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Schema Elements for Granta Annual Report: FY2024

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1 Executive Summary

Granta: Materials Intelligence (Granta: MI) is a commercial database software distributed by Ansys, Inc. that is utilized by the Nuclear Security Enterprise (NSE) to organize and store relevant materials data. Lack of standard and well-documented database schema is the primary obstacle to an NSE materials data management solution, so the objective of this project is to create and document such a schema.

In FY21, an approach for designing, documenting, and managing a standard database schema was described based on the creation of *schema elements* (collections of attributes used to describe particular aspects of the data) to be used as building blocks for creating various database tables without duplication. In FY22, these methods were applied through a multi-site collaboration to create and document the schema elements necessary to build a thermogravimetric analysis (TGA) testing table. In FY23 the schema was expanded to include elements for a differential scanning calorimetry (DSC) table, along with schema for supporting metadata tables including Instruments, Projects, Documents, and Testing Series.

In FY24 the following progress was made, again through multi-site collaboration:

- The existing schema elements were modified to accommodate thermomechanical analysis (TMA) data, and a table, Test Data: TMA, was created for managing TMA data.
- The elements necessary for the following additive manufacturing (AM) data tables (directed at data specific to selective laser sintering AM technology) were created:
 - AM Builds
 - AM Processes
 - AM Part Designs
 - Built AM Parts
 - AM Feedstock Materials
 - AM Feedstock Material Batches
- The elements necessary for creating a Calibrated Material Models table were created, and the Calibrated Material Models table was created.

In FY25 the existing schema will be deployed on the production enterprise Granta instance on the enterprise secure network. Schema elements will be appended, and new elements created as necessary, to allow the creation of tables specifically to support materials testing, AM process development, and design and analysis for modernization programs.

2 Introduction

2.1 Motivation for a standard enterprise database schema

Granta: Materials Intelligence, also known as Granta: MI or Granta, is a commercial database software distributed by Ansys, Inc. that is utilized by the Nuclear Security Enterprise (NSE) to organize and store relevant materials data. For a more complete discussion of the use of Granta: MI at NSE sites, see the FY21 Schema Elements annual report¹ and the FY23 At-Risk Materials report². Strong use-cases for an enterprise repository for materials data include:

- Identification, tracking, and reporting of materials availability issues.
- Understanding the effects of additive manufacturing (AM) build parameters and feedstock material properties on printed parts to provide a path to process-based qualification.
- Consolidation of surveillance materials characterization data to support aging studies, new materials development, and material modeling.
- Establishment of a single-source-of-truth for material specification, properties, and material model parameters to support digital design and engineering of future systems.

Site and NNSA program management recognize that an enterprise instance of Granta is our best hope for satisfying these use cases, and supporting new programs requires a fast implementation. *A prerequisite for the implementation of any enterprise materials data management solution is the deployment of a standard database schema, and this is the objective of the Schema Elements project.*

A schema consists of a set of attributes (a.k.a. ‘data fields’) for each type of data (e.g, AM data, material properties data, materials availability risk data, etc.) as well as documentation of the definitions of each attribute so each site can use the schema consistently. Consistency is key to the ability to pool datasets uploaded by disparate teams across the enterprise, but consistency is challenging to achieve because of the complex nature of materials data. For example, to make use of material test data, the exact pedigree of the material must be documented (including, for example, the material supplier, the age of the material, the AM build parameters, etc.). Furthermore, this complex metadata also must be linked to the specific values of material properties and material model parameters that it supports.

2.2 Approach for developing a standard database schema

As documented in detail in previous reports^{1,3,4}, the approach for designing a well-documented and consistent schema utilizes the concept of a *schema element*: a collection of attributes used to describe a particular aspect of the data. Schema elements are then used, in whole or part, and combined with other schema elements, to construct the attributes that define database tables (e.g. for material properties, AM build parameters, specific types of characterization test, etc.). Re-using schema elements in multiple tables promotes consistency, avoids unnecessary duplication, and simplifies documentation.

¹ LA-UR-21-29682

² LLNL-TR-854668

³ LA-UR-22-30313

⁴ LA-UR-23-32932

Since FY21 a multi-site team has been meeting to draft, discuss, and deploy schema elements. The individuals representing each site in FY24 are shown in Table 1. The attributes, their definitions, and their use-cases are documented in PowerPoint slides archived on the cross-site SharePoint hosted by SNL. The schema is then implemented by LANL on an unclassified Granta instance accessible to all NSE sites and is used as a ‘master’ schema to which production databases will be synchronized.

Table 1. List of regular participants in cross-site Schema Elements project discussions during FY24.
Bolded names represent primary points of contact from each site.

| LANL | SNL | LLNL | KCNSC | PX |
|---|---|--|--|--|
| <ul style="list-style-type: none"> • Jillian O’Neel • Jack Brett • Philip Schembri • Vanessa Feagin • Luis Diaz • Alison Ticknor | <ul style="list-style-type: none"> • Samuel Moran • Inkiad Ahmed • Richard Karnesky • Matthew Witman | <ul style="list-style-type: none"> • Jennifer Cruz • Daniel Gardner | <ul style="list-style-type: none"> • Leslie Embrey • Leslie Lytle • Haley Owens • Jonathan Parman | <ul style="list-style-type: none"> • Frank Cordova |
| NNSS | SRNL | Y-12 | AWE | |
| <ul style="list-style-type: none"> • Travis Bame • Gerald Schotik | <ul style="list-style-type: none"> • Christopher Rasmussen • Paul Korinko • Camden Chatham | <ul style="list-style-type: none"> • Lloyd Arrowood | <ul style="list-style-type: none"> • Craig Lowe | |

2.3 Process for creating schema elements

Schema development usually consists of *both* (a) creating new and/or modifying existing schema elements, *and* (b) arranging schema elements into a new table. As a result of FY22 and FY23 progress on this project, a library of schema elements now exists, and it is becoming more common to simply edit/append existing schema elements rather than to create new ones.

The following is a summary of the process used for creating/modifying schema elements and creating new tables:

1. The site team responsible for creating the table works with the Schema Elements project manager to schedule a presentation of the draft schema element(s) and table on the cross-site meeting agenda.
2. At the meeting, the responsible site team presents the internally reviewed new/modified schema element(s) along with the proposed arrangement of schema elements into a table layout. Note:
 - i. When modifying or appending existing schema elements, the existing slides documenting that schema element should be edited, rather than creating a new slide set.
 - ii. The schema element slide deck for a new schema element should include:
 - Schema element name and definition
 - Brief overview of attributes

- Use-cases and the requirements derived from them
 - Potential discussion points
- iii. The table layout slide deck should include
 - Name and description of the new table
 - Discussion of use-cases for the table, including how the table will relate to other tables to satisfy NSE materials data management needs
 - List of schema elements to be used in the table layout, highlighting which attributes from each schema element will be used or not used
 3. The responsible site team distributes the slide decks to all sites no less than a week after the presentation (preferably the day of the presentation).
 4. Teams at other sites review the slide decks and prepare feedback.
 5. At a meeting 2-weeks from the original presentation, other sites share their feedback, and all sites discuss.
 6. The responsible site team implements changes to the schema element(s), table layout, and slide decks based on the cross-site feedback and discussion, and the updated slides are distributed to the cross-site team.
 7. Steps 2-6 are repeated until there is consensus.
 8. The responsible site team creates the attribute help files – the html files available to users and used to define the attributes - and sends them to the LANL team.
 9. The slides used for discussion are archived on the ECN SharePoint 'Granta MI Materials Database [JOWOG31]' site in the Schema Elements Review Documents folder, with the file name following the naming convention established by existing files.
 10. The schema element is created by the LANL team on the unclassified Granta MI instance, which includes:
 1. Creating the attributes in the Schema Elements table of the Schema Elements database.
 2. Creating a layout titled '[schema element] (released) *schema element name*', where *schema element name* is the name of the schema element. For example, '[schema element] (released) Test Information'.
 3. Copying the help files created by the responsible site to the Schema Elements database and ensuring the attributes are linked to them.
 11. The table is created by the LANL team on the on the unclassified Granta MI instance, which includes:
 1. Creating a layout in the Schema Elements table of the Schema Elements database titled '[table] (released) *table name*', where *table name* is the name of the table. For example, '[table] (released) Test Data: DSC'.
 2. Creating a new table titled *table name* in the Schema Elements database by copying the attributes and layout from the Schema Elements table into this new table.
 3. Syncing (i.e. using the Data Updater utility in Granta MI Admin) the new table into the appropriate destination database from the Schema Elements database.
 4. Copying the attribute help files into the destination databases.
 5. Checking the linked tabular attributes and record links to ensure they work as intended on the production databases and repairing any issues.

3 Summary of schema elements and tables

As of FY24, the schema elements shown in Table 2 have been drafted, reviewed by all sites, documented as PowerPoint files on the SharePoint, and deployed to the unclassified Granta instance into the following three databases⁵:

- NSE Weapons Materials Database (WMD)
- NSE Materials Characterization Database (MCD)
- NSE Additive Manufacturing Database (AMD)

Similarly, the tables deployed into each database on the unclassified instance are shown in Table 3. This schema is that to which the production instance on the ESN will be synchronized.

Note that the NSE WMD contains tables managed by Ansys through the Restricted Substances Database updates, and those are not listed in Table 3. Also, because the schema for the Materials and At-Risk Cases tables have been in use by the At-Risk Materials project since before the Schema Elements project began, the schema in those tables are a hybrid of released schema elements and unreviewed attributes. It is expected that these tables will evolve towards containing only released schema elements once the relevant schema elements are addressed through this project.

