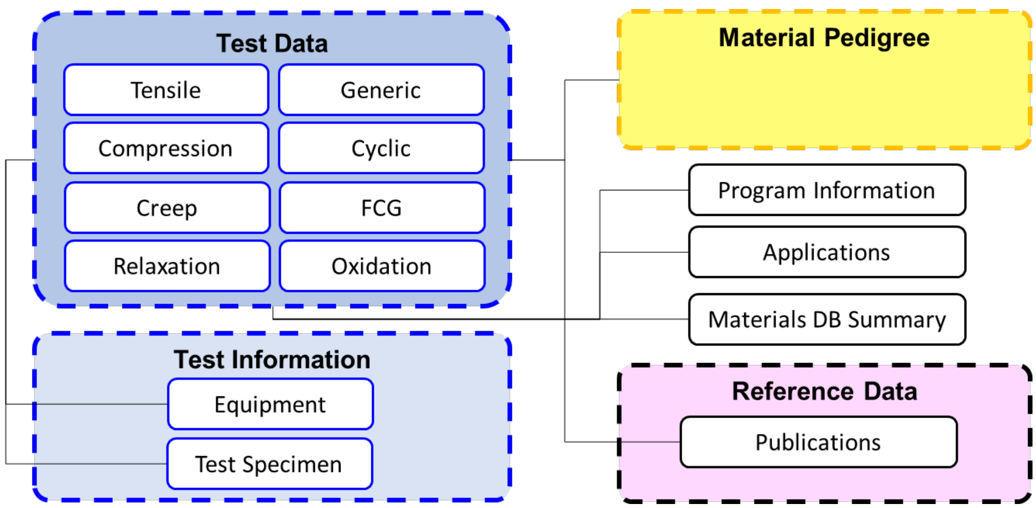


Figure 14.—Test Data Collection and Associated Linkage with Other Collections

3.6 Test Information

The Test Information collection of tables stores information on testing equipment (i.e., destructive, nondestructive, measurement devices, heating devices, and additive manufacturing) and general test specimens used for the various experiments stored in the database. The purpose of these tables is to define information used in multiple tests in one location and link to associated test records, enabling the database best practice of minimizing repeated information. Within the Test Information collection there are currently two tables:

1. **Test Specimens** – This table stores geometric, nominal dimensions for test specimens used in a particular test. Information stored includes the sample geometry, orientation, and schematics of the specimen design.
2. **Equipment** – This table is used to define the testing equipment available both destructive and nondestructive, including measurement and heating equipment, load/testing frames, machines for manufacturing and processing, and equipment for material evaluation. It also defines any equipment used for material processing and manufacturing, such as build

machines for additive manufacturing. Records include information regarding the equipment's name, description, location, calibration history, and any associated schematics or images related to the equipment.

Test Information records are linked to individual tables within the Test Data collection to enable traceability between the samples tested, the execution of the test, and the collection of data. Records can also be linked to the Manufacturing collection to associate a manufacturing method with a physical machine, see Figure 15. For more detailed information on each table the reader is referred to Appendix A.7.

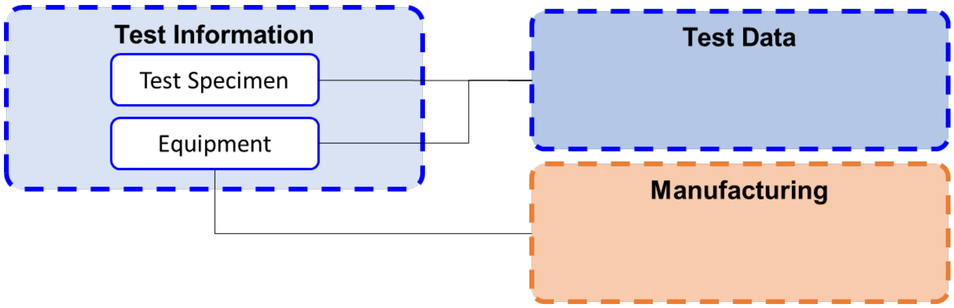


Figure 15.—Test Information Collection and Associated Linkage with Other Collections

4.0 Auxiliary Data Management Toolset

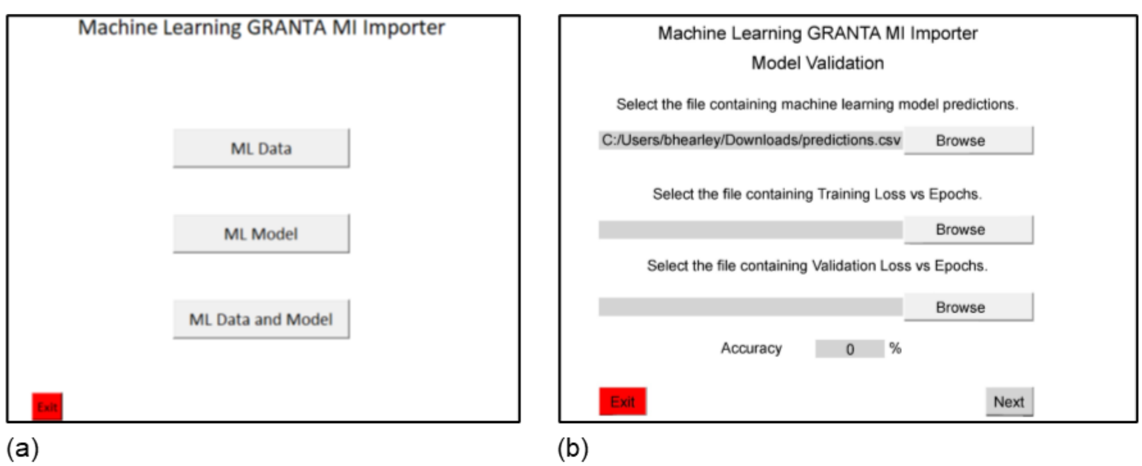
One of the major challenges with implementing an ICME approach is proper maintenance of the digital twins or digital representations (which exist whenever the physical entity no longer matches the virtual entity) at each length scale, and the established traceability between each twin to maintain the application's digital thread. Though the established ICME schema for storing data does provide the means 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 material pedigree, test data, models, and application, and is thus prone to human error that can break the digital thread, thus prohibiting some users in an organization from adopting such tools. 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 optimization 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.

Also, within the context of ICME, experimental data is critical in determining necessary model parameters and validating computational tools that can be used to predict process-property relationships. Therefore, it is necessary for an organization to have an effective means of storing test data, linking the tests performed to the material pedigree and models developed, and to have consistent, reliable means of importing and analyzing data within an information management system. Herein various tools will be described that expedite the capture, analysis, and maintenance of data, both real (experimental) and virtual (simulation). These tools not only help to ensure database administrators that the data entered into the database is correct, consistent, within the guidelines of the database best practices, but also improve the user experience by eliminating manual, time-consuming data entry, thus assisting in overcoming the cultural barriers associated with effective materials data management.

4.1 Data Importers

One key challenge that all organizations will face when implementing data management systems is cultural buy-in from the creators of the data. Many data producers find the process of importing their data to a data management system to be time consuming and unintuitive, and are therefore much more likely to simply keep their data stored in non-shared locations, such as personal hard drives, or in shared folders, such as within cloud-based services, with no means for effectively finding data, using data, or establishing the required traceability to establish the digital thread or digital twins. It is therefore recommended that in addition to a well-defined schema, those who look to effectively introduce materials data management at an organizational level must also develop data import tools to facilitate the process of populating the data, both relieving data creators of the burden of manually importing data and reducing the potential for human error when defining attributes, both by avoiding incorrect entry by the user and providing users with automatic error recognition for invalid data types/entries. Additionally, cultural buy-in can be further increased if data importers can offer users some additional service, including data reduction, analysis, automation of tasks, automatic linking to other records, etc.

At NASA GRC, data importers are generally created via Python scripting, allowing users to convert their raw data to a neutral file format which can then be read and populated into the Granta MI System. Additionally, some data importers have been created with graphical user interfaces (GUI) to further facilitate the importing process. One such example is the importer developed for storing machine learning data (both real and virtual) and models. Figure 16a and Figure 16b show the home page and data page, respectively, for the Machine Learning GRANTA MI Importer GUI. In Figure 16a, the user is able to upload machine learning data, a machine learning model, or both. Once an option is selected, the user is prompted with supplying various files containing the data, the source code for the model, and some additional information used to establish the model pedigree. Data and model records are automatically populated, linked together to establish traceability between the data and the models such that the limitations of the model are well understood and documented, and placed in the database. Additionally, the importer will automatically parse through supplied machine learning code, extract the model architecture and hyper parameters, and populate that information in the database without any user intervention (Figure 16c). Additional information on the machine learning schema and data importer can be found in Ref. [17].



(c)

Figure 16.—Machine Learning Data and Model Importer: (a) GUI Home Page, (b) GUI Data Selection Screen, and (c) Automation of Machine Learning Model Extraction

4.2 Py MILab

Py MILab is a specially designed framework (written in Python) for importing experimental data directly from either test machine or various file formats, performing efficient data analytics on the resulting response spectrum and then storing the resulting data and metadata in the appropriate tables while simultaneously linking material pedigree, specimen geometry, microstructure, test instrumentation and any other pertinent information to the corresponding test record automatically (minimal user interaction). The benefits of such a tool are significant reduction in user effort, full traceability between test machine calibration and test performance, and consistency in data reduction and analysis. Bulk importing begins with all raw data being passed through a machine specific subroutine to convert it to a standard format for analysis and is then followed by data analysis wherein specific automatic parameter extraction for either standard or generic tests is performed. Manual editing of the results and/or stage information is enabled as well as automatic placement of the record containing both pointwise data, functional data, and meta data. Lastly, automatic linking to test equipment and measurement devices ensures that how the data was captured is maintained in the database. The tool not only automatically places test data in the correct location in the database with all required linkages for full test pedigree, but also provides users automatic, consistent, and rapid analysis of various types of test data with minimal user interaction, enabling efficient test characterization for large test programs. Figure 17 illustrates the workflow conducted by Py MILab. Additional details on Py MILAB can be found in Ref [18].

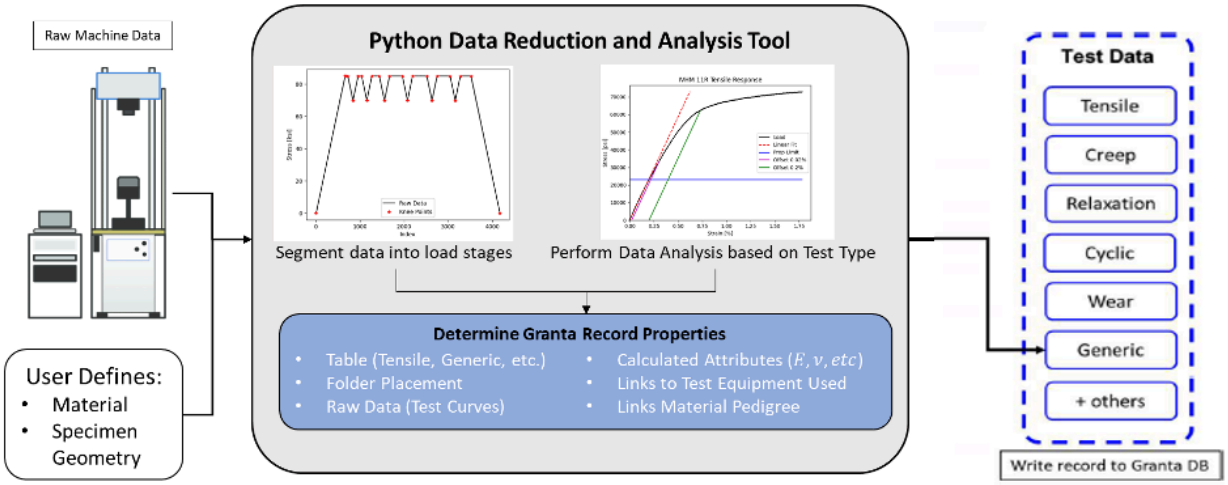


Figure 17.—Py MILab workflow diagram

4.3 AIMAOS (Automated Information Management Across Organizations and Scales)

A 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.

AIMAOS (Automated Information Management Across Organizations and Scales) is a digital thread maintenance tool which orchestrates the ICME process through judicious automation, across organizations and scales, by the updating and propagation of analyses information (both data and metadata) from a given scale to higher and higher length scales, the final product being the design of 'fit-for-purpose' material(s) within a given target application. Users can create material digital twins/representations 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 to accelerate the design of 'fit-for-purpose' materials. AIMAOS offers users an interactive Python-based 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. The associated workflow is illustrated in Figure 18, where 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. For more detailed information see Ref. [19].

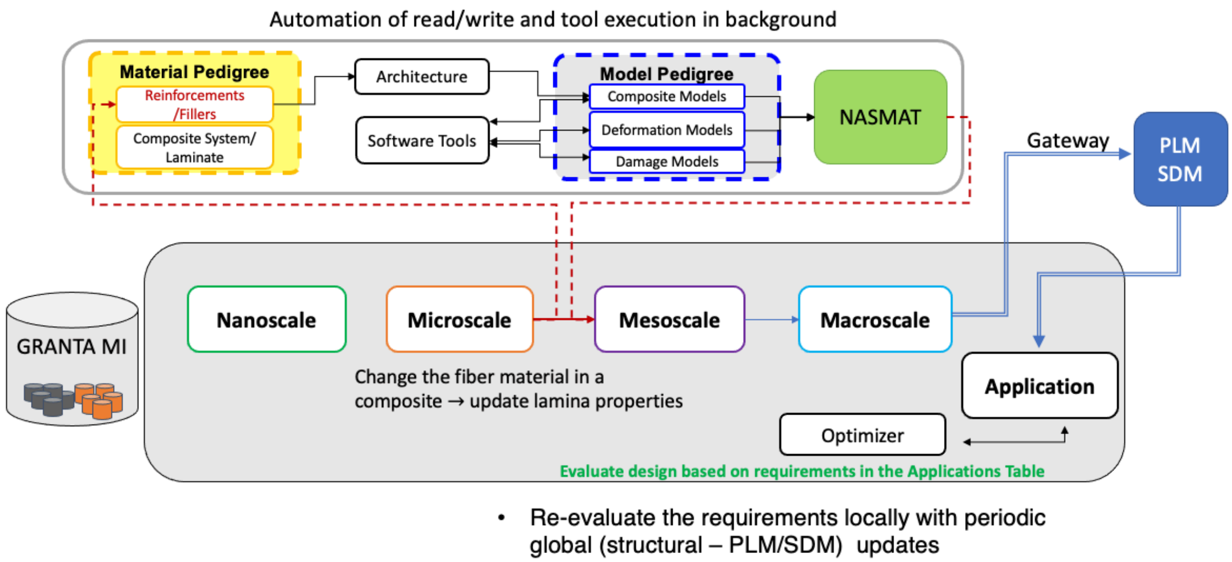


Figure 18.—AIMAOS Workflow

5.0 Conclusions

A robust material information management system that facilitates capturing, analyzing, maintaining, and disseminating materials data is critical to any organization looking to benefit from enabling ICME material design. Design of such a system, however, takes careful consideration - data should be organized to be well defined and easily findable by users of the system and linked across the material lifecycle to establish traceability between material pedigree, experimental data, and associated simulation data, allowing for maintenance of the material digital thread and establishment of process-structure-property-performance relationships. At NASA GRC, a robust schema has been established (within the context of the Granta MI Material Information Management platform offered by Ansys) for effectively capturing all relevant material information for ICME. Utilizing 3rd party software for data management does come with disadvantages, including license fees and limitations on data storage attribute types, but are far outweighed by the advantages of removing organizational burden for maintaining reference databases, import and export tools, and connections to commercial 3rd party software tools. Additionally, Granta MI allows users to write their own auxiliary tools, such as Py MILAB and AIMAOS, to connect in-house analysis codes and workflow management tools to establish intelligent automatic processes for analyzing, maintaining, and storing data. It should be noted that although the schema was presented within the context of Granta MI, the tables defined, organization of data, and linking behavior between database entities is agnostic, and can be readily applied to any relational database platform.

As organizations look to adopt ICME practices for material design, careful thought should be given to the choice of the information management platform, the design of the schema, including the separation of tables, definition of attributes, and linking behavior between attributes and records to establish traceability, and the development of tools that interact with the database to create the "cyberinfrastructure". Each of these elements not only address the technical challenges associated with implementing ICME, but also the cultural challenges revolving around buy-in of the people within organizations in utilizing such tools and methods. The presented schema is inclusive for many types of materials data, but can also be modified by each organization to meet the desired goals for their stakeholders. Additionally, the NASA GRC ICME schema is always evolving as new use cases, data, and users across various fields turn to information management as a solution for effectively capturing, analyzing, maintaining, and disseminating their data. Thus, the NASA GRC ICME schema presented offers as an excellent starting point, rather than a final solution, for any organization looking to implement a material information management system for storing and utilizing data for materials design and discovery.

