Robust Informatics Infrastructure Required For ICME: Combining Virtual and Experimental Data

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With the increased emphasis on reducing the cost and time to market of new materials, the need for robust automated materials information management system(s) enabling sophisticated data mining tools is increasing, as evidenced by the emphasis on Integrated Computational Materials Engineering (ICME) and the recent establishment of the Materials Genome Initiative (MGI). This need is also fueled by the demands for higher efficiency in material testing; consistency, quality and traceability of data; product design; engineering analysis; as well as control of access to proprietary or sensitive information. Further, the use of increasingly sophisticated nonlinear, anisotropic and/or multi-scale models requires both the processing of large volumes of test data and complex materials data necessary to establish processing-microstructure-property-performance relationships.

Fortunately, material information management systems have kept pace with the growing user demands and evolved to enable: (i) the capture of both point wise data and full spectra of raw data curves, (ii) data management functions such as access, version, and quality controls; (iii) a wide range of data import, export and analysis capabilities; (iv) data "pedigree" traceability mechanisms; (v) data searching, reporting and viewing tools; and (vi) access to the information via a wide range of interfaces.

This paper discusses key principles for the development of a robust materials information management system to enable the connections at various length scales to be made between experimental data and corresponding multiscale modeling toolsets to enable ICME. In particular, NASA Glenn's efforts towards establishing such a database for capturing constitutive modeling behavior for both monolithic and composites materials is discussed.

I. Introduction

With the increased emphasis on reducing the cost and time to market of new materials ICME (Integrated Computational Materials Engineering) has become a fast growing discipline within material science and engineering. The vision of ICME is compelling in many respects, not only for the value-added in reducing time to market for new products with advanced, tailored materials, but also for enhanced efficiency and performance. Although the challenges and barriers (both technical and cultural) are formidable; substantial cost, schedule, and technical benefits can result from broad development, implementation, and validation of ICME principles[1]. ICME is an integrated approach to the design of products, and the materials that comprise them, by linking material models at multiple time and length scales. A key ingredient is the linkage with manufacturing processes, which produce internal material structures, which in turn influence material properties and allowables, enabling tailoring (engineering) to specific industrial applications. Figure 1 illustrates the interconnection of these scales and their cause/effect relationships, e.g., processing conditions produce a particular microstructure from which properties are obtained, which then dictate a specific structural performance. Note that the evolution of elliptical line types (i.e., dotted to dashed to solid line) are purposely included to imply the level of maturity/understanding (from immature, semi-mature, mature, respectively) of modeling at each level of scale (both temporal and geometric). Furthermore, the figure illustrates the difference between two non-mutually exclusive viewpoints; that is designing "with-the-material" (structural analyst viewpoint) versus designing "the material" (a materials scientist viewpoint). It is also apparent that the fundamental linkage between these two viewpoints is ultimately the associated constitutive model(s) for a particular material. One cannot overestimate the importance of understanding the input and output at each scale in order to determine

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meaningful properties that are ultimately required by a structural analyst. Equally important is the fact that experiments (whether computational/virtual or laboratory) performed at a given level can be viewed from two perspectives. If one "looks up" to higher scales, then the results can be viewed as exploration or characterization experiments used to identify/obtain the necessary model features or parameters, respectively, operating at the present and/or next higher level. Conversely, if one "looks down", these same results can be used to validate the modeling methods/approaches employed to transition from the lower level(s) to the given level.

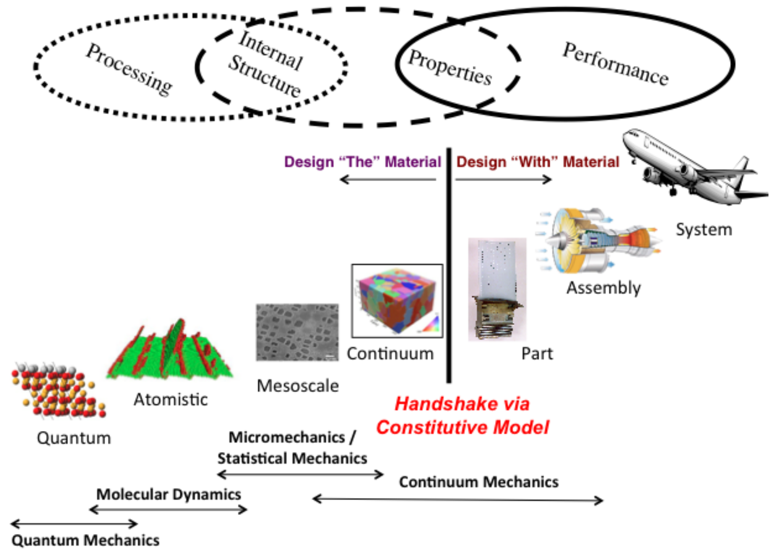


Figure 1: Description of associated length scale dependence and modeling methods in the context of ICME.

While there is a clear indication that ICME is growing, the successful implementation and realization, of ICME in the daily work of researchers and engineers in industry, government and academia is still lacking. One key contributing factor, since ICME is an inherently data intense activity, is the lack of either a robust information management system and/or a digital storage culture within most organizations. This stems from that fact that on the surface, a materials properties database may seem simply like a fancy means of storing, retrieving and distributing materials data; something akin to an electronic file cabinet. However, as discussed by Marsden et al.[2] and Arnold et al.[3], an effective ICME materials database must allow the data inside a database to be seamlessly accessible by analysis tools and allow the results from the analysis to be read back into the database and stored with all of the associated metadata, while keeping track of associations across the full range of length scales.

For example, a physics-based model to predict the yield strength of a nickel-based superalloy may need to draw upon quantum mechanics predictions of stacking fault energies, lattice distortions, and phase equilibria of several different alloying elements. These predictions would be combined with microstructural scale models that either use the quantum mechanics predictions, or are calibrated with experimental data. Phase equilibria models such as CALPHAD models are an example, as well as processing-microstructure models of castings or forgings. Important information necessary for a yield strength model would include not only equilibrium phases but also the kinetics of microstructural evolution (of several features, including γ' precipitate and carbide size and spacing, grain size and grain boundary phases). The maturity of these models already allows semi-quantitative predictions of various parameters. But development of higher fidelity models will require the capture, analysis and dissemination of higher fidelity data as well as all associated pedigree information for calibration and validation. For example, while a current model may utilize an average particle size as a key parameter, future models may require entire particle size distributions to be measured and tracked with respect to various manufacturing methods. Clearly, the enormity of data types (e.g., discrete, functional, structured, and unstructured to name a few) and the shear quantity of data can be overwhelming. Consequently, historical static systems are likely to be gradually phased out, evolving to become an integral part of dynamic materials property databases that are web-accessible and in which data—and the relationships between items of data—can be interactively searched, reorganized, analyzed, and applied. The dynamic databases have great superiorities in satisfying the needs of modern material-related sciences and engineering like ICME. Furthermore, it is critical to understand that ICME is not just developing processing-microstructure (P-M) relationships or microstructure-property (M-P) relationships independently, but rather it is the integration of these various length scale-specific relationships so that linkage from processing all the way up to performance can be made and utilized. This requirement greatly increases the need for data/meta-data and contextual linkage so that knowledge can be both captured and discovered. For example, the variety and complexity of modern materials and their applications necessitate complicated, and often massive, materials testing. As for composite materials, large volumes of test data on the properties of their various constituents, characterization of the constituents' individual and combined mechanical behavior, and development of constitutive models are often required. It is typical to require that data for each constituent can be reliably and conveniently traced back from the final products through their processing steps to the original raw materials. A second example is the need to provide adequate data to support increasingly sophisticated nonlinear, anisotropic and multi-scale engineering analyses. Here again, instead of storing a simple set of reduced, point wise, data, like elastic modulus and yield strength, the entire response (e.g., stress-strain, creep, relaxation, etc.) curve may be required. Collating, storing, processing, interacting with, and finally applying such data and metadata requires advanced dynamic information systems, enabling management of changing proprietary data alongside reference data collections, while ensuring consistency, quality, and traceability