Table 2. Name and description of each schema element created as of the end of FY24.

| Schema element name | Description |
|--------------------------------|---|
| Record Information | Information about the record itself, including when it was created, modified, and reviewed |
| Project Information | Information about the project and links to the project record from other records |
| Data Files | Data files, and information about them, for the purpose of traceability |
| Instrument Parameters | Attributes that describe the setup of the instrument and test program sufficiently to reproduce the test |
| Test Conditions | Attributes that specifically describe the state of the sample material during the test, intended to describe the test data for data consumers |
| Test Information | Non-instrument-specific meta data attributes related to the test data stored in the record |
| Specimen Information | Information about the specimen that was tested, including, geometry, manufacturing information, etc. |
| Test Data & Results | Attributes used to hold the data and results from a test, including X-Y curve data as well as point, range, or tabular attributes |

⁵ Note that Section 3 of the FY23 report (LA-UR-23-32932) discussed the decisions made about which databases should be created and which tables each should house.

| | |
|--|--|
| Calibration Information | Information on the calibration of instruments that are used in testing records |
| Testing Series Information | Information about the testing series and links to the testing series record from other records |
| Document Information | Attributes related to documents, links to documents in external repositories, and an attribute to embed the document directly. |
| Equipment Information | Information about the equipment used to generate materials data, including characteristics like the make, model, and owner of the equipment |
| Build Information | Information associated with an additively manufactured build, including characteristics about the build such as the build ID number, build start date, build end date and name of build operator |
| AM Process Information | Information associated with the process to create an additively manufactured part, including variables such as laser power, scan/laser speed, and hatch spacing. |
| Part Design Information | Information that may be needed to design, create, and/or recreate an AM part (shape, object, specimen, component, etc.) |
| Built Part Information | Information about a specific instance of a realized AM part |
| Calibrated Material Model (CMM) Information | Attributes that describe CMM parameter sets, as used by scientists and engineers performing numerical or analytical calculations |
| Material Properties | Properties of a material, as used by scientists and engineers performing numerical or analytical calculations |
| Reference and Data Basis | Attributes that point the user to the source of data held in various other attributes |
| General Material Information | General materials information that can be used for identification purposes and in searching/reporting. |
| Material Specification Information | General information about the material specification (7DS, MIL spec, etc.) |
| General AM Feedstock Batch Information | Information about an additive manufacturing feedstock material batch that is not specific to material type, AM technology, machine manufacturer, etc. |
| Material Processing Information | Information about how a material was processed for reproducibility and input/output use cases |

Table 3. List of tables, and the database in which they reside, for which schema has been developed as of the end of FY24. Tables developed by Ansys and delivered as part of the Restricted Substances Database package are omitted from this list but are used in the NSE Weapons Materials Database.

| Table name | Database | Records in this table contain... |
|-----------------------------------|---|--|
| Materials | NSE Weapons Materials Database | Data specific to a material, as identified by a specification document number and links to related records |
| Calibrated Material Models | NSE Weapons Materials Database | Parameters and related metadata describing calibrated material models |
| At-Risk - Cases | NSE Weapons Materials Database | Data related to identification and tracking of materials availability risks |
| Test Data: TGA | NSE Materials Characterization Database | Data for thermogravimetric analysis (TGA) tests |
| Test Data: DSC | NSE Materials Characterization Database | Data for differential scanning calorimetry (DSC) tests |
| Test Data: TMA | NSE Materials Characterization Database | Data for thermo-mechanical analysis (TMA) tests used to measure thermal expansion |
| Projects | NSE Materials Characterization Database | Project metadata, with links to all records related to each project |
| Testing Series | NSE Materials Characterization Database | Testing series metadata, with links to all records related to each testing series |
| Documents | NSE Materials Characterization Database | Data for documents, the document files, and/or links to documents in other repositories |
| AM Builds | NSE Additive Manufacturing Database | Data describing a specific instance of an AM build |
| AM Processes | NSE Additive Manufacturing Database | Data describing AM processes that may be used to create one or more AM builds |
| AM Part Designs | NSE Additive Manufacturing Database | Data describing part designs intended for AM build |
| Built AM Parts | NSE Additive Manufacturing Database | Data describing parts built via an AM build |

4 New schema elements and changes to existing schema elements

This section contains a summary of additions and changes to schema elements, along with notable use-cases, discussion points and decisions. However, it is not intended to be complete documentation of the schema. The Schema Elements table in the Schema Elements database on the unclassified enterprise Granta instance contains all the details of the schema. We judge duplication of the full schema into this report to be inefficient and to add little value.

4.1 Instrument Parameters [modified]

4.1.1 Use-cases and discussion

Attributes were added to the Instrument Parameters schema element to accommodate thermomechanical analysis (TMA) testing. The previously documented use-cases for that schema element apply to these new attributes. Attributes being added are instrument parameters necessary to reproduce a test.

4.1.2 New or Modified Attributes

Table 4. Attributes added to the existing Instrument Parameters schema element.

| Attribute Name | Attribute Type | Notes |
|-------------------|----------------|---|
| Probe type | DCT | Value set: [Expansion, Compression, Penetration, Tension] |
| Probe diameter | PNT | |
| Preload force | PNT | |
| Film fiber offset | STXT | |

4.2 Test Data and Results [modified]

4.2.1 Use-cases and discussion

Attributes were added to the Test Data & Results schema element to accommodate thermomechanical analysis (TMA) testing. The previously documented use-cases for that schema element apply to these new attributes. Attributes being added are common columns of data and average results output from a TMA instrument and necessary for characterization of materials.

4.2.2 New or Modified Attributes

Table 5. Attributes added to the existing Test Data & Results schema element.

| Attribute Name | Attribute Type | Notes |
|--|----------------|---|
| Dimension change vs. time | FDA | Parameters: [Time] |
| Dimension change vs. temperature | FDA | Parameters: [Temperature] |
| Dimension change vs. force | FDA | Parameters: [Force] |
| Specimen length vs. time | FDA | Parameters: [Time] |
| Specimen length vs temperature | FDA | Parameters: [Temperature] |
| Coefficient of Thermal Expansion Averaged Over Temperature Range | TAB | Headers: Average Coefficient of Thermal Expansion, Standard Deviation, Temperature Range, Notes |

4.3 Build Information [new]

4.3.1 Definition

This schema element contains metadata information associated with creating an additively manufactured build. It focuses on characteristic information about the build such as the build ID number, build start date, build end date and name of build operator. Note that an “AM build” is defined as all parts, components, coupons, and/or shapes created in a single build instance.

4.3.2 Use-cases and discussion

Use-cases, in the form of ‘user stories’, that drive requirements for the schema element include:

- “As a data consumer, I want to be able to quickly locate my AM build in the database and link between build record and other records.”
 - **Requirement:** An attribute for build ID number, which must be unique in the AM Builds table and helps with linking.
- “As a data consumer, I want to be able to search for builds created on or between certain dates so I can compare against machine health status and/or previous machine calibration date.”
 - **Requirement:** Attributes for build start date and build end.
- “As a manufacturing manager, I want to know duration of builds / how long it takes to create builds so I can more accurately predict capacity/resource planning.”
 - **Requirement:** Attribute for build duration in a standard format.

- “As a data consumer, I want to know who to contact with questions I have about the layout of and operation of the build.”
 - **Requirement:** Attribute to capture appropriate points of contact.
- “As a manufacturing manager, I want to know status of AM builds (how many builds are complete, incomplete, failed, etc). I want to be able to track builds that complete successfully and have access to build notes when builds are incomplete or fail so I can understand, analyze, iterate, and minimize the number of failed builds.”
 - **Requirement:** Attribute to capture build complete status, with the ability to capture failed builds as well as builds successfully completed.
- “As a manufacturing engineer, I want to have access to the build files so I can repeat the build, review the build execution, and/or iterate on the build.”
 - **Requirement:** Attribute(s) to capture appropriate build files.
- “As a data consumer, I want to be able to navigate to associated data (material batch, previous machine calibration, machine on which AM build was created, and parts from build) by way of linked records.”
 - **Requirement:** Links from AM Build table to material batches record, previous machine calibration record, machine record, and parts records.

4.3.3 Attributes

Table 6. Attributes in the General Build Information section of the Build Information schema element.

| Attribute Name | Attribute Type | Notes |
|----------------------------------|----------------|---|
| Build ID | STXT | Unique identifier |
| Build start date | DATE | |
| Build end date | DATE | |
| Name of build operator | STXT | Format must follow the convention: First and last name (DUID from OneID phonebook) |
| Name of build requestor | STXT | Format must follow the convention: First and last name (DUID from OneID phonebook) |
| Name of build contact | STXT | Format must follow the convention: First and last name (DUID from OneID phonebook) |
| Build iteration objective | LTXT | Purpose of build instance |

Table 7. Attributes in the Build Characterization Information section of the Build Information schema element.

| Attribute Name | Attribute Type | Notes |
|---------------------|----------------|--|
| Software | TAB | Columns: [Software Name, Vendor, Manufacturer, Version, Software Notes] |
| Build files | TAB | Columns: [File Type, File Name, File Notes] |
| Build time | PNT | Amount of time taken for build instance to complete |
| Build pauses | TAB | Columns: [Layer Number, Pause Duration, Cause, Pause Notes] |

Table 8. Attributes in the Build Status Information section of the Build Information schema element.

| Attribute Name | Attribute Type | Notes |
|----------------------------|----------------|---|
| Build complete? | LOGIC | This does not pertain to whether the build instance was successful |
| % build complete | RNG | Percent of build instance completion calculated by (number of completed layers / number of total layers) x 100. |
| Build status | DCT | Indicates whether the build instance met requirements and/or specifications. |
| Build failure type | DCT | Value set: [Powder shortage, Lack of sufficient supports, Inadequate process parameters, Poor part design, Poor build orientation, Machine failure, Other] |
| Build failure notes | LTXT | Notes specifically about build failure |

| | | |
|----------------------------------|-------|--|
| Build needs optimization? | LOGIC | |
| Build information notes | LTXT | Information not captured in other attribute fields |

Table 9. Attributes in the Links to Build section of the Build Information schema element.

| Attribute Name | Attribute Type | Notes |
|---------------------------------|---------------------------------|---------------------|
| AM Builds | Static link to AM Builds table | |
| AM Builds | Smart link to AM Builds table | |
| Linked build information | Tabular link to AM Builds table | Columns: TBD |

4.4 AM Processes Information [new]

4.4.1 Definition

This schema element contains data and information associated with laser powder bed fusion (LPBF) and selective laser sintering (SLS) processes to create an additively manufactured part. It focuses on the variables that shall be controlled build-to-build to additively manufacture a part, such as laser power, scan/laser speed, and hatch spacing. This schema element focuses on process parameter “set points” rather than process parameter in situ monitoring / measurements at this time. Machine settings and machine calibration information will be captured in separate schema elements.

