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Schema Elements for Granta Annual Report: FY2022

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Contents

Tables

1 Background and Motivation

Granta: Materials Intelligence, also known as Granta:MI or Granta, is a commercial database software by Ansys, Inc. that is utilized by the Nuclear Security Enterprise (NSE) to organize and store relevant materials data. For a complete discussion of the use of Granta:MI at NSE sites, see the FY21 annual report[1]. Granta:MI is used by five NSE sites locally, and all NSE sites have access to an enterprise instance on the Enterprise Secure Network (ESN) as well as an unclassified development instance. It has been recognized by NNSA management that a shared repository for additive manufacturing (AM) data would not only ensure data and knowledge is not lost but would provide a pool of information relating AM inputs (build parameters, raw materials properties, post-processing information) to the as-built properties of AM parts. Such a pool of data would enable optimization of AM build design and help NNSA achieve the goals of shortening fielding times for new components.

An obstacle to sites sharing AM data in enterprise Granta:MI instances is the lack of a standard database schema, and it is the objective of this project to create and document this schema. A schema consists of a set of attributes (a.k.a. 'data fields') for each type of data (e.g. build process, post-process information, raw materials information, specimen test information, etc) as well as documentation of the definitions of each attribute so each site can use the schema consistently.

This document summarizes the objectives and approach for FY22 work in Section 2. Section 3 describes the schema elements released in FY22. Section 4 describes how the schema elements project relates to the newly released ASTM F3490-21. Section 5 presents a list of conventions and best practices, updated from the list presented in the FY21 report. Finally, Section 6 summarizes the FY22 work and describes the work to be performed in FY23.

2 FY22 Objective and Approach

The objective for FY22 was to complete the creation, documentation, and release on the ESN of a schema for thermogravimetric analysis (TGA) material characterization testing, which was begun in FY21. The decision to prioritize creating this *TGA Testing* schema was made by collecting, through cross-site teleconference meetings, a list of testing types used by each site and the site-specific priority for each of those data types. The entire list, and discussion relating to the decision to choose TGA Testing is documented on the Jowog 31 Granta SharePoint site[2] hosted by Sandia National Laboratories.

The TGA Testing schema elements, which together comprise the entire TGA Testing database table sufficient for managing TGA data, were drafted, reviewed, and released consistent with the process described in the FY21 annual report. Additionally, the following process for drafting, reviewing, and releasing schema elements was followed:

[1] LA-UR-21-29682
[2] https://collaborate.sandia.gov/sites/grantadatabase_J31/default.aspx

1. A schema element was drafted by a member of the LANL team. This draft is documented in a PowerPoint file that includes:
    a. Schema element definition
    b. Attributes and their types
    c. Use-cases for the schema element and its attributes
    d. Discussion points
    e. Relation to ASTM F3490-21
2. The PowerPoint document was presented at the cross-site Schema Elements meeting, allowing some time for discussion.
3. Each site was given two weeks to review the draft and provide comments.
4. The LANL team incorporated comments into a final draft, which was reviewed and approved by each site at a subsequent cross-site meeting.

Through this process, the 10 schema elements comprising the TGA Testing database table, described in the following section, were completed.

The process described above is inherently collaborative across many NSE sites. In particular, Sandia National Laboratories (SNL) and Kansas City Nuclear Security Campus (KCNSC) each received modest funding to enable their participation. In general, this participation consisted of:

- TGA subject matter expert input to compile a list of metadata needed to reproduce a TGA test and data used by the consumers of such test data
- Cross-referencing proposed schema elements against local Granta database schema to generate feedback and suggestions for improvement
- Discussion at twice-monthly cross-site Schema Elements telecons

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

LANL	SNL	LLNL	KCNSC	PX	Y-12
• **Jillian O'Neel** • Jack Brett • Philip Schembri • Rachel Waggoner • Lisa Hughey • Robin Pacheco	• **Samuel Moran** • Inkiad Ahmed • Richard Karnesky • Matthew Witman	• Ryan Whitmore • **Daniel Gardner**	• **Leslie Embrey** • Juanita Stephen	• **Frank Cordova** • Paul Aguirre • Timothy Sanchez	• **Lloyd Arrowood**
NNSA	**NNSS**	**PNNL**	**SRNL**	**AWE**	
• Matthew York • Samuel Perry	• **Michele Arcade** • Travis Bame	• **Kriste Henson**	• **Paul Korinko** • Christopher Rasmussen • Camden Chatham	• **Craig Lowe** • Fred Moran	

The contribution of personnel, listed in Table 1, from other sites to this project has proved valuable in constructing schema that is useful for data management across the NSE. The effort needed by all sites to

support this project will need to be increased as the project progresses so that (a) sites can upload data to test the schema, (b) sites can aid in the development of uploading tools, and (c) sites can develop schema in parallel with LANL, increasing the bandwidth and shortening the timeline of the project.

3 TGA Testing Schema Elements

This section lists, for each schema element necessary to construct a TGA Testing database table, the definition of the schema element, the attributes (including their types, as defined in Table 2, and value sets if applicable), and any notable decisions and discussion points that arose during their creation.

Table 2. Definition of attribute types referenced in this section.

Abbreviation	Attribute Type
PNT	Floating point value
RNG	Two floating point values; one for minimum and one for maximum
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.

3.1 Record Information

3.1.1 *Definition*

This schema element contains information about the record itself, including when it was created, modified, and reviewed, and who did those things. It does not contain any information about materials or data. As such, it is likely to be used in the same way (all attributes in the same order) in all tables (maybe even all databases). Some information in this schema element, such as *Record create date*, should be available in the Record Properties Granta object; however, we are duplicating in these attributes because not all users have access to record property information.

3.1.2 *Discussion Points & Important Decisions*

1. **Naming of people:** A discrete list of names will be too difficult for a database administrator to manage and too long for write users to navigate. However, a short text attribute allows for unintentional non-unique entries (ex: *Phil Schembri* and *Philip Schembri*). The ideal solution would be to integrate Granta with an existing personnel database like the OneID phonebook. The LANL team had some preliminary discussions with the OneID phonebook team and came to the conclusion that such integration will be technically difficult and not possible with the current level of resources, although it would be worth revisiting in the future. The current compromise is to use short text attributes for names and define a format for write users to follow in the help file for the attribute (See Section 5 *Conventions and Best Practices*). These name attributes will have to be manually validated when records are reviewed for release, but it may be possible to code a tool to provide automatic validation in the future.
2. **Data Sensitivity discrete list options:** The choices provided in the *Data Sensitivity* attribute discrete list were taken from existing Department of Energy (DOE) guidance including O 471.3, M 471.3, O 471.1B, and M 471.1-1. See Table 3 for the provided choices. Note that none of our current databases are rated for Unclassified Controlled Nuclear Information (UCNI) so that option has been omitted from the list. Additionally, options pertaining to classified information should be removed from the discrete list if the schema element is being deployed on an unclassified server. Finally, this attribute is not intended to function as document marking. It is only meant to inform data consumers as to the sensitivity of the data they are viewing. Databases are treated as working documents at the highest classification level present in the database and are marked as such.

3.1.3 *Attributes*

Table 3. Record Information Schema Element Attributes

Attribute Name	Attribute Type	Value Set
Data sensitivity	DCT w/ meta LTXT (for notes)	Unclassified – Not Approved for Unlimited Release, Unclassified – Approved for Unlimited Release, Official Use Only, Official Use Only – Export Controlled Information, Classified – CRD, Classified – CFRD, Classified – SRD, Classified - SFRD
Record create date	DAT	
Record last modified date	DAT	
Name of data originator	STXT	
Name of record creator	STXT	
Name of modifier	STXT	
Record owner	DCT	LANL, LLNL, SNL, KCNSC, PX, SRNL, SRS, Y-12, NNSO, PNNL, NNSA
Record review	LTXT	
Record information notes	LTXT	

3.2 Project Information

3.2.1 *Definition*

This schema element contains information about the project that the record is a part of. Most of the attributes are actually links since the information about projects is contained natively in the Projects table, and we want to avoid duplication.

3.2.2 *Discussion Points & Important Decisions*

1. **Existence of a Projects table:** A Projects table will exist and be used to group test records performed as part of the same project. This table will be made by the schema elements project team at a later date.
2. **Required attributes:** *Project ID* and *Linked project information* are required for testing tables. This is specified in the help file and will be enforced when layouts are created.

3.2.3 *Attributes*

Table 4. Project Information Schema Elements Attributes

Attribute Name	Attribute Type	Value Set
Project ID	STXT	Unique in *Projects* table
Project	Static link to *Projects* table	
Project	Smart link to *Projects* table	
Linked project information	Linked TABL	Linking Value = Project ID
Project information notes	LTXT	

3.3 Data Files

3.3.1 *Definition*

This schema element contains data files and information about them for the purpose of traceability.

3.3.2 *Discussion Points & Important Decisions*

1. **Data quality:** Data quality rating attributes were initially discussed in version 1 of this schema element; however, it became clear that there is still a lot of work to do in terms of standardizing how data quality is assessed across the NSE. We decided to omit these kinds of attributes for now with the plan to reassess once the data producer/consumer community decides how to move forward with cross-site data quality assessments.

3.3.3 *Attributes*

Table 5. Data Files Schema Element Attributes

Attribute Name	Attribute Type	Value Set
Raw data file	FIL	
Final data file	FIL	
Other data file	FIL	
Raw data file link	HYP	
Final data file link	HYP	
Other data file link	HYP	
Data files notes	LTXT	

3.4 Instrument Parameters

3.4.1 *Definition*

This schema element contains attributes that describe the setup of the instrument and test program sufficiently for an operator to reproduce the test. This also includes hardware and accessory information, as well as instrument/software settings such as gas flow rate, signal gain, etc. Finally, it includes test program information such that a test operator can replicate the test on their own instrument (ex: Step 1 – Ramp from 30°C to 150°C at 5°C/min, Step 2 – Isothermal hold for 5 mins, etc.).

3.4.2 *Discussion Points & Important Decisions*

1. **Existence of an Instruments table:** An instruments table will contain records for individual instruments that include information such as the manufacturer, model, serial number, etc. Each instrument will have a unique *Instrument ID*. A test record will be linked to a single instrument record; therefore, an instrument may consist of a custom collection of hardware, but the set-up will be treated as a single object. This Instrument table will be developed by the schema elements team in the future.
2. **Instrument configuration:** A long text *Instrument configuration* attribute will be used to record test specific instrument information. For example, the exact accessories, filters, gauges, or other hardware used during the test.
3. **Test method description:** This long text attribute will replace previously created tabular attributes such as *Heating Schedule* that are used in some local site databases. This is because long text attributes are easier to upload into and are flexible enough to allow data uploaders to describe any sort of test program. The help file for this attribute guides uploaders to include whatever would be reasonably needed for another test operator to replicate the test on their own instrument.
4. **Specific TGA test setup attributes:** Attributes specific to TGA testing setup and software settings were collected from the cross-site TGA subject matter experts (SMEs) that participated in the schema elements meetings.
5. **Pre-test instrument verification:** It is expected that the Instruments table will contain information about instrument calibration. However, there is a testing workflow that involves verifying the instrument's calibration before each test. To hold this information, the *Pre-test instrument verification file* and *Pre-test instrument verification notes* attributes were created.