In prior publications[3,4] the data scheme, best practices, and informatics requirements to establish a robust, 21st century, information management system for capturing and analyzing material information necessary to enable: 1) generalized constitutive modeling and 2) data-mining to establish microstructure /property/failure relationships for monolithic and composite materials, was discussed. The proposed schema/requirements for ICME were demonstrated using a turbine disk Ni-based superalloy, i.e., ME3 material in Arnold et al.[3]. Furthermore, the requirement of integrating both virtual and experimental data, over the entire material data life cycle and at various length scales, in the same information management system was posited as being essential for ICME becoming a reality and permeating the material and engineering cultures within a given organization. For example, Figure 2 illustrates the interaction between experimental data and virtual data (that data resulting from simulation tools) in that some experimental processing data (A) serves as input to a process model which then in turn outputs some microstructure feature (W), which is stored in the database. This virtual microstructure data is then combined with measured microstructural data (B) and provided as input to a micromechanics and/or statistical mechanics analysis package, which then generates material property data (X and Y), which again is stored in the database. This property data (X,Y) is then subject to experimental validation, as well as used in some continuum level analysis package (e.g., finite element analysis (FEA)) to assess some performance criteria (e.g., fatigue life, creep rupture, buckling load, etc.) Z; which is stored in the database. Clearly such an information management infrastructure not only enables the capture, analysis, dissemination and maintenance of various types of data, but also facilitates the verification and validation of model output, and certification of toolsets at multiple length scales. Also, once all of the input/output protocols are established, it can enable the seamless integration of these toolsets with optimization algorithms that will provide the final linkage of processing to performance criteria—thus making true ICME a reality.

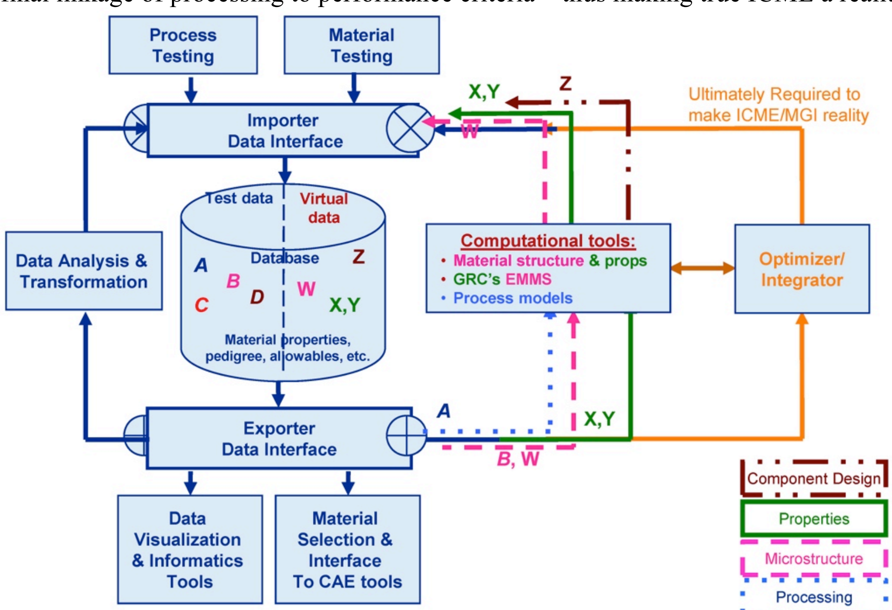


Figure 2: ICME Infrastructure for housing Modeling and Testing Information.

In this paper, our interests lie in identifying the challenges, best practices, and required schema with associated attributes to make the integration of virtual data and test data, described in Fig. 2, a reality. Specifically we will discuss and demonstrate the information management system, based on the Granta MI system, being developed at NASA Glenn for storing not only its experimental data, but also the simulation data (both correlation and predictions) resulting from constitutive modeling activities of both monolithic metals and composite materials. This integration is the first step in our attempt to connect both simulation and experimental data at various scales. Consequently, illustrative emphasis will be placed on the requirements (schema and attributes) for the material/model information management *software*, rather than on the *data* contained within the systems.

II. Requirements for Best Practice

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, regulatory compliance, and quality control. Although not specifically addressed in this paper, the general experience gained from these more general applications will be added to the identification and discussion of the features required for best practice materials information management with an eye toward ICME; which implies characterization and validation of models (e.g., constitutive, life, processing, etc.). The Material Data Management Consortium (MDMC)[§] has defined the material data *lifecycle* (see Figure 3) 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 life cycle 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 as well as 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); with the last but crucial step being the deployment (dissemination) of the right information, to the right people, at the right time and in the right format. Note that the middle ring of Figure 3 provides additional information regarding the type of data utilized and functions performed during each phase in the data life cycle; while the outer most ring details the individuals most likely responsible for these functions.

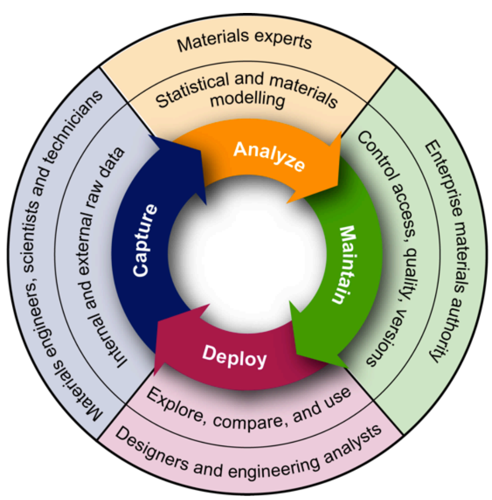


Figure 3: Four aspects of material data lifecycle.

[§]A group of aerospace and energy sector organizations (both industrial and governmental) that have 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. This group was established in 2002 (through collaboration) with ASM International, NASA Glenn Research Center and Granta Design Limited, see www.mdmc.net.

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 (as depicted in Fig. 2) range from i) data input; 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'; viii) product life management tools (PLM); and ix) to structural analysis codes that utilize a central database. Note that the models and tools listed in (iv) and (v) can operate on a variety of different length scales, thus potentially requiring scale-specific attributes. 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 as an efficient, reliable and user-friendly way as possible. Finally, these tools should also enable enterprise-wide (even world-wide) solution or access.

A. Capture

To maximize the impact on material and structural discipline practitioner and/or researcher, more than just 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) have the ability to capture a materials 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) have the ability to capture the application potential of a given material system, be it monolithic, composite, multifunctional, etc.; and iii) enable 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[3].

B. Analyzing Materials Data

For most organizations a corporate materials database is a dynamic resource—they want to continually add data and to 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 in order 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. Such tools are highly specialized and may be developed in-house, come from academic or commercial collaborators, or be purchased. Table 1 lists some examples.

Table 1: Examples of analysis tools needed by materials experts

Property Estimation Tools	Thermo-Cal, CALPHAD, EMMS, etc.
Processing Test Data	Tensile tests, compression tests, creep, fatigue crack growth, E399 fracture toughness…
Deformation Models	Fit test load/stress, total strain and/or inelastic strain as a function of time at various constant temperatures (tensile, creep, relaxation, cyclic, step tests, etc). For example elastic, viscoelastic or generalized viscoelastoplastic models.
Damage/Life Models	Stress vs. life curves for stress controlled cyclic tests using models such as: the Basquin model, the Life power model, the Ramberg-Osgood model. Creep strain vs. time, for creep and creep rupture: Larson Miller model or Kachanov type continuum damage mechanics (CDM) model.