4.4.2 Use-cases and discussion

Use-cases, in the form of ‘user stories’, that drive requirements for the schema element include:

- “As a materials engineer, I want to be able to search process parameter sets by technology, name, etc.”
 - **Requirement:** Attribute for categorizing process parameters sets by technology type and attribute for a unique identifier.
- “As a materials engineer, I want to be able to analyze material properties as a function of process parameters.”
 - **Requirement:** Attributes for all relevant process parameters.
- “As a materials engineer, I want to be able to analyze material properties as a function of build environment variables.”
 - **Requirement:** Attributes for all relevant build environment variables.
- “As a process engineer, I want to be able to track anomalies so I can understand process successes and failures, and then iterate on process parameter development.”
 - **Requirement:** Attributes to describe and explain anomalies.

- “As a manufacturing engineer, I want to be able to reproduce a build using the same process parameters that were used previously.”
 - **Requirement:** Attributes to store full process parameter files/records for reference for future processing/development.
- “As a process engineer, I want to be able to search all process parameter sets within a single build.”
 - **Requirement:** Links to associated build(s) such that multiple builds may link to a given process record.

4.4.3 Attributes

Table 10. Attributes in the AM Processes Information schema element.

| Attribute Name | Attribute Type | Notes |
|----------------------|----------------|---|
| AM process ID | STXT | Unique in the AM Process table |
| XY beam offset | PNT | |
| Hatching laser power | PNT | Hatching refers to filler scans |
| Hatching laser speed | PNT | Hatching refers to filler scans |
| Contour laser power | PNT | Contour refers to scans near outermost border |
| Contour laser speed | PNT | Contour refers to scans near outermost border |
| Edge laser power | PNT | Edge refers to outermost border scans |
| Edge laser speed | PNT | Edge refers to outermost border scans |
| Upskin laser power | PNT | Upskin refers to areas of layers not covered by vectors of following layers |
| Upskin laser speed | PNT | Upskin refers to areas of layers not covered by vectors of following layers |
| Downskin laser power | PNT | Downskin refers to underside of overhangs |
| Downskin laser speed | PNT | Downskin refers to underside of overhangs |
| Scan pattern | DCT | Value set: [Chessboard/Checkerboard |

| | | |
|---------------------------|------|--|
| | | Island Serpentine Stripe] |
| Layer thickness | PNT | |
| Powder dosing | RNG | Increased packing does not change layer thickness. |
| Build chamber temperature | PNT | |
| Build surface temperature | PNT | |
| Gas flow | RNG | |
| Build atmosphere | DCT | Value set: [Argon, Helium, Nitrogen] |
| Recoater | DCT | Value set: TBD in Phase 2 of AM Processes schema |
| Recoater speed | PNT | |
| Files | TAB | Columns: [File Type, File Name, File Notes] |
| Process information notes | LTXT | |
| Energy density | RNG | |
| Exposure | DCT | Value set: [Single, Double] |
| Initial Z | PNT | Elevator height at start of build |
| Material set | DCT | Value set: [PA2105_060_000, PA2200_060_102, PA2200_100_100, PA2200_100_102, PA2200_100_EOS, PA2200_120_102, PA2200_120_EOS, PA2201_100_000, PA2201GB_100_000, PA2203AIG_100_000, PA2210FR_100_000, PP1101_100_000, PS3302_100_000,] |

| | | |
|--|------------------------------------|--|
| Minimum layer time | PNT | Amount of time a stationary laser beam is applied to substrate |
| Shrinkage scaling – pre-process | DCT | Value set: [Pre-processing X, Pre-processing Y, Pre-processing Z] |
| Shrinkage scaling | PNT | Process control scaling X, Y, Z |
| AM Processes | Static link to AM Processes table | |
| AM Processes | Smart link to AM Processes table | |
| Linked AM process information | Tabular link to AM Processes table | Columns: TBD |

4.5 Part Design Information [new]

4.5.1 Definition

This schema element contains design information needed to manufacture a part. This includes data associated with the nominal dimensions of a part. Dimensions/measurements of already manufactured or ‘built parts’ are captured in the Built Part Information Schema Element.

4.5.2 Use-cases and discussion

Use-cases, in the form of ‘user stories’, that drive requirements for the schema element include:

- “As a product engineer, I want to be able to have a robust nomenclature/naming convention for my part design so I can identify, locate, and search for parts built based off this design.”
 - **Requirement:** Attribute for Part ID, to be unique in the AM Part Designs table.
- “As a product engineer, I want to know my part type so I can refer to associated specification and check adherence to specification and so I can further understand the purpose of part creation.”
 - **Requirement:** Attribute to categorize part designs by type.
- “As a product engineer, I want to know the dimensions of my part design so I can analyze nominal dimensions versus actual part dimensions.”
 - **Requirement:** Attribute for part dimensions that can be compared directly to measured dimensions in the Built AM Parts table.
- “As a process/product engineer, I want all design/build/process files associated with part creation so I may replicate my part.”
 - **Requirement:** Links to design, build, and process parameters.

4.5.3 Attributes

Table 11. Attributes in the Part Design Information schema element.

| Attribute Name | Attribute Type | Notes |
|--------------------------------|--------------------------------------|--|
| Part design ID | STXT | Unique in AM Part Designs table |
| Part type | DCT | Value set: [Component, Process sample, Product sample, Tensile, Torsion, Density, Micrograph, Witness (generic), Other] |
| Part dimensions | TAB | Columns: [Dimension Label, Measured Dimension, Standard Deviation, Target Dimension, Difference, Pass/Fail, Measurement Technique, Notes] |
| Part design information notes | LTXT | |
| Part design files | TAB | Columns: [File Type, File Name, File Location, Notes] |
| AM Part Designs | Static link to AM Part Designs table | |
| AM Part Designs | Smart link to AM Part Designs table | |
| Linked part design information | Tabular link to AM Part Design table | Columns: TBD |

4.6 Built Part Information [new]

4.6.1 Definition

This schema element contains information associated with measured data for parts in the as-built state prior to post-processing operations. Part design information containing nominal part dimensions is contained in the Part Design Information Schema Element.

4.6.2 Use-cases and discussion

Use-cases, in the form of ‘user stories’, that drive requirements for the schema element include:

- “As a product engineer, I want to be able to have a robust nomenclature/naming convention for my part so I can identify, locate, and search my part.”
 - **Requirement:** Attribute for built part ID unique in the Built AM Parts table.
- “As a process engineer, I want to know the location of my part on the build plate, so I can understand the effects various parameters (gas flow, laser positioning, etc) of part location and analyze optimal buildable locations on the build plate.”
 - **Requirement:** Attributes to describe the location of a built part with respect to a coordinate system, understanding that not all projects or build series will refer to the same coordinate system (e.g. a coordinate system may be x, y, z coordinates of part (center of mass, center of part), 0°, Θ coordinates, quadrant identification, or other).
- “As a product engineer, I want to know the dimensions of my part so I can analyze nominal dimensions versus actual part dimensions and analyze other parameters as a function of part dimensions.”
 - **Requirement:** Attribute for built part dimensions such that they can be compared to nominal dimensions stored in the AM Part Designs record .

4.6.3 Attributes

Table 12. Attributes in the Built Part Information schema element.

| Attribute Name | Attribute Type | Notes |
|-------------------------------------|----------------|--|
| Built part ID | STXT | Unique identifier. No two built parts shall have the same Part number ID |
| Part location on build | STXT | Including reference to coordinate systems |
| Part orientation | DCT | Value set: [Vertical, Horizontal, 45 Degree, Other] |
| Built part dimensions | TAB | Columns: [Dimension Label, Measured Dimension, Standard Deviation, Target Dimension, Difference, Pass/Fail, Measurement Technique, Notes] |
| Built part information notes | LTXT | |
| Built part files | TAB | Columns: [File Type, File Name, File Location, Notes] |

| | | |
|--------------------------------------|-------------------------------------|---------------------|
| Built AM Parts | Static link to AM Built Parts table | |
| Built AM Parts | Smart link to AM Built Parts table | |
| Linked built part information | Tabular link to AM Built Part table | Columns: TBD |

4.7 Calibrated Material Model Information [new]

4.7.1 Definition

This schema element contains attributes that describe CMM parameter sets, as used by scientists and engineers performing numerical or analytical calculations involving weapon system materials. This information includes:

- The values of the CMM parameters.
- The 'data basis' (a.k.a. 'pedigree' or 'provenance') of the parameter set.
- Information sufficient to determine which material model formulation/version the parameters correspond to.
- Information about the performance of the material model and parameter set; i.e., how much, and under what conditions, it is likely to be a sufficient representation of actual material response.

4.7.2 Use-cases and discussion

Discussions about the design of an enterprise Calibrated Material Models table began in 2019, more than 2 years prior to the inception of the Schema Elements project. These occurred over a period of about 2 years as part of the Calibrated Material Models Working Group (CMMWoG) meetings, which formed as a working group of the Jowog 31 engineering analysis and testing Hocwog. There is much documentation⁶ of the discussions, decisions, and compromises made, and so we refer the reader to those for full details. Here we give only a summary.

The CMMWoG covered many topics, including:

- How CMM records should be linked to test data
- The structure of the schema, e.g.:
 - Separating 'properties' and CMM tables
 - Using a single CMM table for all material models
 - Using a separate record for each material model used for a specific material (i.e. a one-to-many relationship between 'Materials' and CMMs)
- Differences in CMM parameter meanings between analysis codes or formulations (e.g. 'yield stress')

⁶ See the Calibrated Material Models folder in the Granta MI Materials Database [JOWOG31] SharePoint site: [https://collaborate.sandia.gov/sites/grantadatabase_J31/Documents/Calibrated Material Models/Notes](https://collaborate.sandia.gov/sites/grantadatabase_J31/Documents/Calibrated%20Material%20Models/Notes)

- CMM ‘quality’ ratings/rubrics to help users filter records (and other use-cases), and how they could be mis-used or misinterpreted
- Independent variables, including material age, lot/batch, etc
- How statistical information should be stored
- How/where to capture calibration scripts and source code
- How data will be integrated with design (e.g. Creo) and analysis (e.g. Abaqus, Sierra) tools

The first draft of the CMM schema element represented the LANL team’s interpretation of the compromises to many of the problems documented in the CMMWoG notes. Feedback, especially from the SNL and KCNSC teams, helped to further refine the schema.