Acknowledgements

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Appendix A: Details of Table Collections

A.1 Additional Tables

The tables in Section A.1. are individual tables that do not belong to any one collection. The tables include:

1. Microstructure
2. Software Tools
3. Materials Summary
4. Applications
5. Program Information

A.1.1 Microstructure

The Microstructure table is used to store microstructure images and analysis of images, regardless of whether the imaging was performed in-house or taken from the literature. Records in the Microstructure table contain material information, cutout diagrams at the macroscale to specify where images are taken, micrograph images of the material microstructure, information on the imaging, including magnification, microscopy technique, image size, etc., and extracted analysis parameters, such as phase compositions and sizes and grain sizes and shapes. Records are organized by material class (e.g., Metals, PMC), material base (e.g., Titanium-based Alloys, Nickel-based Alloys), material name (e.g., Ti-6Al-4V, Timetal 21S), and then the individual batch of the material (Figure 19). Note that in Figure 19, a generic record is used at the material name level, which summarizes statistical information on the microstructure analysis in the individual records. At the material batch record level, the schema is able to support multiple images for an individual record, such that all microstructure images for an associated material pedigree can be stored in one location.

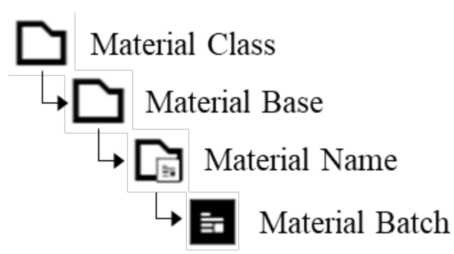

Figure 19.—Microstructure Tree Structure

To associate micrograph images with an associated material pedigree, the Microstructure table can be linked to any table in the Material Pedigree collection. Because both in-house micrographs and images from the literature are stored in the Microstructure table, records can also be linked to the References: Materials and References: Publications tables. Program information is viewed in the Microstructure table by linking to the Program Information table. Finally, for microstructure analysis of manufactured parts or assemblies, records can be linked to the Application table (Figure 20).

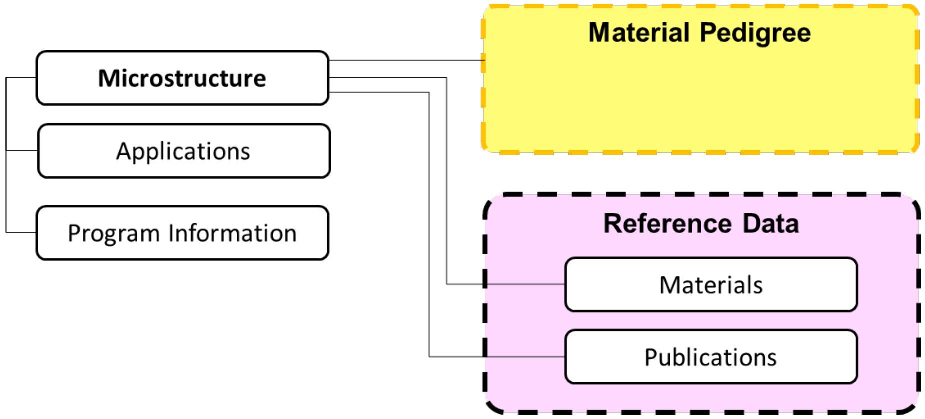

Figure 20.—Microstructure Linking Behavior

A.1.2 Software Tools

The Software Tools table is used to establish traceability between generated simulation data and the software tools used in the data creation. It is also used as a reference for the organization on what software tools are available for future simulations. Records in the Software Tools table contain a description and characterization of the tool, including potential use cases, available operating systems supported, tool limitations and assumptions, etc., and hyperlink/file attributes for the tool location, user manuals, references, etc. Records are organized by the tool use case (e.g., Simulation, Design/Optimization, Database Management, etc.) at the highest level. Each high-level folder contains a unique subfolder architecture that best organizes that type of tool (Figure 21).

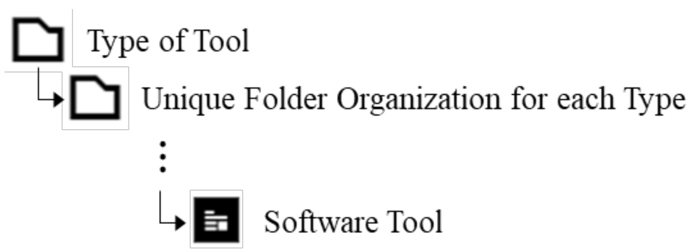

Figure 21.—Software Tools Tree Structure

Records in the Software Tools table can be linked to any of the records in the Models Pedigree collection to establish the relationship between simulation data and the tool used in generating the data. Similarly, records can be linked to the References: Machine Learning Data table for tools used in generating virtual training data. For parts and assemblies, records in the Software Tools table can be linked to those in the Application table for any simulation-based analyses performed. Finally, References: Publications records can be linked to the Software Tools table if a tool was used in published generated data (Figure 22).

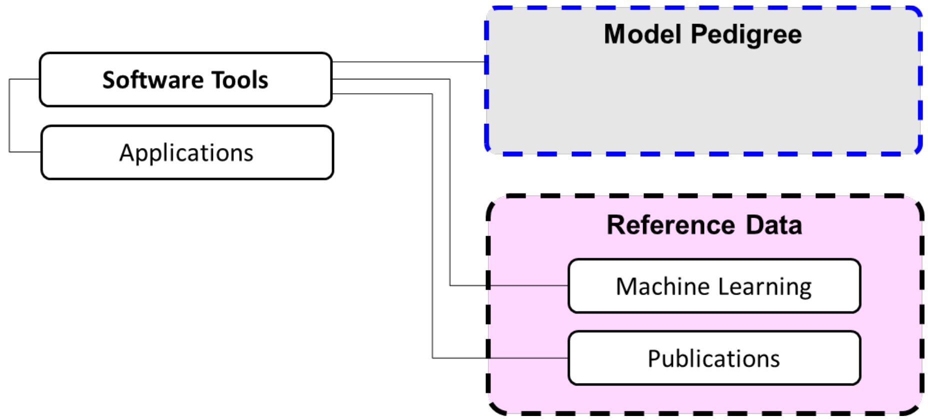

Figure 22.—Software Tools Linking Behavior

A.1.3 Materials Summary

The Materials Summary table provides a summary of the in-house testing that has been or will be performed and the material availability (inventory) for potential use in applications. Records in the Materials Summary table are sorted by test program, and thus offer program managers a unique location to store a test program matrix and monitor the progress of the testing program over time. Records contain information on the material name, availability, form (e.g., plate, sheet, rod, etc.), and available dimensions. Furthermore, through the linked tabular attribute, records contain summaries of the various tests outlined in the Test Data collection, including test type, temperature, batch number (to establish material pedigree), and relevant results to each test. Records are organized by material class (e.g., Metals, PMC, CMC, etc.), material base (e.g., Titanium-based Alloys, Nickel-based Alloys), material name (e.g., Ti-6Al-4V, Timetal 21S), and then individual test series (Figure 23). Note that in Figure 23, a generic record is used at the material name level. In these generic records, information from each different test series can be concatenated together, such that pedigree is maintained between individual test series while still providing an overall summary of the material testing that has been performed.

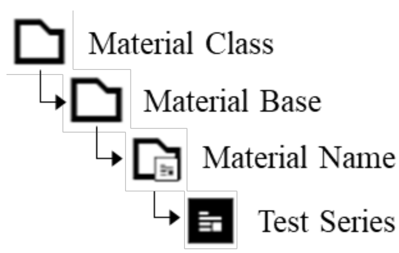

Figure 23.—Materials Summary Tree Structure

As stated previously, records are dynamically pulled from the Test Data collection and viewed in the Materials Summary table, thus inherently linking records between the two tables. For each individual test, the pedigree record is also linked to the Materials Summary table for full traceability between material manufacturing and test results. Program information is viewed in the Material Summary table by linking to the Program Information table. Finally, the References: Publications table can be linked to the Materials Summary table for published information on the testing of the material (for either an individual test series or the material as a whole) (Figure 24).

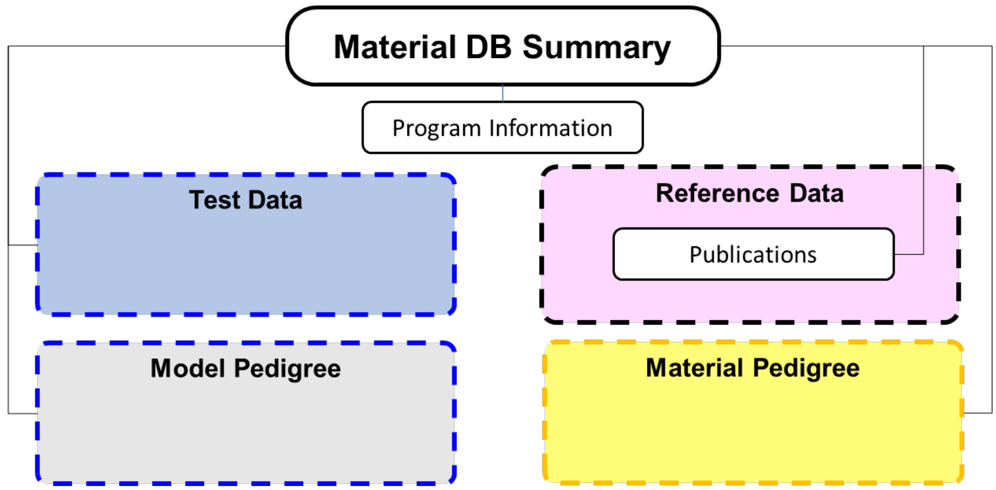

Figure 24.—Materials Summary Linking Behavior

A.1.4 Application

The Application table serves as the bridge between the materials paradigm and the structural paradigm, providing a unique place in the database to link 1) material pedigree, 2) properties, and 3) models to design both materials, parts, and assemblies, thus providing the necessary information, pedigree, and traceability to establish a digital twin/representation for the material or application. Records in the Application table contain information on the application's geometry/manufacturing requirements, performance requirements, analysis results, failure information, material requirements/selection, inspection, and readiness levels. Geometry/manufacturing requirements includes identification of the spacial and temporal geometric design, material zones, and microstructure profile, which allows the record to track both variations within the structure and over time as the part endures its lifecycle. Performance requirements include the identification of any standards for the part and its mechanical, thermal, and environmental requirements. Analysis results includes a summary of any analyses, either virtual or experimental, performed on the application and a location to link to Product Lifecycle Management (PLM) and Simulation Data Management (SMD) systems that are outside of the scope of a materials database. Failure information refers to tracking the potential failure modes and mechanisms, their likelihood, and their impact. Material Requirements/Selection includes any material requirements, the bill of materials (for parts) or parts list (for assemblies), and documentation of the selection criteria. Inspection includes any examination, be it destructive or non-destructive, in certifying the application. Finally, the Readiness Levels section documents the Technology Readiness Level (TRL), Manufacturing Readiness Level (MRL) Integration Readiness Level (IRL), and System Readiness Level (SRL), as defined in Ref. [13]. Records in the Application table record are organized by a generic record that captures general information on the application class (e.g., disk, vane, combustion dome), then records on specific applications (Figure 25). For example, a generic record may contain typical dimensions, approved organizational materials, expected analyses, etc. for a turbine disc, whereas the record within contains specific information on the design, analysis, and materials used for a real part.

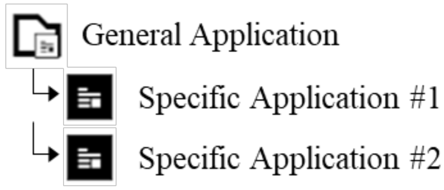

Figure 25.—Application Table Tree Structure

Due to the roll that the Application table plays in establishing a bridge between the materials database and product management systems and the desire for the Application table record to serve as an integral part of an application's digital thread, the Application table features extensive linking with the other tables in the database. Material Pedigree records can be linked to the Application table to establish traceability for any material selection performed. Similarly, if reference material data is used in part design, the Application table links to the References: Materials table. Manufacturing records can be linked to the Application table to define any processing or manufacturing done on the application. Records can also link to the Test Data collection, either to establish traceability between tests performed for material properties or for testing of the application itself. Records in the Model Pedigree collection and Software Tools table can be linked to the Application table for any material models implemented in the analysis of the application or simulations performed. Records in the remainder of the References collection (i.e., Standards, Information/Resources, Schematics, Publications) can all be linked to the Application table to track any publications/documents created on the application, view any relevant schematics, and identify and track the status of specific requirements in any associated standard. Program information is viewed in the Application table by linking to the Program Information table. Finally, records in the Application table can link to other records in the Application table, allowing part records to link to an assembly, enabling a system-of-systems organization of the records in the database (Figure 26).

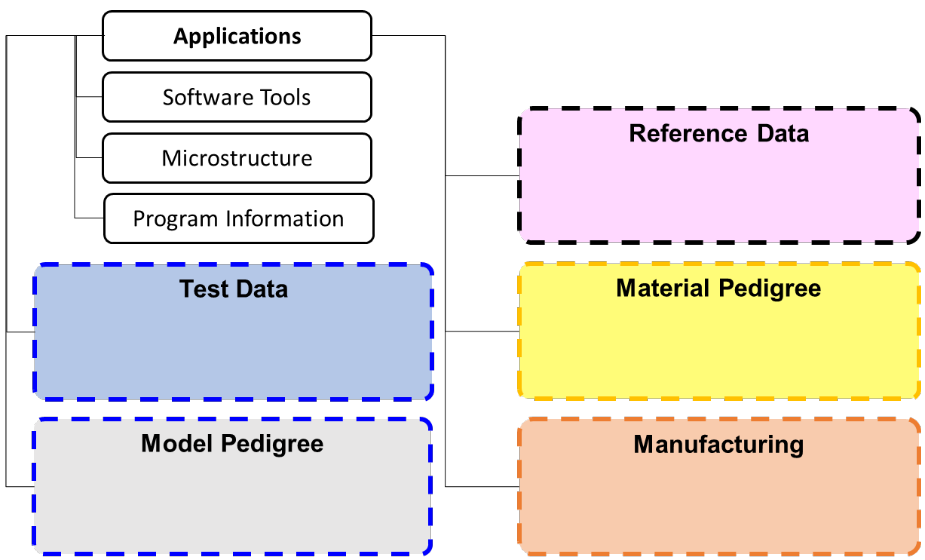

Figure 26.—Application Table Linking Behavior

A.1.5 Program Information

The Program Information table provides a single location to store all program or project information associated with data creation, initial intention for the data, funding, contact information, and access. Records in the Program Information table include the project name, a description of the project, the funding source for the project, point of contacts, and discrete attributes for the owners of the data and distribution rights of the data. It should be noted that the last two items are not used in place of security controls for each attribute, but rather provide project-level information to data consumers on who data is owned by and can be shared with. Information in these records can then be viewed in the other tables in the database via the tabular attribute, eliminating the need to repeatedly define such attributes, both saving time and following the database best practices outlined in Section 1.1. The Program Information table organization will likely vary from organization to organization, but at NASA GRC records are organized first by the NASA Mission Directorates (e.g., ARMD, STMD), and then the individual programs within each Mission Directorate (e.g., TACP, HyTec, Hypersonic, etc.) see (Figure 27).

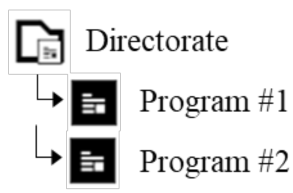

Figure 27.—Program Information Tree Structure

As stated previously, records are dynamically pulled from the Project Information table and viewed in the various other tables in the database, thus inherently linking records between the two tables while displaying relevant program information for that data. Specifically, the Program Information table data can be viewed in the Materials Summary table, Microstructure table, the Test Data collection, the Model Pedigree collection, and the Application table (Figure 28).