Whatever the exact nature or source of such software tools, best practice materials information management requires that these tools:

- Be able to be used together so that they combine 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 is extracted directly into the analysis tool and results are saved directly back into the correct locations in the database (see Section III);
- Their results be permanently linked to raw input data and the details of the analyses performed, so as to maintain full traceability.

C. Maintaining Materials Information

Establishing a "gold source" of materials information is not enough; as this source must also be protected, nurtured, and maintained. A number of data management features are critical to this process; i) traceability, ii) access control, iii) version control, iv) data quality control.

1. Traceability

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 "materials pedigree" information can help users understand and correctly apply the materials 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. Most importantly, it is *impossible* to be confident in the use of mission-critical data if its pedigree is unknown; as using un-pedigreed data involves an extreme risk. Raw, statistical, and design data are considered to be the core data categories, while pedigree, microstructure, testing, application, in-service environment and exposure, and reference data are normally deemed background information. However, it is precisely this background data that are essential to capture, analyze, and maintain if ICME is to become a reality. 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, NASA Glenn's Granta MI® system being an example, see Figure 4. For example, in NASA Glenn's data schema (see Fig. 5) the microstructure information category (table), is separated, 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. The proposed schema, and attributes associated with the Model and Software tool portions of Figure 5, will be discussed in greater detail in Section III.

2. Access Control

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 relevant data. 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. For maximum flexibility, it should operate at as low a level as possible in the database, i.e., 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, specific access control, 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 data based level system) would make significant portions, if not all, of the database unavailable to the larger community.

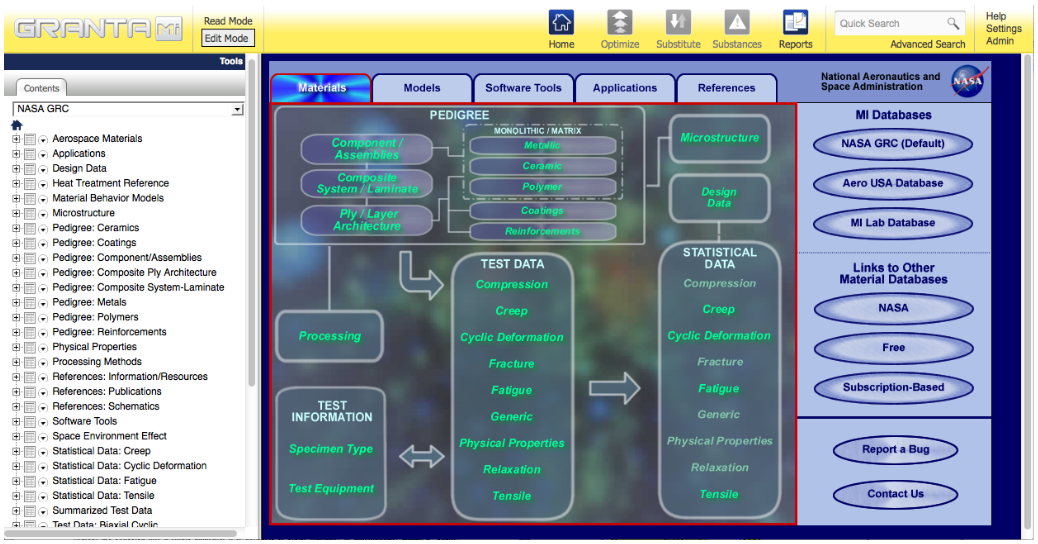


Figure 4: NASA Glenn's Customization of GRANTA MI Materials Information Management System.

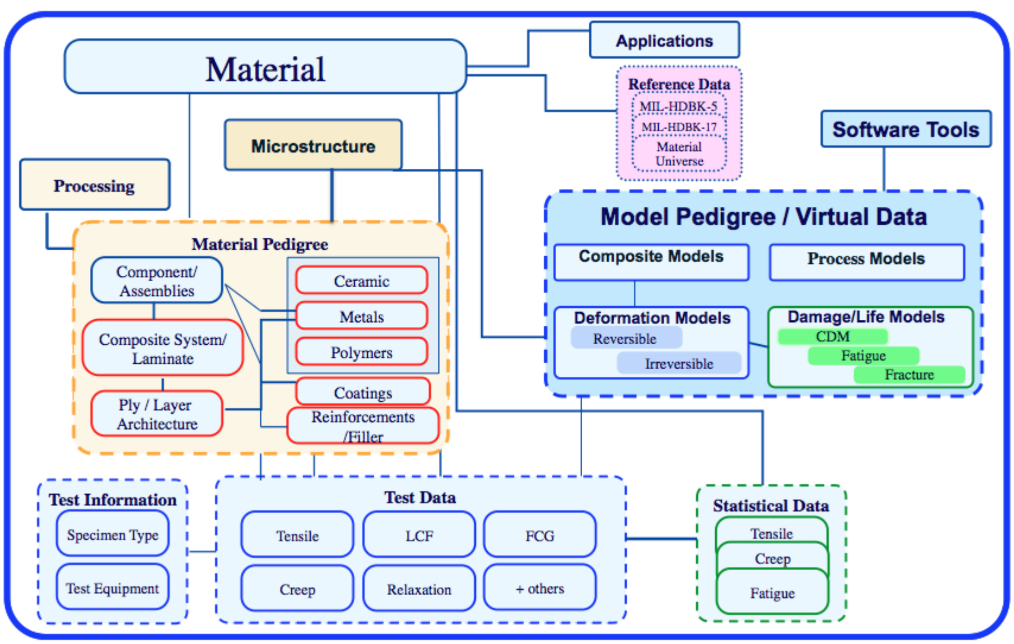


Figure 2 NASA Glenn's Schema Modified to Incorporate Virtual data to enable ICME

3. Version Control

Change management can be a major issue in any dynamic 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.

4. *Data Quality 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 or P-index to indicate when a given parameter or "property" is calculated (or predicted—thus the P designation) is particularly important to consider. 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., down grading of quality, epistemic uncertainty) on higher scale calculations. Such a concept should also facilitate the specification / utilization of needed verification experiments. 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.

III. Linkage of Experimental and Virtual Data Via Establishment of Model Tables

As stated previously, foundational to any ICME endeavor is a robust information management system in which both experimental and model simulation (virtual) data coexist, preferably in a single database, at various levels of scale. Just as in the case of experimental data, capturing the pedigree of the material tested is an essential step to enable proper interpretation of results, so too is tracking the pedigree of any simulation (virtual) data entered into the database. Virtual data is an outcome from running some form of model/analysis software tool. In the case of mechanics of materials, this can be as simple as exercising a given constitutive model (the easiest being isotropic Hooke's Law, which involves only 2 parameters (i.e., Young's Modulus and Poisson ratio) representing a volume element of material, and as complex as a general nonlinear finite element analysis of a complex structural component. In either case it is essential to understand/record the fundamental assumptions (material system, material anisotropy, linear, nonlinear behavior, boundary conditions, etc.), pertinent model parameters, loading conditions, etc. in order to properly connect experimental data with simulation data. One might ask, "Why should I store the resulting simulation data?" The benefits of storing simulation data along with their pedigree information are four fold: 1) it allows immediate comparison between experiment and simulation, thus enabling an assessment of the accuracy of both the correlation ability and predictive ability of the model, 2) it enables periodic re-assessment of the model's accuracy as the experimental data set grows, thus indicating when the model's characterization needs to be updated, 3) it provides future generations with benchmark curves to confirm the version of the model being used or to verify its re-implementation by someone else, and 4) it allows complete traceability; from model version to experimental data used for correlation. Obviously, ICME involves a wide variety of models (e.g., process models, internal structure models, constitutive, etc.) as indicated in Section II.B and thus necessitates a versatile schema.