Use-cases, in the form of ‘user stories’, that drive requirements for the CMM schema element (and the CMM table) include:

- “As an analyst, I want access to the trusted set of material model parameters so I can ensure I’m using the same material models as other analysts working on the same or similar systems.”
 - **Requirement:** CMM table with record review/release process to ensure duplicate parameter sets are resolved/documented.
 - Note that use of the same set of CMM parameters acts as a quality control mechanism – the more a CMM is used, the more likely a problem, if it exists, will be found.
- “As an analyst, I want to know the pedigree of the material model parameters I am using in case my system model is particularly sensitive to some of them.”
 - **Requirement:** Information, or links to information, about the calibration process and source test data.
 - Note that links to test data will be accommodated by using the schema elements that contain those links in the CMM table layout.
- “As an analyst, I want to make sure that the parameter set I’m using corresponds to my analysis code and material model formulation so I don’t introduce errors.”
 - **Requirement:** attributes clearly communicating the analysis code and/or material model formulation/code version appropriate for the parameter set.
- “As an engineering analyst and/or design engineer, I want to ensure the CMM I’m using corresponds to the appropriate drawing/specification, so I don’t accidentally model the part with the wrong material.”
 - **Requirement:** Link between the ‘Materials’ record (which contains the product definition information and the material properties) and the CMM record.
 - This requirement is satisfied by incorporating the linked tabular attribute in the Material Properties schema element into the CMM table.
- “As an analyst, I want to know for which range of conditions (e.g. strains, rates, temperatures) each CMM is applicable, so I don’t apply a CMM in the wrong conditions, causing errors in my system simulation.”
 - **Requirement:** attributes for ‘applicable range’ of strain/strain rate/temperature.
- “As an analyst, I want to be able to access a trusted source of uncertainty information (e.g. parameter ranges or distributions) I can use to understand sensitivities and uncertainties in my simulations”
 - **Requirement:** attributes or meta-attributes for parameter ranges in addition to nominal values and ability to store files for more complicated uncertainty information.

- “As an engineering analyst, I want to know the ‘quality’ of a CMM (a.k.a. how ‘realistic’, how ‘validated’, etc) so I can make some judgement about the ‘predictiveness’ of my system simulation.”
 - **Requirement:** attributes that store, even if qualitatively, the characteristics that define ‘quality’. This includes:
 - How ‘good’ was the data to which the model was calibrated?
 - How does the CMM output compare to the test data it was calibrated to? To other test data?
 - How much ‘fidelity’ is included in the formulation of the CMM? I.e., how much of the physical phenomena governing the material’s macroscopic behavior does it account for?

The attributes in the CMM Information schema element were divided into four sections:

- CMM General Information
- CMM Performance Information
- Links to CMM Table
- CMM Parameters

The first three are documented in Table 13 through Table 15. The CMM Parameters schema element consists of an extensive list of CMM parameter attributes, and this list is not included here. The parameter attributes for each model type (e.g. ‘Johnson-Cook’) are collected into sections and named with the following convention:

<Material Model Name>: <Parameter Name>, <Parameter Symbol (optional)>

For example:

- Crushable Foam: yield stress ratio for hydrostatic loading, k_t
- Hyperfoam: nu

The following material model types are currently accommodated, mostly to satisfy LANL requirements, and it is expected that others will be added to satisfy the requirements of other sites:

- Tabulated Uniaxial Stress Hardening Curve
- Thermorheologically simple (TRS) Parameters: Williams-Landel-Ferry (WLF) form
- CHIPFoam
- Preston Tonks Wallace (PTW)
- Johnson-Cook
- Hyperelastic
- VIPor
- Abaqus: Hyperfoam
- Abaqus: Mullins Effect
- Abaqus: Crushable Foam

The ‘quality’ use-case above was the topic of much discussion at the CMMWoG meetings. It was proposed that a single ‘quality score’ be created based on a well-documented rubric, but there was concern that rolling up the strengths and weaknesses of a CMM parameter set into too few measures would risk incorrectly guiding a user of the data. The compromise that LANL implemented was to attempt to capture

as many of the features of the rubric as possible in individual attributes and leave it to the user to decide how to filter and report those measures. When discrete types were used, the approach was to keep the number of choices low to promote consistency. The attributes in the CMM Performance section are primarily intended to address this ‘quality’ use-case.

There was much discussion at the CMMWoG meetings of ways to store CMM parameter uncertainty information since this is required to study sensitivities and uncertainties in simulations. The current schema element does not fully implement the proposed ‘4 levels of uncertainty’ solution (refer to the CMMWoG notes⁶ for details) but we propose the implementation should consist of storing the nominal parameter values in parameter attributes, which are point or functional attributes, and then adding meta-attributes to store ranges, prior distributions, and joint distributions as necessary. Range meta-attributes were added to the CHIPFoam material model parameter attributes as a demonstration of the concept.

4.7.3 Attributes

Table 13. Attributes in the CMM General Information section of the Calibrated Material Model Information schema element.

| Attribute Name | Attribute Type | Notes |
|---------------------------------------|----------------|---|
| Applicable analysis code | DCT | Value set: [Abaqus, Ansys, ParaDyn, Sierra/SM, Sierra/SD, Sierra/Aria] |
| CMM name used in analysis code | STXT | Value set: [CHIPFoam, Crushable Foam, Elastic Plastic, Johnson-Cook Hardening, Elastic Plastic, PTW Hardening, Elastic Plastic, Tabular Hardening, Hyperelastic, Hyperfoam, Linear Elastic, Linear Elastic, Anisotropic, VIPor, Viscoelastic, ViscoPlastic ViscoDamage (VPVD)] |
| CMM source code version | STXT | |
| CMM source code link | HYP | |
| CMM formulation information | TABL | Columns: [Notes, Image, Link] |
| CMM calibration date | DAT | |
| CMM calibration method | DCT | Value set: [Manual, Optimized, Other (see analysis files)] |

| | | |
|---------------------------------------|------|--|
| CMM calibration analysis files | TABL | Columns: [Name, File, Image, Description] |
| CMM uncertainty level | DCT | Value set: [Level 1: nominal values, Level 2: nominal and some range values, Level 3: nominal and some marginal (independent) distributions, Level 4: nominal and some joint (co-varying) distributions] |
| CMM notes | LTXT | |

Table 14. Attributes in the CMM Performance section of the Calibrated Material Model Information schema element.

| Attribute Name | Attribute Type | Notes |
|--|----------------|---|
| CMM intended application | LTXT | The specific analysis scenario (e.g. welding, blast, g-loading, etc) that the CMM was intended for. |
| Sufficiency of calibration data | DCT | Value set: [Insufficient, Sufficient, More than sufficient] |
| Examples of CMM performance | TABL | Columns: [Name, File, Image, Description] |
| Applicable range of strains for this CMM | RNG | |
| Applicable range of strain rates for this CMM | RNG | |
| Applicable range of temperatures for this CMM | RNG | |
| Mechanical fidelity in this CMM | DCT | Value set: [None, Low fidelity, Medium fidelity, High fidelity] |
| Thermal fidelity in this CMM | DCT | Value set: [None, Low fidelity, Medium fidelity, High fidelity] |
| Aging fidelity in this CMM | DCT | Value set: [None, Low fidelity, Medium fidelity, High fidelity] |
| CMM performance notes | LTXT | |

Table 15. Attributes in the Links to CMM Table section of the Calibrated Material Model Information schema element.

| Attribute Name | Attribute Type | Notes |
|-----------------------------------|--|-------|
| Calibrated Material Models | Smart link from Materials to CMM table using Material ID | |

4.8 Material Properties [new]

4.8.1 Definition

This schema element contains attributes that store the properties of a material. Nominally, a ‘material’ is one corresponding to a particular material specification.

4.8.2 Use-cases and discussion

Use-cases, in the form of ‘user stories’, that drive requirements for the Material Properties schema element (and some requirements for the Materials table) include:

- “As an engineering analyst, system engineer, or designer I want access to a trusted set of material properties so I can ensure I’m using the same properties as others working on the same materials.”
 - **Requirement:** Materials table, linked to product definition, with attributes for material properties.
- “As an engineering analyst, I want to know about the variability of the properties, not just the nominal value, so I can see how sensitive my simulation is to material properties.”
 - **Requirement:** Ability to store a nominal property value that is not the mean (i.e. for strength values subjected to an acceptance criterion, which results in a non-Gaussian distribution).
 - **Requirement:** Meta-attributes for variability information, including range (i.e. uniform distribution).
 - **Requirement:** Ability to add other meta-attributes for more sophisticated variability information.
- “As an engineering analyst, I want to ensure all CMMs for a given material contain the same properties.”
 - **Requirement:** Links for property data to populate in CMM records and thus be exported to analysis codes.
- “As an engineering analyst, I want properties spanning the common temperatures experienced in engineering environments.”
 - **Requirement:** Functional attributes for properties in addition to nominal values.

The CMMWoG discussions described in section 4.7.2 also covered these use-cases and requirements, and so many of the requirements on material property attributes are similar to those described for CMM parameters, such as the need for uncertainty information.

It is a potential point of confusion that both ‘Material’ records and test data records may contain what look like properties. For example, a Differential Scanning Calorimetry (DSC) test record may contain an attribute for the specific heat capacity in the Test Data and Results section, while there may also be an attribute for the specific heat capacity in the Material Properties section of a ‘Material’ record. We propose that ‘properties’ and ‘test results’ are differentiated by the fact that while test results apply to a specific *sample* of a material, the properties are intended to represent an entire population of material samples. When it is necessary to differentiate between the two, attributes for test results may be named with the prefix ‘Specimen’. For example, ‘Specimen yield strength’ may be the yield stress measured in a particular test, while ‘Yield strength in tension’ may be the expected value of the yield strength of any material sample from materials meeting a defined specification.

Attributes in the Material Properties schema element are divided into the following four sections:

- Linked Material Properties
- Physical Properties
- Mechanical Properties
- Thermal Properties

The Linked Material Properties section accommodates the linked tabular attribute used to ‘map’ the properties of a material into a related record where those properties can be displayed and exported. This satisfies the use-case for CMM records where, in general, both properties and CMM parameters are needed by an analysis code and materials may be modeled with multiple CMM types or parameter sets.

The Physical Properties section houses the attributes that are not exclusively thermal or mechanical properties, including Density and Degree of crystallinity.