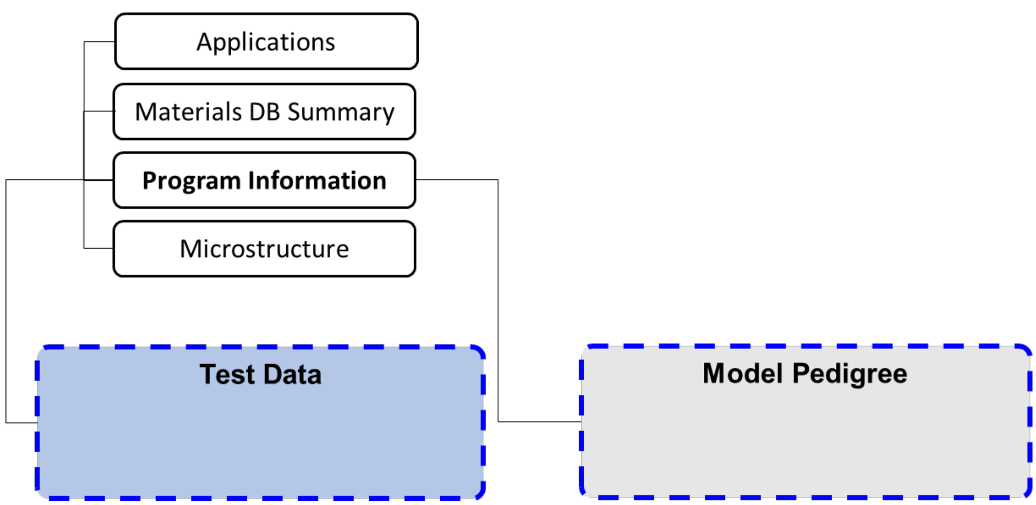

Figure 28.—Program Information Table Linking Behavior

A.2 Manufacturing

The Manufacturing stores the various manufacturing and processing methods (both subtractive and additive) used on either batch materials or individual test specimens within the database. Records in this collection contain information describing the process, a list of approved materials for the process, typical ranges of parameters that must be defined for a given material, and associated schematics and references. Manufacturing records are used to define a general description of a given method, rather than specific information related to an individual material. For individual batch material processing, records are linked to those in either the Materials Pedigree or References: Materials tables, with material specific information defined in the latter. Within the Manufacturing collection, there are currently two tables:

1. Subtractive Manufacturing
2. Additive Manufacturing

A.2.1 Manufacturing: Subtractive Manufacturing

Records in the Manufacturing: Subtractive Manufacturing table store general information on the various processing methods that can be applied to a material that change the expected behavior to external loading using traditional or subtractive methods. Such records contain a detailed description of the process, associated schematics outlining the process, physical attributes, attributes related to the economics and cost modeling of the process, and geometric descriptors, and any additional characteristics. Records are organized in this table by a processing class (e.g., Deposition, MMC Processing) and then the actual method (e.g., Wire Winding, HIP) (Figure 29).

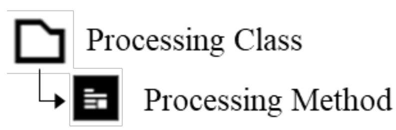

Figure 29.—Manufacturing: Subtractive Manufacturing Tree Structure

Records in the Manufacturing: Subtractive Manufacturing are used to serve as a reference for a manufacturing method, as opposed to describing a specific instance of the process applied to a material. Rather, information on specific material processing is defined in the pedigree tables, where it is expected that each new processing method applied to a batch or test specimen would result in a new record in the pedigree tables. The processing method(s) applied should then be linked to the corresponding pedigree record. Subtractive Manufacturing records can also be linked to the Test Information: Equipment table to link any machines or tools used for the given processing method (Figure 30).

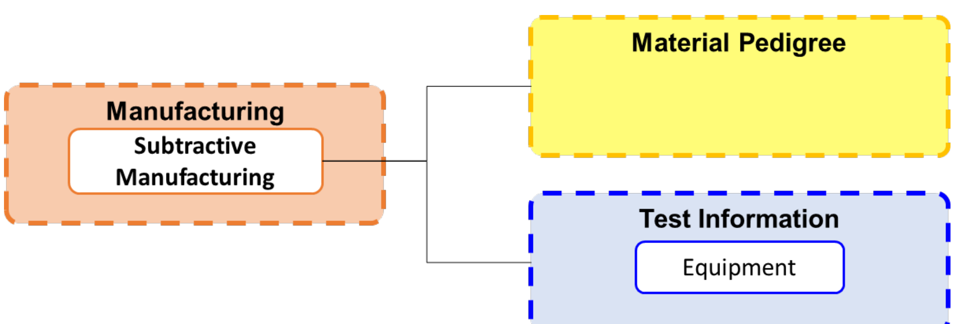

Figure 30.—Manufacturing: Subtractive Manufacturing Linking Behavior

A.2.2 Manufacturing: Additive Manufacturing

Records in the Manufacturing: Additive Manufacturing table store general information on the various manufacturing, pre-processing, and post-processing methods for additively manufactured materials. Records contain a description of the process, geometric parameters relating to the build size, information on the feedstock, a list of the parameters used to define the build with typical ranges for each parameter, associated pre- and post-processing methods typically employed for that process, and list of compatible materials, linked to the pedigree tables. Records in the Manufacturing: Additive Manufacturing table are organized first by classification (i.e., Additive Manufacturing Process, Post-Processing, Pre-Processing), then by designation of melt-based or non-melt based, then by feedstock type (e.g., powder, wire), and finally by the method (Figure 31).

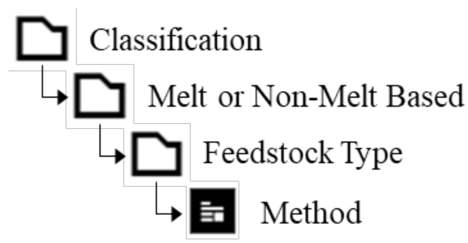

Figure 31.—Manufacturing: Additive Manufacturing Tree Structure

Similar to the Manufacturing: Subtractive Manufacturing table, Manufacturing: Additive Manufacturing records are used to serve as a reference for a manufacturing method, as opposed to describing a specific instance of the process applied to a material. For specific additive builds, information on specific material processing and actual additive manufacturing parameters used in production of the material are defined in the pedigree tables, where a link to the manufacturing method is used to provide the parameters necessary to define the build. Manufacturing records are also linked to the build machine, stored in the Test Information: Equipment table, such that the relationship between the method and the actual build, as well as pedigree information on the machine calibration, maximum build geometry, and machine location, can be established. Additionally, pre- and post-processing records can be linked to a given manufacturing method to establish best practices for part production (Figure 32).

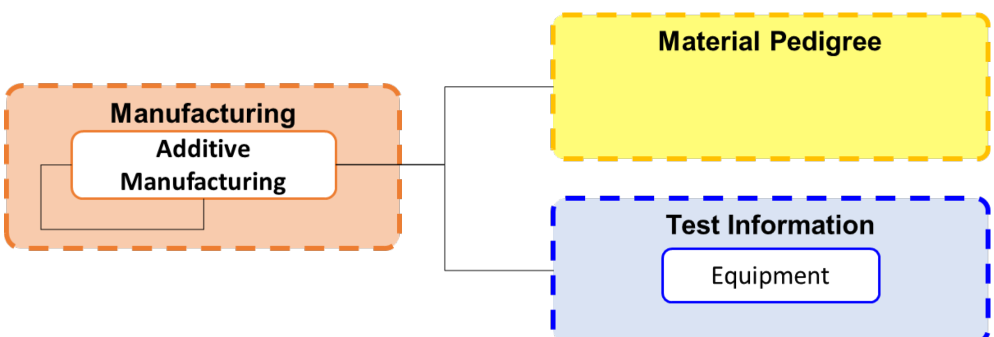

Figure 32.—Manufacturing: Additive Manufacturing Linking Behavior

A.3 Materials Pedigree

The Materials Pedigree collection is used to store pedigree information for metal, ceramic, polymer, composite, and coating materials used in subsequent experimental testing. Records within the Materials Pedigree collection represent specific batch productions of material characterized, associated chemistry and processing of the material, cutout diagrams for individual specimens used for experimental testing, and performed inspection data on the material. Record links are used to provide traceability between records within the Material Pedigree collection and associated experimental testing, published literature data, and the Materials Summary table. Within the Materials Pedigree collection, there are currently eight tables:

1. Ceramics
2. Coatings
3. Metals
4. Polymers
5. Reinforcements
6. Composite Ply Architecture
7. Composite System-Laminate
8. Component/Assemblies

A.3.1 Pedigree: Ceramics

The Pedigree: Ceramics table stores material pedigree information for ceramic materials. Records in the Pedigree: Ceramics table are organized by material class, the base ceramic material, and then the individual materials (Figure 33). Each record contains data on the ceramic material composition, manufacturing and processing information, and physical properties from the manufacturer.

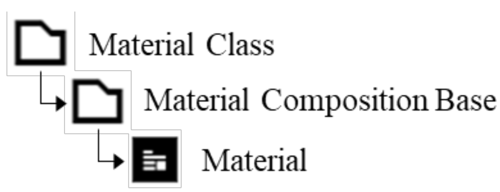

Figure 33.—Pedigree: Ceramics Tree Structure

Records in the Pedigree: Ceramics table can be linked to the Pedigree: Composite Ply Architecture table, Pedigree: Composite System Laminate table, and/or Pedigree: Component/Assemblies table if the ceramic material is used in a ceramic matrix composite (CMC), as well as the Manufacturing: Subtractive Manufacturing for any information related to the processing of the ceramic material. Records can also be linked to any of the Test Data tables in the database for any corresponding tests that were conducted from the batch of material represented in that record. For any microstructure images or characterization, records can also be linked to the Microstructure table. Finally, records can be linked to the References: Publications table for any associated publications with the material (Figure 34).

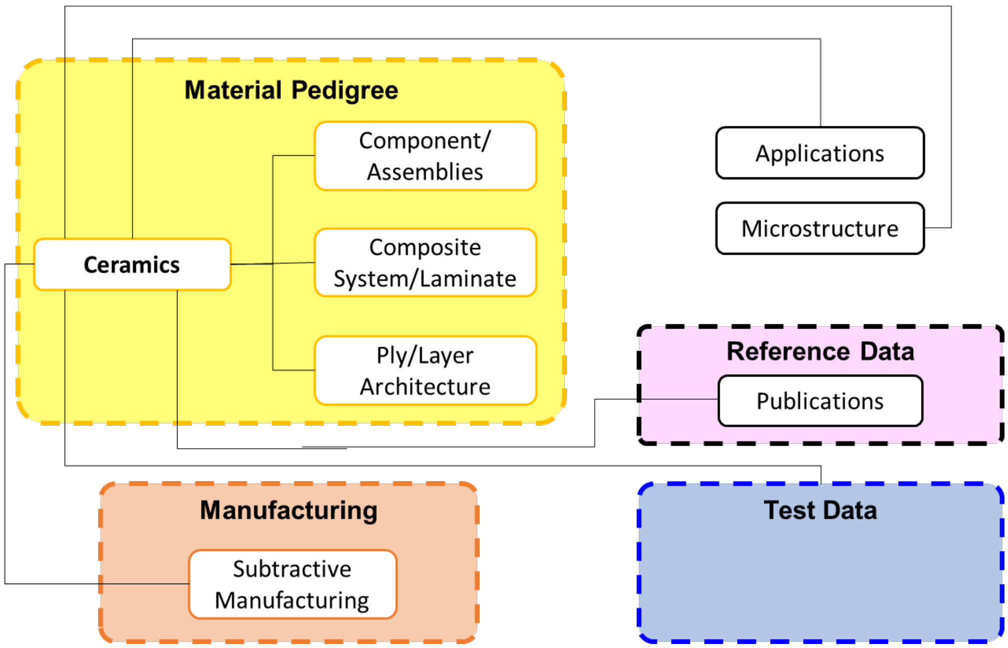

Figure 34.—Pedigree: Ceramics Linking Behavior

A.3.2 Pedigree: Coatings

The Pedigree: Coatings table stores material pedigree information for coatings. Records in the Pedigree: Coatings table are organized by use case (e.g., External Coatings, Reinforcement Coatings, etc.), the base material, and then the individual materials (Figure 35). Each record contains data on the material composition, manufacturing, processing information, and layer thickness.

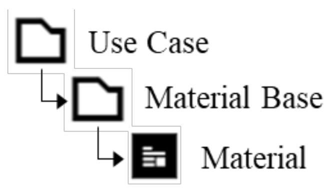

Figure 35.—Pedigree: Coatings Tree Structure

Records in the Pedigree: Coatings table can be linked to the Pedigree: Composite Ply Architecture table, Pedigree: Composite System Laminate table, or Pedigree: Component/Assemblies table if the coating is used in a composite material, as well as the Manufacturing: Subtractive Manufacturing for any information related to the processing of the coating. Records can also be linked to any of the Test Data tables in the database for any corresponding tests that were conducted from the batch of material represented in that record. For any microstructure images or characterization, records can also be linked to the Microstructure table. Finally, records can be linked to the References: Publications table for any associated publications with the material (Figure 36).

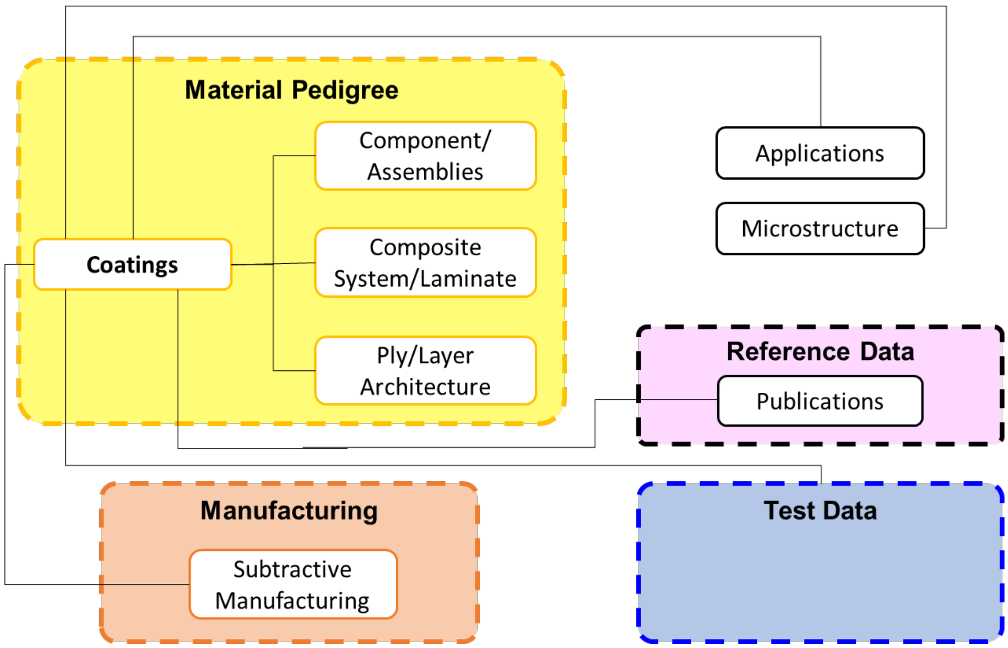

Figure 36.—Pedigree: Coatings Linking Behavior

A.3.3 Pedigree: Metals

Records in the Pedigree: Metals table store metallic material information, including the alloy chemistry, raw material processing, intermediate processing, final processing, heat treatment, and material properties. Records are organized first by the alloy base, or the element with the highest percentage in the alloy chemistry (e.g., Nickel, Titanium, etc.), then by the alloy name (e.g., Ti-6Al-4V, Ti-6Al-7Nb, etc.), then by processing method (e.g., Extruded, Rolled, etc.), and then by the material (Figure 37).

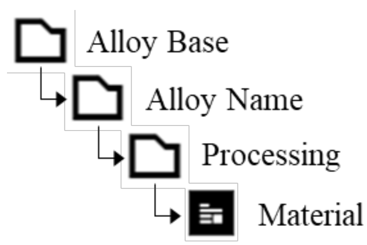

Figure 37.—Pedigree: Metals Tree Structure

Records in the Pedigree: Metals table can be linked to the Manufacturing: Subtractive Manufacturing table to define the processing method for the material, the Microstructure table to link microstructure images and characterization available, the Pedigree: Composite System/Laminate table or Pedigree: Component/Assemblies table if the metal is used in a composite system, and the Manufacturing collection for any information related to the processing of the metal, albeit additive or subtractive. Records can also be linked to any of the Test Data tables in the database for any corresponding tests that were conducted from the batch of material represented in that record. For any microstructure images or characterization, records can also be linked to the Microstructure table. Finally, records can be linked to the References: Publications table for any associated publications with the material (Figure 38).