3.4.3 *Attributes*

Table 6. Instrument Parameters Schema Element Attributes

Attribute Name	Attribute Type	Value Set
Test method file	FIL	
Test method description	LTXT	
Balance gas	DCT, multi-value	Air, Argon, Helium, Nitrogen
Balance gas flow rate	PNT, multi-value	
Specimen gas	DCT, multi-value	Air, Argon, Helium, Nitrogen
Specimen gas flow rate	PNT, multi-value	
Pan material	DCT	Aluminum, Ceramic, Platinum
Pan volume	DCT	50µL, 80µL, 100µL, 250µL
Furnace type	DCT	Evolved Gas Analysis (EGA) Furnace, Infrared (IR) Furnace, Wire Wound (Pt/Rh) Furnace
Instrument ID	STXT	Unique to specific instrument
Linked instrument information	Linked TABL	Linking value = Instrument ID
Instrument	Smart link to *Instruments* table	
Instrument configuration	LTXT	
Pre-test instrument verification file	FIL	
Pre-test instrument verification notes	LTXT	
Instrument parameters notes	LTXT	

3.5 Test Conditions

3.5.1 *Definition*

This schema element contains attributes that specifically describe the state of the specimen material during the test. These are things like test temperature, strain rate, etc. that impact the response of the material. They are intended to describe the test data for data consumers. It is acknowledged that these

attributes may partially duplicate some of the information in the Instrument Parameters schema element, which may describe the test in more detail but are not as useful for data consumers.

3.5.2 *Discussion Points & Important Decisions*

1. **Overlap with Instrument Parameters Schema Element:** The LANL team acknowledges that this Test Conditions schema element may appear to overlap with the Instrument Parameters schema element; however, they have different use cases/requirements and serve different roles. For example, the *Test method description* attribute in the Instrument Parameters schema element may say, for example, "Step 1 – Ramp 10°C/min from -80°C to 150°C, Step 2 – Isothermal for 5 mins, Step 3 – Ramp 5°C/min from 150°C to 20°C". As described in the definition for the Instrument Parameters schema element, this provides a TGA operator with the information that they need to replicate the test on their own instrument. In this same example, the *Test temperature* attribute in the Test Conditions schema element will say "-80 to 150°C" and the *Test temperature ramp rate* attribute will say "5°C/min" & "10°C/min". As described in the definition for the Test Conditions schema element, this allows data consumers to easily search for tests done at specific temperatures or temperature ramp rates without having to parse through the long text *Test method description* attribute.

3.5.3 *Attributes*

Table 7. Test Conditions Schema Element Attributes

Attribute Name	Attribute Type	Value Set
Test atmosphere	DCT, multi-value	Air, Argon, Helium, Nitrogen
Test temperature	RNG	
Test temperature ramp rate	PNT, multi-value	
Test conditions notes	LTXT	

3.6 Test Information

3.6.1 *Definition*

This schema element contains non-instrument-specific meta data attributes related to the test data stored in the record. This includes personnel, organizations, and documents associated with the test, as well as the time and date of the test.

3.6.2 *Discussion Points & Important Decisions*

1. **Test group value domains:** Test group will be a short text attribute because a cross-site discrete list would be too cumbersome for administrators and data uploaders. However, the attribute definition will contain a table of "valid" test groups provided by each site. See point 8 of the *Conventions & Best Practices* section for more discussion. Review of data entered into *Test group*

will be a manual process at first, but the team sees an opportunity to use the table of "valid" test groups as the basis for an automated validation tool in the future.

3.6.3 *Attributes*

Table 8. Test Information Schema Elements Attributes

Attribute Name	Attribute Type	Value Set
Test ID	STXT	Unique
Test site	DCT	KCNSC, LANL, LLNL, NNSA, NNSS, PNNL, PX, SNL/CA, SNL/NM, SRNL, SRS, Y-12, Non-NSE site
Test group	STXT	"Valid" options provided in help file
Name of requester	STXT	
Name of test contact	STXT	
Name of operator	STXT	
Date test performed	DAT	
Time test performed	STXT	
Test type	DCT	Thermogravimetric Analysis (TGA)
Document number of work order	STXT	
Document number of test standard	STXT	
Document number of test plan	STXT	
Document number of test report	STXT	
Document numbers of other documents	STXT	
Documents	Static link to *Documents* table	
Test information notes	LTXT	

3.7 Specimen Information

3.7.1 *Definition*

This schema element contains information about the specimen that was tested. For example, attributes may describe size, geometry, manufacturing information, etc.

3.7.2 *Discussion Points & Important Decisions*

1. **"Specimen" vs. "Sample":** It was decided to use the term "specimen" instead of "sample" because: 1) The ASM definition is that a sample is a quantity of material that represents a larger lot and a sample is usually made into multiple specimens for testing, and 2) In statistics, a sample is a subset taken to represent a larger population and a specimen is an individual member of the sample. Additionally, ASTM F3490-21 uses "specimen" to refer to test articles.
2. **Specimen features/dimensions:** The specimen geometry options and corresponding features/dimensions were compiled in collaboration with cross-site TGA SMEs. Each feature/dimension is a point attribute with a long text meta-attribute called *Method measurement description*. Nominal values such as values from drawings should be marked "Estimated". Measured values should use the long text meta attribute to describe how the measurement was taken.

3.7.3 *Attributes*

Table 9. Specimen Information Schema Elements Attributes

Attribute Name	Attribute Type	Value Set
Specimen ID	STXT	
Specimen description	LTXT	
Specimen location	STXT	
Name of specimen preparer	STXT	
Specimen manufacturing description	LTXT	
Specimen form	DCT	Liquid, Powder, Solid
Specimen geometry	DCT	Cubic, Cylindrical, Rectangular, Irregular
Specimen length	PNT w/ LTXT meta (for measurement method description)	
Specimen width	PNT w/ LTXT meta (for measurement method description)	
Specimen height	PNT w/ LTXT meta (for measurement method description)	
Specimen diameter	PNT w/ LTXT meta (for measurement method description)	
Specimen mass	PNT w/ LTXT meta (for measurement method description)	
Specimen density	PNT w/ LTXT meta (for measurement method description)	
Specimen information notes	LTXT	

3.8 Test Data & Results

3.8.1 *Definition*

This schema element contains attributes used to hold the data and results from a test. Generally, this schema element consists of functional data attributes that hold X-Y curve data as well as point, range, or tabular attributes that hold specific values. Data may be uploaded directly from test instrument sensors (e.g. Load) or may be calculated (e.g. Stress). Results are usually, but not always, determined by analyzing curve data (e.g. Young's Modulus).

3.8.2 *Discussion Points & Important Decisions*

1. **One Test record = One Test performed:** Test records hold one test performed on one specimen. There are use cases around statistics and "roll-ups" (e.g. averages) that will need to be addressed in a future schema element.
2. **Point vs. Tabular Attributes for "Results":** TGA results can include: weight changes over a certain temperature range or at one specific temperature, onsets of weight changes, maximum rates of weight change, and residual mass. Depending on the material and experiment, the weight changes and temperatures of interest will vary, resulting in a potentially large number of point attributes needed. Therefore, it was decided to create "general" tabular attributes to hold the results listed above, even though it slightly complicates data uploading.

3.8.3 *Attributes*

Table 10. Test Data & Results Schema Element Attributes

Attribute Name	Attribute Type	Value Set
Weight percent vs. time	FDA	Parameter = Time
Weight percent vs. temperature	FDA	Parameter = Temperature
Derivative of weight percent vs. temperature	FDA	Parameter = Temperature
Weight changes	TABL	
Temperatures at onsets of weight change	TABL	
Temperatures at maximum rates of weight change	TABL	
Residual weight	PNT	
Analysis method	LTXT	
Name of analyzer	STXT	
Document number of analysis document	STXT	
Analysis document	Static link to *Documents* table	
Test data & results notes	LTXT	

3.9 Testing Series Information

3.9.1 *Definition*

This schema element contains information about the testing series that the record is a part of. Most of the attributes are actually links since the information about testing series is contained natively in the Testing Series table, and we want to avoid duplication.

3.9.2 *Discussion Points & Important Decisions*

1. **Existence of a Testing Series table:** A Testing series table will exist and be used to group test records together. This table will be made by the schema elements project at a later date.

3.9.3 *Attributes*

Table 11. Testing Series Information Schema Element Attributes

Attribute Name	Attribute Type	Value Set
Testing series ID	STXT	Unique in *Testing Series* table
Testing series	Static link to *Testing Series* table	
Testing series	Smart link to *Testing Series* table	
Linked testing series information	Linked TABL	Linking value = Testing Series ID
Testing series information notes	LTXT	

3.10 Material Pedigree Information

3.10.1 *Definition*

This schema element contains information about the material pedigree that the record is a part of. Most of the attributes are actually links since the information about material pedigree is contained natively in the Material Pedigree table, and we want to avoid duplication.

3.10.2 *Discussion Points & Important Decisions*

1. **Existence of a Material Pedigree table:** A Material Pedigree table will exist and will hold information about the "flavor" (i.e. specific instance) of material that was tested. It will hold information like lot number, origin, and specific processing/aging details. This table will be made by the schema elements project at a later date.

3.10.3 *Attributes*

Table 12. Material Pedigree Information Schema Element Attributes

Attribute Name	Attribute Type	Value Set
Material pedigree ID	STXT	Unique in *Material Pedigree* table
Material pedigree	Static link to *Material Pedigree* table	
Material pedigree	Smart link to *Material Pedigree* table	
Linked material pedigree information	Linked TABL	Linking value = Material Pedigree ID
Material pedigree information notes	LTXT	

4 Discussion of ASTM F3490-21 as it relates to released schema elements

During FY22, the American Society for Testing and Materials (ASTM) released a standard, F3490-21, proposing standard practices for managing AM data pedigree. This is essentially a proposed schema for an AM database, so it is very relevant to the work of this project. Conforming to an industry standard practice may allow data sharing/pooling beyond NSE sites in the future.

The standard describes schema for AM data at a high level, not including attributes for process-specific AM build data. Like Granta:MI it organizes data into tables (which it calls *modules*) and attributes (which is calls *elements*). A review of the document showed that there is a large degree of overlap between the schema elements proposed for this project and those proposed by ASTM. Some points where they differ include:

- F3490-21 includes some data types that our project has not yet established use cases for. For example, it includes simulation data and product definition data (i.e. drawings) that this project treats as residing in other repositories and could be linked to AM data.
- F3490-21 separates attributes about the AM build from those describing the process parameters used in the build. This is seen as advantageous since multiple builds may be created using, nominally, the same process parameters, and so linking build data to process data avoids duplication. This will be considered when this project begins designing the schema elements specific to builds.

Going forward, when the schema elements team drafts a new schema element, it will be cross-referenced against the ASTM standard. If there are significant differences, justification will be documented.

5 Conventions and best practices (updated from FY21)

During the FY21 Schema Elements work, the team developed conventions, standards, and best practices for the NSE implementation of Granta:MI. 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 name)
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 the objects listed below. While the schema element should contain all objects, implementation into a production 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 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 to from test records to a Documents record since a test may reference multiple documents and each document may be referenced by multiple tests.
   - Schema elements for links will include:
     - 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 *Project ID* or testing series records contain a unique, short text *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
     - A smart record link
     - A tabular attribute with the previously mentioned short text ID attribute as the linking value and relevant linked columns defined.
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.

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. Jack Brett (338217) - 3/8/2021 - Granta Review
6. **Files in Data Files section:**
    - 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. ASCI) 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 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.
    - If a discrete list is not ordered, 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.

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 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.

6 Summary and FY23 plans

In FY22 the schema elements necessary for the creation of a standardized NSE TGA Testing database table were drafted, reviewed, and released. This was a collaborative process in which all NSE sites participated. Attribute definitions, critical decisions, and best practices resulting from many cross-site telecons have been documented to be used as reference going forward.

In FY23 a TGA Testing database table will be available for all sites to 'proof test'. This will uncover opportunities for improving the schema, and so the schema will need to be revised. This proof testing will also allow sites to identify their site-specific workflows for uploading data, aiding the team in planning for the development of standardized data-upload tools.