In this section, it is our intent to present an appropriate schema (see Fig. 5) not only to store model information and model parameters in a location that is easily accessible by FEA or other analysis codes through some type of interface software (e.g., Material Gateway®), but also to store any associated simulation data necessary to assist in the evaluation/utilization of these models. In other words, we want to establish what constitutes this pedigree (i.e., required attributes) and the format (e.g, attribute type and record layout) for best storing this information. The focus in this paper will be limited to constitutive models for both monolithic and composite materials; since to date the experimental data stored in NASA Glenn's Granta MI® database is limited to coupon level data. In the case of monolithic materials, three tables and their associated attributes need only be defined to enable the complete data life cycle to be handled, these are: Deformation Table, Damage-Life Table, and Software Tools Table. Whereas, in the case of composite materials, one must think more broadly as multiple length scales can be involved depending upon the approach taken (i.e., macromechanics or micromechanics) to define the material's "constitutive model". Consequently, this additional meso or macro scale beyond that of the constituent scale (e.g., that associated with monolithic material) necessitates the introduction of a fourth table, the Composite Table. Clearly, extension to other scales (e.g., atomistic, processing, microstructure modeling, structural) should be no more difficult than adding additional tables with appropriate attributes to the Model pedigree group within Fig. 5 to represent each new scale considered.

A. Deformation Model Table

Constitutive material models (be they simple or complex) provide the required mathematical link between stress and strain. The most well-known and widely used constitutive model is the generalized Hooke's law

$$\sigma_{ij} = \mathrm{C}_{ijkl} e_{kl} \tag{1}$$

which describes time-independent, linear (proportional) reversible material behavior. For the case of isotropy, the proportionality tensor C_{ijkl} contains only two independent material parameters, E and ν. Extension into the irreversible regime has been accomplished by assuming an additive decomposition of the total strain tensor, ε_{ij} ,

$$\varepsilon_{ij} = e_{ij} + \varepsilon_{ij}^{I} + \varepsilon_{ij}^{th} \tag{2}$$

or

$$e_{ij} = \varepsilon_{ij} - \varepsilon_{ij}^{I} - \varepsilon_{ij}^{th} \tag{3}$$

into three components, that is, a reversible mechanical strain, e_{ij} , (i.e., elastic/viscoelastic); an irreversible strain, ε_{ij}^{I} , (i.e., inelastic (plastic and/or creep, or viscoplastic)); and a reversible thermal strain, ε_{ij}^{th}. After substituting expression (3) into equation (1) one arrives at a stress-strain relation that incorporates irreversible strains as well as reversible ones, that is:

$$\sigma_{ij} = \mathrm{C}_{ijkl}(\varepsilon_{kl} - \varepsilon_{kl}^{I} - \varepsilon_{kl}^{th}) \tag{4}$$

where numerous models describing the evolution of the inelastic strain have been proposed in the literature[8-11]. Given this traditional separation into reversible and irreversible constitutive models it is conceived that the Deformation Table be comprised of two primary, top level, folders (i.e., reversible and irreversible) which are further subdivided into folders/records associated with specific materials and constitutive models, respectively for each domain. Table 2 illustrates the current attributes and associated data type, as well as the corresponding layout of information for the Deformation Table. This layout is separated into ten basic sections. The first section is associated with the project information. The second, material description, section, is where the model record is connected to the specific material (or system) that the model is attempting to represent. This is accomplished by linking the material pedigree (via the various attributes in this section, see Table 2, and specifically the material pedigree record link) to the model idealization information contained in the current Deformation Table record.. The model description section gives the general features of the model, while the next two sections (Characterization Information/Parameter Estimation Method and Test Data Used In Parameter Estimation) describe when, who and how the model material parameters were arrived at and what test data were used during the correlation of the specific model. Note the attributes 'Software Tool Used' and 'Regression Software/Version Used' allow the best practice of only defining information in one location, yet enabling viewing in multiple locations, to be followed as these attributes link the current model record to the Software Tools Table which contains all the pertinent information regarding the specific model/tool being utilized; i.e., its source code and executable – see Table 3 for the associated attributes and layout. Next comes that actual model specific area, where, depending upon the type of record (reversible or irreversible), one or more of these highlighted (model specific) sections will be filled out. For instance, assuming reversible material behavior, then either the 'Thermo-Elastic Model Parameters' section or 'Viscoelastic Model Parameters' section will be filled out, depending upon whether the material behavior is rate and time-independent or not, respectively. If the material behavior exhibits irreversible deformation, then an irreversible record would be required, and in this case, reversible parameters would merely be "viewed" in one of the above sections depending on the material's reversible behavior, while either the 'Plasticity Model Parameters' or 'Viscoplastic Model Parameters' would be defined, again depending upon the material's observed behavior. Note that, in the elastic and plastic sections' attributes, almost identical names are listed (e.g., yield stress and yield stress (T)). This is to demonstrated that, within a given Table, multiple attributes can be defined, which enable the user to decide how he/she would like to store a particular model parameter, that is, as a single point value or as a function of temperature, for example. Granta MI® allows the user to choose to display all attributes or only those attributes that are not empty in a given record. Lastly, the 'Simulation Responses' section is where all virtual data will be store. Currently, these functional data attributes (e.g., Stress vs. Strain Response (11 axis)) have been assigned ten parameters (i.e., Specimen ID, Test Type, Loading Rate Type, Loading Rate Stress Magnitude, Loading Rate Strain Magnitude, Target Type, Target Value, Hold Duration, Simulation Classification, and Temperature), with four being identified as discrete (i.e., those associated with type and classification). In this way multiple loading histories can be stored in a single attribute that represents a given graphical plotting space, for example, stress-strain, stress-time, strain-time.

Table 2: Layout and Attributes for Deformation Model Table

	Attributes	Type
	Project Information	
	Performing Organization	STXT
	Project Name/Funding Source	STXT
	Point of Contact (POC)	STXT
	Material Description	
	Material	STXT
	Material Class	DCT
	Commercial Name	STXT
	Specific Name	STXT
	Process	DCT
	Material Pedigree Record	Link
	Batch Number	STXT
	Material Notes	LTXT
	Description of Deformation Model	
	Model Name	STXT
	Version	PNT
	Model Class	STXT
	Model ID	STXT
	Deformation Regime	DCT
	Software Tool Used	STXT
	Assumptions	LTXT
	Description	LTXT
	Hardening Form	DCT
	Characterization Information/Parameter Estimation Method	
	Characterization/Analysis Date	DAT
	Analyst Name	STXT
	Characterization Notes	LTXT
	Computation Method	DCT
	Regression Analysis Method	STXT
	Optimization Method	STXT
	Regression Software/Version Used	STXT
	Temperature	PNT
	Temperature Range	RNG
	Test Data Used In Parameter Estimation	
	Tensile Test Data (Linked Records location in layout)	Links
	Creep Test Data (Linked Records location in layout)	Links
	RelaxationTest Data (Linked Records location in layout)	Links
	Cyclic Test Data (Linked Records location in layout)	Links
	Generic Test Data (Linked Records location in layout)	Links
	Summarized Test Data (Linked Records location in layout)	Links
Reversible	**Thermo-Elastic Model Parameters**	
	Young's Modulus, E (T)	FDA
	Poisson's Ratio, ν (T)	FDA
	CTE, α (T)	FDA
	Thermal Conductivity (T)	FDA
	Specific Heat (T)	FDA
	Thermo-Elastic Properties (Define)	TABL
	Thermo-Elastic Properties (View)	TABL
	Viscoelastic Model Parameters	
	No. of Reversible Mechanisms, M	INT
	Maxwell Mechanisms (Define)	TABL
	Maxwell Mechanisms (View)	TABL