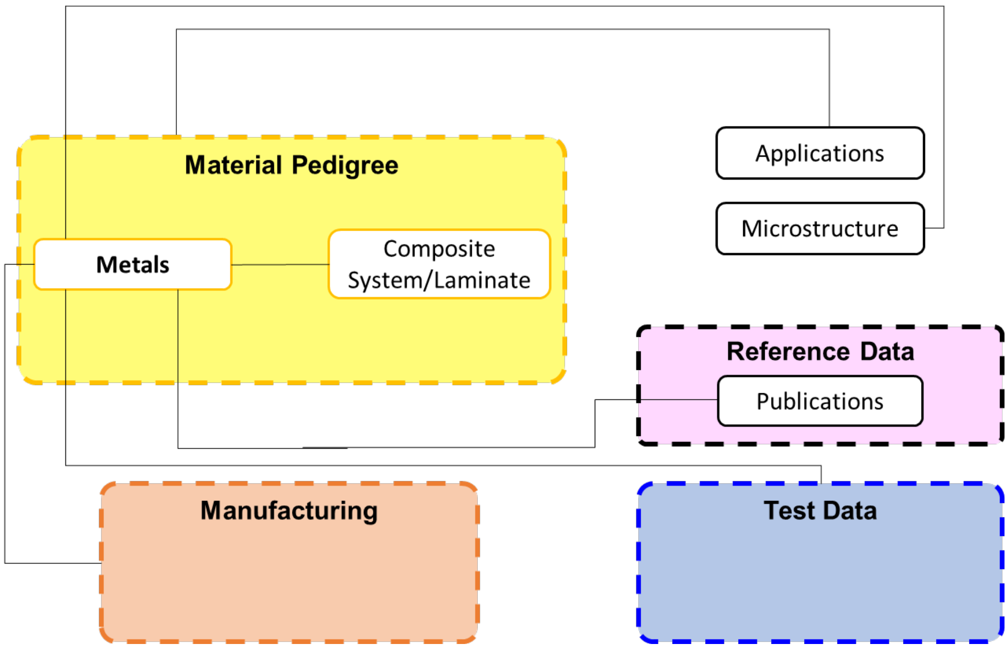

Figure 38.—Pedigree: Metals Linking Behavior

A.3.4 Pedigree: Polymers

Records in the Pedigree: Polymers table store material information for polymer matrix materials, including the polymer chemistry, constituent (i.e., the resin and hardener) information, mixing ratios, and vendor material properties. Records in the Pedigree: Polymers table are organized by the polymer matrix class (e.g., Epoxy, Bismaleimide, etc.) and then the polymer material (Figure 39).

Figure 39.—Pedigree: Polymers Tree Structure

Records in the Pedigree: Polymers table can be linked to the Pedigree: Ply/Layer Architecture and Pedigree: Composite System/Laminate tables as a defined constituent of a composite material, and the Manufacturing: Subtractive Manufacturing table for any information related to the processing of the polymer. Records can also be linked to any of the Test Data tables in the database for any corresponding tests that were conducted from the batch of material represented in that record. For any microstructure images or characterization, records can also be linked to the Microstructure table. Finally, records can be linked to the References: Publications table for any associated publications with the material (Figure 40).

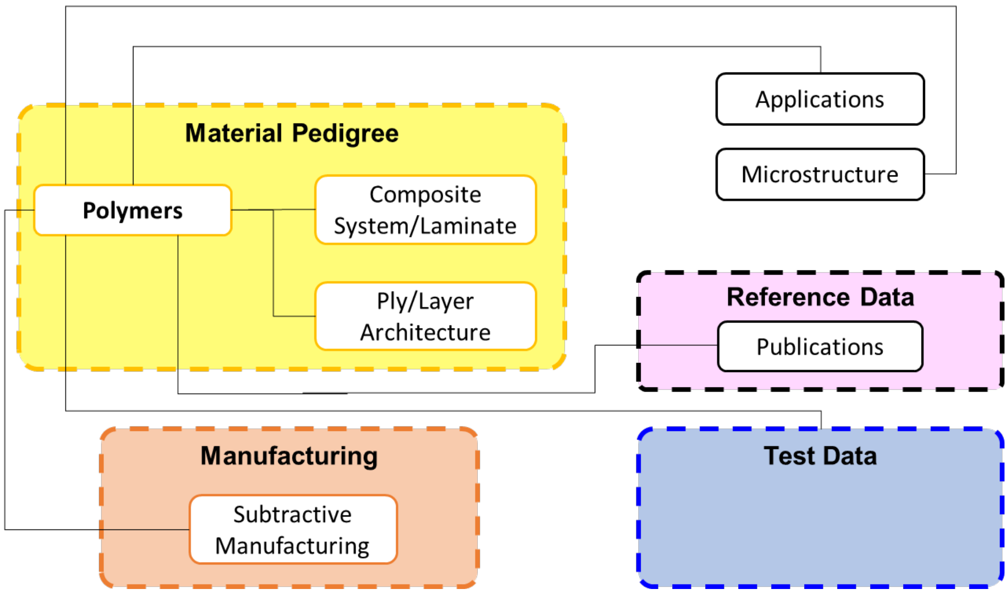

Figure 40.—Pedigree: Polymers Linking Behavior

A.3.5 Pedigree: Reinforcements

Records in the Pedigree: Reinforcements table store material information for reinforcement materials used in composites, including weaves, fiber tows, monofilaments, and particulates. Records store information including the name and manufacturer of the material, geometric descriptors, processing information from the manufacturer, and coating information from the manufacturer, if applicable. Records are organized by the type of reinforcement (e.g., Fiber, Particulate, Wire), then by the material class (e.g., Carbon Fiber, E-Glass), and finally by the specific material (e.g., IM7 Carbon Fiber, T700S Carbon Fiber) (Figure 41).

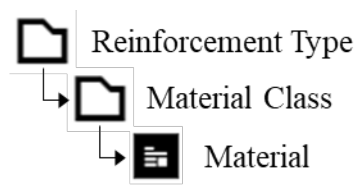

Figure 41.—Pedigree: Reinforcements Tree Structure

Similar to the Pedigree: Polymers table, records in the Pedigree: Reinforcements table can be linked to the Pedigree: Ply/Layer Architecture and Pedigree: Composite System/Laminate tables as a defined constituent of a composite material and to the Manufacturing: Subtractive Manufacturing table for any information related to the processing of the reinforcement. Records can also be linked to any of the Test Data tables in the database for any corresponding tests that were conducted from the batch of material represented in that record. For any microstructure images or characterization, records can also be linked to the Microstructure table. Finally, records can be linked to the References: Publications table for any associated publications with the material (Figure 42).

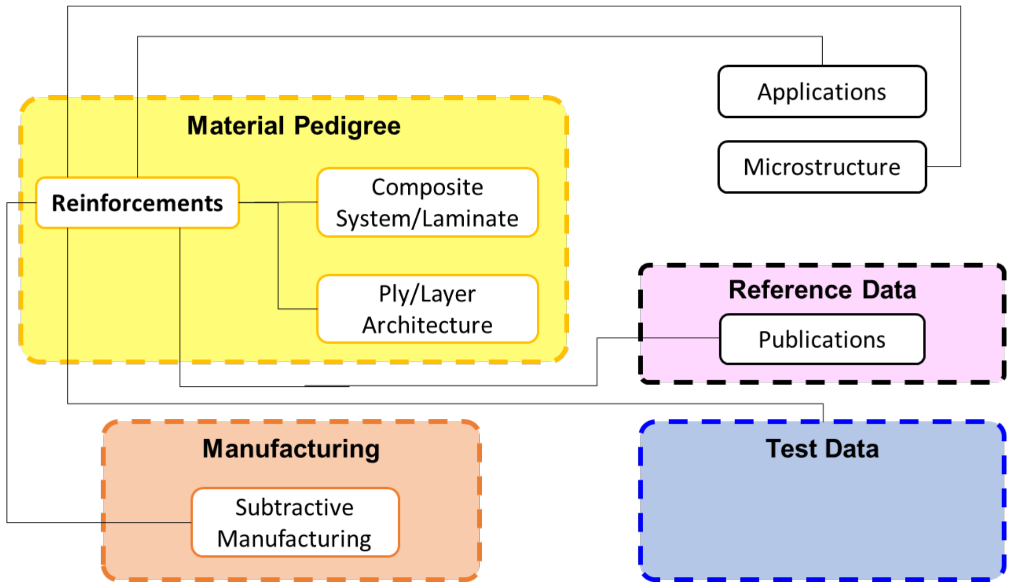

Figure 42.—Pedigree: Reinforcements Linking Behavior

A.3.6 Pedigree: Composite Ply Architecture

Records in the Pedigree: Composite Ply Architecture table store material information for a single ply or lamina made from a reinforcement material and matrix material also stored in the database. Records are organized first by composite type (i.e., Ceramic Matrix Composite (CMC), Metal Matrix Composite (MMC), or Polymer Matrix Composite (PMC)), then by the general composite name (e.g., Titanium Matrix Composite, Epoxy/Carbon, etc.), and then by the specific material (e.g., IM7/8502 Epoxy Unidirectional). Generic records are used to summarize information for a given material, with child records used to store the pedigree of individual batches of said material (Figure 43).

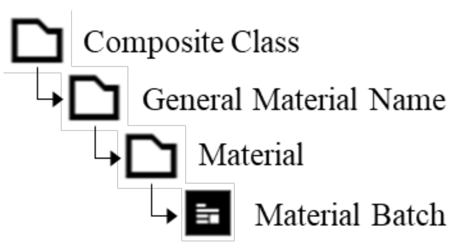

Figure 43.—Pedigree: Composite Ply Architecture Tree Structure

Records in the Pedigree: Composite Ply Architecture table can be linked to the Pedigree: Reinforcements, Pedigree: Ceramics, Pedigree: Metals, and Pedigree: Polymers tables if a material in one or more of those tables is used as a constituent in a ply, as well as the Pedigree: Coatings table if a coating is applied at the ply level, as well as the Manufacturing: Subtractive Manufacturing table for any information related to the processing of the ply. Records can also be linked to any of the Test Data tables in the database for any corresponding tests that were conducted from the batch of material represented in that record. For any microstructure images or characterization, records can also be linked to the Microstructure table. Finally, records can be linked to the References: Publications table for any associated publications with the material (Figure 44).

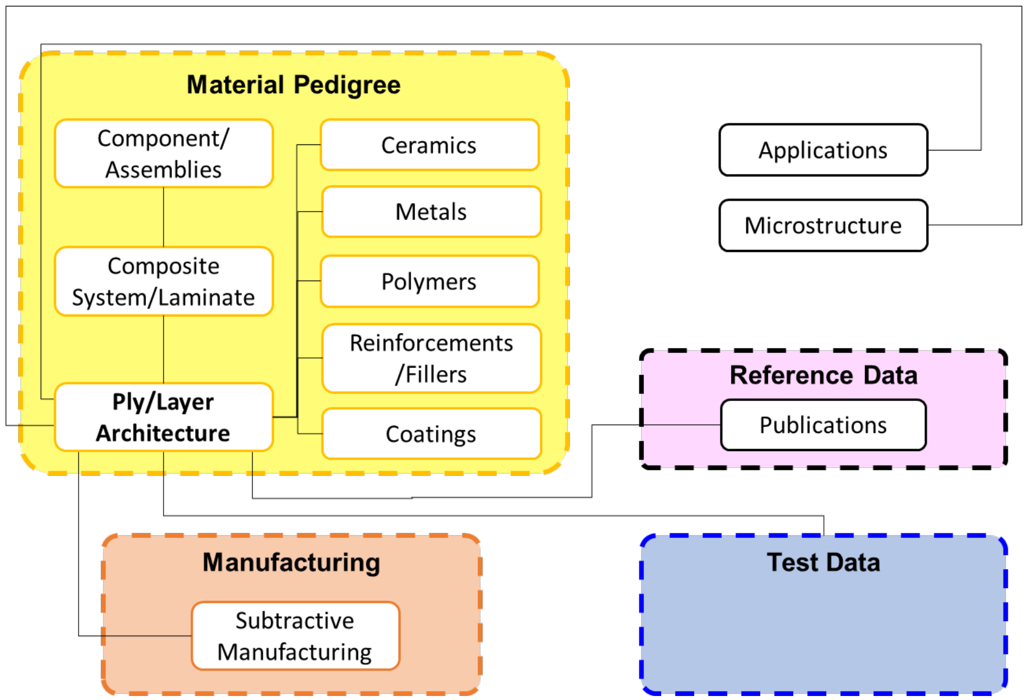

Figure 44.—Pedigree: Composite Ply Architecture Linking Behavior

A.3.7 Pedigree: Composite System-Laminate

Records in the Pedigree: Composite System Laminate table store material information for a laminate system whose laminate is made from single laminas, or plies, defined in the Pedigree: Composite Ply Architecture table. The Pedigree: Composite System Laminate table contains information on the laminate architecture, dimensions, properties, and defects, the ply stacking sequence, the matrix material and reinforcement pedigree, the laminate processing/cure cycle, applied coating, and vendor supplied properties. Records are organized first by composite type (i.e., Ceramic Matrix Composite (CMC), Metal Matrix Composite (MMC), or Polymer Matrix Composite (PMC)), then by the general composite name (e.g., Titanium Matrix Composite, Epoxy/Carbon, etc.), and then by the specific material (e.g., 8 Ply Quasi-Isotropic IM7/8502). Generic records are used to summarize Information for a given material, with child records used to store the pedigree of individual batches of said material (Figure 45).

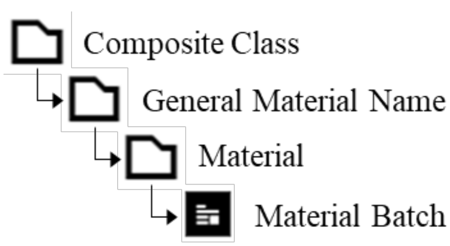

Figure 45.—Pedigree: Composite System-Laminate Tree Structure

The ply stacking sequence is defined via a linked tabular attribute, where each row of the table represents a ply oriented at a given angle. The values in the tabular attribute are populated by linking each ply to the Pedigree: Composite Ply Architecture table. Records can be linked to the Pedigree: Reinforcements, Pedigree: Ceramics, Pedigree: Metals, and Pedigree: Polymers tables if a material in one or more of those tables is used as a monolithic ply in the composite, as well as the Pedigree: Coatings table if a coating is applied to the composite system as a whole. Records can also be linked to the Manufacturing: Subtractive Manufacturing table for any information related to the processing of the laminate, as well as to any of the Test Data tables in the Test Data collection for any corresponding tests that were conducted from the batch of material represented in that record. For any microstructure images or characterization, records can also be linked to the Microstructure table. Finally, records can be linked to the References: Publications table for any associated publications with the material (Figure 46).

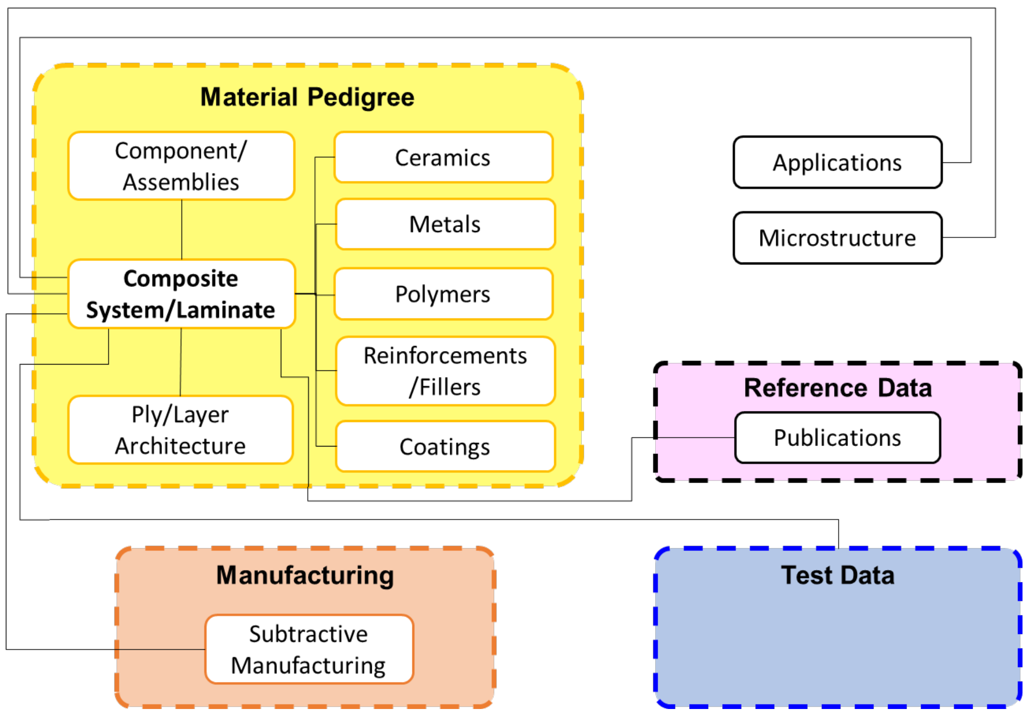

Figure 46. —Pedigree: Composite System-Laminate Linking Behavior

A.3.8 Pedigree: Component/Assemblies

Records in the Pedigree: Component/Assemblies table store pedigree information on typical components or assemblies used in manufacturing, such as sandwich panels and stiffened panels. Records contain information on the material system used and the component geometry. Pedigree: Component/Assemblies records are organized by the type of component (e.g., Panel Structure, Stiffened Structure), then the shape or configuration of the structure (e.g., hat stiffener, I-Stiffened panel, T-Stiffened panel), and then the actual component (Figure 47).