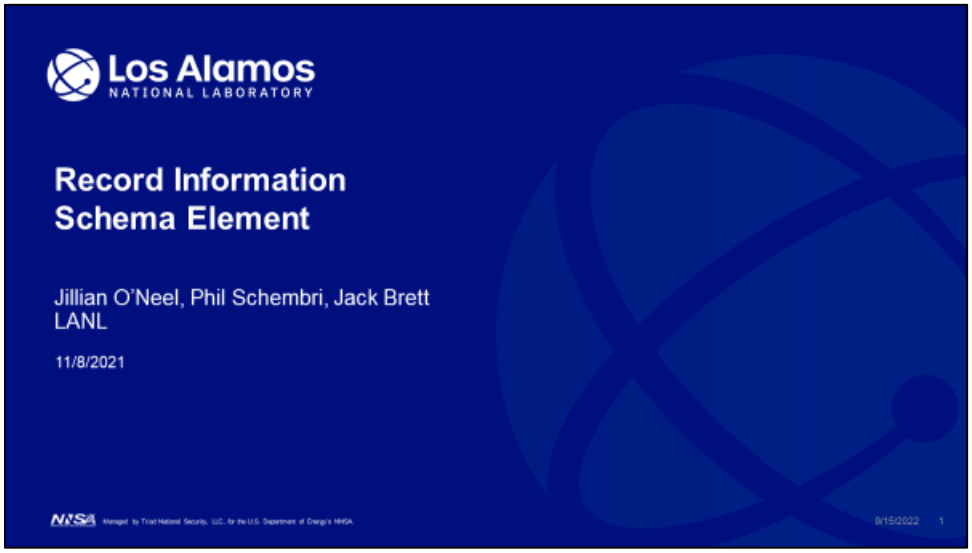
Further database tables will also be developed following the same process as for the TGA Testing table, including Project, Testing Series, and Instruments tables. If funding is sufficient, either the LANL team or teams at other sites will begin development of schema elements for other test types. Because development of the TGA Testing table established many attributes common to all testing types, adding new test types will take much less effort.

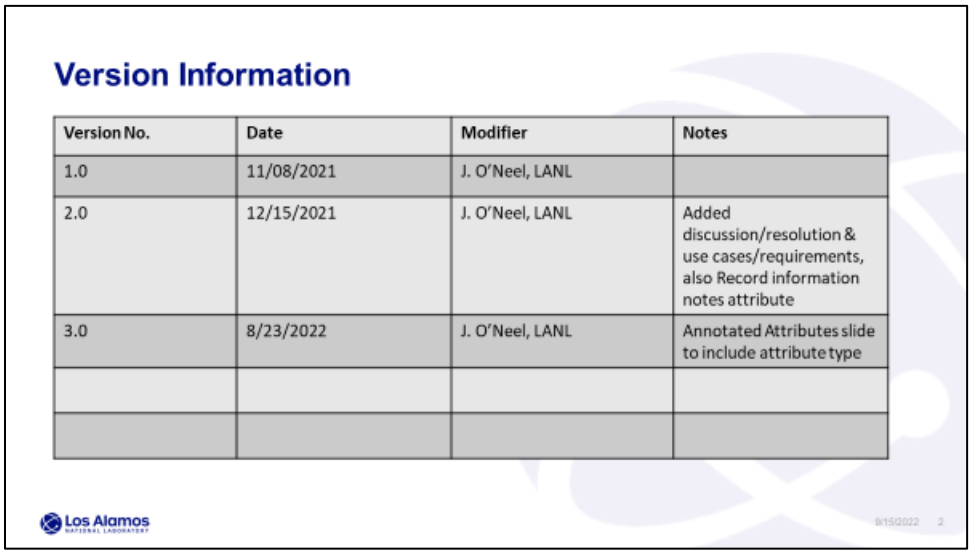
Development of standardized database schema is very time consuming because of the collaboration and careful documentation involved. However, the task is also very parallelizable – teams at each site could

lead the development of schema elements or entire tables. Thus, the most efficient way to speed up the creation of the cross-site AM database is for sufficient funding to exist for all sites to participate; i.e., for all sites to lead the development of specific schema elements.

7 Appendix: Schema Element Discussion Slides

7.1 Record Information





Schema Element name & definition

- Name = Record Information
- Definition = This schema element contains information about the record itself, including when it was created, modified, and reviewed, and who did those things. It does not contain any information about materials or data. As such, it is likely to be used in the same way (all attributes in the same order) in all tables (maybe even all databases). Some information in this schema element, such as *Record create date*, should be available in the Record Properties Granta object; however, we are duplicating in these attributes because not all users have access to record property information.

Attributes

Record Information	
Data sensitivity	(Discrete w/ LTXT meta)
Record create date	(Date)
Record last modified date	(Date)
Name of data originator	(STXT)
Name of record creator	(STXT)
Name of modifier	(STXT)
Record owner	(Discrete)
Record review	(LTXT)
Record information notes	(LTXT)

Uses cases & Requirements

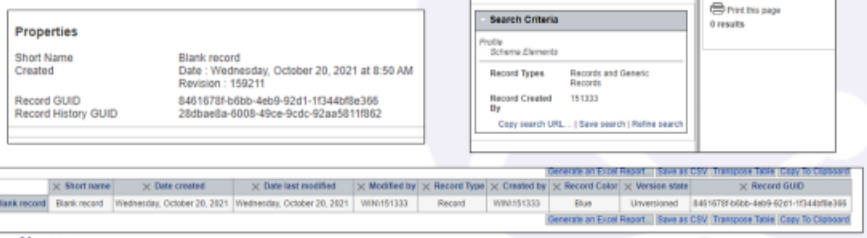
- As a manager, I want to be able to search and report on which and how many records were created/modified by my team members over a specified time period so I can measure progress/performance.
  - **Requirement**: attributes for 'record creator', 'record modifier', 'create date', and 'modified date'
  - **Requirement**: Searching on a person's name in a 'name of' attribute should return all instances of that person appearing the attribute. (Using a single source, e.g. OneID phonebook, for name format could meet this requirement)
  - **Requirement**: Searching on a person's name in a 'name of' attribute should not return instances of people with similar or identical names appearing in that attribute. (The unique ID could meet this requirement)
- As a data consumer, I would like to know who, besides the people who produced the data, were responsible for the data being entered into the database in case I have questions about it.
  - **Requirement**: attributes for 'data originator', 'record creator', 'record modifier'.
- As a technical SME, I want to know who to contact to request data, that didn't produce and I suspect contains errors, be reviewed and/or corrected.
  - **Requirement**: attributes for 'Record owner' and 'Record review'
- As a data consumer I want to know how much and what type of review the data has received so I know how much confidence I can have in it.
  - **Requirement**: attribute for 'Record review'
- As a data consumer wanting to export data from the database, I would like some guidance as to how to treat the data until I can get it DC reviewed.
  - **Requirement**: attribute for 'Data sensitivity'

Discussion points

- See help files for *Name* attributes
  - Note that the standards & best practices are intended to apply to other "name" attributes that we will encounter in the database (ex: *Operator*)
  - We are currently using first & last name from OneID phonebook listings
    - Should we allow the use of nicknames? (We lean towards "No" for consistency)
  - What should we use as a unique ID?
    - Email address?
      - Pro: Accommodates people not in DOE, ex: Universities
      - Con: Some people have multiple email addresses, people might send unwanted emails
    - DUID from OneID Phonebook?
      - Pro: Unique ID that spans all DOE sites
      - Con: Only DOE sites

Discussion points cont.

- Reasons for duplication of Granta Record Properties object
  - Not easy to see
  - Reverted records don't revert "Date last modified"
  - Names are not recognizable



Discussion & Resolution

Discussion and feedback took place via email and at the 11/22/21 Cross-Site Schema Elements Webex Meeting. The following slides contain a summary.

- Granta functionality (i.e., "Record Properties") does not currently meet the use cases identified. We will proceed with the attributes in this schema element under the understanding that we may move away from them if Granta's functionality improves.
  - Modified dates can increment without versions incrementing
  - Usernames are not easily and universally identifiable
- Data sensitivity
  - Marking & Derivative Classifier (DC) review
    - From previous discussions with classification offices, databases are treated as a working document of the highest "level" (ex: OUO-ECI, SRD, etc.) therefore, individual records do not need to be DC reviewed and marked because they are automatically considered working documents of the highest "level".
    - When data is pulled out of the database and into another document (printed records, reports, spreadsheets, etc.), the exported data needs to be reviewed by a DC and marked appropriately.
    - The data sensitivity attribute is intended to help inform data consumers & DCs, but is not considered 'document marking'. Therefore, population of this attribute is strongly encouraged, but not required.

Discussion & Resolution

- Data sensitivity
  - The discrete list was edited based on DOE guidance (O 471.3, M 471.3, O 471.1B, and M 471.1-1) and includes the following options.
    - Unclassified - Approved for Unlimited Release
    - Unclassified - Not Approved for Unlimited Release
    - Official Use Only
    - Official Use Only - Export Controlled Information
    - Unclassified Controlled Nuclear Information
    - Classified - CRD
    - Classified - CFRD
    - Classified - SRD
    - Classified - SFRD
  - Some notes:
    - The unclassified option was modified to differentiate between data that has been reviewed for unlimited release (ex: LA-UR) and data that is unclassified, but has not been reviewed for unlimited release.
    - UCNI & OUO are independent and UCNI is considered "higher" than OUO.
    - OUO Freedom of Information Act (FOIA) exemptions do not need to be included because they don't affect how the OUO data is handled. However, OUO additional markings, such as "Export Controlled Information", do require a separate option because they have additional handling requirements than just OUO.
    - When this schema element is deployed to production databases, options that are not permitted in the database should not be copied over. For example, "Classified – SRD" should not appear as an option for databases on the Unclassified Network. Also, none of our unclassified databases are currently rated for UCNI.

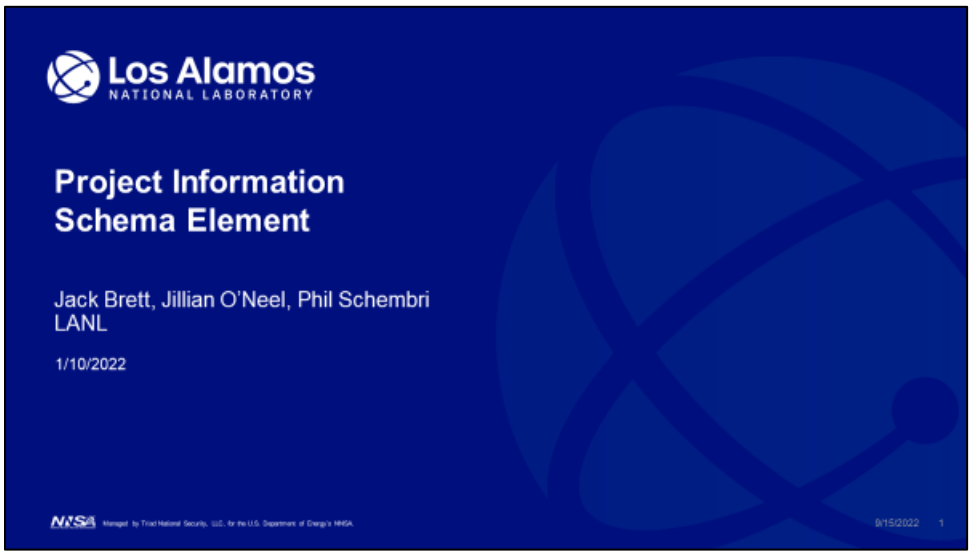
Discussion & Resolution

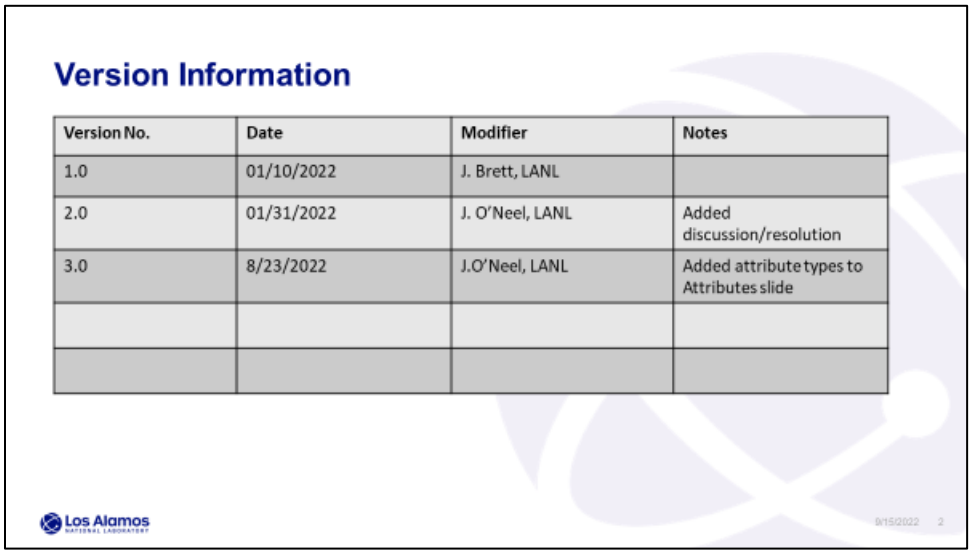
- Names and Unique IDs
  - People's names are required to be populated as "FirstName LastName (DUID#)" as they appear in the OneID Phonebook (no nicknames)
    - For example: Philip Schembri (139424520)
  - If the person is not in the OneID Phonebook or does not have a DUID#, just their first and last name may be used.
    - For example: Olivia Trautschold
- Record create date & Name of record creator
  - We reviewed the definitions for these attributes and felt they did a good job of differentiating between created, modified, and released. They required no editing at this time.
- Do we need attributes for Release date and Name of releaser?
  - No, the "Record Properties" and "Version History" information that Granta provides meets the use cases identified and appears to increment properly.