4.8.3 Attributes

Table 16. Attributes in the Linked Material Properties section of the Material Properties schema element.

| Attribute Name | Attribute Type | Notes |
|----------------------------|----------------|---|
| Linked material properties | TAB | Columns: [Material ID, Material name, Density, Young’s modulus, Poisson’s ratio, Thermal conductivity, Specific heat capacity, Linear thermal expansion coefficient, Thermal expansion reference temperature] |

Table 17. Attributes in the Physical Properties section of the Material Properties schema element.

| Attribute Name | Attribute Type | Notes |
|--------------------------------------|----------------|--|
| Tapped density | PNT | |
| Tapped density range | RNG | Parent: Tapped density |
| Untapped density | PNT | |
| Untapped density range | RNG | Parent: Untapped density |
| Density | PNT | |
| Density range | RNG | Parent: Density |
| Degree of crystallinity | PNT | |
| Degree of crystallinity range | RNG | Parent: Degree of crystallinity |

Table 18. Attributes in the Mechanical Properties section of the Material Properties schema element.

| Attribute Name | Attribute Type | Notes |
|--|----------------|---|
| True stress vs. true strain (tension) | FDA | Parameters: [Strain, Temperature, Strain Rate, Specimen Orientation, Load Segment] |
| True stress vs. true strain (compression) | FDA | Parameters: [Strain, Temperature, Strain Rate, Specimen Orientation, Load Segment] |
| Young's modulus | PNT | |
| Young's modulus range | RNG | Parent: Young's modulus |
| Young's modulus vs. temperature | FDA | Parameters: [Temperature] |
| Poisson's ratio | PNT | |
| Poisson's ratio range | RNG | Parent: Poisson's ratio |
| Poisson's ratio vs. temperature | FDA | Parameters: [Temperature] |

| | | |
|---|-----|---|
| Bulk modulus | PNT | |
| Bulk modulus range | RNG | Parent: Bulk modulus |
| Shear modulus | PNT | |
| Shear modulus range | RNG | Parent: Shear modulus |
| Yield strength in tension | PNT | |
| Yield strength in tension range | RNG | Parent: Yield strength in tension |
| Yield strength in compression | PNT | |
| Yield strength in compression range | RNG | Parent: Yield strength in compression |
| Ultimate strength in tension | PNT | |
| Ultimate strength in tension range | RNG | Parent: Ultimate strength in tension |
| Ultimate strength in compression | PNT | |
| Ultimate strength in compression range | RNG | Parent: Ultimate strength in compression |
| Elongation | PNT | |
| Elongation range | RNG | Parent: Elongation |
| Uniform elongation | PNT | |
| Uniform elongation range | RNG | Parent: Uniform elongation |

Table 19. Attributes in the Thermal Properties section of the Material Properties schema element.

| Attribute Name | Attribute Type | Notes |
|---|-----------------------|---|
| Melting point | PNT | |
| Melting temperature range | RNG | Parent: Melting temperature |
| Glass transition temperature | PNT | |
| Glass transition temperature range | RNG | Parent: Glass transition temperature |
| Thermal conductivity | PNT | |

| | | |
|--|-----|---|
| Thermal conductivity range | RNG | Parent: Thermal conductivity |
| Thermal conductivity vs. temperature | FDA | Parameters: [Temperature] |
| Specific heat capacity | PNT | |
| Specific heat capacity range | RNG | Parent: Specific heat capacity |
| Specific heat capacity vs. temperature | FDA | Parameters: [Temperature] |
| Thermal strain vs. temperature | FDA | Parameters: [Temperature] |
| Linear thermal expansion coefficient | PNT | |
| Linear thermal expansion coefficient range | RNG | Parent: Linear thermal expansion coefficient |
| Linear thermal expansion coefficient vs. temperature | FDA | Parameters: [Temperature] |
| Thermal expansion reference temperature | PNT | For thermal expansion coefficient, which is assumed to be calculated as the secant (a.k.a. 'mean') curve. |

4.9 References and Data Basis [new]

4.9.1 Definition

This schema element contains attributes that point the user to the source of data stored in other attributes. This is particularly important for material property and CMM parameter attributes, where the source of data may not be in-house and thus may not be obvious through links to other parts of the database.

4.9.2 Use-cases and discussion

Use-cases, in the form of 'user stories', that drive requirements for the References and Data Basis schema element include:

- "As a data consumer, I want to trace the original source of a data attribute to ensure the data is appropriate for my application."
 - **Requirement:** Attributes that allow the data uploader to clearly specify the source of data in other attributes (e.g. property or CMM parameter attributes).
- "As an engineering analyst, I want to know if the sources of property or CMM parameter attributes sufficiently represent my material so I can make a judgement about the predictiveness of my simulation."

- **Requirement:** Attribute for ‘quality’ of the reference data. Specifically, how much fidelity the references include (e.g. temperature and rate dependence) and how specific the data is to a particular material specification.
- “As an engineering analyst responsible for a model of an assembly or system, I want to know which CMM or property records have ‘weak’ reference sources so I can plan to improve them if necessary.”
 - **Requirement:** Attribute for ‘quality’ of the reference data. Specifically, how much fidelity the references include (e.g. temperature and rate dependence) and how specific the data is to a particular material specification.
- “As a data consumer, I want to know which reference sources are common and/or to find records that reference particular sources.”
 - **Requirement:** Attribute for a list of references (like a bibliography).
 - **Requirement:** Links to reference databases in Granta.

Ideally, the data basis should be documented as completely and as clearly as possible, sufficiently to reproduce the same data from the referenced sources. In practice, this will depend on the rigor of the user uploading the information. These are the limitations of relegating such important information to a long text attribute, but better solutions do not appear to be available in Granta.

The Reference quality attribute is somewhat subjective, but the following definitions for the levels of reference quality are provided in the discrete list and in the help file:

0 = No reference - parameters are an educated guess.

1 = References need much improvement - some parameters have traceable and applicable references, but others have no such reference.

2 = References need some improvement - most parameters have traceable and applicable references, but some do not. Or, temperature dependence is not accounted for in a parameter for which temperature dependence is known to be strong.

3 = References are good - all parameters have traceable and applicable references but could be improved. For example, temperature dependence could be included for a parameter for which temperature dependence is moderate.

4 = References are exemplary - all parameters come from traceable and applicable references, and corresponding data is available and appropriate for WR material. Temperature dependence is included for all parameters that may require it.

These options and definitions are deemed sufficient to satisfy the use-cases

4.9.3 Attributes

Table 20. Attributes in the References and Data Basis schema element.

| Attribute Name | Attribute Type | Notes |
|----------------------|----------------|--|
| Attribute data basis | LTXT | |
| References | LTXT | |
| Reference quality | DCT | Value set: [0, 1, 2, 3, 4] (see discussion for definitions) |

| | | |
|---------------------------------|------|--|
| References and data basis notes | LTXT | |
|---------------------------------|------|--|

4.10 General Material Information [new]

Note: This schema element was developed in the context of creating a minimum viable schema for powder-laser bed additive manufacturing in the Additive Manufacturing Database; therefore, it mostly contains attributes that support AM use-cases and is expected to be expanded to support additional use-cases in the future.

4.10.1 Definition

This schema element contains general materials information that can be used for identification purposes and in searching/reporting.

4.10.2 Use-cases and discussion

Use-cases, in the form of ‘user stories’, that drive requirements for the General Material Information schema element include:

- “As a data consumer, I would like to be able to see all builds/parts that were made with a certain AM feedstock material.”
 - **Requirement:** ID attribute that is unique per AM feedstock material, Links to AM feedstock material records
- “As a data consumer, I would like to find an AM feedstock material regardless of which name I might know it by.”
 - **Requirement:** Attributes for all types of names including specification name, alternative names, trade names, etc.
- “As a data consumer, I want to search and/or sort materials by supplier”.
 - **Requirement:** Attribute for supplier information
- “As an AM PI, I want to be able to link parts, builds, batches, etc. to the AM feedstock material that was used so I can relate built part properties to feedstock material characteristics”.
 - **Requirement:** Link attributes to AM feedstock material records
- “As a data consumer, I want to be able to filter records by material type so that I can separate metals from polymers, etc.”
 - **Requirement:** Attribute for material type
- “As a data consumer, I want to be able to distinguish different materials made to the same specification, for example when the material varies with location in a part”.
 - **Requirement:** Attribute for other material qualifier.

4.10.3 Attributes

Table 11. Attributes in the General Material Information schema element.

| Attribute Name | Attribute Type | Notes |
|--------------------|----------------|--------------------------------------|
| Material ID | STXT | Unique in the <i>Materials</i> table |

| | | |
|---------------------------------------|--|---|
| AM feedstock material ID | STXT | Unique in the <i>AM Feedstock Materials</i> table |
| Material name | STXT | |
| Material name on specification | STXT | |
| Alternate material names | LTXT | |
| Other material qualifier | STXT | |
| Trade names | STXT | |
| Designation | STXT | |
| Material type | DCT | Value set: [Polymer Polymer Composite High Explosive Mock High Explosive Aluminum alloys Copper alloys Heat Resistant Alloys High alloy steels Nickel alloys Stainless steels Titanium alloys] |
| Suppliers | TABL, linked (to <i>Suppliers</i> table) & local | Columns: [Supplier ID (linking value, from linked <i>Suppliers</i> table), Supplier name (from linked <i>Suppliers</i> table), Supplier item name (local), Supplier item number (local), Percentage of supply (local)] |
| Materials | Static link to <i>Materials</i> table | |
| Materials | Smart link to <i>Materials</i> table | |
| AM Feedstock Materials | Static link to <i>AM Feedstock Materials</i> table | |
| AM Feedstock Materials | Smart link to <i>AM Feedstock Materials</i> table | |

| | | |
|---|---|--|
| Linked AM feedstock material information | TABL, linked (to <i>AM Feedstock Materials</i> table) | Linking value = AM feedstock material ID Columns: TBD |
| Linked material information | TABL, linked (to <i>Materials</i> table) | Linking value = Material ID Columns: TBD |
| Link to datasheet | HYP | |
| Link to safety datasheet (SDS) | HYP | |
| General material information notes | LTXT | |

4.11 Material Specification Information [new]

4.11.1 Definition

This schema element contains general information about the material specification (7DS, MIL spec, etc).