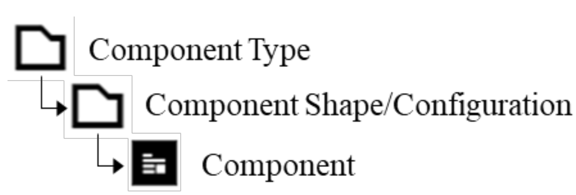

Figure 47.—Pedigree: Component/Assemblies Tree Structure

Records in the Component/Assemblies table can be linked to those in the remainder of the Material Pedigree collection to establish the pedigree of the individual materials or system of materials that make up the component, as well as to the Manufacturing: Subtractive Manufacturing table for any information related to the processing of the component. Records can also be linked to any of the Test Data tables in the database for any corresponding tests that were conducted from the batch of material represented in that record. For any microstructure images or characterization, records can also be linked to the Microstructure table. Finally, records can be linked to the References: Publications table for any associated publications with the component (Figure 48).

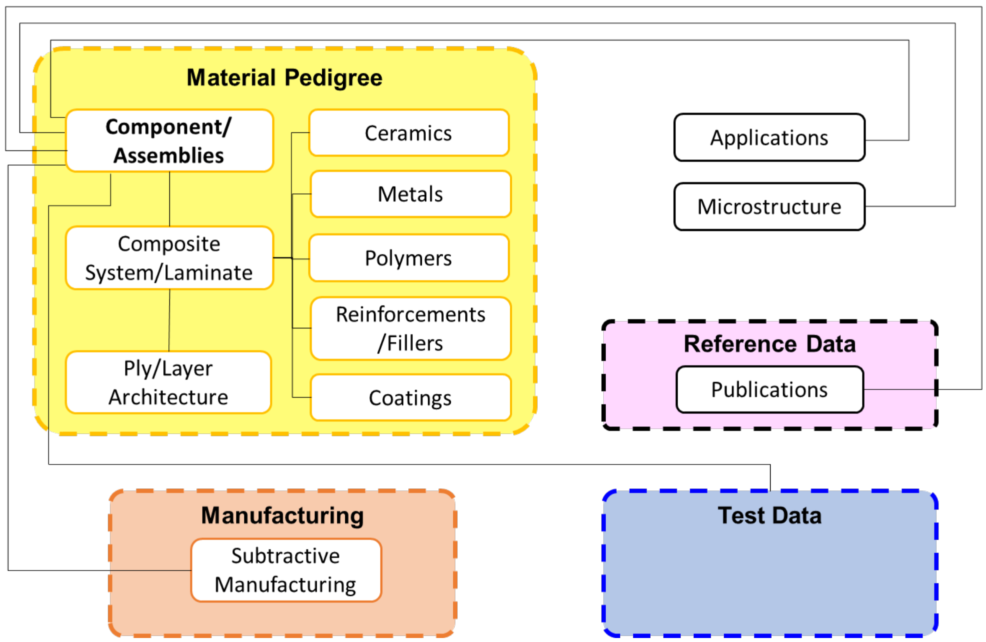

Figure 48.—Pedigree: Component/Assemblies Linking Behavior

A.4 Models Pedigree

The Model Pedigree collection stores all information related to simulations performed at various length scales of a material. Records in the Model Pedigree collection are used to relate information between experimental tests conducted to determine model parameters and simulation results. As such, records in this collection typically contain some description of the material, a description of the model implemented, the methodology for material characterization and parameter estimation within the context of the employed model, the material/model parameters, the simulation results, associated references and links to establish traceability between the material pedigree, testing, and any resultant publications. Within the Model Pedigree collection, there are currently four tables:

1. Composite
2. Deformation
3. Damage/Life
4. Machine Learning

A.4.1 Models: Composite

The Models: Composite table is used to store material models for composite materials at various length scales. At the microscale, records can contain simulations of the microstructure of a single ply or lamina (i.e., the material response of the constituents to applied loading). At the mesoscale, simulations of laminate behavior and homogenized properties can be stored. Records in the Models: Composite table contain material information, modeling information for both the micromechanics and macromechanics (e.g., laminate) approaches, information on the software tools used to conduct the simulation, the simulation results, information on the tests used in model parameter determination, and additional information. Material information includes that of both the composite and the constituent properties, the volume fraction, and the void volume fraction, if applicable. Micromechanics modeling information refers to the micromechanics method, the tool used for micromechanics analysis, associated input and output files that serve as the digital twin for the material, and a description of the microstructure or repeating unit cell (RUC)/repeating volume element (RVE). Laminate modeling information refers to the laminate architecture, software tools used for analysis, input and output files that serve as the laminate-level digital twin for the material, the ABD matrix components, and material allowables determined from the simulation. The simulation response section contains functional attributes for stress/load vs strain/displacement in the normal directions, stress vs time in the normal and shear directions, and strain vs time in the normal and shear directions. The additional information section allows for linking to other models, reports, and definition of general notes on the simulation. Records in the Models: Composite table are organized by composite class (i.e., CMC, MMC, PMC), material name (e.g., IM7/977-3, E-glass/Epoxy), scale (i.e., RUC or Laminate), and then the simulation (Figure 49).

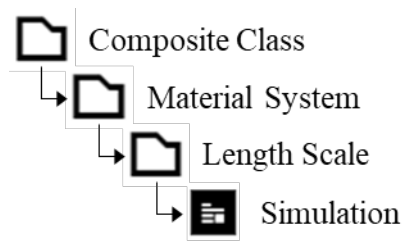

Figure 49.—Models: Composite Tree Structure

Records in the Models: Composites table are able to link to the various Test Data tables to establish the traceability between experimental tests utilized within the database for characterization (determination of model parameters) and validation. They can also link to the Software Tools table to reference any software used to conduct the simulation at any length scale, as well as link to records in the Models: Deformation table if multiple models were used during the simulation. Records can also be linked to the Application table to relate any material models used in the design and analysis of parts or assemblies, thus ensuring maintenance of that application's digital twin. Program information is viewed in the Model Pedigree: Composites table by linking to the Program Information table. Finally, records can be linked to the References: Publications table for any associated publications or reports that feature the simulation performed (Figure 50).

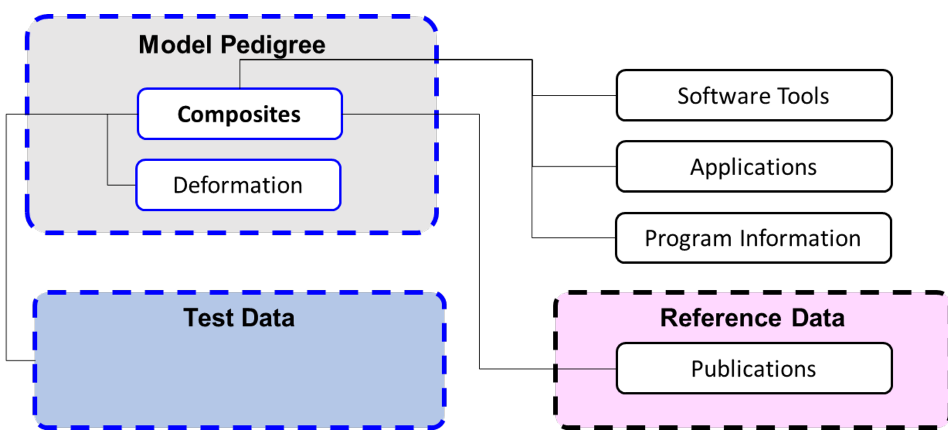

Figure 50.—Models: Composites Linking Behavior

A.4.2 Models: Deformation

The Models: Deformation table is used to store material models and parameters for simulating linear and nonlinear deformation to applied loading. Records contain material information, a model description, material characterization information/parameter estimation methods, model parameters, simulation responses, and additional information. Material description includes the material name, processing, and pedigree information. Model description includes the model's name and description, assumptions made, the deformation regime (i.e., elastic, plastic, elastoplastic, viscoelastic, viscoplastic, or viscoelastoplastic), and the software tools used in employing the model. Characterization information/parameter estimation method refers to the methodology by which the model parameters were determined and the software tools used in parameter estimation. Model parameters can be defined for a thermo-elastic model, viscoelastic model, plastic model, and viscoplastic model. The simulation response section contains functional attributes for stress vs strain in the normal directions, stress vs time in the normal and shear directions, and strain vs time in the normal and shear directions. Finally, additional information allows for definition of the test data used in parameter estimation and links to any associated records in the database. Records in the Models: Deformation table are organized first by reversible or irreversible models, then deformation regime, then material class, then material model (e.g., Ti-6Al-4V GVIPS Viscoplastic Model), and finally the individual material model, which can vary based on temperature, strain rate, etc. for a given material and model choice (Figure 51).

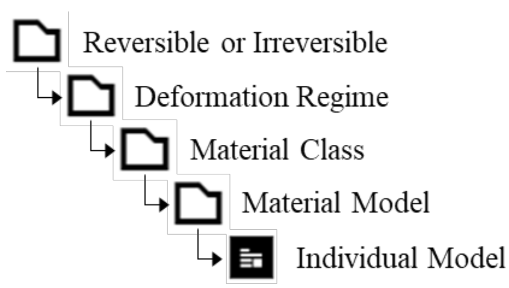

Figure 51.—Models: Deformation Tree Structure

Records in the Models: Deformation table are able to link to the various Test Data tables to establish the traceability between experimental tests performed/stored in the database and determination of model parameters. For material traceability, model records can be linked to any of the Material Pedigree tables as well. They can also link to the Software Tools table to reference any software used to conduct the simulation or in parameter determination, as well as link to records in the Models: Composite table if the deformation model was used as a constituent model or a composites model. Records can be linked to the Application table to relate any material models used in the design and analysis of parts or assemblies, thus ensuring maintenance of that application's digital twin. Program information is viewed in the Model Pedigree: Deformation table by linking to the Program Information table. Finally, records can be linked to the References: Publications table for any associated publications or reports that feature the simulation performed (Figure 52).

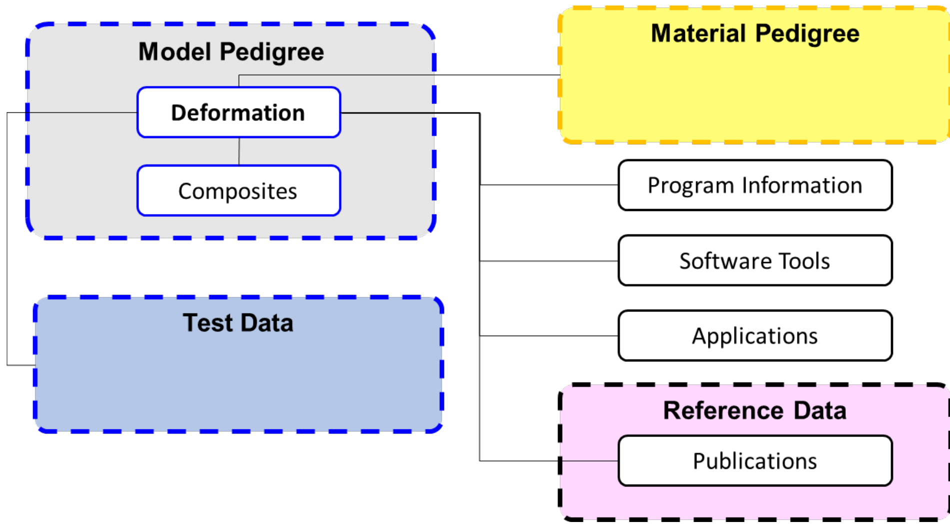

Figure 52.—Models: Deformation Linking Behavior

A.4.3 Models: Damage/Life

The Models: Damage/Life table is used to store material models and parameters for simulating damage and property degradation due to fatigue loading. Records contain general information on the damage mode, the temperature range applicable, and any other analysis notes, as well as the ability to store material parameters and simulation results for various models, including the Basquin model, Coffin-Manson model, Life Power model, Ramberg-Osgood, and ONERA fatigue models. Records in the Models: Damage/Life table are organized first by the type of model (e.g., Fracture, Fatigue), then the damage mode/mechanism (e.g., high frequency cyclic fatigue, low frequency cyclic fatigue), then the material class (e.g., PMC, CMC, Titanium Alloy), then the material name, and then the individual model (Figure 53).

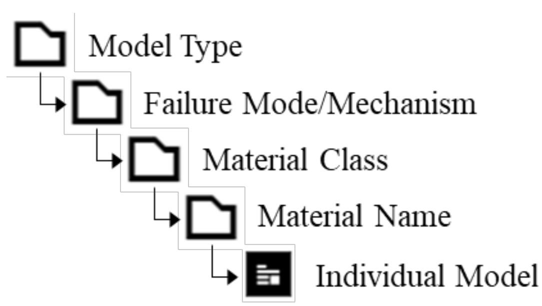

Figure 53.—Models: Damage/Life Tree Structure

Records in the Models: Damage/Life table are able to link to the various Test Data tables to establish the traceability between experimental tests performed in the database and determination of model parameters. For material traceability, model records can be linked to any of the Material Pedigree tables as well. They can also link to the Software Tools table to reference any software used to conduct the simulation or in parameter determination, as well as link to records in the Models: Deformation table if a deformation model was used in the simulation prior to failure. Records can also be linked to the Application table to relate any material models used in the design and analysis of parts or assemblies, thus ensuring maintenance of that application's digital twin. Program information is viewed in the Model Pedigree: Damage/Life table by linking to the Program Information table. Finally, records can be linked to the References: Publications table for any associated publications or reports that feature the simulation performed (Figure 54).

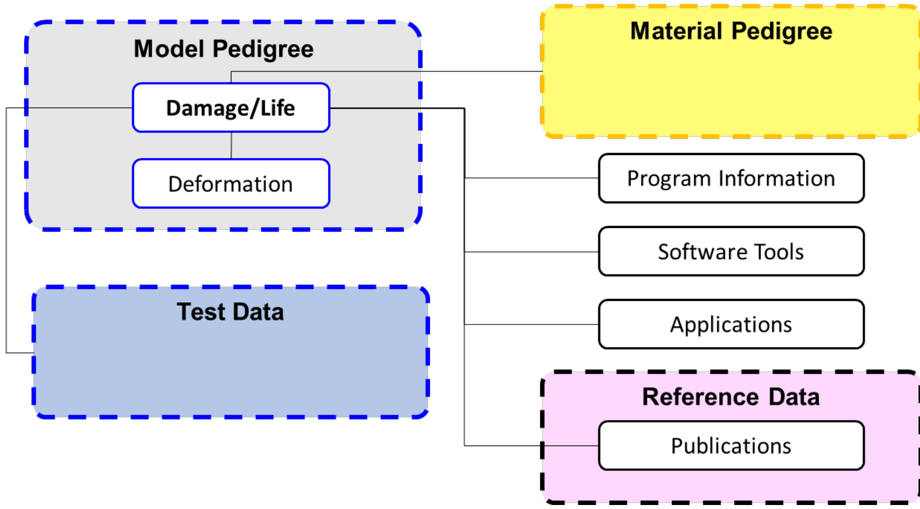

Figure 54.—Models: Damage/Life Linking Behavior

A.4.4 Models: Machine Learning

The Models: Machine Learning table is used to store machine learning models/surrogate models developed for material simulation. Records in the Models: Machine Learning table contain model information, model architecture, data definition, validation information, and further information sections. Model information includes the model's name, a detailed description of the model, the model location for downloading/use, and the required software to run the model. An accurate model definition is particularly important for machine learning models, in which the model can act as a "black box" and mimic physical phenomena without explicitly modeling the physics occurring. Thus, understanding the limitations of the model is paramount in ensuring the model is not used incorrectly. The model architecture section defines the model architecture, including the type of machine learning model, the number of layers, hidden units, activation functions, etc. such that the model can be recreated in any programming language. The data definition section allows for definition of the model inputs and outputs, as well as the definition of training, validation, and test data used in the model creation, all of which are dynamically viewed from the References: Machine Learning Data table if the data was created virtually or from the Test Data collection if the data was collected from physical experiments. The model validation section allows for definition of the accuracy of the model, including functional attributes for the learning curves and tabular attributes for the model predictions of the validation and test sets. The further information section provides links to any software tools used in the model development or employment, as well as any other references in the database. Due to the generic nature of the machine learning table, the record organization is much more fluid than in the other Models tables. In general, however, at the highest level machine learning models are characterized by the existing counterparts in the Models collection (i.e., Composites, Deformation, Damage/Life). Within each of the top level folders, record organization mimics that of the physics-based schema (Figure 55).