	Attributes	Type
Irreversible	**Plasticity Model Parameters**	
	Yield Stress	PNT
	Hardening Modulus	PNT
	Incremental Plasticity Data Pairs	PNT
	Yield Stress (T)	FDA
	Hardening Modulus (T)	FDA
	Incremental Plasticity Data Pairs (T)	FDA
	Viscoplastic Model Parameters	
	Threshold Stress, κ	PNT
	Material Exponent, n	PNT
	Viscosity Parameter, μ	PNT
	No. of Irreversible Mechanisms, N	INT
	Viscoplastic Multi-Mechanisms Parameters (Define)	TABL
	Viscoplastic Multi-Mechanisms Parameters (View)	TABL
	Shear threshold Ratio $\eta = (K_L/K_T)$	PNT
	Shear strength Ratio ξ	PNT
	Shear threshold Ratio $\omega = (Y_L/Y_T)$	PNT
	Normal strength Ratio ζ	PNT
	Simulation Responses	
	Stress vs. Strain Response (11 axis)	FDA
	Stress vs. Strain Response (22 axis)	FDA
	Stress vs. Strain Response (33 axis)	FDA
	Stress (11 axis) vs. Time	FDA
	Stress (22 axis) vs. Time	FDA
	Stress (33 axis) vs. Time	FDA
	Total Strain (11 axis) vs. Time	FDA
	Total Strain (22 axis) vs. Time	FDA
	Total Strain (33 axis) vs. Time	FDA
	Creep Strain (11 axis) vs. Time	FDA
	Creep Strain (22 axis) vs. Time	FDA
	Creep Strain (33 axis) vs. Time	FDA
	Shear Stress vs. Shear Strain Response (12 axis)	FDA
	Shear Stress vs. Shear Strain Response (13 axis)	FDA
	Shear Stress vs. Shear Strain Response (23 axis)	FDA
	Shear Stress (12 axis) vs. Time	FDA
	Shear Stress (13 axis) vs. Time	FDA
	Shear Stress (23 axis) vs. Time	FDA
	Total Shear Strain (12 axis) vs. Time	FDA
	Total Shear Strain (13 axis) vs. Time	FDA
	Total Shear Strain (23 axis) vs. Time	FDA
	Creep Shear Strain (12 axis) vs. Time	FDA
	Creep Shear Strain (13 axis) vs. Time	FDA
	Creep Shear Strain (23 axis) vs. Time	FDA
	Additional Information	
	General Modeling Notes	LTXT
	Application Links	Links
	References	
	Model References	Links
	Model Reports	FIL

DCT Discrete Text (specified choices)
FDA Functional Data Attribute (with associated parameters)
INT Integer Value
LOG Logical
LTXT Long Text Field
PNT Point value
RNG Range variable
STXT Short Text Field
TABL Tabular Attribute (multiple columns of data - PNT, STXT, DCT,

Table 3 Layout and Attributes for Software Tools Table

Attributes	Type
General Description	
Tool Name	STXT
Version	STXT
Description	STXT
Component/System Application	STXT
Tool Scope	DCT
Method	DCT
Software Required to Execute Code	DCT
Other Software Required to Execute Code	STXT
Integration With Other Software	STXT
Website	HYP
Availability	DCT
Late Update (Year)	DCT
Description Notes	LTXT
Classification	STXT
Analysis Design	LOG
Lifing	LOG
Optimization	LOG
Thermal / Heat Transfer	LOG
Thermodynamics	LOG
CFD	LOG
Data Analysis	LOG
Other Classification	STXT
Domain	
Length Scale	DCT
Temporal Scale	DCT
Multiaxiality	DCT
Variables	DCT
Domain Notes	LTXT
Material System Applicability	PNT
Material Independent	LOG
Metallic	LOG
Ceramic	LOG
Polymer	LOG
Composite/Continuous	LOG
Composite/Discontinuous	LOG
Composite/Woven	LOG
Multifunctional	LOG
Smart	LOG
Nano	LOG
Other Material(s)	STXT
Material System Notes	LTXT
Material Description	
Material Directionality	DCT
Material Scope	DCT
Material Response	DCT
Geometric Description	DCT
Reversible	LOG
Irreversible	LOG
Material Description Notes	LTXT

Attributes	Type
Platform Supported	
PC	LOG
Mac	LOG
Operating System Supported	
Windows 8	LOG
Windows 7	LOG
Windows NT	LOG
MacOS	LOG
Unix	LOG
Linux	LOG
Operating System Notes	LTXT
Documentation	
Reference Manual	LOG
User's Manual	LOG
References	LTXT
Verification/Validation Method	
Analytical	DCT
Computation	DCT
Experimental	DCT
Verification Notes	LTXT
Software Technology Readiness Level (TRL)	
TRL (1-9)	DCT
Readiness Notes	LTXT
Availability	
Approved for General Release	LOG
Security Classification	DCT
Availability Category	DCT
Sensitivity	DCT
Distribution Limitations	DCT
Limited Until (month/year)	STXT
Point of Contact (POC)	STXT
POC's Organization	STXT
Availability Notes	LTXT
Source Code	
Development Language	DCT
Development Language (other)	STXT
Source Code Available	LOG
Source Code Availability Cat.	DCT
Source Code POC	STXT
Source Code Location	HYP
Source Code Notes	LTXT
Ownership Rights	
Developer/Performing Org.	STXT
Sponsoring Organization	STXT
Intellectual Property	DCT
Invention Disclosure Filed	LOG
NASA Case No.	STXT
Distribution Category	DCT
Notes	LTXT
Program	
Project Name/Funding Source	STXT
Contract No.	STXT
Grant No.	STXT
Year Inititated	STXT
Software Development Status	DCT
Year Completed/Terminated	STXT
Project Notes	LTXT
Further Information	
Software Reports No Linked Records	Links

DCT Discrete Text (specified choices)
FDA Functional Data Attribute (with associated parameters)
HYP Hyperlink
INT Integer Value
LOG Logical
LTXT Long Text Field
PNT Point value
RNG Range variable
STXT Short Text Field
TABL Tabular Attribute (multiple columns of data - PNT, STXT, DCT, INT, link)

B. Damage – Life Model Table

Similar to the Deformation Table, the Damage-Life Table is divided into nine basic sections where the sixth section contains model specific highlighted subsections (e.g., ECI – Debond Model, Curtin – Fiber Breakage Model, ADEAL (Anisotropic Damage Evolution and Life) Model, and Coffin-Manson Model), only one of which would appear in any given record. Note that the fact that only four specific models are shown in Table 4 is due to space limitations only and not because these are the only models of use or concern. Such a statement also applies to the two reversible and irreversible models shown in Table 2. To enable representations of different stress (e.g., amplitude, maximum, equivalent, range) and strain (e.g., total, elastic, plastic, range) entities that are model-dependent, three additional parameters were added (above and beyond those in the Deformation Table) to the simulation response attributes, these are: Model type, Stress Type, and Strain Type. Using parameters for these various simulation response attributes, representing various graphical spaces (e.g., stress-strain, stress vs. cycle, strain vs. cycle), enables consolidations of a significant amount of data into a few functional data locations, therefore simplifying/standardizing any required importer/exporter tools.