4.11.2 Use-cases and discussion

Use-cases, in the form of ‘user stories’, that drive requirements for the Material Specification Information schema element include:

- “As a data consumer, I would like to be able to review specification documentation for a specific material.”
 - **Requirement:** ID attribute that is unique for the specification, link to a *Specifications* table
- “As a data consumer, I would like to assign materials, use properties, and use calibrated material model parameters for materials as identified by their specification because that is how the product definition relates materials to parts”.
 - **Requirement:** ID attribute that is unique for the specification, link to a *Specifications* table

4.11.3 Attributes

| Attribute Name | Attribute Type | Notes |
|--------------------------------------|---|---|
| Material specification number | STXT | Unique in the <i>Specifications</i> table |
| Control suffix | STXT | |
| Material specification | Smart link to the <i>Specifications</i> table | |

| | | |
|-------------------------------|--|--|
| Material specification | Static link to the <i>Specifications</i> table | |
|-------------------------------|--|--|

4.12 General AM Feedstock Batch Information [new]

Note: This schema element was developed in the context of creating a minimum viable schema for powder-laser bed additive manufacturing in the Additive Manufacturing Database. It will most likely be expanded to support additional use-cases in the future.

4.12.1 Definition

This schema element contains information about an additive manufacturing feedstock material batch that is not specific to the material type, AM technology, or machine manufacturer. This includes information such as Batch ID, Date Prepared, Lot number, etc.

4.12.2 Use-cases and discussion

Use-cases, in the form of ‘user stories’, that drive requirements for the General AM Feedstock Batch Information schema element include:

- “As a data consumer, I would like to be able to link batch-to-batch variability to built part properties.”
 - **Requirement:** ID attribute that is unique for each material batch, link to AM Feedstock Material Batches
- “As an AM project lead, I would like to know when a batch was prepared and by whom for traceability.”
 - **Requirement:** Name of batch preparer, Date batch prepared
- “As an AM project lead, I would like to be able to track AM feedstock batch “history” or “lineage” as material is recycled, blended with other materials, etc.”
 - **Requirement:** Batch-to-batch links in order to link “child” batches to “parent” batches, local columns in order to describe quantities of blends.

4.12.3 Attributes

| Attribute Name | Attribute Type | Notes |
|--|----------------|--|
| AM feedstock batch ID | STXT | Unique in the <i>AM Feedstock Material Batches</i> table |
| AM feedstock batch type | DCT | Value set: [Powder] |
| Date AM feedstock batch prepared | DAT | |
| Name of AM feedstock batch preparer | STXT | |
| AM feedstock batch lot number | STXT | |

| | | |
|---|--|---|
| AM feedstock batch size | PNT | Unit = g |
| AM feedstock batch parents | TABL, linked (to <i>AM Feedstock Material Batches</i> table) & local | Columns: AM feedstock batch ID of parent (linked, linking value = <i>AM feedstock batch ID</i>), Percent by weight (local), Percent by volume (local), Notes (local)] |
| AM Feedstock Material Batches | Static link to <i>AM Feedstock Material Batches</i> | |
| AM Feedstock Material Batches | Smart link to <i>AM Feedstock Material Batches</i> | |
| General AM feedstock batch information notes | LTXT | |

4.13 Material Processing Information [new]

4.13.1 Definition

This schema element contains information about how a material was processed for reproducibility and input/output use cases. Examples of material processing including mixing, sieving, heat treatment, etc.

4.13.2 Use-cases and discussion

Use-cases, in the form of ‘user stories’, that drive requirements for the Material Processing Information schema element:

- “As an AM SME, I would like to track how AM SLS powder is processed for reproducibility purposes.”
 - **Requirement:** Need attributes to describe powder processing and they need to be able to accommodate multi-step processes.

4.13.3 Attributes

| Attribute Name | Attribute Type | Notes |
|----------------------------------|----------------|---|
| Heat treatment parameters | TABL, local | Columns: [Step number (INT), Equipment (STXT), Temperature (RNG), Temperature ramp rate (PNT), Duration (PNT), Notes (LTXT) |

| | | |
|---------------------------|-------------|---|
| | |] |
| Mixing parameters | TABL, local | Columns: Step number (INT), Equipment (STXT), Mixing method (DCT)] |
| Sieving parameters | TABL, local | Columns: Step number (INT), Equipment (STXT), Temperature (RNG, K), Temperature ramp rate (PNT, °C/min), Duration (PNT, min), Notes (LTX)] |

5 New tables and changes to existing tables

This section contains a summary of additions and changes to database tables, along with notable discussion points and decisions. However, it is not intended to be complete documentation of the schema. The Schema Elements table in the Schema Elements database on the unclassified enterprise Granta instance contains all the details of the schema. We judge duplication of the full schema into this report to be inefficient and to add little value.

5.1 Materials [modified]

The Materials table was in use by the At-Risk Materials project before the process to standardize schema using schema elements began. Thus, the schema will be merged with the standard enterprise schema whenever opportunities arise to do this. In FY24, the following changes were made:

- The Record Information schema element was added.
- Property attributes were modified to be consistent with the Material Properties schema element. This includes:
 - Range attributes were changed to be point attributes with a range meta-attribute.
 - Property attributes were added to include all those in the Material Properties schema element.
- References and Data Basis attributes were replaced by those from the corresponding schema element.
- A 'Lead time' attribute was added to support the At-Risk Materials project. This attribute was added to the unreleased 'Unavailability Likelihood Information' schema element.

The parts of the layout for the Materials table that overlap with reviewed and released schema elements is shown in Table 21. Work will need to be done in the near future to:

- Create, review, and release schema elements for all other attributes in the Materials table.
- If necessary, map data from legacy attributes to newly created ones.

Table 21. Layout for Materials table, including only the attributes that overlap with reviewed and released schema elements (other attributes exist and are in use by At-Risk Materials).

| Schema element | Section | Attribute or link group |
|---|------------------------------|--|
| Record Information | Record Information | <i>{All attributes from this section are used}</i> |
| General Material Information | General Material Information | Material ID |
| | | Material name |
| | | Material name on specification |
| | | Alternate material names |
| | | Other material qualifier |
| | | Trade names |
| | | Material type |
| | | Suppliers |
| Material Properties | Physical Properties | Density |
| | Mechanical Properties | <i>{All attributes from this section are used}</i> |
| | Thermal Properties | <i>{All attributes from this section are used}</i> |
| References and Data Basis | References and Data Basis | <i>{All attributes from this section are used}</i> |
| Calibrated Material Models Information | Links to CMM Table | <i>{All attributes from this section are used}</i> |

5.2 AM Builds [new]

Table 22. Layout for AM Builds table.

| Schema element | Section | Attribute or link group |
|-------------------------------------|------------------------------------|--|
| Record Information | Record Information | <i>{All attributes from this section are used}</i> |
| Project Information | Project Information | Project ID |
| | | Projects (smart link using Project ID) |
| | | Linked project information |
| | | Project information notes |
| Build Information | Build General Information | <i>{All attributes from this section are used}</i> |
| | Build Characterization Information | <i>{All attributes from this section are used}</i> |
| | Build Status Information | <i>{All attributes from this section are used}</i> |
| AM Process Information | AM Process Information | AM Process ID |
| | | AM Processes (smart link using AM process ID) |
| | | Linked AM process information |
| Part Design Information | Part Design Information | AM Part Designs (static link) |
| | | Linked part design information |
| Built Part Information | Built Part Information | Built AM Parts (smart link using Build ID) |
| | | Linked built part information |
| General Material Information | General Material Information | AM Feedstock Materials (static link) |
| | | Linked AM feedstock information |

| | | |
|---|--|---|
| General AM Feedstock Batch Information | General AM Feedstock Batch Information | AM Feedstock Material Batches (static link) |
|---|--|---|

5.3 AM Processes [new]

Table 23. Layout for AM Processes table.

| Schema element | Section | Attribute or link group |
|-------------------------------|------------------------|--|
| Record Information | Record Information | <i>{All attributes from this section are used}</i> |
| Project Information | Project Information | Projects (static link) |
| | | Linked project information |
| | | Project information notes |
| AM Process Information | AM Process Information | <i>{All attributes from this section are used}</i> |
| Build Information | Links to Build | AM Builds (smart link using AM process ID) |
| | | Linked build information |

5.4 AM Part Designs [new]

Table 24. Layout for AM Part Designs table.

| Schema element | Section | Attribute or link group |
|--------------------------------|-------------------------|--|
| Record Information | Record Information | <i>{All attributes from this section are used}</i> |
| Project Information | Project Information | Projects (static link) |
| | | Linked project information |
| | | Project information notes |
| Part Design Information | Part Design Information | <i>{All attributes from this section are used}</i> |
| Build Information | Links to Build | AM Builds (static link) |

5.5 Built AM Parts [new]

Table 25. Layout for Built AM Parts table.

| Schema element | Section | Attribute or link group |
|-------------------------------|------------------------|--|
| Record Information | Record Information | <i>{All attributes from this section are used}</i> |
| Project Information | Project Information | Project ID |
| | | Projects (smart link using Project ID) |
| | | Linked project information |
| | | Project information notes |
| Built part Information | Built part Information | <i>{All attributes from this section are used}</i> |
| Build Information | Links to Build | Build ID |
| | | AM Builds (smart link using Build ID) |
| | | Linked build information |
| AM Process Information | AM Process Information | AM process ID |

| | | |
|--------------------------------|-------------------------|---|
| | | AM Processes (smart link using AM process ID) |
| | | Linked AM process information |
| Part design information | Part design information | Part design ID |
| | | Linked part design information |
| | | AM Part Designs (smart link using Part design ID) |

5.6 Test Data: TMA [new]

This table element contains attributes used to hold the data and results from a TMA test. TMA studies measures changes in the dimensions of a sample as a function of time, temperature and force in a controlled atmosphere. The TMA test is frequently used to characterize materials to inform design decisions, to study how they age, and to provide data used for material model calibration. The schema elements, sections, attributes, and link groups used to build this table are shown in Table 26.