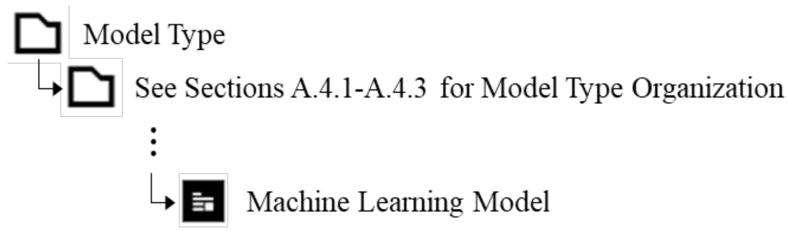

Figure 55.—Models: Machine Learning Tree Structure

Records in the Models: Machine Learning table are able to link to the various Test Data tables if the data used for training, validation, and testing came from experimental data and the References: Machine Learning Data table if the data was generated virtually solely for the purpose of training the model. Records can also link to the Software Tools table to reference any software used to train the model or use the model in practice. Program information is viewed in the Model Pedigree: Machine Learning table by linking to the Program Information table. Finally, records can be linked to the References: Publications table for any associated publications or reports that feature the simulation performed (Figure 56).

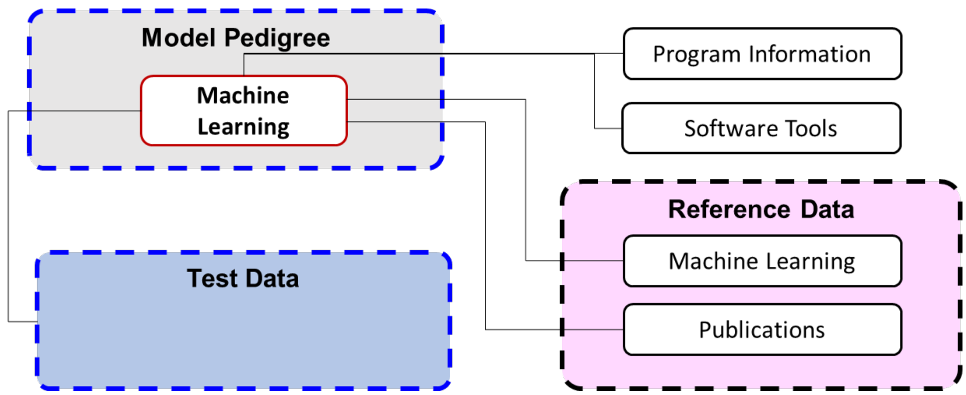

Figure 56.—Models: Machine Learning Linking Behavior

A.5 References

The Reference Data collection stores various forms of reference data in the database, including literature data, virtual data, access to other databases and resources, and different standards. Within the Reference Data collection, there are currently six tables:

1. Materials
2. Machine Learning Data
3. Publications
4. Schematics
5. Information/Resources
6. Standards

A.5.1 References: Materials

The References: Materials table is used to store material information from the literature, including material composition, material properties, functional data curves for properties that vary with temperature, physical characteristics of the material, and manufacturing/commercial availability of the material. Records in the References: Materials table are organized by material class (e.g., ceramics, polymers, metals), material base (e.g., titanium-based alloys, nickel-based alloys), material name (e.g., Ti-

6Al-4V) and then individual sources on that material (Figure 57). Note that in Figure 57, a generic record is used at the Material level. The generic records contain a tabular attribute that automatically calculates the average, maximum, minimum, and standard deviation of the various material properties stored in each individual source for the material, which can be useful when applying reference materials to models and analyses.

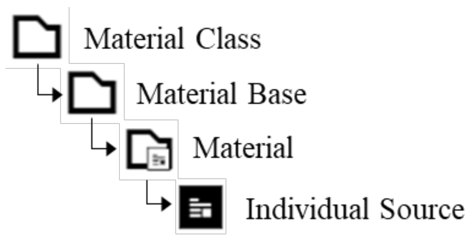

Figure 57.—References: Materials Tree Structure

Due to the lack of definitive pedigree data associated with reference data, it is assumed that any available material pedigree, testing information, etc. is stored in the References: Materials individual source record, with the exception of microstructure images and analysis, which is stored in the Microstructure table, regardless of whether the microstructure images were captured in-house or from the literature, due to the required schema infrastructure needed to effectively capture such data. Thus, records in the References: Materials table can be linked to the Microstructure table to establish the traceability between microstructure images and their source. Records can also be linked to the Models collection if reference data was used in model parameter determination or validation and the Application table if reference material properties are used in material models or analyses (Figure 58).

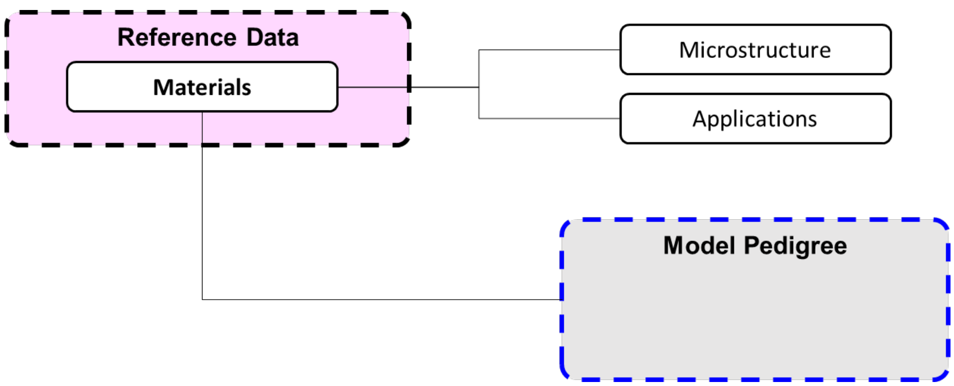

Figure 58.—References: Materials Linking Behavior

A.5.2 References: Machine Learning Data

The References: Machine Learning Data table is used to store virtual (simulation) data created solely for the purpose of training a machine learning model. Records include information on the data series information, the data itself, and links to associated records. Data series information includes a description of the data generated, any software tools used in generating the data, and an attribute to store the raw data file if desired. The data section allows for storage of the input and output values used in training the machine learning model. Due to the general structure required for storing any type of data for a machine learning model, and that the data used as inputs or outputs can take various forms (e.g., point values, data series, images, text, etc.), each input and output is stored as either long text attribute or image type in the record. The data section therefore also contains a tabular attribute to define each long text attribute, including the name of the property and any associated units. Records in the References: Machine

Learning Data use a generic record to store information about the entire data set used for training a machine learning model, with individual records within the generic record for each member of the data set (Figure 59). This methodology is used due to limitations imposed by the Granta MI system with regards to viewing data in other records, and the desire to define data in one location and view it in potentially multiple developed machine learning models.

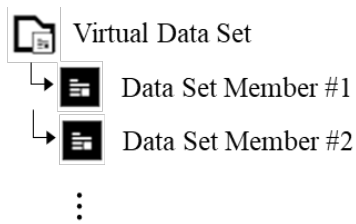

Figure 59.—References: Machine Learning Data Tree Structure

Records in the References: Machine Learning Data table can be linked to Models: Machine Learning records to define the individual training, validation, and test examples used in the model training. Data can be dynamically viewed in the model record, such that the data can be defined once in the reference table and viewed elsewhere, following the previously established database best practices. Software Tools records can also be linked to the References: Machine Learning Data records to provide information on the software used in generating the virtual data set (Figure 60).

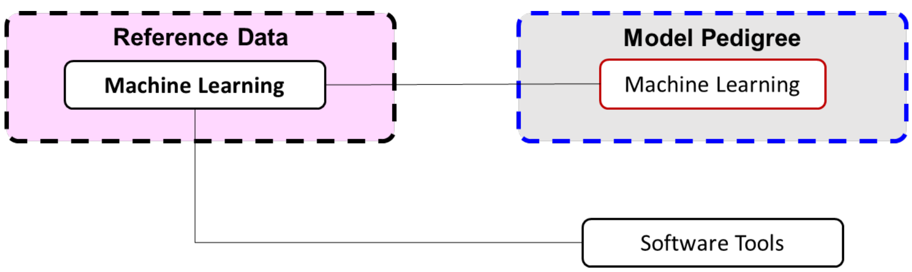

Figure 60.—References: Machine Learning Data Linking Behavior

A.5.3 References: Publications

The References: Publications table stores published papers and reports, along with associated publication metadata, related to all information in the database produced in-house. Records contain direct links to the publication (i.e., the pdf file), point of contact information, project/funding information, and links to associated data throughout the database. Records in the Reference: Publications table are organized by material at the highest level (e.g., Ceramics, Composites, Metals, etc.). For each sublevel, folder organization follows that of the matching pedigree schema described in Section A.2 (Figure 61).

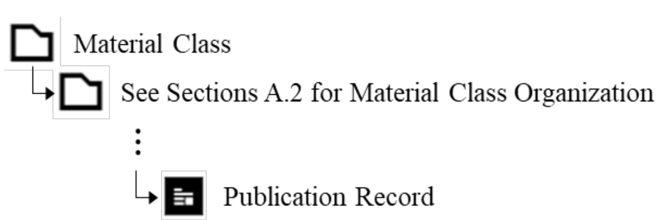

Figure 61.—References: References: Publications Tree Structure

As described in the above sections, tables in the Material Pedigree, Test Data, and Model Pedigree collections can all be linked to the References: Publications table to associate data with published information. Additionally, the Software Tools table, Microstructure table, Program Information Table, and Application table can all be linked to a References: Publications record (Figure 62).

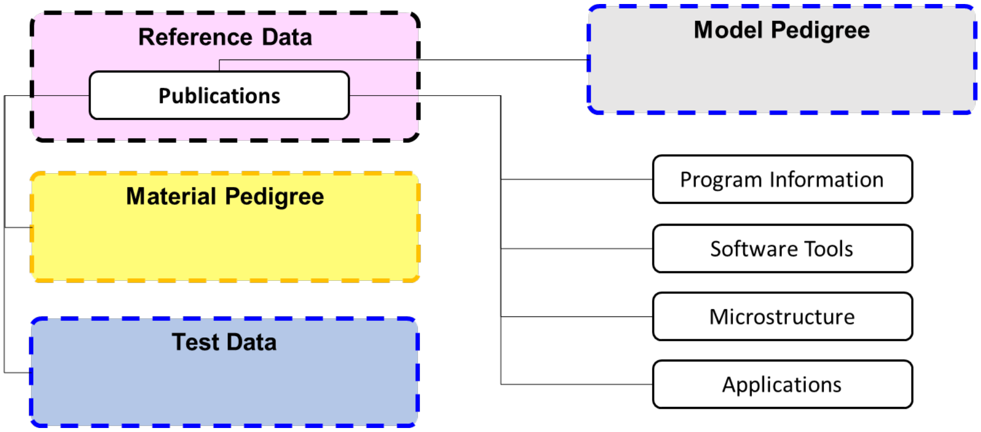

Figure 62.—References: Publications Linking Behavior

A.5.4 References: Schematics

The References: Schematics table is used to store general schematics that are not specific to any given application. Rather, schematics stored in this table can be used as a reference for general applications (e.g., typical rolling bearings vs. a specific rolling bearing for an engine). Records in the References: Schematics table are organized by application (Figure 63).

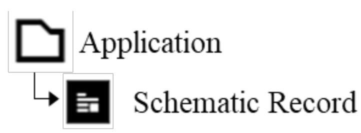

Figure 63.—References: Schematics Tree Structure

Record links to the References: Schematics table are used to establish typical applications that a material can be used for. Therefore, the References: Schematics table can be linked to any record in the Material Pedigree collection (Figure 64).

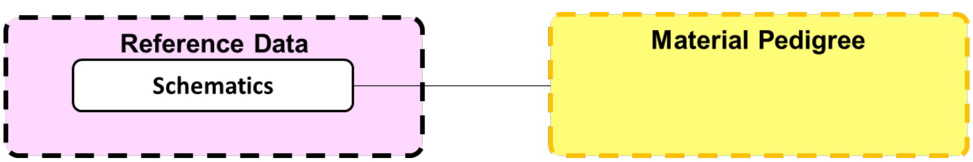

Figure 64.—References: Schematics Linking Behavior

A.5.5 References: Information/Resources

The References: Information/Resources table is used to store reference information on other available databases, research organizations, laboratories, societies, and conferences, publishing information (i.e., materials journals and publishers), material suppliers, and other reports that are not published for the general public. Records are organized by the type of resources (i.e., material databases, technical reports, suppliers, publishing, etc.) at the highest level. Each high-level folder contains a unique subfolder architecture that best organizes that type of resource (Figure 65).

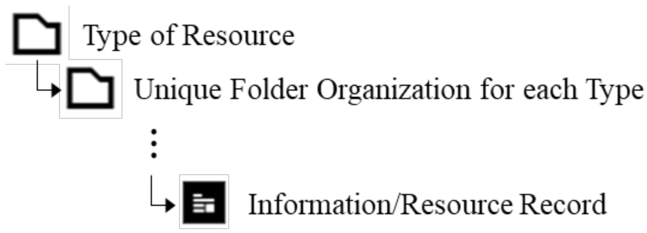

Figure 65.—References: Information/Resources Tree Structure

Records in the References: Information/Resources can be linked to the various material pedigree tables, test data tables, the Materials Summary table, and the Application table to associate any resource with existing data in the database (Figure 66).

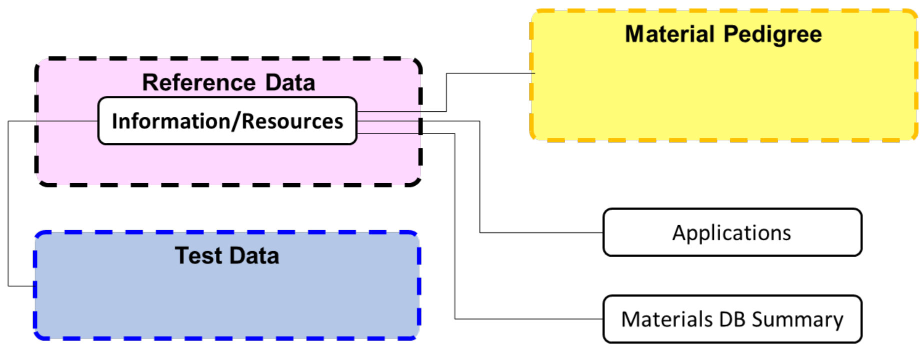

Figure 66.—References: Information/Resources Linking Behavior

A.5.6 References: Standards

The References: Standards table is used to store various standards for material and application testing, manufacturing, and evaluation. Records contain the individual elements of a given standard such that they can be individually viewed and evaluated for a given material or application via the viewed tabular attribute. Records are organized by the type of standard (e.g., Testing Standards, Manufacturing Standards, Evaluation Standards, etc.), then a subcategory of that type (e.g., tensile test standards, creep test standards, etc.), and then the individual standard (Figure 67).

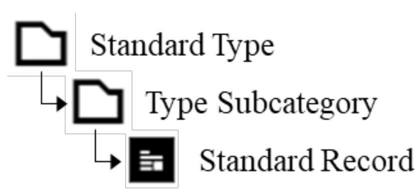

Figure 67.—References: Standards Tree Structure

Records in the References: Standards table can be linked to the Test Data collection for any implemented testing standard, the Manufacturing collection for any manufacturing standards, and the Application table for any standard implemented in the manufacturing, testing, analysis, and evaluation of a part or assembly (Figure 68).

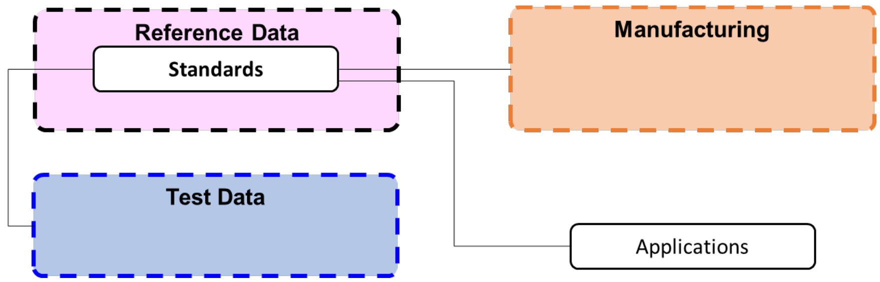

Figure 68.—References: Standards Linking Behavior

A.6 Test Data

The Test Data collection is used to store in-house test data and associated test pedigree. In general, records within the Test Data collection contain data pertaining to the test information, material/processing information, specimen information, test conditions, test response, test results, and data collection. Test information includes a test description, associated standards, the test operator and date, and any additional test notes. Material/processing information includes information on the bulk material prior to the creation of individual test samples. The specimen information includes the actual geometry and orientation of the specimen and any processing/conditioning applied to the individual specimen. The test conditions include the test environment, control mode, and specified strain/loading rate. The test response contains functional data for the displacement, load, strain, stress, and Poisson's ratio for each normal axis as a function of time. The test results section contains the calculated properties from the conducted test, including modulus, yield behavior, creep zones, and failure behavior. In general test response and test result attributes are separated by direction to allow for anisotropic material definition. Unless otherwise stated, it is assumed that for any uniaxial test, the 11 direction aligns with the direction of loading, the 22 direction is transverse to the loading direction, and the 33 direction is normal to both the 11 and 22 directions, measured in the global coordinate system (Figure 69). Each table in the Test Data collection contains an 'Orientation" attribute to define the rotation angle θ to transform global measurements to the material coordinate system, denoted by L, T, and Z. Herein, the *normal directions* will refer to the 11, 22, and 33 directions and the *shear directions* will refer to the 12, 13, and 23 directions.