Discussion & Resolution

- Record Review
  - This attribute type was switched to long text (LTXT).
    - The team decided that a tabular attribute would make importing and exporting too difficult and a short text (STXT) does not allow enough characters for multiple reviewers with long names.
    - Markdown to make the formatting nice is strongly encouraged.
- Record information notes
  - All schema elements should have an accompanying long text notes attribute at the end
  - Meant to contain any notes about the data in the schema element attributes
  - For example, "LANL is listed as the **Record owner** because they commissioned this testing that was done by KCNSC."

7.2 Project Information





Schema Element name & definition

- Name = Project Information
- Definition = This schema element contains information about the project that the record is a part of. Most of the attributes are actually links since the information about projects is contained natively in the Projects table, and we want to avoid duplication.

Attributes

Project Information	
Project ID	(STXT, unique when in Projects table)
Project (static link to Projects table)	(static link)
Project (smart link to Projects table)	(smart link)
Linked project information	(Linked Tabular, linking value = Project ID)
Project information notes	(LTXT)

Use Cases and Requirements

- As a data consumer I would like to see all records related to a specific project (without having to perform a search) so I can ensure I have a complete data set.
  - Requirement: complete links from tests to project and from project to tests. Project ID required for uniqueness.
- As a data consumer I would like to see all records related to a specific project (without having to perform a search) so I can discover data related to records I found using a search. E.g. I search for mechanical test data for SX358 and I discover thermal test data for SX358 because it's part of the same project.
- As a funding manager I would like to see all records related to a specific project (without having to perform a search) so I can gather statistics on test data I have funded.
- As a data consumer I would like to see summary information about the project a test record is associated with so I can judge whether the test data is applicable for my needs. E.g. was the project objective comparison of materials or material model calibration/validation?
  - Requirement: tabular attribute (**Linked project information**)

Discussion Points

- Should we require a Project ID?
  - For all testing tables, we propose requiring a Project ID, a linked tabular attribute, either a static or smart link, and a corresponding project record for linking
    - Smart links will automatically populate
  - Attributes can be set to "required" on a per-layout basis on MI:Admin
- The Project ID is required to be unique, no two projects can have the same Project ID
- Tables using this schema element will choose between either the static or the smart links:
  - Smart links when one-to-many relationship is expected between Projects table and the table using this schema element
  - Static links when many-to-many relationship is expected between Projects table and the table using this schema element
  - **Linked project information** can be used in both cases
- **Project information notes** is not for notes about the project (which would be entered in the Project record itself); it's for notes about the Project Information attributes. E.g. "This test was originally intended to be part of Project A, but the specimen was not used for that project and was used for Project B instead."
  - Any project-specific information displayed in the record using this schema element should be linked through **Linked project information**

Discussion Points cont.

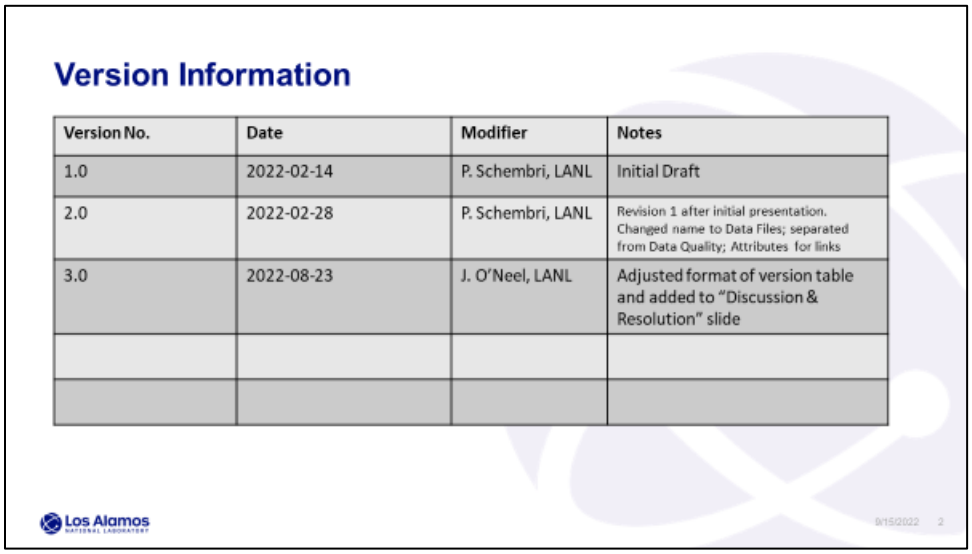
- The structure of links established in this schema element will likely be used as a template for other similar schema elements.
  - Template
    - "ID" short text attribute (e.g. **Project ID**)
    - Tabular link (e.g. **Linked project information**)
    - Smart link or Static link
  - Other tables probably using similar structure
    - AM Builds
    - Materials
    - Testing Series
    - Etc.

Discussion & Resolution

Discussion and feedback took place via email and at the 1/24/2022 Cross-Site Schema Elements Webex Meeting. The following slides contain a summary.

- Project ID will be a required attribute for all testing tables
  - Recommended (but not required) format is as follows:
    - **Project Name - Year or FY of Project**
    - Example: "Investigation of 304L Stainless Steel - FY19". It is recommended that the "Project Name" be short, concise, and derived from a work package or report. It is encouraged to include the names or types of materials studied in the "Project Name".
- General format for linking between tables is established and will use the following attributes:
  - Short text attribute for a Unique ID
  - Smart or Static Link
  - Linked tabular attribute

7.3 Data Files



Note

- The schema element was originally proposed as 'Data Information' and included attributes for data files and data quality. After the 2/14/22 discussion, we split this schema element into the following two:
  - Data Files
  - Data Quality
- The subsequent slides are related only to the Data Files schema element

Schema Element name & definition

- Name = Data Files
- Definition = This schema element contains data files, and information about them, for the purpose of traceability.

Attributes

Data Files		
	Raw data file	*(File)*
	Final data file	*(File)*
	Other data file	*(File)*
	Raw data file link	*(hyperlink)*
	Final data file link	*(hyperlink)*
	Other data file link	*(hyperlink)*
	Data files notes	*(Long text)*

Attributes

- **Raw data file** – data file from instrument, or earliest data file
- **Final data file** – file uploaded to Granta attributes
- **Other data file** – any other/intermediate file; zipped if multiple

- **Raw data file link** – hyperlink to raw data file
- **Final data file link** – hyperlink to final data file
- **Other data file link** – hyperlink to other data file

- **Data files notes** – information *about* the data/file not captured in other attributes. There will probably be other attributes to capture, e.g., data analysis procedures.

Uses cases & Requirements

- As a data-consumer, I have a question about (or suspect an error in) the data stored in the point or functional attributes, so I would like to view the original files.
  - **Requirement:** Need attributes to store raw data files
- As a data-consumer, I suspect an error was made (e.g. in the units) while the data was uploaded. I'd like to see the file that was uploaded to check.
  - **Requirement:** Need attributes to store the 'final' data file that was uploaded.
- As a data-consumer, I would like to see any other metadata associated with this record that might not be stored as attributes.
  - **Requirement:** Need attributes to store any data files that might contain metadata.

Other uses cases (not fully addressed by Data Information)

- As a data-consumer, I have a question about (or suspect an error in) the data stored in the point or functional attributes, so I would like to know the process by which the final stored data was created based on the raw data files.
  - **Requirement:** Need attributes to store intermediate data files and **information about data analysis/regression**.
  - This use case may be further addressed in a schema element related to analyzed test results

Discussion points

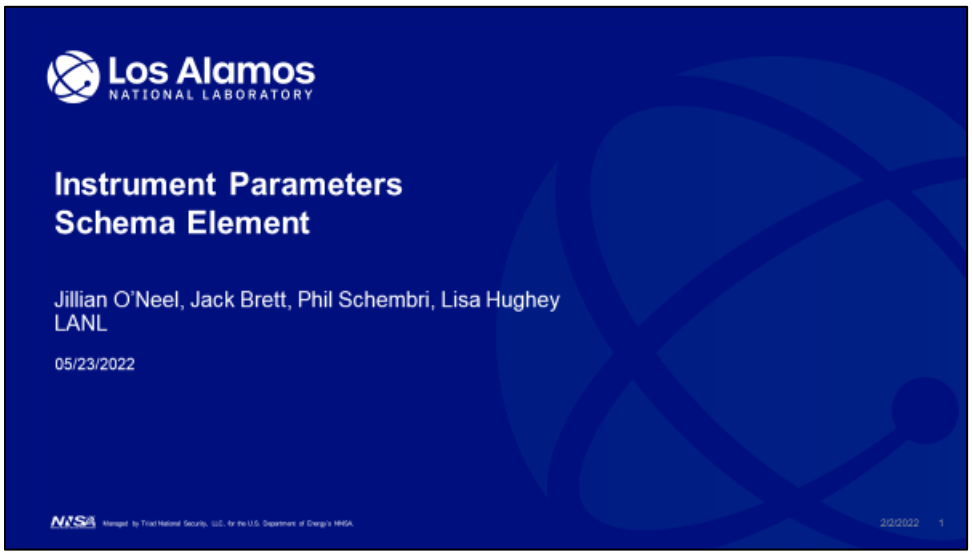
(original slide related to Data Information schema element)

- **Files**:
  - **Data information notes** should be sparse in most cases. There should be dedicated attributes (in other schema elements) for frequently stored information.
  - File attribute vs. tabular?
    - **Tabular**: Difficult to upload (bad); arbitrary number of files (good); not tied to particular definition (good?).
    - **File**: Easy to upload (good); fixed number of files (bad); interpreted to match definitions (bad?).
    - **We weighted ease-of-upload heavily**. Unlike for some tables (e.g. AM Builds) text importers are very often used for importing, so we need the file uploaded during import.
  - **Other data file**
    - We initially used more specific attributes ('corrected file', 'analyzed file') but decided they were difficult to define.
    - This attribute *could* be tabular
- **Data quality rating**
  - There has been much previous discussion; we tried to capture use cases & show how to include rubric.
  - Why can this (and not the files) be tabular? Quality rating probably added after initial import, unlike files
    - Should this attribute be multiple discrete attributes instead of Tabular? Ease of upload vs. ease of visualization?