C. Composite Model Table

In its broadest context, a composite is anything comprised of two or more entities with a recognizable interface (i.e., distinct internal boundaries) between them. If these internal boundaries are ignored, continuum mechanics can be used to model composite materials as pseudo-homogenous anisotropic materials with directionally dependent "effective," "homogenized," or "smeared" material properties. Micromechanics, on the other hand, attempts to account for the internal boundaries within a composite material and capture the effects of the composite's internal arrangement. In micromechanics, the individual materials (typically referred to as constituents or phases) that make up a composite are each treated as continua via continuum mechanics models, with their individual representative properties and arrangement dictating the overall behavior of the composite material. Consequently, by developing a schema capable of handling a micromechanics approach enables demonstration of an ICME capable (multiscale) framework. For a detailed, comprehensive discussion on modeling of composite materials, the reader is referred to the book entitled *Micromechanics of Composite Materials: A Generalized Multiscale Analysis Approach*[12].

The Composite Model table (see Table 5) consists of similar sections as describe in Section III.A; yet in this table there is no explicit section entitled 'Characterization Information/Parameter Estimation Method'. As this information would be contained in the Deformation Table associated with the various constituent constitutive models, in the case of a micromechanics approach; or in the case of a macromechanics approach, the anisotropic (transversely isotropic at a minimum) models representing a given unidirectional "ply" level material, would be stored (along with characterization information and material parameters) in their corresponding records in the Deformation Model Table as well. However, three new sections, specific to composite materials, are present: 'Micromechanics Modeling Information', 'Laminate Level Modeling Information', and 'Multiscale Modeling Information', with only one section per record being populated – depending upon the type of composite analysis being performed. Note that in each of these sections, not only is the analysis tool (again, uniquely defined in the Software Tool table) identified, but also now the associated input file required to perform the simulations whose results are stored in the Simulation Response section is required. This is due to the fact that composites are in essence like little structures (with stress redistributions occurring internally) and require typically more than a single set of constitutive model parameter information (e.g., in the case of micromechanics geometric and processing information) to be available to reproduce the simulation results. Two new tabular attributes are defined to represent the repeating unit cell (RUC) or representative volume element (RVE) information or the laminate level information. Figure 6 illustrates both types of tabular attributes where each column heading represents a parameter associated with the given tabular attribute. Fig 6a provides an example of a unidirectional, 35% fiber volume fraction, titanium matrix composite (SCS-6/Ti-15-3) represented using a micromechanics approach. Immediately one sees that two phases are present (Fiber and Matrix) and that the Fiber phase is modeled as an elastic material with its strength being represented by the Curtin fiber breakage model[12]. The matrix phase is modeled as an elastic/plastic material with its fatigue life represented using the anisotropic nonlinear cumulative damage rule– ADEAL[12]. Similarly, the ECI debond criterion[12] is used between the fiber and matrix phase.

Fig. 6b illustrates a fictitious laminate in which a monolithic Ti-15-3 layer is surrounded by a unidirectional SCS-6/Ti-15-3 ply oriented at +45 on the bottom and -45 on the top. Note that the parameter "Scale" identifies whether a micromechanics approach (indicated by "RUC") or macromechanics approach (indicated by "Effective") is being applied to given layer. In the case of layers 1 and 3, information regarding the modeling of this composite material would be contained in the RUC composite record named SCS6/Ti15-3 whose constitutive description was shown in

Fig. 6a. Therefore each record referenced can depict a given scale with the interconnection between the constituent scale and the laminate (meso) scale occurring within the laminate information tabular attribute.

Table 4 Layout and Attributes for Damage-Life Model Table

Attributes	Type
Project Information	
Performing Organization	STXT
Project Name/Funding Source	STXT
Point of Contact (POC)	STXT
Material Description	
Material	STXT
Material Class	DCT
Commercial Name	STXT
Specific Name	STXT
Process	DCT
Material Pedigree Record	Link
Batch Number	STXT
Material Notes	LTXT
Description of Deformation Model	
Model Name	STXT
Version	PNT
Model Class	STXT
Model ID	STXT
Software Tool Used	STXT
Assumptions	LTXT
Description	LTXT
Characterization Information/Parameter Estimation Method	
Characterization/Analysis Date	DAT
Analyst Name	STXT
Characterization Notes	LTXT
Computation Method	DCT
Regression Analysis Method	STXT
Optimization Method	STXT
Regression Software/Version Used	STXT
Temperature	PNT
Temperature Range	RNG
Control Mode	DCT
Cyclic Fequency Range	RNG
Kt Range	RNG
Test Data Used In Parameter Estimation	
Tensile Test Data (Linked Records location in layout)	Links
Creep Test Data (Linked Records location in layout)	Links
RelaxationTest Data (Linked Records location in layout)	Links
Cyclic Test Data (Linked Records location in layout)	Links
Generic Test Data (Linked Records location in layout)	Links
Summarized Test Data (Linked Records location in layout)	Links
ECI - Debond Model	
Normal debond strength (σ_{DB})	FDA
Gamma normal (Λ_n)	FDA
B - normal	FDA
Debond time - normal	FDA
Tangential debond strength(σ_{DB})	FDA
Gamma tangential (Λ_t)	FDA
B - tangential	FDA
Debond time - tangential	FDA
Curtin - Fiber Breakage Model	
Mean fiber strength (σ_o)	FDA
Frictional sliding resistance (τ)	FDA
Fiber gauge length (Lo)	FDA
Fiber diameter (d)	FDA
Stress exponnet (m)	FDA

Attributes	Type
ADEAL(Anisotropic Damage Evolution and Life) Model Parameters	
Beta	PNT
A coff	PNT
Sigmanot-fl	PNT
Mnot	PNT
Sigma u	PNT
b-meanstress	PNT
bp-meanstress	PNT
omega u	PNT
omega fl	PNT
omega M	PNT
eta u	PNT
eta fl	PNT
eta M	PNT
Coffin-Manson Model	
Fat. Ductility Coeff. (Coff.-Mans.)	PNT
Plastic Fat. Ductility Coeff. (Coff.-Mans.)	PNT
Model Fit R^2 (Coff.-Mans.)	PNT
Plastic Model Fit R^2 (Coff.-Mans.)	PNT
Half Life Data Used (Coff.-Mans.)	LOG
X or Y Std. Err. Used (Coff.-Mans.)	DCT
No. of Std. Err. (Coff.-Mans.)	PNT
Simulation Responses	
Stress vs. Strain Response (11 axis)	FDA
Stress vs. Strain Response (22 axis)	FDA
Stress vs. Strain Response (33 axis)	FDA
Stress (11 axis) vs. Cycles	FDA
Stress (22 axis) vs. Cycles	FDA
Stress (33 axis) vs. Cycles	FDA
Strain (11 axis) Amplitude vs. Cycles	FDA
Strain (22 axis) Amplitude vs. Cycles	FDA
Strain (33 axis) Amplitude vs. Cycles	FDA
Strain (11 axis) vs. Cycles	FDA
Strain (22 axis) vs. Cycles	FDA
Strain (33 axis) vs. Cycles	FDA
Shear Stress vs. Shear Strain Response (12 axis)	FDA
Shear Stress vs. Shear Strain Response (13 axis)	FDA
Shear Stress vs. Shear Strain Response (23 axis)	FDA
Shear Stress (12 axis) vs. Cycles	FDA
Shear Stress (13 axis) vs. Cycles	FDA
Shear Stress (23 axis) vs. Cycles	FDA
Shear Strain (12 axis) Amplitude vs. Cycles	FDA
Shear Strain (13 axis) Amplitude vs. Cycles	FDA
Shear Strain (23 axis) Amplitude vs. Cycles	FDA
Additional Information	
General Modeling Notes	LTXT
Application Links	Links
References	
Model References	Links
Model Reports	FIL