Table 26. Layout for Test Data:TMA table.

| Schema element | Section | Attribute or link group |
|--------------------------------------|-------------------------------|--|
| Record Information | Record Information | <i>{All attributes from this section are used}</i> |
| Project Information | Project Information | Project ID |
| | | Linked project information |
| | | Project information notes |
| Testing Series Information | Testing series Information | Testing series ID |
| | | Linked Testing series information |
| | | Testing series information notes |
| Data Files | Data Files | <i>{All attributes from this section are used}</i> |
| Document Information | Document Information | Documents |
| Test Information | Test Information | <i>{All attributes⁷ from this section are used}</i> |
| Test Conditions | Test Conditions | <i>{All attributes from this section are used}</i> |
| Material Pedigree Information | Material Pedigree Information | <i>{All attributes⁷ from this section are used}</i> |
| Specimen Information | Specimen Information | <i>{All attributes from this section are used}</i> |
| Equipment Information | Equipment Information | Instrument ID |
| | | Linked instrument information |
| Instrument Parameters | Instrument Parameters | Test method file |
| | | Test method description |
| | | Gas |
| | | Gas flow rate |
| | | Probe type |

⁷ Not including record link groups.

| | | |
|--------------------------------|-------------------------|---|
| | | Preload force |
| | | Film fiber offset |
| | | Instrument configuration |
| | | Pre-test instrument verification file |
| | | Pre-test instrument verification notes |
| | | Instrument parameter notes |
| Calibration Information | Calibration Information | <i>{All attributes from this section are used}</i> |
| Test Data & Results | Test Data & Results | Dimension change vs. time |
| | | Dimension change vs. temperature |
| | | Dimension change vs. force |
| | | Specimen length vs. time |
| | | Specimen length vs temperature |
| | | Coefficient of Thermal Expansion Averaged Over Temperature Range |
| | | Analysis method |
| | | Name of analyzer |
| | | Document number of analysis document |
| | | Test data & results notes |

5.7 AM Feedstock Materials [new]

The AM Feedstock Materials table was developed to support a minimum viable product for the NSE Additive Manufacturing Database for powder laser bed printing (SLS/SLM). The AM Feedstock Materials table will hold records for the general material that goes into the AM machine. Different formulations of feedstock materials will have their own records. Specific instances (batches) of a feedstock material will be held in the AM Feedstock Material Batches table (section 5.8) and will be linked to the general material record.

Table 27. Layout for AM Feedstock Materials table.

| Schema element | Section | Attribute or link group |
|-------------------------------------|------------------------------|--|
| Record Information | Record Information | <i>{All attributes from this section are used}</i> |
| General Material Information | General Material Information | AM feedstock material ID |
| | | Material name |
| | | Material name on specification |
| | | Alternate material names |
| | | Other material qualifier |
| | | Trade names |
| | | Material type |
| | | Suppliers |
| | | Link to datasheet |
| | | General material information notes |

| | | |
|---|------------------------------------|--|
| Specification Information | Material Specification Information | Material specification number |
| | | Control suffix |
| | | Specifications (Static link) |
| Material Properties | Material Properties | Density |
| | | Tapped density |
| | | Degree of crystallinity |
| | | Young's modulus |
| | | Melting point |
| | | Glass transition temperature |
| | | Thermal conductivity |
| | | Thermal conductivity vs. temperature |
| | | Specific heat capacity |
| | | Specific heat capacity vs. temperature |
| References and Data Basis | References and Data Basis | <i>{All attributes from this section are used}</i> |
| Project Information | Project Information | Projects (static link to Projects table) |
| | | Linked project information |
| Build Information | Build Information | AM Builds (smart link to AM Builds table using AM feedstock material ID) |
| General AM Feedstock Batch Information | AM Feedstock Material Batches | AM Feedstock Material Batches (smart link to AM Feedstock Material Batches table using AM feedstock material ID) |
| Test Information | Links to Test Data | Test Data: DSC (static link to Test Data: DSC table) |
| | | Test Data: TGA (static link to Test Data: TGA table) |
| | | Test Data: TMA (static link to Test Data: TMA table) |

5.8 AM Feedstock Material Batches [new]

The AM Feedstock Material Batches table was developed to support a minimum viable product for the NSE Additive Manufacturing Database for powder laser bed printing (SLS/SLM). The AM Feedstock Material Batches table will hold records for the specific instances (or batches) of a material that goes into the AM machine.

Table 28. Layout for AM Feedstock Material Batches table.

| Schema element | Section | Attribute or link group |
|---|--|--|
| Record Information | Record Information | <i>{All attributes from this section are used}</i> |
| General AM Feedstock Batch Information | General AM Feedstock Batch Information | AM feedstock batch ID |
| | | AM feedstock batch type |
| | | Date AM feedstock batch prepared |
| | | Name of AM feedstock batch preparer |
| | | AM feedstock batch lot number |
| | | AM feedstock batch size |

| | | |
|--|---------------------------------|---|
| | | AM feedstock batch parents |
| | | General AM feedstock batch information notes |
| General Materials Information | General Materials Information | AM feedstock material ID |
| | | AM Feedstock Materials (smart link to AM Feedstock Material table using AM feedstock material ID) |
| | | Linked AM feedstock material information |
| Material Processing Information | Material Processing Information | <i>{All attributes from this section are used}</i> |
| Material Properties | Material Properties | Tapped density |
| | | Melting point |
| | | Glass transition temperature |
| | | Degree of crystallinity |
| References and Data Basis | References and Data Basis | <i>{All attributes from this section are used}</i> |
| Project Information | Project Information | Projects (static link to Projects table) |
| Build Information | Build Information | AM Builds (smart link to AM Builds table using AM feedstock material ID) |
| Test Information | Links to Test Data | Test Data: DSC (static link to Test Data: DSC table) |
| | | Test Data: TGA (static link to Test Data: TGA table) |
| | | Test Data: TMA (static link to Test Data: TMA table) |

5.9 Calibrated Material Models [new]

Table 29. Layout for Calibrated Material Models table.

| Schema element | Section | Attribute or link group |
|--|-------------------------------|---|
| Record Information | Record Information | <i>{All attributes from this section are used}</i> |
| Project Information | Project Information | Projects (static link) |
| | | Linked project information |
| | | Project information notes |
| Materials Information | General Materials Information | Material ID |
| | | Materials (smart link to Materials table using Material ID) |
| Material Properties | Linked Material Properties | Linked material properties |
| | Physical Properties | <i>{All attributes from this section are used but renamed as 'override' properties}</i> |
| | Mechanical Properties | <i>{All attributes from this section are used but renamed as 'override' properties}</i> |
| | Thermal Properties | <i>{All attributes from this section are used but renamed as 'override' properties}</i> |
| Calibrated Material Model Information | CMM General Information | <i>{All attributes from this section are used}</i> |
| | CMM Performance | <i>{All attributes from this section are used}</i> |

| | | |
|---------------------------|------------------|--|
| | CMM Parameters | <i>{All attributes from this section are used}</i> |
| Test Information | Test Information | Test Data: TGA (static link) |
| | | Test Data: DSC (static link) |
| | | Test Data: TMA (static link) |
| References and Data Basis | | <i>{All attributes from this section are used}</i> |

6 Conventions, standards, and best practices

The following list of conventions, standards, and best practices for the NSE implementation of Granta: MI has been updated to include FY24 developments. These conventions and best practices are intended to be utilized across all schema elements, and they will be communicated to users through the *help files* available to users as a URL link on the attribute name.

1. Attribute Naming:

- Attributes will not have identical names if they are not intended to be used in a functionally identical way.
- In a name with more than one word, the first word is capitalized, and the rest is lowercase.
- Attributes containing people's names should be named "Name of xyz".
- Functional attributes should be named 'y-axis quantity vs. x-axis quantity'.
- Linked tabular attributes should be named 'Linked xyz information' where 'xyz' is the type of data linked from the linked table (which could, but is not required to be, the linked table or schema element name).
- Attributes containing dates should be named "Date of xyz"
- See also: 19

2. Notes Attributes: Each schema element will contain a long text attribute called "*Schema element name*" notes (ex: Record information notes) that is intended to serve as a catch-all notes attribute for that section of the table.

3. Linking conventions: Links between records will, in general, consist of one or more of the following:

- A short text attribute corresponding to the unique 'ID' in the table that is being linked to. For example, project records contain a unique, short text attribute called Project ID and testing series records contain a unique, short text attribute called Testing series ID. This is useful for automating static or smart link generation.
 - 'ID' attributes used for linking should be enforced to be unique in their native tables (i.e., Project ID should be unique in the Projects table), except in special cases.
- A static record link
 - If applicable, It is recommended the name of the link be the name of the table being linked to.
- A smart record link

- If applicable, It is recommended the name of the link be the name of the table being linked to⁸.
- A tabular attribute with the previously mentioned short text ID attribute as the linking value and relevant linked columns defined.

While the schema element may contain all the above objects, implementation into a database table may involve down-selecting objects. For example, either a static *or* a smart record link, but not both, should be implemented based on whether the links will be one-to-one or one-to-many.

- For example:
 - A smart link can be used to link a test record to a Pedigree record by matching the Pedigree ID in both records since a test record can correspond to only a single Pedigree (although a Pedigree may correspond to many tests).
 - A static link would be used to link test records to a Documents record since a test may reference multiple documents and each document may be referenced by multiple tests, precluding the ability to create links by matching Document ID or Test ID in both records.

Linking attributes (or link groups) should be part of the schema element describing the information being linked *to*. For example, links *to* the Documents table, and the Document ID attribute, should be part of the Document Information schema element. This ensures they are captured in exactly one schema element.

- 4. Naming of people:** To aid in searching, people's names in short text attributes must be written consistently. The following convention is proposed.
 - First name and last name as they appear in the [OneID phonebook](#).
 - For NSE personnel, the DUID from the OneID phonebook in parentheses following the name.
 - E.g., Jillian O'Neel (123456789)
- 5. Reviewer Convention:** Rather than using separate attributes for each different kind of record review, which isn't flexible enough, a long text attribute will be used with the format described below. Each reviewer will append with their own entry on a new line. Current review types include "Technical Review" for data accuracy, "Granta Review" for conformation to database conventions, and "Classification Review" for review by a Derivative Classifier. The format will be:
 - First name and last name (unique ID) - date - review type
 - E.g., Jillian O'Neel (123456789) - 08/08/2024 - Granta Review
- 6. Files in Data Files schema element:**
 - Files in this schema element will be stored in individual attributes rather than in a flexible, tabular 'Files' attribute. This facilitates ease of uploading.
 - Unless otherwise specified, files are understood to be retained for traceability purposes only. Data consumers should only take data from attributes.
 - Human readable (e.g., ASCII) files are preferred. If binary files must be used, they must be excluded from the Granta search engine by unchecking the 'allow file contents to be searched' option.
 - A data file is required if one exists and is not too big to upload.
 - If files are too big to be uploaded, they may be stored externally (for example, in an institutional large file store) and a hyperlink to the file's location may be uploaded to the file

⁸ It has been noted that multiple smart links, each using different linking values, may be needed to link to a table, depending on which table is being linked from. A new naming convention may be needed to account for multiple smart links with different linking values. For example, "AM Builds with the same Build ID" or "AM Builds with the same AM Feedstock Material ID".

link attributes (ex: *Raw data file link*). It is understood that these links could break if directories on the external system change; therefore, it is recommended that data uploaders establish a directory structure on the external system that is as robust and standardized as possible.