Discussion & Resolution

- **Files**:
  - **File attribute vs. tabular**?
    - Individual file attribute types were chosen over a single 'Files' tabular attribute (which would allow storage of an arbitrary number of files) because we prioritized ease of upload over flexibility. This priority applies to testing records because we need to be able to upload them efficiently; priority may be different for other tables (e.g. AM Builds).
  - **File size and location**
    - Large data files may not 'fit' in Granta. We should allow for files to be stored in a separate system and linked to Granta.
- **Data quality rating**
  - Data quality attributes were initially included in this schema element, but discussion at the cross-site meeting prompted separation of those attributes into their own schema element for discussion later.

7.4 Instrument Parameters



Version Information

Version No.	Date	Modifier	Notes
1.0	5/23/2022	J. O'Neel, LANL	Initial version presented
2.0	8/23/2022	J.O'Neel, LANL	Added attribute types to Attributes slide and Discussion & Resolution slides
3.0	9/14/2022	J. O'Neel, LANL	Updated to include pre-test verification attributes

Los Alamos
2/2/2022 2

Schema Element name & definition

- Name = Instrument Parameters
- Definition = This schema element contains attributes that describe the setup of the instrument and test program sufficiently enough for an operator to reproduce the test. This includes hardware and accessory information as well as instrument/software settings such as gas flow rate, signal gain, etc. Finally, it includes test program information such that a test operator can replicate the test on their own instrument (ex: Step 1-Ramp from 30°C to 150°C at 5°C/min. Step 2-Isothermal hold for 5 mins….).

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2/2/2022 3

Attributes

Instrument Parameters

Test method file	(File)
Test method description	(LTXT)
Balance gas	(Discrete, multi-value)
Balance gas flow rate	(Point, multi-value)
Specimen gas	(Discrete, multi-value)
Specimen gas flow rate	(Point, multi-value)
Pan material	(Discrete)
Pan volume	(Discrete)
Furnace type	(Discrete)
Instrument ID	(STXT, unique if in Instruments table)
Linked instrument information	(Linked tabular, linking value = Instrument ID)
Instrument (smart link to Instruments table)	(smart link)
Instrument configuration	(LTXT)
Pre-test instrument verification file	(File)
Pre-test instrument verification notes	(LTXT)
Instrument parameters notes	(LTXT)

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2/2/2022 4

Uses cases & Requirements

Use cases

1. As a material scientist wanting to reproduce the conditions in a series of tests, I want to know details of the instrument and related hardware used and how it was configured.
2. As a manager, I want to know how many and which tests were performed with certain instruments.
3. As a data consumer, I suspect some test data may depend on the instrument used, so I want to see which instrument make/model/serial number was used for each test.
4. As a test operator, I want to know which instrument/software settings were used in a test in order to replicate the test.
5. As a test operator, I want to know the "procedure" used in a test in order to replicate the test.

Requirements

- Links between Test record and Instrument record
- Tabular links so some instrument information can be viewed in the test record
- Ability to report all tests linked to a piece of Instrument
- Attributes for relevant instrument/software settings
- Attributes for procedure/test method

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2/2/2022 5

Discussion Points - Link to Instruments (already discussed)

- *Are the use-cases strong enough to motivate an Instruments table?*
  Other options:
  - LTXT attribute to describe 'the instrument'
    - May satisfy use case 1, but not others.
    - May be difficult to guide users to input sufficient information
  - Discrete (pull-down menu) for, e.g. 'Manufacturer', 'Model'. Or maybe for 'system', consisting of particular instruments/configurations
    - May satisfy all use cases
    - Lists may be too long to manage & need frequent appending (admin maintenance)

- We have assumed an Instruments table will exist.
  - Until we get to that table, we won't know exactly what's in it, but we assume it will include:
    - Manufacturer, Model, Serial Number, Instrument ID (unique)
  - We also assume this is different from the Machines table in the AM database

Discussion Points – Link to Instruments (already discussed)

- We have assumed a Test record is linked to a **single** Instrument record.
  - Distinction between 'instrument' (required for test) and 'accessories' (optional)
  - 'Instrument' may consist of a custom collection of hardware but is still treated as single object

- Importing tabular links for multiple records is non-trivial:
  - Excel importers can be modified to allow a column in the Data sheet (e.g. containing Instrument ID) to be copied to the sheet for tabular attributes, allowing *relatively* easy population of the tabular attribute.

- We propose only one LTXT attribute: Instrument configuration
  - Might there be other test-record-specific instrument information?
  - If there is, we propose it still goes in this attribute. Multiple similar LTXT attributes confuse people uploading data

Discussion points

- Test Method Description
  - Used to be called "Heating Schedule" or "Thermal Schedule"
  - Used to be tabular
  - Now = Long text
  - Pros:
    - Flexible
      - General enough to hold any information without needing to add tabular columns
      - Can easily accommodate variations in experiments, available parameters that can be changed, etc.
    - Data can be imported more easily (ex: via text importer)
  - Cons:
    - Doesn't guide the user to upload in a certain format
    - Difficult to review and ensure sufficient population, therefore…
    - We probably need to be okay with losing some "test reproducibility"

Discussion points

- Discrete menus
  - Gases = Air, Argon, Nitrogen, Helium
  - Pan material = Aluminum, Ceramic, Platinum
  - Pan volume = 50µL, 80µL, 100µL, 250µL
  - Furnace type = Infrared (IR) Furnace, Evolved gas (EGA) Furnace, Wire wound (Pt/Rh) Furnace

Discussion & Resolution

- Decided to use the term "Instrument" instead of Test Equipment
- We achieved agreement on the ideas on slides 6 & 7.
  - There will be an Instruments table
  - A test record will link to a single instrument record
  - **Instrument configuration** attribute (LTXT) used to describe instrument set-ups, hardware, etc.
- After some back-and-forth discussion, we also decided to continue with the long text attribute **Test method description** as a replacement for the previously tabular "Heating Schedule" attribute. (Slide 8)

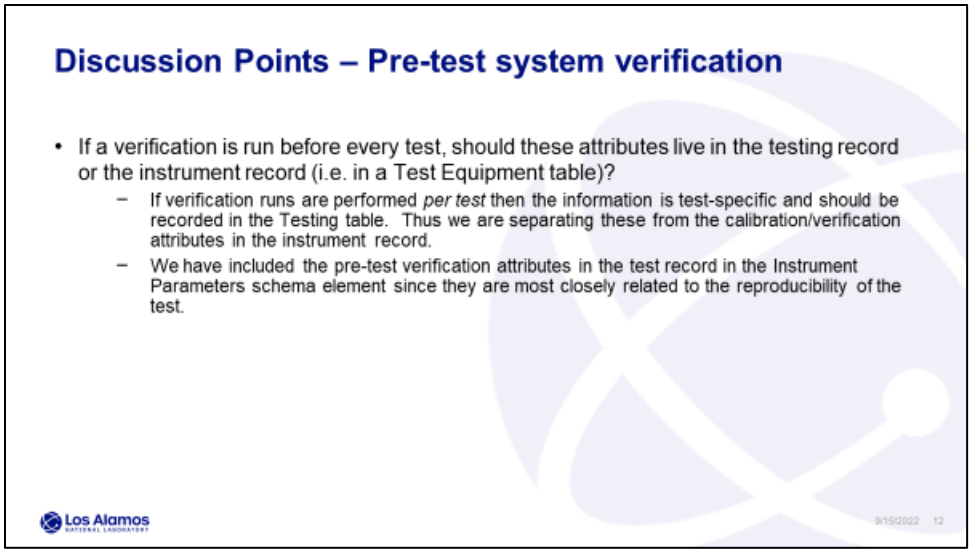
Pre-test verification: Uses cases & Requirements

Use cases

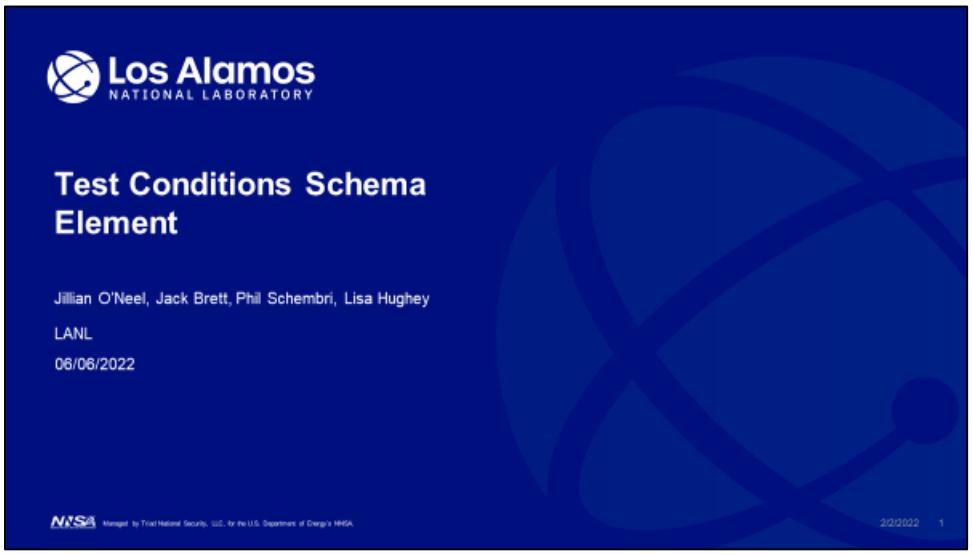
1. As a test operator, I want to store how a system verification was performed before each test run so I can reproduce it if necessary. There may be a verification before each test, not just at after the less-frequent instrument calibration.
   - Ex: TGA/DSC standards or FTIR background measurements.
2. As a data consumer, I would like to know if an instrument verification has been performed before each test because that gives me greater confidence in the test data.

Requirements

- Pre-test verification attributes that will live in the test record in addition to calibration/verification attributes in the Test Equipment (instruments) table.



7.5 Test Conditions



Version Information

Version No.	Date	Modifier	Notes
1.0	06/08/2022	J. Brett, LANL	
2.0	08/23/2022	J. O'Neel, LANL	Added attribute types to Attributes slide

2/2/2022 2

Schema Element name & definition

- Name = Test Conditions
- Definition = This schema element contains attributes that specifically describe the state of the sample material during the test. These are things like test temperature, strain rate, etc. that impact the response of the material. They are intended to describe the test data for data consumers. It is acknowledged that these attributes may partially duplicate some of the information in the Instrument Parameters schema element, which may describe the test in more detail but are not as useful for data consumers.

2/2/2022 3

Attributes

Test Conditions	
Test atmosphere	(Discrete, multi-value)
Test temperature	(Range)
Test temperature ramp rate	(Point, multi-value)
Test conditions notes	(LTXT)

2/2/2022 4

Uses cases & Requirements

- Use case: As a materials scientist, I want to quickly see testing conditions, such as the test's overall temperature range or the testing atmosphere, in order to more easily determine if the test is relevant to me.
  - **Requirement:** Need individual attributes for Test conditions and these attributes should be attribute types that facilitate standardized uploading of the data and filtering/searching (i.e., not long text).
- Use case: As a data consumer, I would like to be able to search for TGA tests performed under specific temperatures and/or atmospheres.
  - **Requirement:** Need individual attributes for test temperature and atmosphere, need them to be structured like point or range or discrete.
- Use case: As a data consumer, I want to know the 'state' of the material as it was being tested without a need to understand how the test parameters affect that state.
  - **Requirement:** Need specific attributes to describe the environment and atmposphere the material experiences.

Discussion points

- Some of these attributes may overlap with Instrument Parameter attributes
  - In this case, the attributes may seem redundant, but it is necessary to have these atributes to keep track of the material's state during the test.
  - For example, Instrument Parameters may contain an attribute for **Test method description** that describes how the instrument thermally cycled the sample, while Test Conditions may contain the range attribute **Test temperature,** which describes the range of states the material experienced during the test. The two should be consistent with each other but are populated slightly different and are used for slightly different purposes.
- The use case for this schema element might be more obvious for mechanical tests, in which case attributes would include 'Strain rate', 'Test temperature', etc. For TGA, the use case may be less immediate.
- Test atmosphere
  - Should be included since the environment of a TGA test can be changed and searchable.
  - Multivalued because in some cases, the atmosphere in a TGA expermient can be changed mid-test.