DCT Discrete Text (specified choices)
FDA Functional Data Attribute (with associated parameters)
INT Integer Value
LOG Logical
LTXT Long Text Field
PNT Point value
RNG Range variable
STXT Short Text Field
TABL Tabular Attribute (multiple columns of data - PNT, STXT, DCT, INT, link)

Table 5 Layout and Attributes for Composite Model Table

Attributes	Type
Project Information	
Performing Organization	STXT
Project Name/Funding Source	STXT
Point of Contact (POC)	STXT
Material Description	
Material	STXT
Material Class	DCT
Commercial Name	STXT
Specific Name	STXT
Material Pedigree Record	Link
Batch Number	STXT
Material Notes	LTXT
General Modeling Information	
Model ID	STXT
Characterization/Analysis Date	DAT
Temperature	PNT
Temperature Range	RNG
Assumptions	LTXT
Micromechanics Modeling Information	
Micromechanics Method	DCT
Micromechanics Analysis Tool	STXT
Micromechanics Tool Information	Link
Micromechanics Input File	FIL
No. of Constituents	INT
RUC/RVE Constituitve Description	TABL
RUC/RVE Image	PIC
Fiber Packing Arrangement	DCT
Effective Thermo-Elastic Composite Properties	TABL
Micromechanics Notes	LTXT
Laminate Level Modeling Information	
Laminate Name	STXT
Laminate Specification	STXT
Architecture Type	DCT
Laminate Pattern	DCT
Laminate Thickness	PNT
Ply Thickness (avg)	PNT
No. of Plies	INT
Laminate Definition	TABL
Laminate Analysis Tool	STXT
Laminate Analysis Tool Information	Link
Composite Laminate Analysis Input File	FIL
Laminate Notes	LTXT
Laminate Extensional Stiffness Matrix (A)	TABL
Laminate Coupling Stiffness Matrix (B)	TABL
Laminate Bending Stiffness Matrix (D)	TABL
Volume Fractions	
Total Matrix Volume Fraction	PNT
Total Reinforcement Volume Fraction	PNT
Total Void/Porosity Voume Fraction	PNT

Attributes	Type
Multiscale Modeling Information	
Multiscale Analysis Tool	DCT
Multiscale Analysis Tool Information	Links
Multiscale Analysis Input File	FIL
Multiscale Modeling Notes	LTXT
Composite Test Data Used for Characterization/Vaildation	
Tensile Test Data (Linked Records location in layout)	Links
Creep Test Data (Linked Records location in layout)	Links
RelaxationTest Data (Linked Records location in layout)	Links
Cyclic Test Data (Linked Records location in layout)	Links
Generic Test Data (Linked Records location in layout)	Links
Simulation Responses	
Stress vs. Strain Response (11 axis)	FDA
Stress vs. Strain Response (22 axis)	FDA
Stress vs. Strain Response (33 axis)	FDA
Stress (11 axis) vs. Time	FDA
Stress (22 axis) vs. Time	FDA
Stress (33 axis) vs. Time	FDA
Total Strain (11 axis) vs. Time	FDA
Total Strain (22 axis) vs. Time	FDA
Total Strain (33 axis) vs. Time	FDA
Creep Strain (11 axis) vs. Time	FDA
Creep Strain (22 axis) vs. Time	FDA
Creep Strain (33 axis) vs. Time	FDA
Shear Stress vs. Shear Strain Response (12 axis)	FDA
Shear Stress vs. Shear Strain Response (13 axis)	FDA
Shear Stress vs. Shear Strain Response (23 axis)	FDA
Shear Stress (12 axis) vs. Time	FDA
Shear Stress (13 axis) vs. Time	FDA
Shear Stress (23 axis) vs. Time	FDA
Total Shear Strain (12 axis) vs. Time	FDA
Total Shear Strain (13 axis) vs. Time	FDA
Total Shear Strain (23 axis) vs. Time	FDA
Creep Shear Strain (12 axis) vs. Time	FDA
Creep Shear Strain (13 axis) vs. Time	FDA
Creep Shear Strain (23 axis) vs. Time	FDA
References	
General Modeling Notes	LTXT
Model References	LTXT

DCT Discrete Text (specified choices)
FDA Functional Data Attribute (with associated parameters)
INT Integer Value
LOG Logical
LTXT Long Text Field
PNT Point value
RNG Range variable
STXT Short Text Field
TABL Tabular Attribute (multiple columns of data - PNT, STXT, DCT, INT, link)

Phase	Type	Def. Rev.	Def. Irrev.	Damage/Life	Volume Fraction
1	Fiber	SCS-6		Curtin:SCS-6	35
2	Matrix	Ti-15-3E	InPlas:Ti-15-3	ADEAL-Ti15-3	65
	Debond			ECI-SCS6/Ti-15-3	

Note: Type is DCT parameter (Fiber/Fill/Debond/Interface/Matrix)

a) Example of the RUC/RVE Constitutive Discription attribute filled out.

Ply No.	Ply thickness	Ply Angle	Scale	RUC Record	Def. Rev.	Def. Irrev.	Damage/Life	Architecture	Fiber Volume Fraction
1	0.04	-45	RUC	SCS6/Ti15-3				Square	35
2	0.02	0	Effective		Ti-15-3E	InPlas:Ti-15-3	ADEAL-Ti15-3		
3	0.04	45	RUC	SCS6/Ti15-3				Hexagonal	35

b) Example of the Laminate Definition attribute filled out.

Figure 6 Example of new tabular attributes to describe the composite pedigree

IV. Supporting Infrastructure: Importers/Exporters

To assist those populating the database, as well as those extracting information from the database, specialized importers and exporters must be developed. Typically, each interface is "fit-for-purpose" and in that spirit we have created an Excel-based model importer to assist the user/analyst in populating records within each Model Table. This enables non-experts with the Granta MI® system to not only know what information is required but to efficiently load that information/data into the system. Therefore distributing such an Excel file out to the analyst community provides them with a standard format to capture their simulation data while at the same time ensuring that sufficient pedigree information is captured to make this information meaningful. Figure 7 illustrates the "record data" sheet, which contains the basic general information necessary to create a given record in the Deformation Table. Toward the bottom of the figure one can see how the reversible and irreversible model specific parameters are grouped into sections. Figure 8 shows an example simulation data sheet in which the time, stress, and strain response for a given analysis is to be captured. The corresponding graphic representation of this data, in the stress-strain, stress-time and strain-time space, is display on the left.