- If more than one “other data files” exist, they should be zipped together and the .zip folder should be uploaded to the *Other data file* attribute.

7. Guidelines for discrete attributes:

- A discrete list can be ‘ordered’ (by checking the appropriate box in MI: Admin), meaning that Granta: MI assigns value to each choice. For example, the list consisting of the values ‘red’, ‘yellow’, and ‘green’ can be ordered so a user can search for values ‘above’ yellow. Care should be taken to order the choices in a way that would make the most sense to a data consumer. For example, is a user searching for all values ‘above’ yellow looking for records with yellow & green or yellow & red?
- If a discrete list is not ordered (ex: a list of all NSE sites), the values in the discrete type should be sorted in alphabetical order (“Arrange by Name” in MI: Admin) and the “Ordered” box should not be checked.

8. Guidelines for managing value domains:

- Discrete types are recommended when the list of choices is not too long and when the list doesn't change too much (since it must be managed by a database administrator).
- A linked table (or linked database) is recommended when values can/should practically be added by users and/or when metadata about the value are useful to capture. Note that this option:
 - Requires effort from the database administrator to set up but not to maintain.
 - May require effort from the user to ensure data is entered into the correct table.
- Text attributes are recommended when discrete types and linked tables are not practical. If possible, a value domain should be created by each site and documented to aid review process. Examples of attributes where this method is used include ‘Organization’ and ‘Location’, as well as attributes for people’s names.
 - Note that Text attributes with no documented or enforced value domain should be considered of primary use for ‘reproducibility’ use-cases, not for searching/reporting use-cases since data may be entered differently by different users. This applies to long text attributes like ‘Test method description’ that describe how a test is performed (for reproducibility) but doesn’t support searching or sorting based on the data.
 - More specifically, data stored in text attributes with no documented or enforced value domain should be assumed *not* to be consumed as an independent variable. E.g., it will not be possible to study the DSC behavior of specimens in a testing series as a function of the data in the (short text) Pan type attribute.

9. Unit Systems

- Attributes that have units should be assigned the applicable unit in the mm-N-s consistent unit system as the default unit.
- As units are assigned to attributes, admins should verify that the selected unit is consistently and correctly set-up in MI: Admin. This includes using “Derived from other units” whenever possible and correctly inputted “Unit System Equivalents”.
- When reviewing schema elements, units and equivalent units will also be reviewed for consistency.

- 10. Help Files:** A help file is required for each attribute and must be in the standardized format, which consists of the four sections below. If any of these sections do not apply, they will contain 'N/A'.
- Definition: the definition of the attribute
 - Standards: conventions that must be adhered to
 - Best Practices: recommended conventions
 - Image: an image to clarify any of the above
- 11. Required attributes:** The Granta: MI software can force an attribute to be required, based on the layout. Since the decision to require attribute data may depend on the project uploading the data, it is proposed that a layout only require data if omission of that attribute data would significantly diminish the value of the record data. Required attributes are noted as such in the Standards section of the help file.
- 12. Conventions for 'ID' values:** Attributes such as Specimen ID and Project ID are used to identify linked records. There is no required format for the short text in these attributes since sites may have existing conventions. However, help files should recommend a format to help when an existing convention does not exist.
- 13. External Data Management Standards & Practices:** Integration with other established data management standards and practices is preferred; however, the team has noted instances where deviation is necessary due to the database use cases and/or Granta: MI software limitations. These standards include ASTM F3490-21 for Additive Manufacturing Data as well as internal practices such as documentation for the treatment of Official Use Only / Controlled Unclassified Information. Specific deviations are noted in the PowerPoint slides for the schema element which are available on the project SharePoint. Any deviations that require action from a data uploader or are helpful for interpretation for a data consumer are communicated via the specific attribute's html help file.
- 14. Owner vs. Point-of-Contact⁹:** It is often desired to have a name listed alongside data and metadata in Granta so that data consumers know who to contact for more information. Upon discussion, the term "owner" is often suggested for the attribute name that contains this information (e.g., Instrument owner, Data owner, Project owner, etc.). However, it was determined that "owner" implies a level of control over the data that does not reflect the paradigm of the database. Therefore, we often chose to use the term "point-of-contact" which better reflects the actual purpose of the metadata.
- 15. Test Results vs. Material Properties:** It is often a point of confusion that test results for an individual test contain attributes that seem to be material properties. For example, a single tensile test record may contain a 'Yield Strength' that is calculated from the data. Meanwhile, a material property record may also contain a 'Yield Strength' value. We propose that 'properties' and 'test results' are differentiated by the fact that while test results apply to a specific *sample* of a material, the properties are intended to represent an entire population of material samples. When it is necessary to differentiate between the two, attributes for test results may be named with the prefix 'Specimen'. For example, 'Specimen yield strength' may be the yield stress

⁹ This convention may need to be updated to be consistent with the At-Risk Materials 'Cases' table, in which 'Record owner' is specified as the site (not person) ultimately responsible for the accuracy of the data in the record, especially in cases where records are being edited by multiple sites.

measured in a particular test, while 'Yield strength in tension' may be the expected value of the yield strength of any material sample from materials meeting a defined specification.

- 16. Tabular File Attributes:** There are some places in the database (such as the AM Builds table) where we would like to use a tabular attribute to store files. This is usually used when the number of files that a data producer wants to upload varies from record-to-record. A tabular attribute provides the flexibility of being able to upload any number of files to one record in one attribute. For these kinds of attributes, we propose the following structure.
- 1st Column = "File", FIL datatype (required)
 - 2nd Column = "File type", DCT datatype, contains a list of acceptable categories of file for the intended use (optional, can be used when a variety of kinds of files may be uploaded)
 - 3rd column = "Notes", LTXT datatype (required)
- 17. One X per Record:** In many tables of the database, we have decided that one of something (X) will correspond to one record in the database. See below for a list of these decisions.
- 1 test specimen per test record
 - 1 calibrated material model per calibrated material model record
 - 1 feedstock material per AM feedstock material record
 - 1 feedstock material batch per AM feedstock material batch record
 - 1 part per AM built part record
 - 1 AM machine per machine record
- 18. Table Name Convention:** Table names should almost always be plural. For example, *Documents, Machines, AM Feedstock Materials*, etc. The exception to this is test data tables which should follow the convention of "Test Data: Test Type". For example, "Test Data: TMA".
- 19. Brevity vs. Clarity of Object Names:** When choosing attribute names, there should be a balance between clarity and brevity. For example, the attribute name 'Build ID' was used rather than 'AM Build ID' because it was shorter, and it was judged that 'Build' was unlikely to be used outside of the 'AM' context.

7 Glossary

This section contains a list of definitions necessary for correct and consistent interpretation of enterprise Granta schema. In addition, Table 30 is a list of abbreviations used to describe Granta attribute types.

- **Build:** The application of a process to a set of AM feedstock materials using a machine to create a particular instance of a part or parts.
- **Calibrated Material Model:** a.k.a. 'CMM' A set of equations used to simulate a class of materials combined with the parameters determined (through a calibration process) to represent a specific material.
- **Equipment:** A piece of hardware or system of hardware. Machines and instruments are both types of equipment.
- **Instrument:** Hardware or a system of hardware used to generate data that characterizes the response of a material to a controlled environment.
- **Machine:** a.k.a. 'Printer'. The system of hardware used to create AM parts from AM feedstock material using a defined process.
- **Material:** In the context of the NSE databases a material is one specified by one or more specifications, including material specification, product specifications, or other specification.

- **Material Pedigree:** a.k.a. 'Pedigree'. This term is used to specify a particular instance of a material, often with a known history that may affect its response in characterization testing. For example, materials subjected to 'aging and compatibility' testing are usually subjected to well characterized environments, and those instances of a material are considered to have a particular pedigree.
- **Project:** A collection of tasks to achieve a well-defined objective, often funded by a single program.
- **Testing Series:** A set of related material characterization tests, usually with the objective of learning how a material (or set of related materials) responds when one or more independent variables (e.g. temperature, strain rate, hydrogen content) is varied.
- **Uniaxial Test:** A mechanical test performed with the intent of maintaining a uniaxial state of stress or strain throughout some portion of the loading using a traditional servo-mechanical or hydraulically actuated load frame. Other test types, such as split Hopkinson pressure bar testing, may also produce a uniaxial state of stress and strain but are referred to by other terms.

Table 30. List of abbreviations for Granta attribute types

| Abbreviation | Attribute Type |
|--------------|--|
| PNT | Floating point value |
| RNG | Two floating point values; one for minimum and one for maximum |
| INT | Integer |
| STXT | Short text (<256 characters) |
| LTXT | Long text |
| DCT | Discrete type, a.k.a. 'drop down menu' with pre-defined choices |
| DAT | Date |
| FIL | File |
| TABL | Table with rows and columns consisting of other attribute types. Data could be linked from other tables. |
| HYP | Hyperlink |
| FDA | Series float functional data, a.k.a. curve data with a primary 'x-axis' parameter and other parameters possible. |
| IMG | Image file |

8 Summary and path forward

In FY24 the following progress was made on the Schema Element project:

- The existing schema elements were modified to accommodate thermal-mechanical analysis (TMA) data, and a table, Test Data: TMA, was created for managing TMA data.
- The elements necessary for the following additive manufacturing (AM) data tables (directed at data specific to selective laser sintering AM technology) were created:
 - Builds
 - AM Processes
 - AM Part Designs
 - Built AM Parts
 - Machines
 - AM Feedstock Materials
 - AM Feedstock Material Batches
- The elements necessary for creating a Calibrated Material Models table were created, and the Calibrated Material Models table was created.

In FY25 the existing schema will be deployed on the production enterprise Granta instance on the enterprise secure network. Schema elements will be appended, and new elements created as necessary, to allow the creation of tables specifically to support materials testing, AM process development, and design and analysis for modernization programs.