Discussion Points (cont.)

- Test temperature ramp rate
  - Chose units of °C/min
  - This input should be positve, even during cooling (where the temp is decreasing but the rate is still a postive number, not negative)
  - Multi-valued attributes a little harder to upload, goes into a new sheet when exported into excel. No way around this since ramp rate changes in the same test are common in other types of testing.

Example of Difference between Instrument Parameters & Test Conditions

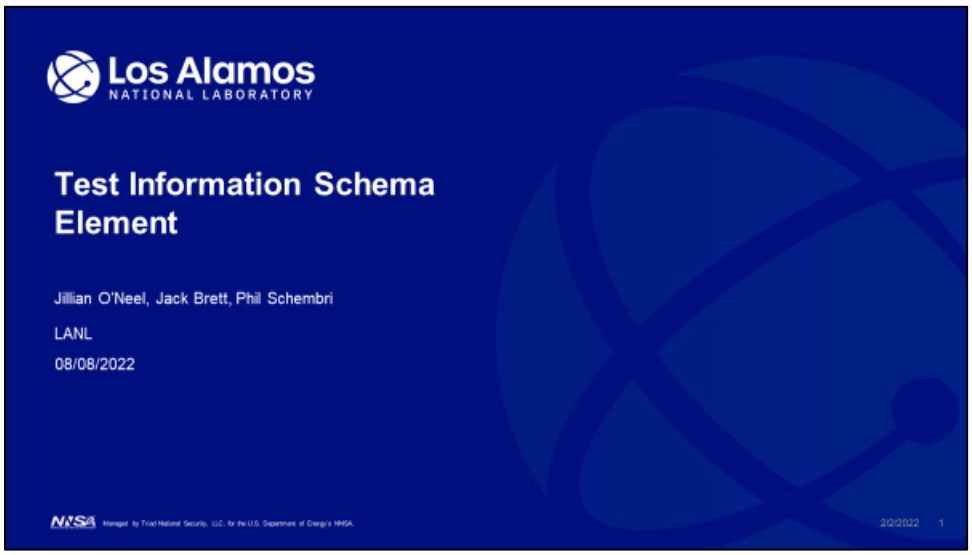
Instrument Parameters vs. Test conditions

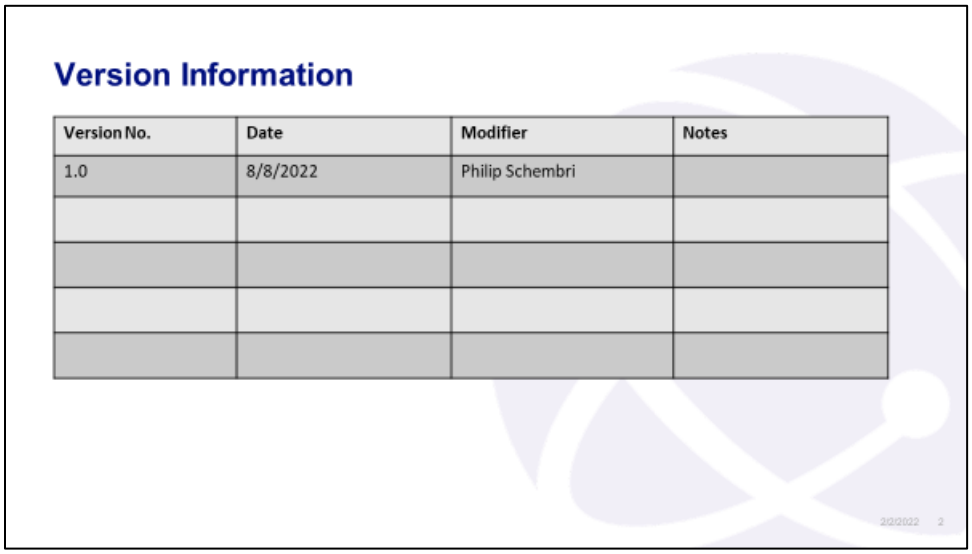
Point attributes			
	Test temperature ramp rate	5.00	°C/min
		10.00	°C/min
Range attributes			
	Test temperature	-80 to 150	°C
Long text attributes			
	Test method description		
	OrgMethod 1: Equilibrate at -80.00 °C		
	OrgMethod 2: Ramp 10.00 °C/min to 150.00 °C		
	OrgMethod 3: Isothermal for 5.00 min		
	OrgMethod 4: Ramp 5.00 °C/min to -20.00 °C		

Discussion & Resolution

- General agreement amongst sites with these attributes and how they are implemented.

7.6 Test Information





Schema Element name & definition

- Name = Test Information
- Definition = This schema element contains non-instrument-specific meta data attributes related to the test data stored in the record. This includes personnel, organizations, and documents associated with the test, as well as the time and date of the test.

2/2/2022 3

Attributes

Test Information	
Test ID	(STXT; unique)
Test site	(Discrete)
Test group	(STXT)
Name of requester	(STXT)
Name of test contact	(STXT)
Name of operator	(STXT)
Date test performed	(DATE)
Time test performed	(STXT)
Test type	(Discrete)
Document number of work order	(STXT)
Document number of test standard	(STXT)
Document number of test plan	(STXT)
Document number of test report	(STXT)
Document numbers of other documents	(STXT)
Documents (static link to Documents table)	(Static Link)
Test information notes	(LTXT)

2/2/2022 4

Uses cases & Requirements

(There are probably many more use-cases. This list is to ensure there are sufficient credible use cases to justify the schema.)

- **Use case**: As a data consumer, I want to know who to contact with questions I have about the test data, methods, and/or analysis.
  - **Requirement**: Need attributes to store personnel and organizations associated with the test
- **Use case**: As a data consumer, I would like to be able to search for tests performed or requested by certain people so I can find similar data and/or data on similar materials/projects.
  - **Requirement**: Attributes containing names and organizations must be in a consistent format.
- **Use case**: As a data producer uploading data, I need a way to group related tests.
  - **Requirement**: Testing Series ID and Test ID attributes must be included in test records.

2/2/2022 5

Uses cases & Requirements

- **Use case**: As a data consumer, I would like to find all tests (on a particular material) perfomed within a certain time window since this corresponds to the time a particular formulation of material was being used or to the time a particular part was being manufactured.
  - **Requirement**: Attributes for test date.
- **Use case**: As a data consumer, I want to be able to search for tests of a certain type without relying on the predefined database hierarchy (in case that hierarchy changes)
  - **Requirement**: Attribute for test type.
- **Use case**: As a data consumer, I would like to be able to easily find documents associated with a test record since they contain further information useful to interpret the data.
  - **Requirement**: Attributes for document numbers and links to documents.
- **Use case**: As a data producer uploading data, I would like to be able to associate documents with test records efficiently and with minimal duplication.
  - **Requirement**: Attribute for document number included in both test record and document record to enable linking.

Discussion points

- Test ID vs. Specimen ID
  - LANL has used Specimen ID as a unique test identifier, but we might want to perform multiple tests on the same specimen, so it would help to track test and specimen independently
  - No standardized format. Need to accommodate existing standards across multiple organizations.
- Note that **Test group** is short text, not discrete:
  - Need to maintain consistency to satisfy use cases. We propose each site maintain a 'valid test group' list and validate the data after upload, before release. E.g.:

LANL	LLNL	SNL/NM	SNL/CA	KCNSC	PX	SRNL	Y12	NNSS	PNNL
C-CDE									
Q-5									
Q-14									
M-9									
MPA-CINT									
MST-7									
MST-8									
MST-16									

Discussion points

- Attributes for 'test location' were considered but it was decided a Test Equipment table should house those.
  - The data can be linked into the test record.
  - Information about location might be difficult to track if equipment moves, and this risk was accepted.
- Based on TGA data examples from sites, we propose the following personnel are sufficient to capture
  - Requester, test contact, operator.
  - We propose to allow for multiple test contacts, comma separated.
- Based on TGA data examples from sites, we propose the following documents are sufficient to capture
  - Work order, test plan, test standards, test report.
  - We also include 'other documents', with document numbers comma separated.
    - There is not yet a nice way to automate link population with comma-separated link values. Python could do it though.

Discussion points

- We moved **Testing series ID** and links to Testing Series record to a separate Testing Series Information (almost identical to Project Information, which we discussed previously)

We propose only these Testing Series Information attributes be used in testing records

- **Test type**: it's not obvious why we need it now, but we might want it in the future
  - It essentially duplicates the testing table name, so we don't have to rely on the location of the record to know what type of test it is.
  - For other test types we might also add a test 'sub-type'. E.g.:
    - For 'Uniaxial' tests we might add 'monotonic compression'
    - For 'Gas Gun' experiments we might add sub-types 'shock', 'spall', 'recover', etc
    - **Do any sites have multiple test sub-types for TGA?**
- **Work center**: Is it sufficient to capture this in **Test information notes**?

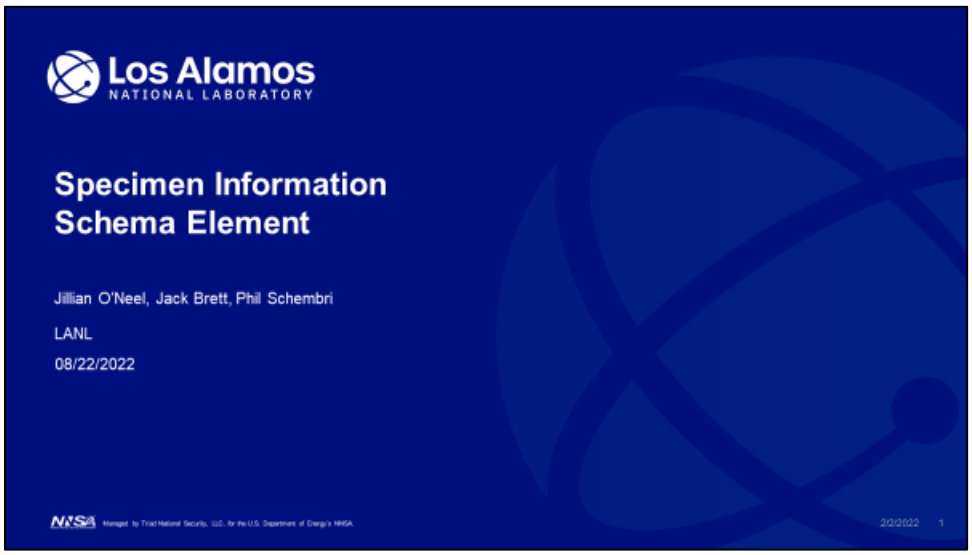
2/2/2022 9

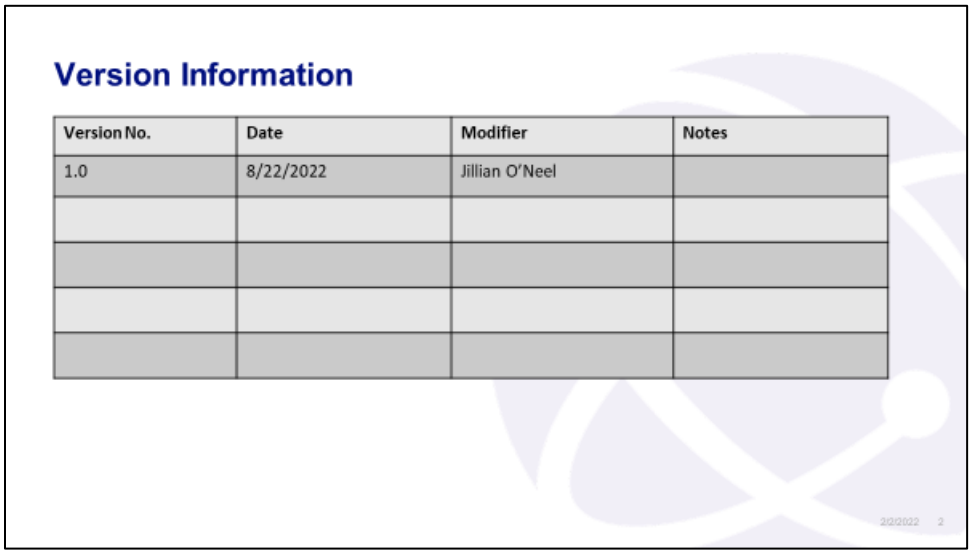
Relationship to ASTM F3490-21

Granta (Test Information)	ASTM (Table 15)	Notes
Test ID	TIC ID	
Test site	TIC Vendor/Supplier/ Contractor	If non-NSE site, vendor name is in 'Test information notes'
Test group	TIC Vendor/Supplier/ Contractor	
Name of requester		Not included in ASTM
Name of test contact	TIC Point of Contact	
Name of operator	TIC Operator	
Date test performed	TIC Start Time and Date	In Granta, duration and/or end date/time can be stored in 'Test information notes'. (No use-case for storing them in structured attributes)
Time test performed	TIC Start Time and Date	In Granta, duration and/or end date/time can be stored in 'Test information notes'. (No use-case for storing them in structured attributes)
Test type	TIC Type	
Document number of work order		Not included in ASTM
Document number of test standard	TIC Standard	
Document number of test plan	TIC Procedure	These might not be identical, but close.
Document number of test report		Not included in ASTM
Document numbers of other documents		Not included in ASTM
Documents (static link to Documents table)		Note that ASTM stores 'TIC Procedure' as document but 'TIC Standard as string. In Granta we allow for both for all documents.
Test information notes	TIC Name and TIC Notes/Comments/ Description	Note that there is possibility of overlap with Instrument Parameters schema element