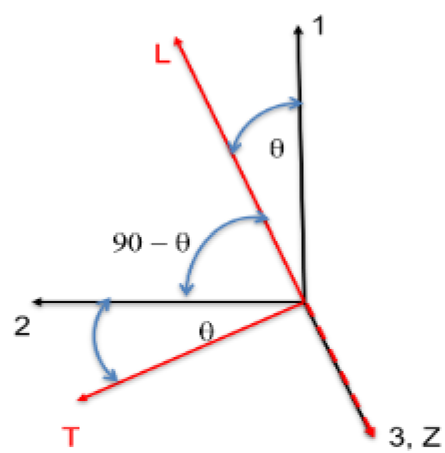

Figure 69.—Coordinate System Definition in the Database

Finally, the data collection section contains information on the testing frame, measurement devices, and any other devices used to conduct the test. For the remainder of Section A.6, each table contains the aforementioned information unless otherwise specified, and will not be repeated in the individual table descriptions for brevity. Within the Test Data collection, there are currently eight tables:

1. Tensile
2. Compression
3. Creep
4. Relaxation
5. Generic
6. Cyclic
7. Fatigue Crack Growth
8. Oxidation

A.6.1 Test Data: Tensile

The Test Data: Tensile table stores in-house test data for uniaxial tensile tests. Records include the above information described in Section A.6. The test response section stores functional data for strain vs time in the normal directions, stress vs time in the normal directions, stress vs strain in the normal directions, and Poisson's Ratio vs Strain (11 axis) in the shear planes. The test results section stores calculated Young's modulus in the normal directions, the method for calculating the modulus, the elastic Poisson's ratio for the shear planes, the proportional limit and yield stress offsets at 0.02% and 0.2%, the ultimate strength and associated strain, and the failure strength and associated strain. Records in the Test Data: Tensile table are organized by material class/base (e.g., PMC, CMC, Titanium Alloy, Nickel Alloy), material name (e.g., Ti-6Al-4V, Timetal 21S), test temperature, strain rate, and then the individual test. Generic records are used at each folder level between the material class/base and the individual test to summarize the tests performed, extracted material properties from each test, and display average and standard deviations of material properties automatically calculated by Granta MI (Figure 70).

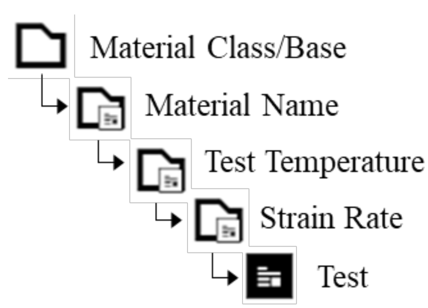

Figure 70.—Test Data: Tensile Tree Structure

To establish the traceability between the bulk material and individual test specimens used for a given test, records in the Test Data: Tensile test can link to any table in the Material Pedigree collection. Records in both the Test Specimen and Equipment tables can also link to the Test Data: Tensile table to establish the pedigree of the nominal specimen dimensions, data collection equipment, and test execution. Records can also be linked to the Applications table for testing performed on a part or assembly. Program information is viewed in the Test Data: Tensile table by linking to the Program Information table. Finally, the Test Data: Tensile table can link to the References: Publications table to provide any literature available that contains the test data (Figure 71).

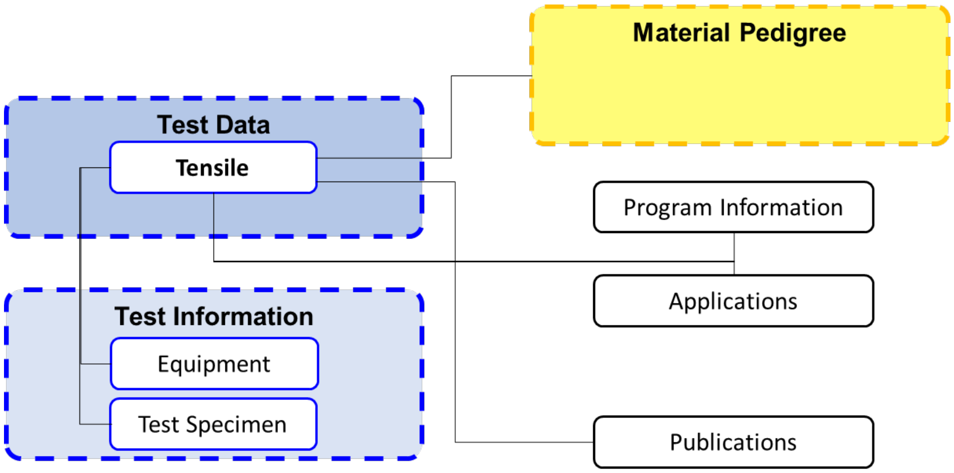

Figure 71.—Test Data: Tensile Linking Behavior

A.6.2 Test Data: Compression

The Test Data: Compression table stores in-house test data for uniaxial compression tests. Records include the above information described in Section A.6. Similar to the Test Data: Tensile table, the test response section stores functional data for strain vs time in the normal directions, stress vs time in the normal directions, stress vs strain in the normal directions, and Poisson's Ratio vs strain (11 axis) in the shear planes. The test results section stores calculated Young's modulus in the normal directions, the method for calculating the modulus, the elastic Poisson's ratio in the shear planes, the proportional limit and yield stress offsets at 0.02% and 0.2%, the compressive strength and associated strain, and the failure strength and associated strain. Records in the Test Data: Compression table are organized by material class/base (e.g., PMC, CMC, Titanium Alloy, Nickel Alloy), material name (e.g., Ti-6Al-4V, Timetal 21S), test temperature, strain rate, and then the individual test. Generic records are used at each folder level between the material class/base and the individual test to summarize the tests performed, extracted material properties from each test, and display average and standard deviations of material properties automatically calculated by Granta MI (Figure 72).

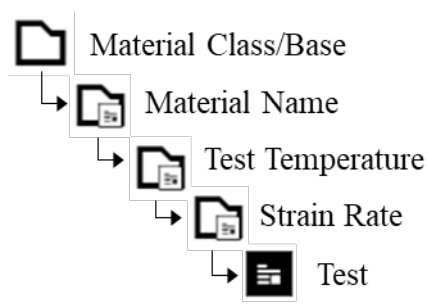

Figure 72.—Test Data: Compression Tree Structure

The Test Data: Compression table exhibits the same linking behavior as the Test Data: Tensile table shown in Section A.6.1 (Figure 73).

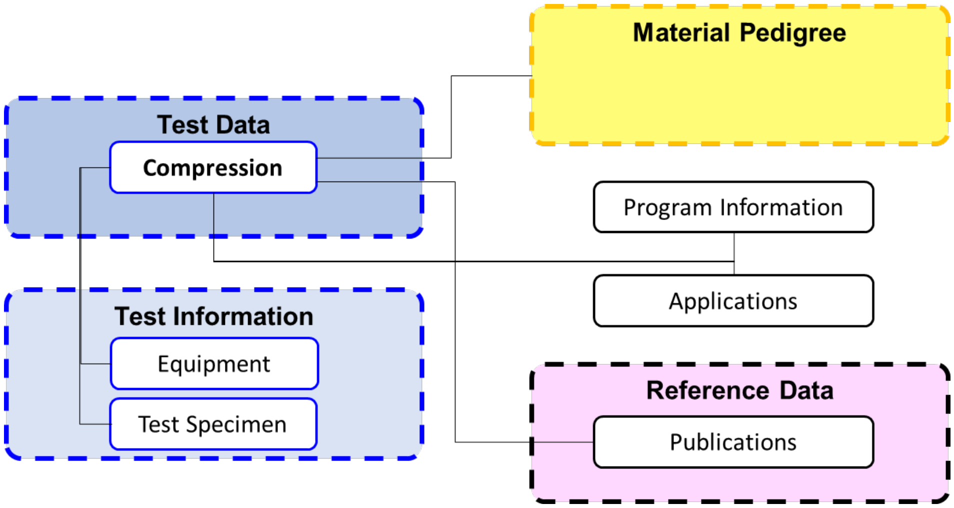

Figure 73.—Test Data: Compression Linking Behavior

A.6.3 Test Data: Creep

The Test Data: Creep table stores in-house test data for single stage creep tests. Records include the above information described in Section A.6. The test response section stores functional data for strain and stress vs time in the normal directions, stress vs strain in the normal directions, creep strain vs time in the 11 direction (i.e., the direction of loading), the strain rate vs time, and the Poisson's Ratio vs Strain (11 axis) in the shear planes. The test results section stores calculated Young's modulus in the normal directions, the method for calculating the modulus, the elastic Poisson's ratio in the shear planes, the proportional limit and yield stress offsets at 0.02% and 0.2%, all of which are calculated during the initial tensile response only. Furthermore, records also contain information on the primary, secondary, and tertiary creep zones. Records in the Test Data: Creep table are organized by material class/base (e.g., PMC, CMC, Titanium Alloy, Nickel Alloy), material name (e.g., Ti-6Al-4V, Timetal 21S), test temperature, creep stress, and then the individual test. Generic records are used at each folder level between the material class/base and the individual test to summarize the tests performed, extracted material properties from each test, and display average and standard deviations of material properties automatically calculated by Granta MI (Figure 74).

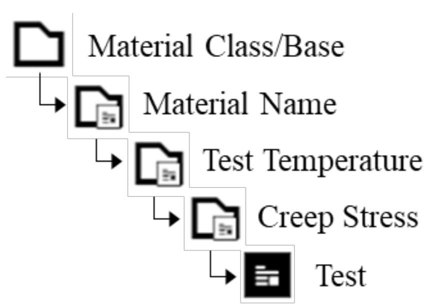

Figure 74.—Test Data: Creep Tree Structure

The Test Data: Creep table exhibits the same linking behavior as the Test Data: Tensile table shown in Section A.6.1 (Figure 75).

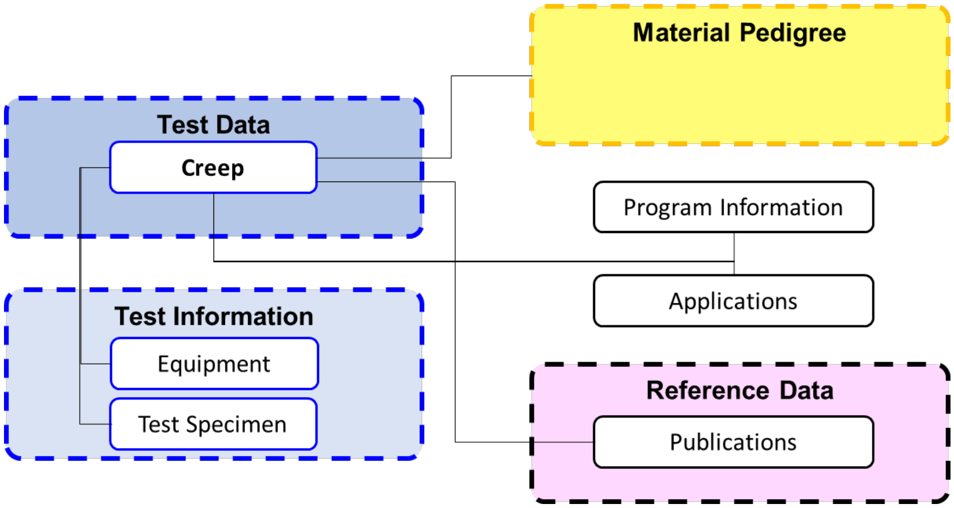

Figure 75.—Test Data: Creep Linking Behavior

A.6.4 Test Data: Relaxation

The Test Data: Relaxation table stores in-house test data for single stage relaxation tests. Records include the above information described in Section A.6. The test response section includes stress vs strain in the normal directions, relaxation stress vs strain in the normal directions, and the Poisson's Ratio vs Strain (11 axis) in the shear planes. The test results section stores calculated Young's modulus in the normal directions, the method for calculating the modulus, the elastic Poisson's ratio in the shear planes, the proportional limit and yield stress offsets at 0.02% and 0.2%, all of which are calculated during the initial tensile response only. Furthermore, records also contain information on the constant strain zone, the unloading behavior after the relaxation, and the recoverable and unrecoverable strain. Records in the Test Data: Relaxation table are organized by material class/base (e.g., PMC, CMC, Titanium Alloy, Nickel Alloy), material name (e.g., Ti-6Al-4V, Timetal 21S), test temperature, constant strain, and then the individual test. Generic records are used at each folder level between the material class/base and the individual test to summarize the tests performed, extracted material properties from each test, and display average and standard deviations of material properties automatically calculated by Granta MI (Figure 76).

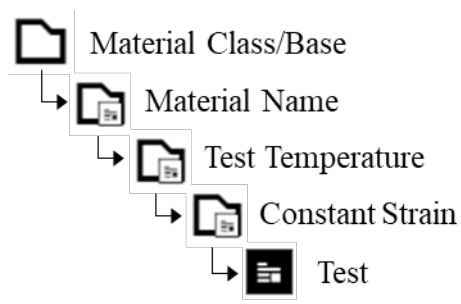

Figure 76.—Test Data: Relaxation Tree Structure

The Test Data: Relaxation table exhibits the same linking behavior as the Test Data: Tensile table shown in Section A.6.1 (Figure 77).

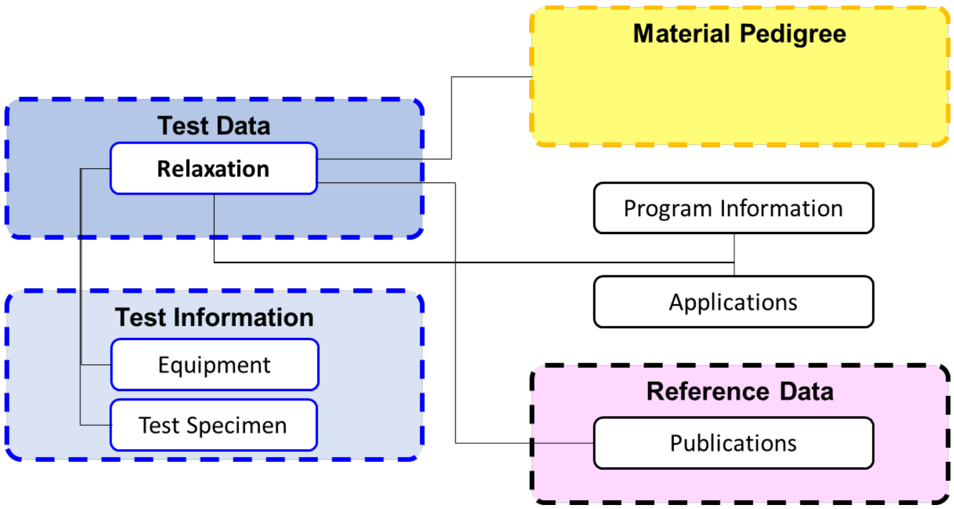

Figure 77.—Test Data: Relaxation Linking Behavior

A.6.5 Test Data: Generic

The Test Data: Generic table stores in-house test data for multistage uniaxial and multiaxial tests. Tests stored in the Test Data: Generic table can contain tensile loading and unloading, compressive loading and unloading, creep (i.e., constant stress), and relaxation (i.e., constant strain) stages, defined below in Table 2.