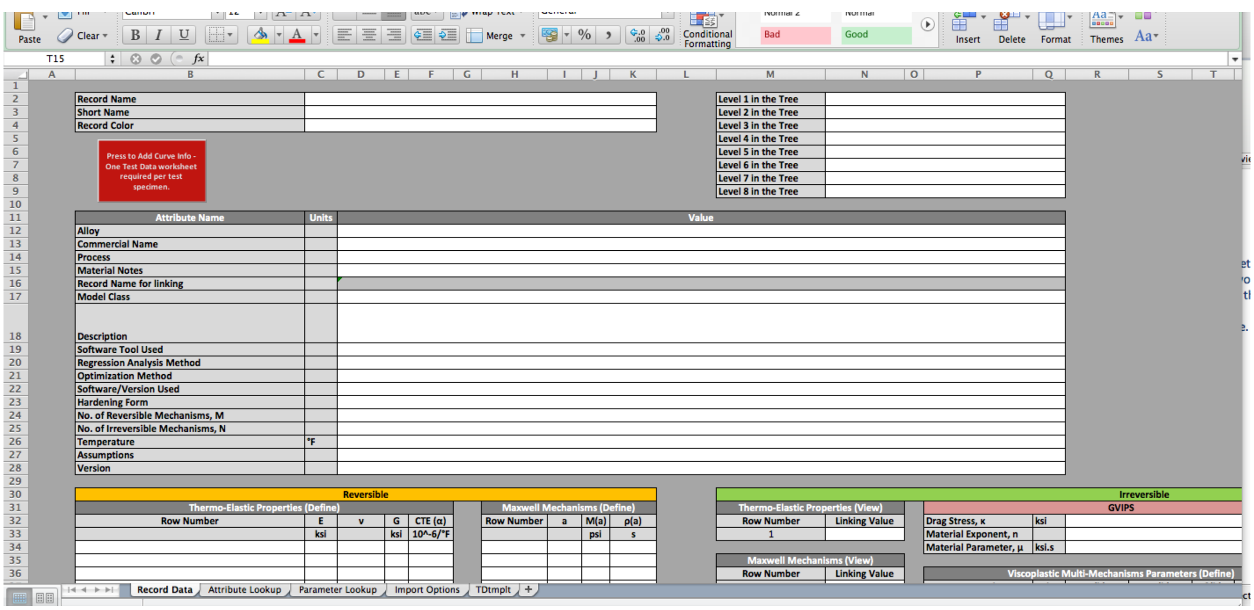
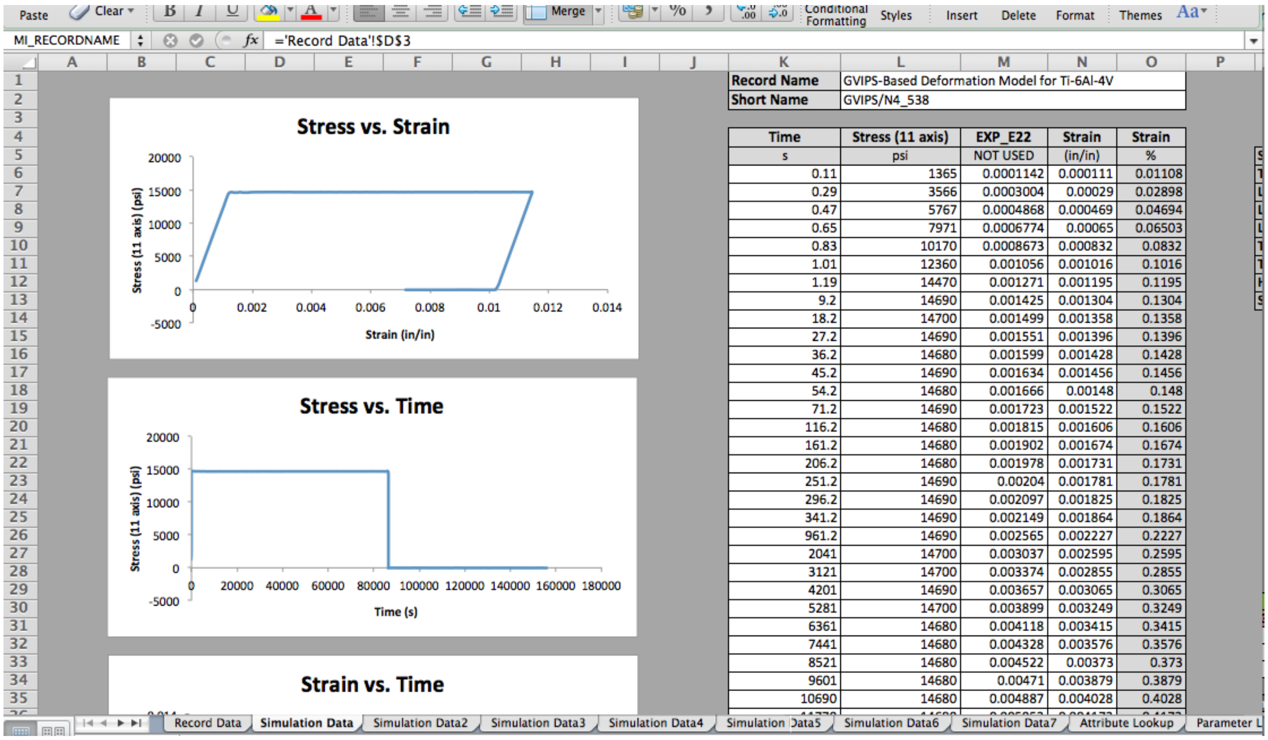


Figure 7 Deformation Model Table Excel Importer: Record Data sheet



Record Name	GVIPS-Based Deformation Model for Ti-6Al-4V
Short Name	GVIPS/N4_538

Time	Stress (11 axis)	EXP_E22	Strain	Strain
s	psi	NOT USED	(in/in)	%
0.11	1365	0.0001142	0.000111	0.01108
0.29	3566	0.0003004	0.00029	0.02898
0.47	5767	0.0004868	0.000469	0.04694
0.65	7971	0.0006774	0.00065	0.06503
0.83	10170	0.0008673	0.000832	0.0832
1.01	12360	0.001056	0.001016	0.1016
1.19	14470	0.001271	0.001195	0.1195
9.2	14690	0.001425	0.001304	0.1304
18.2	14700	0.001499	0.001358	0.1358
27.2	14690	0.001551	0.001396	0.1396
36.2	14680	0.001599	0.001428	0.1428
45.2	14690	0.001634	0.001456	0.1456
54.2	14680	0.001666	0.00148	0.148
71.2	14690	0.001723	0.001522	0.1522
116.2	14680	0.001815	0.001606	0.1606
161.2	14680	0.001902	0.001674	0.1674
206.2	14680	0.001978	0.001731	0.1731
251.2	14690	0.00204	0.001781	0.1781
296.2	14690	0.002097	0.001825	0.1825
341.2	14690	0.002149	0.001864	0.1864
961.2	14690	0.002565	0.002227	0.2227
2041	14700	0.003037	0.002595	0.2595
3121	14700	0.003374	0.002855	0.2855
4201	14690	0.003657	0.003065	0.3065
5281	14700	0.003899	0.003249	0.3249
6361	14680	0.004118	0.003415	0.3415
7441	14680	0.004328	0.003576	0.3576
8521	14680	0.004522	0.00373	0.373
9601	14680	0.00471	0.003879	0.3879
10690	14680	0.004887	0.004028	0.4028

Figure 8 Deformation Model Table Excel Importer: Typical simulation data sheet

V. Conclusions

As models become more accurate, their complexity tends to increase, as they rely less and less on simplifying assumptions. This complexity drives the need for more data to be measured, predicted, compared, stored, and tracked. The goals of ICME, to link models at multiple scales, drives these same needs and underscores the value of a robust information management system. Often overlooked as a "mere database," this information management system should be viewed as a "necessary" or an "enabling" infrastructural aspect to ICME. In this paper, we have taken the first step in implementing a robust model pedigree infrastructure for integrating experimental data with simulation data resulting from constitutive models being applied at various scales. Further some of the key requirements for best practice in materials informatics were discussed. Examples of many of the functionalities and approaches described above already exist, and are now widely applied. As a result, materials property information management has become increasingly effective in recent years, responding to the demands of new material and engineering applications and the pressures of operating in a globalized engineering environment. But many hurdles are yet to be overcome, and further challenges are to be expected, particularly in the area of ICME information management.

Nonetheless, these challenges are likely to be met as materials information management and ICME in general becomes mainstream, particularly in industries like aerospace, defense, and energy, and as more organizations demonstrate a return on their investment in technology and manpower in this area. Other technology trends also support expansion of materials information management capabilities— computationally aided engineering (CAE) is becoming more embedded in engineering processes, simulations are becoming more sophisticated, and thus demands for materials property data are becoming increasingly complicated and frequent.

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