2/2/2022 10

7.7 Specimen Information





Schema Element name & definition

- Name = Specimen Information
- Definition = This schema element contains information about the specimen that was tested. For example, size, geometry, manufacturing information, etc.

2/2/2022 3

Attributes

Specimen Information	
Specimen ID	(STXT)
Specimen description	(LTXT)
Specimen location	(STXT)
Name of specimen preparer	(STXT)
Specimen manufacturing technique	(Discrete multi-value, w/ LTXT meta)
Specimen form	(Discrete)
Specimen geometry	(Discrete)
Specimen length	(Point, w/ LTXT meta)
Specimen width	(Point, w/ LTXT meta)
Specimen height	(Point, w/ LTXT meta)
Specimen diameter	(Point, w/ LTXT meta)
Specimen mass	(Point, w/ LTXT meta)
Specimen density	(Point, w/ LTXT meta)
Specimen information notes	(LTXT)

2/2/2022 4

Uses cases & Requirements

(There are probably many more use-cases. This list is to ensure there are sufficient credible use cases to justify the schema.)

- **Use case**: As a test operator, I want to know detailed information about the specimen that was tested (such as geometry, manufacturing info, and size) so that I can replicate the test.
  - **Requirement**: Need attributes to store geometry, dimensions, manufacturing info, etc.
- **Use case**: As a data consumer, I would like to relate specimen features (such as density) to test results.
  - **Requirement**: Need attributes for specimen features such as mass, density, dimensions, location, etc..
- **Use case**: As a data consumer, I want to find all tests done on a specific specimen.
  - **Requirement**: Need attribute for Specimen ID. Should be unique to an individual test specimen, but shouldn't be set as unique in Granta because multiple test records could have the same Specimen ID (ex: FT-IR then TGA)

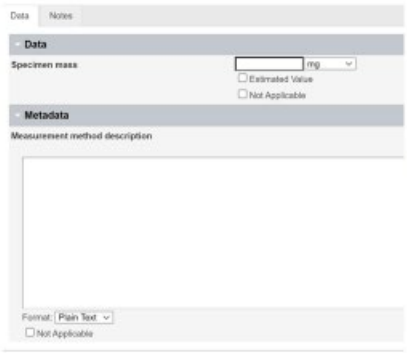
2/2/2022 5

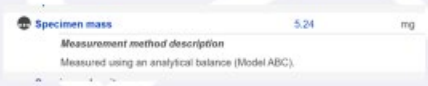
Discussion points

- There is some information we want to know about a specimen that falls under "Material Pedigree Information". This is usually information about where a specimen came from. For example, did it come from a part? Or a specific lot/batch? Material name? etc.
  - We think that this kind of information should live natively in the Material Pedigree table and get linked into the test table via linked tabular data.
  - We will make a separate schema element for the links to Material Pedigree.
- Specimen ID
  - Not unique in Admin, but should be unique to one "test article"
  - No standard naming convention
- Specimen dimensions/features
  - Specimen length, Specimen width, Speciment height, Specimen diameter, Specimen height, Specimen mass, Specimen density
  - Point attributes
    - Nominal values should be marked "Estimated"
    - "Method measurement description" = meta long text attribute meant to describe how the dimension/feature was measured (ex: Measured by hand using calipers.)

2/2/2022 6

Discussion points, Cont.





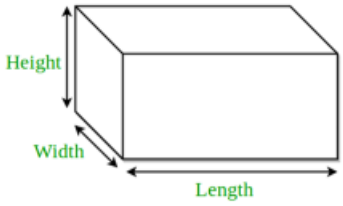
2/2/2022 7

Discussion Points Cont.

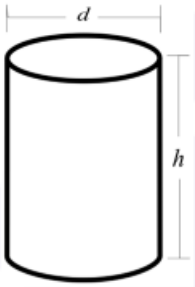
- Specimen form (discrete list)
  - Liquid, Powder, Solid
- Specimen geometry (discrete list)
  - Cubic, Cylindrical, Rectangular, Irregular
- Specimen manufacturing technique (discrete list)
  - Additive Manufacturing, Cored, Cut Off, Drilled, Electrical Discharge Machining (EDM), End Milled, Ground, Laser Cut, Milled, Polished, Pressed, Stamped, Turned, Water Jet

2/2/2022 8

Discussion points, Cont.



Cubic/Rectangular



Cylindrical

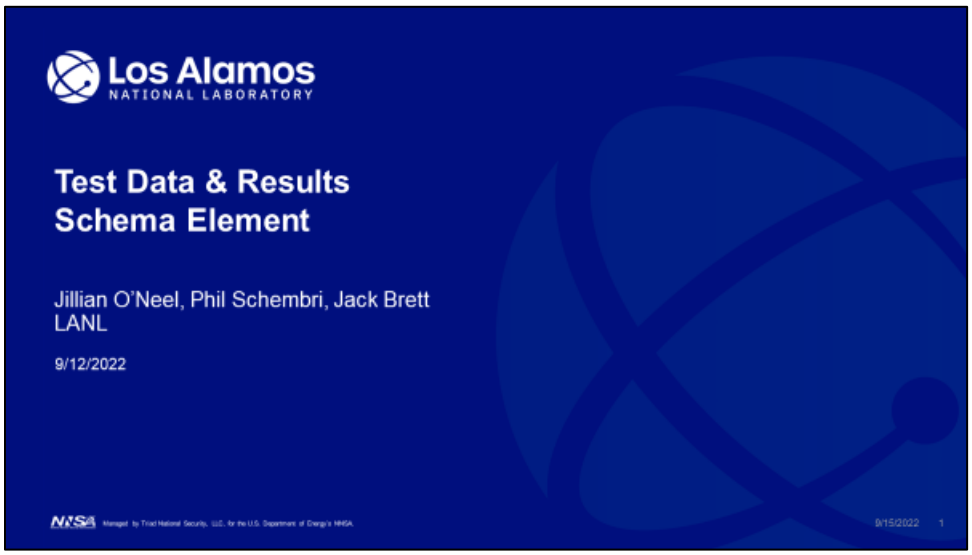
2/2/2022 9

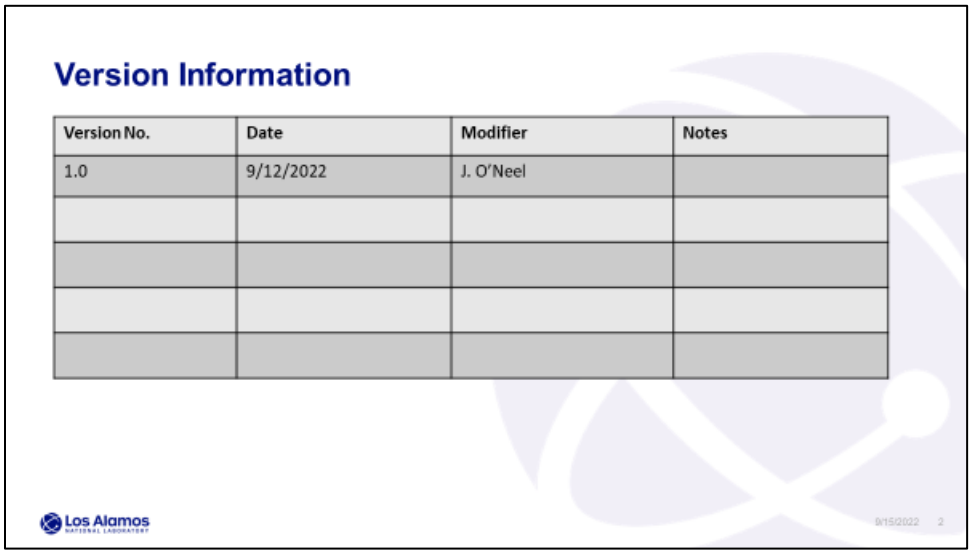
Relationship to ASTM F3490-21

Granta Attribute	ASTM Version (from Table 16)	Notes
Specimen ID	Specimen ID	
Specimen description	Specimen description	
Specimen location	Specimen location	ASTM uses "document" data type, Granta uses short text
Name of specimen preparer		Not in ASTM
Specimen manufacturing technique	Specimen Sampling Extraction Fabrication Method	
Specimen form	Specimen type	ASTM uses free text, Granta uses discrete
Specimen geometry	Specimen type	ASTM uses free text, Granta uses discrete
Specimen length		Not in ASTM
Specimen width		Not in ASTM
Specimen height		Not in ASTM
Specimen diameter		Not in ASTM
Specimen mass		Not in ASTM
Specimen density		Not in ASTM
Specimen information notes		Not in ASTM

2/2/2022 10

7.8 Test Data and Results





Schema Element name & definition

- Name = Test Data & Results
- Definition = This schema element contains attributes used to hold the data and results from a test. Generally, this schema element consists of functional data attributes that hold X-Y curve data as well as point, range, or tabular attributes that hold specific values. Data may be directly from test instrument sensors (ex: Load) or may be calculated (ex: Stress). Results are usually, but not always, determined by analyzing curve data (ex: Young's Modulus).

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9/15/2022 3

Attributes

Test Data & Results	
Mass percent vs. time	(float functional, series, parameter = Time)
Mass percent vs. temperature	(float functional, series, parameter = Temperature)
Derivative of mass percent vs. temperature	(float functional, series, parameter = Temperature)
Weight changes	(TABL)
Temperatures at onsets of weight change	(TABL)
Temperatures at maximum rates of weight change	(TABL)
Residual mass	(point)
Analysis method	(LTXT)
Name of analyzer	(STXT)
Document number of analysis document	(STXT)
Analysis document (static link to Documents table)	(static link)
Test data & results notes	(LTXT)

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9/15/2022 4

Uses cases & Requirements

- Use Case: As a data consumer, I would like to be able to plot TGA curves for multiple tests on one plot.
  - **Requirement:** Need functional attributes for all TGA curve data.
- Use Case: As a TGA data analyst, I would like to store results such as weight loss over a specified temperature range, onset of weight loss, maximum rate of weight loss, and temperature at X% weight loss.
  - **Requirement:** Need attributes to accommodate the above types of analysis, understanding that analysis varies from material-to-material and project-to-project.
- Use Case: As a data consumer, I would like to gather and report TGA analysis from multiple samples.
  - **Requirement:** Attributes should work with Granta reporting tools
- Use Case: As a TGA data analyst, I would like to replicate analysis performed previously.
  - **Requirement:** Need attributes to describe analysis.