TABLE 2.—LOAD STAGE DEFINITON FOR MULISTAGE GENERIC TESTS

Control Mode	Rule	Stage Type
Stress	$\lvert\dot{\sigma}\rvert < 10^{-3}\ ksi/s$	Creep
Strain	$\dot{\varepsilon} < 10^{-8}\%/s$	Relaxation
Stress or Strain	$\dot{\sigma} > 0\ and\ \sigma_{end} > 0\ or\ \dot{\varepsilon} > 0\ and\ \varepsilon_{end} > 0$	Tensile Loading
Stress or Strain	$\dot{\sigma} < 0\ and\ \sigma_{end} > 0\ or\ \dot{\varepsilon} < 0\ and\ \varepsilon_{end} > 0$	Tensile Unloading
Stress or Strain	$\dot{\sigma} < 0\ and\ \sigma_{end} < 0\ or\ \dot{\varepsilon} < 0\ and\ \varepsilon_{end} < 0$	Compressive Loading
Stress or Strain	$\dot{\sigma} > 0\ and\ \sigma_{end} < 0\ or\ \dot{\varepsilon} > 0\ and\ \varepsilon_{end} < 0$	Compressive Unloading

Records include the above information described in Section A.6. The test response section stores functional data for stress vs strain, stress vs time, stress vs test temperature, strain vs time and strain vs test temperature, all in the normal directions. It also stores stress in the 11 and 22 direction vs shear strain in the 12 direction, shear stress (12 direction) vs time, shear strain (12 direction) vs time, shear stress (12 direction) vs strain in the normal directions, and shear stress vs shear strain in 12 direction. The test results section stores the Young's Modulus in the normal directions, the shear modulus in the 12 direction, the yield behavior in the normal directions and the 12 direction, ultimate strength and strain in the normal directions, and the Poisson's ratio in the shear planes. Additionally, the Test Data: Generic table contains a Stage Information section, in which a tabular attribute is used to define individual stages, including the stage type (see Table 2), control mode, strain rate, stress rate, and the beginning and end time, stress, strain, rotation, and/or temperature. The section also contains functional attributes to plot the control stress, strain, and temperature as a function of time for more complex loading histories. Records in the Test Data: Generic table are organized by material class/base (e.g., PMC, CMC, Titanium Alloy, Nickel Alloy), material name (e.g., Ti-6Al-4V, Timetal 21S), test temperature, and then the individual test. Generic records are used at each folder level between the material class/base and the individual test to summarize the tests performed, extracted material properties from each test, and display average and standard deviations of material properties automatically calculated by Granta MI (Figure 78).

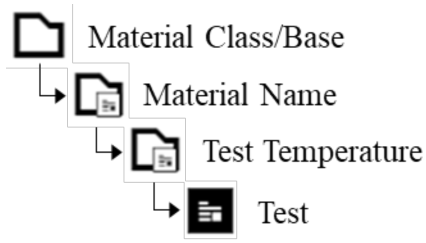

Figure 78. —Test Data: Generic Tree Structure

The Test Data: Generic table exhibits similar linking behavior as the Test Data: Tensile table shown in Section A.6.1 (Figure 77).

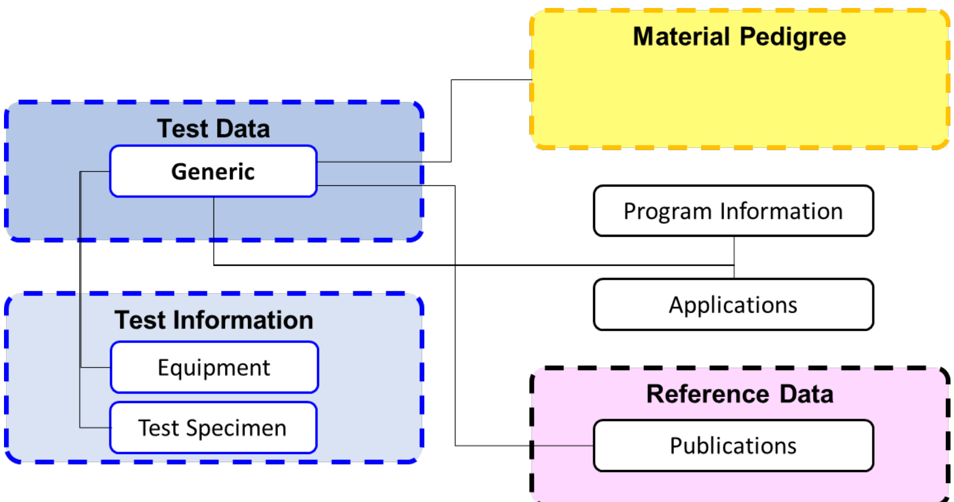

Figure 79.—Test Data: Generic Linking Behavior

A.6.6 Test Data: Cyclic

The Test Data: Cyclic table stores in-house test data for cyclic/fatigue tests. Records include the above information described in Section A.6. The test response section includes the stress vs strain in the three normal directions, the tensile strain vs time in the normal directions, hysteresis loops in the normal directions, the cyclic strain vs time in the normal directions, and the stress R-ratio, stress A-ratio, stress V-ratio, strain R-ratio, strain A-ratio, and strain V-ratio all as a function of cycles. The test results section stores the Young's modulus in the normal directions, the Poisson's ratio in the shear planes, the fatigue life, cyclic life, cyclic frequency, stress range, and strain range. Records in the Test Data: Cyclic table are organized by material class/base (e.g., PMC, CMC, Titanium Alloy, Nickel Alloy), material name (e.g., Ti-6Al-4V, Timetal 21S), test temperature, stress or strain range, and then the individual test. Generic records are used at each folder level between the material class/base and the individual test to summarize the tests performed, extracted material properties from each test, and display average and standard deviations of material properties automatically calculated by Granta MI (Figure 80).

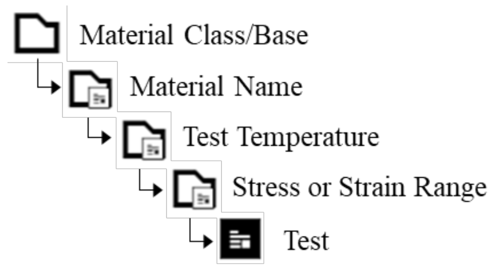

Figure 80.—Test Data: Cyclic Tree Structure

The Test Data: Cyclic table exhibits the same linking behavior as the Test Data: Tensile table shown in Section A.6.1 (Figure 81).

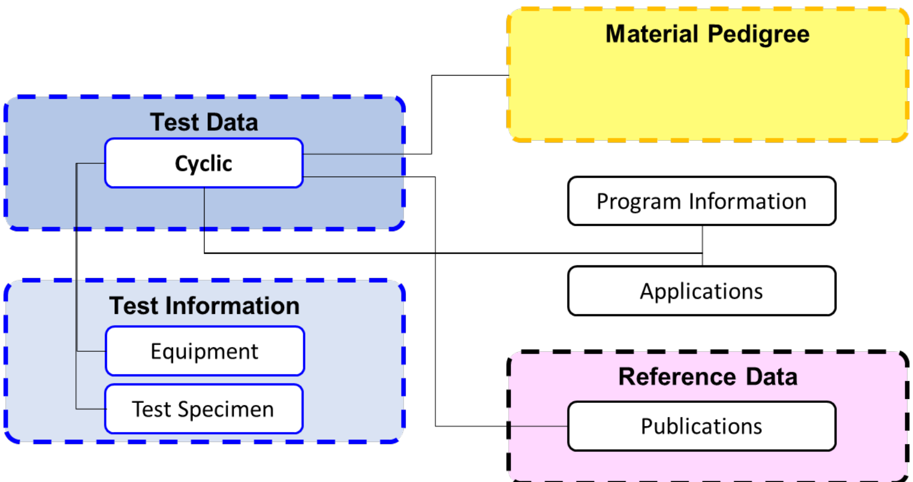

Figure 81.—Test Data: Cyclic Linking Behavior

A.6.7 Test Data: Fatigue Crack Growth (FCG)

The Test Data: Fatigue Crack Growth (FCG) table stores in-house test data for fatigue crack growth tests. Records include the above information described in Section A.6. The test response section includes the crack length, maximum load, and load range as a function of the number of cycles, as well as the change in crack length per load cycle as a function of the stress intensity range. The test results section contains various characteristics used to model the crack growth as a function of the fatigue loading. Records in the Test Data: Fatigue Crack Growth table are organized by material class/base (e.g., Titanium Alloy, Nickel Alloy), material name (e.g., Ti-6Al-4V, Timetal 21S), test temperature and then the individual test. Generic records are used at each folder level between the material class/base and the individual test to summarize the tests performed, extracted material properties from each test, and display average and standard deviations of material properties automatically calculated by Granta MI (Figure 82).

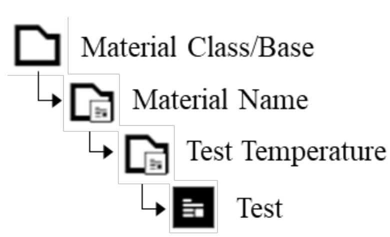

Figure 82.—Test Data: Fatigue Crack Growth Tree Structure

The Test Data: Fatigue Crack Growth table exhibits the same linking behavior as the Test Data: Tensile table shown in Section A.6.1 (Figure 83).

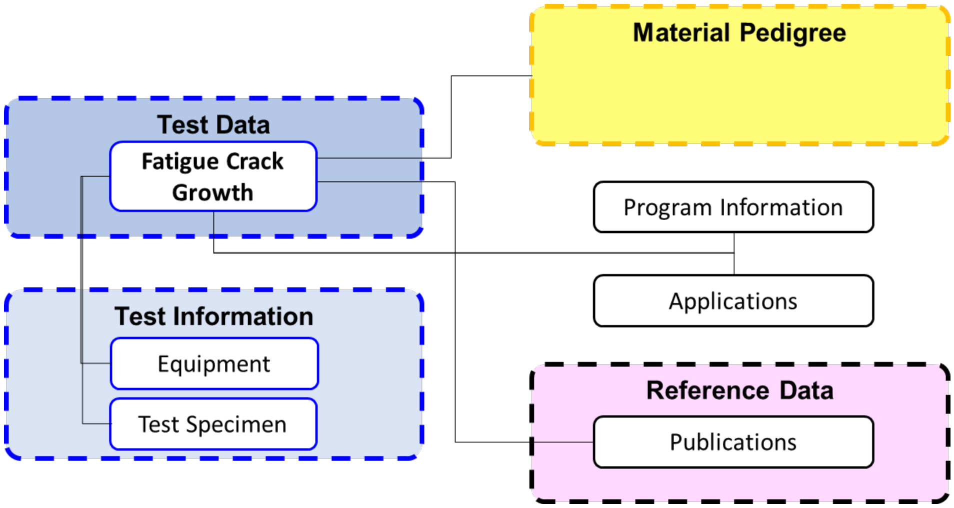

Figure 83.—Test Data: Fatigue Crack Growth Linking Behavior

A.6.8 Test Data: Oxidation

The Test Data: Oxidation table stores in-house test data for oxidation of different metals. Records include material information, and test information. Material information includes the alloy composition and processing of the material tested. Testing information includes the test temperature, cyclic information, and various functional attributes to track the weight vs time as the material is subject to thermal cyclic loading. Records in the Test Data: Oxidation table are organized by material class/base (e.g., Titanium Alloy, Nickel Alloy), material name (e.g., Ti-6Al-4V, Timetal 21S), test temperature and then the individual test. Generic records are used at each folder level between the material class/base and the individual test to summarize the tests performed, extracted material properties from each test, and display average and standard deviations of material properties automatically calculated by Granta MI (Figure 84).

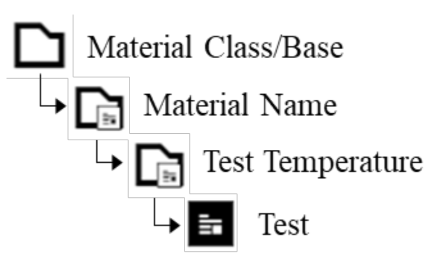

Figure 84.—Test Data: Oxidation Tree Structure

The Test Data: Oxidation table exhibits the same linking behavior as the Test Data: Tensile table shown in Section A.6.1 (Figure 85).

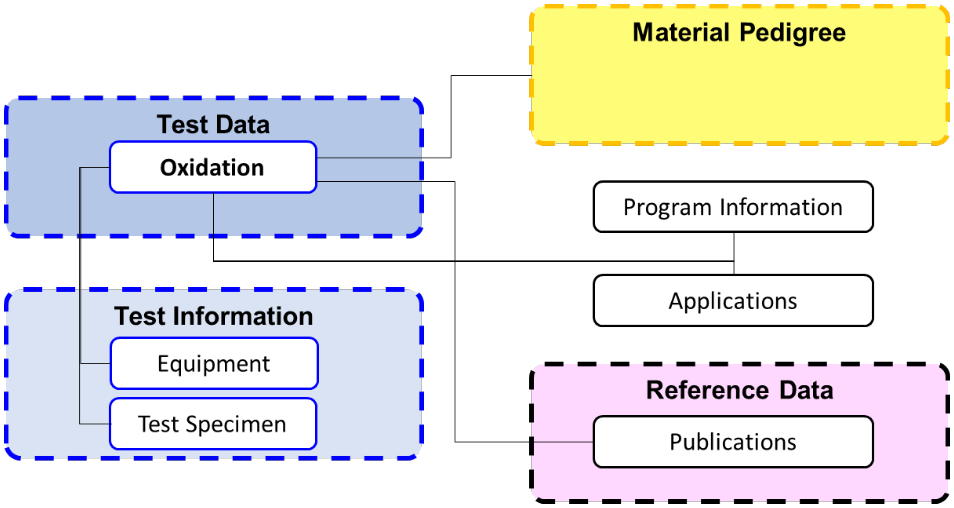

Figure 85.—Test Data: Oxidation Linking Behavior

A.7 Test Information

The Test Information collection of tables stores information on equipment (both destructive, nondestructive, and manufacturing) and general test specimens used for the various experiments stored in the database. The purpose of these tables is to define information used in multiple tests in one location and link to associated test records, enabling the database best practice of minimizing repeated information. Within the Test Information collection there are currently two tables:

1. Test Specimens
2. Equipment

A.7.1 Test Specimens

Records in the Test Specimens table store geometric, nominal dimensions for test specimens used in a particular test. Information stored includes the sample geometry, orientation, and schematics of the specimen design. Records are organized by the type of loading, the type of test, and then the individual specimen design (Figure 86).

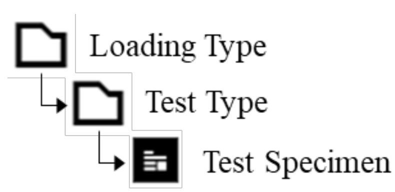

Figure 86.—Test Specimen Tree Structure

Test Specimen records are linked to the individual tables within the Test Data collection to provide nominal dimensions for the test specimen geometry (Figure 87). However, within the Test Data records, the actual dimensions of the sample are stored for proper calculation of stress and strain and to maintain the sample pedigree.

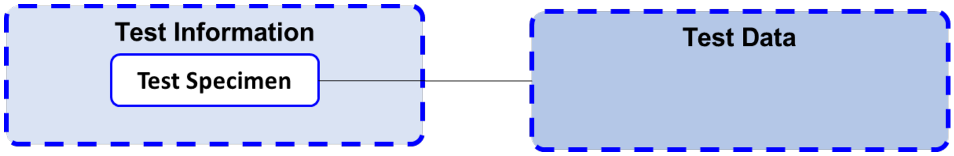

Figure 87.—Test Specimen Linking Behavior

A.7.2 Equipment

The Equipment table is used to define the testing equipment available, including measurement equipment, load/testing frames, machines for manufacturing and processing, and equipment for material evaluation. Records include information regarding the equipment's name, description, location, calibration history, and any associated schematics or images related to the equipment. Records are organized by the type of equipment (e.g., Measurement Device, Heating Device, Load Frame), then the use case (e.g., creep, Cyclic, Tension), and finally the individual piece of equipment (Figure 88).

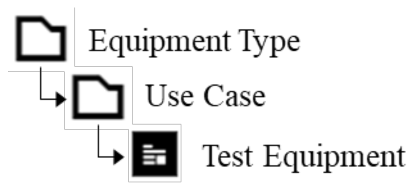

Figure 88.—Equipment Tree Structure

Similar to the Test Specimen table, Equipment records are linked to the individual tables within the Test Data collection to establish traceability between the samples tested, the execution of the test, and the collection of data. Equipment records can also be linked to the Manufacturing collection to associate a manufacturing method with a physical machine (Figure 89).

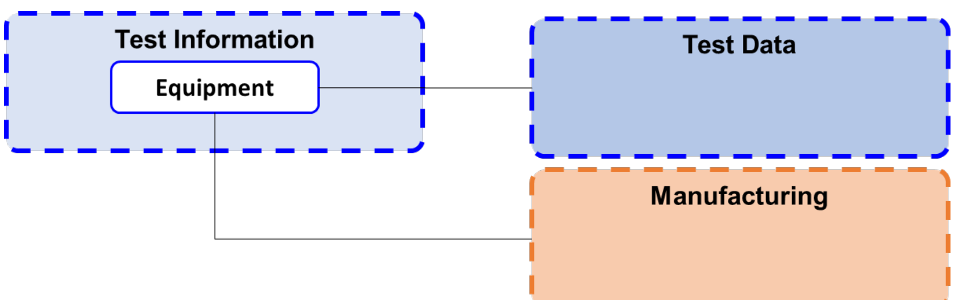

Figure 89.—Equipment Linking Behavior