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9/15/2022 5

Discussion points

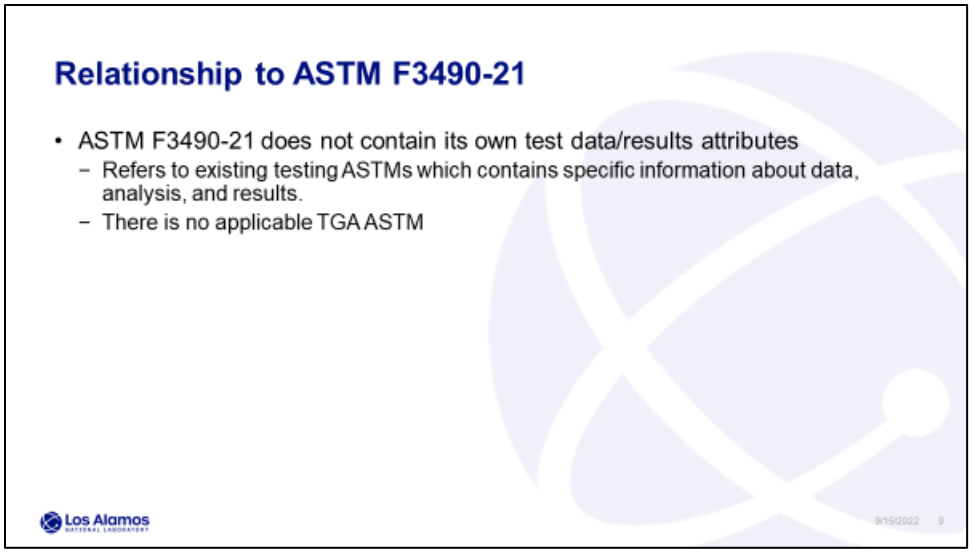
- Test records hold one test performed on one specimen
  - There are use cases around statistics and "roll-ups" (ex: averages) that will need to be addressed in the future, but not in this schema element.
- Best practices for functional data attributes
  - Naming:
    - 'Y-axis Quantity' vs. 'X-axis Quantity' (ex: Mass percent vs. temperature)
    - As with all other attributes, only first word is capitalized
    - 'vs.' = lower case with period
  - In MI:Admin:
    - Float Functional, Series
    - Do not select "Attribute can be used as search filter"
    - Add parameters thoughtfully (messes with python uploading)
      - These TGA attributes only have 1 parameter for 'X-axis quantity'

Discussion points

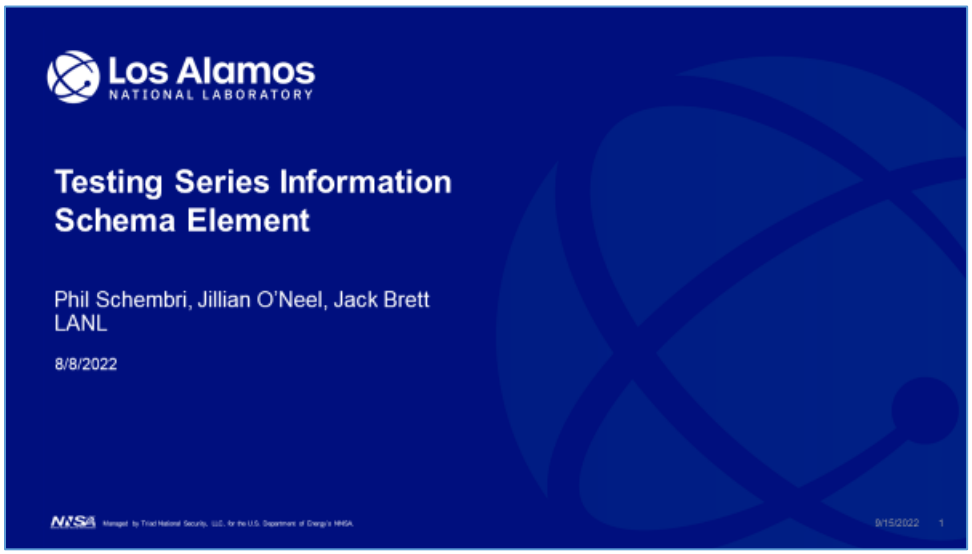
- Results Attributes (Point vs. Tabular)
  - Point:
    - Pros: Easier to import (text importer), Easier to report (comparison chart)
    - Cons: Will need separate attributes for all potential analysis scenarios (ex: Weight Loss (%) by 325°C, Temperature at 5% Weight Loss, First Weight Loss Onset, Second Weight Loss Onset, etc.) = a lot of attributes, Harder to combine and compare datasets (when exporting or comparing data sets will need to know which analysis attributes are populated)
  - Tabular:
    - Pros: 4 attributes cover all potential data analysis scenarios (production, R&D, new materials, etc.)
    - Cons: Harder to import (no text importers, a little extra formatting for excel importers), Harder to report (Excel reports)

Discussion & Resolution

TBD



7.9 Testing Series Information



Schema Element name & definition

- Name = Testing Series Information
- Definition = This schema element contains information about the testing series that the record is a part of. Most of the attributes are actually links since the information about testing series is contained natively in the Testing Series table, and we want to avoid duplication.

- What is a 'Testing Series'?
  - E.g. compression tests on a material at various temperatures & rates
  - Loose definition: *A set of tests in which some independent variables are being varied*
  - A Testing Series might just be convenient to organize tests into sets (e.g. acceptance tests performed in FY23Q1).
  - There could be one or more Testing Series in a project

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9/15/2022 2

Attributes

Testing Series Information	
Testing series ID	Short text (unique to testing series)
Testing series (static link to Testing Series table)	Static link
Testing series (smart link to Testing Series table)	Smart link
Linked testing series information	Linked tabular
Testing series information notes	Long text

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9/15/2022 3

Use Cases and Requirements

- **Use case**: As a data consumer I would like to see which series of tests a test record belongs to so I can find related test data; e.g. replicate tests and/or tests at neighboring conditions.
  - **Requirement**: complete links from tests to Testing Series and from Testing Series to tests. Testing Series ID required to be unique to each testing series.
- **Use case**: As a material modeler, I would like to know which testing series' a material model was calibrated with and metadata about those series'
  - **Requirement**: complete links from tests to Testing Series and from Testing Series to tests. Testing Series ID required to be unique to each testing series.

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9/15/2022 4

Discussion Points

- Should we require a Testing series ID in a test record? (i.e. should all test records be linked to a Testing Series record?)
  - Note that we required Project ID for testing records
  - We propose *not* requiring **Testing series ID** to remove unnecessary overhead for one-off tests, although it should be highly recommended in every other case.
- The **Testing series ID** is required to be unique to a testing series, no two Testing Series records can have the same **Testing series ID**.
  - Obviously, multiple test records can contain the same **Testing Series ID**.
- Tables using this schema element will choose between either the static or the smart links:
  - Smart links when one-to-many relationship is expected between Testing Series table and the table using this schema element (e.g. for testing tables)
  - Static links when many-to-one relationship is expected between Testing Series table and the table using this schema element (e.g. for Calibrated Material Models tables)
  - **Linked testing series information** can be used in both cases

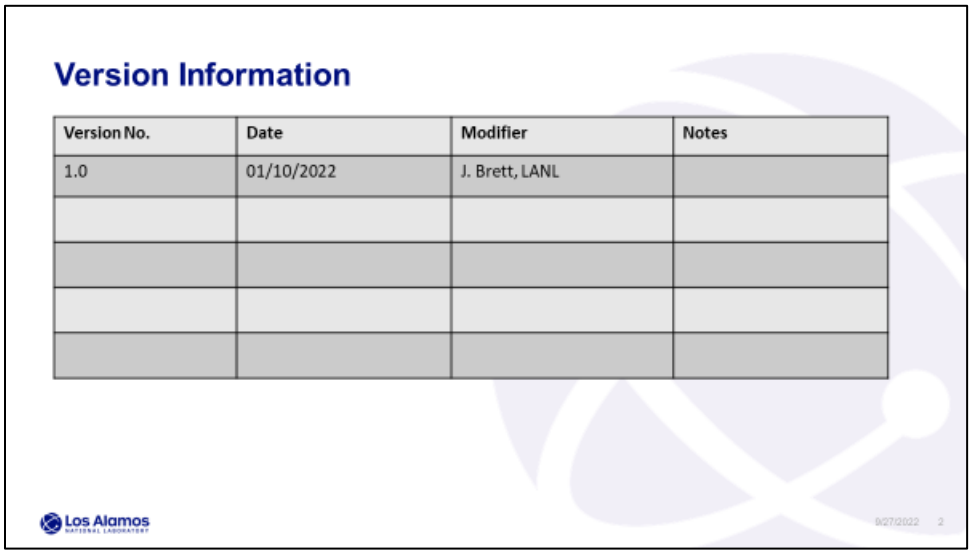
Discussion Points cont.

- **Testing series information notes** is not for notes about the testing series (which would be entered in the Testing Series record itself); it's for notes about the Testing Series Information attributes. E.g. "This test was originally intended to be part of Testing Series A, but the specimen was not used for that series and was used for Testing Series B instead."
- Reminder: The structure of links established in this schema element follows that for other similar schema elements.
  - Template
    - 'ID' short text attribute (e.g. **Project ID**)
    - Tabular link (e.g. **Linked project information**)
    - Smart link or Static link
  - Other tables probably using similar structure
    - Projects
    - AM Builds
    - Materials
    - Testing Series
    - Etc.

Relationship to ASTM F3490-21

- The Testing Series Information schema element is judged to be consistent with F3490-21 because:
  - F3490-21 doesn't use the any object between 'Project' and 'test'.
  - Testing Series Information is not required.
  - Data could be transferred between a database with Testing Series and one without, and not inconsistencies would be introduced.

7.10 Material Pedigree Information



Schema Element name & definition

- Name = Material Pedigree Information
- Definition = This schema element contains information about the material pedigree that the test specimen is a part of. Most of the attributes are actually links since the information about material pedigree is contained natively in the Material Pedigree table, and we want to avoid duplication.

Attributes

Attribute Name	Attribute Type	Value Set
Material pedigree ID	STXT	Unique in Material Pedigree table
Material pedigree	Static link to Material Pedigree table	
Material pedigree	Smart link to Material Pedigree table	
Linked material pedigree information	Linked TABL	Linking value = Material Pedigree ID
Material pedigree information notes	LTXT	

Use Cases and Requirements

- As a data consumer I would like to see all records related to a specific material pedigree (without having to perform a search) so I can ensure I have a complete data set.
  - Requirement: complete links from tests to material pedigree and from material pedigree to tests. Material Pedigree ID required for uniqueness.
- As a data consumer I would like to see all records related to a specific material pedigree (without having to perform a search) so I can discover data related to records I found using a search. E.g. I search for mechanical test data for SX358 Lot#12345 and I discover thermal test data for SX358 Lot# 12345 because it's part of the same project.
- As a data consumer I would like to see summary information about the material pedigree that a test record is associated with so I can judge whether the test data is applicable for my needs. E.g. Was the test performed on pristine or aged material?
  - Requirement: tabular attribute (**Linked material pedigree information**)

Discussion Points

- The Material Pedigree ID is required to be unique, no two instances of a material can have the same Material Pedigree ID
- Tables using this schema element will choose between either the static or the smart links:
  - Smart links when one-to-many relationship is expected between Material Pedigree table and the table using this schema element (probably most common for testing tables)
  - Static links when many-to-many relationship is expected between Material Pedigree table and the table using this schema element (probably most common for projects, testing series, etc.)
  - **Linked material pedigree information** can be used in both cases
- **Material pedigree information notes** is not for notes about the material pedigree (which would be entered in the Material Pedigree record itself); it's for notes about the Material Pedigree Information attributes.
  - Any material pedigree-specific information displayed in the record using this schema element should be linked through **Linked material pedigree information**