

LA-UR-22-28376

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Title: Granta upload bottlenecks at LANL

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Intended for: Discussion with uncleared vendor via webex

Issued: 2022-08-10



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Granta upload bottlenecks at LANL

Phil Schembri, Jillian O'Neel

8/17/2022

Agenda

- Brief overview of LANL database
- Use-case 1: Material Properties records
- Use-case 2: Aging & compatibility test records
- Tools that might be useful

Brief overview of LANL database

Weapons Materials

- LANL Weapon Systems Engineering Materials Data
 - Calibrated Material Models
 - Common Material Properties
 - Isotopic MCNP Cards
 - Documents
 - Test Equipment
 - Pedigree
 - Projects
 - Testing Series
 - Testing - Specimen Measurements
 - Testing - DMA
 - Testing - Torsional DMA
 - Testing - PVT
 - Testing - Shear
 - Testing - Triaxial
 - Testing - Biaxial
 - Testing - Uniaxial
 - Testing - SHPB
 - Testing - Gun Experiments
 - Testing - Taylor Impact
 - Testing - Onion Skin
 - Testing - TMA and Dilatometry
 - Testing - TGA
 - Testing - TCA
 - Testing - DSC and MDSC
 - Testing - Fourier-Transform Infrared Spectroscopy
 - Testing - Time Domain NMR (MOUSE)
 - Testing - Imaging
 - Tools
 - Isotopes

LANL Weapon Systems Engineering Materials Database

Database Homepage

Home Properties Material Models Test Data Documents Parts Export to Abaqus Help

Home: Database Map

```

graph TD
    Parts --> MaterialPedigree
    Parts --> MaterialProperties
    TestData --> MaterialProperties
    TestData --> MaterialModels
    Documents --> MaterialProperties
    Documents --> MaterialModels
    MaterialProperties --> MaterialModels
    MaterialModels --> ExportCode
    
```

- **Parts** are associated with **material properties** through the material specification. Multiple parts may be associated with a single material.
- **Test data** and/or **documents** provide supporting data for both material properties and **material models**.
- Material property information feeds into the material model.
- There may be more than one material model for each material, but each material model will share the same material property information.
- Material models can be exported to a text file in **Abaqus format**.
- Links between records (record links, tabular data links, or both) represent the arrows in this diagram.
- *Note that this unclassified version of the database does not contain all the functionality or data of the classified version. Data/functionality missing here and available on the classified database is pointed out using this red italic font.*

- Several organizations upload **test data**
 - Tools and workflows specific to instruments
- Several organizations upload material **property** & calibrated material model (**CMM**) data, linked to test data
- **Many users** upload data; no centralized 'Granta group'
- Data must be **reviewed** for consistency before release

Use case 1: Material properties

- Primary producer and consumer is Engineering Analysis group.
- Relatively small number of Properties records.
 - Usually created manually in Viewer
- Even ‘frequent’ Granta users struggle to make records consistent with standards.
 - Standards documented in help files and Confluence
- Creating/editing records is high-effort.
- Not fun for users to be told to revise their records many times after review.

Use case 1: Material properties; example record

Contents

Weapons Materials

- LANL Weapon Systems Engineering Materials Database
 - Calibrated Material Models
 - Common Material Properties
 - Subset:Material Properties (Default)
 - Ceramics [v1 Unreleased]
 - Elastomers [v1 Unreleased]
 - Foams [v1]
 - High Explosives [v1]
 - Metals [v1]
 - Aluminum [v1]
 - Beryllium [v1]
 - Gold [v1]
 - Silver [v1]
 - Steels [v1]
 - Titanium [v1]
 - Ti6Al4V [v1]
 - Ti6Al4V [AMS4928] [v4]**
 - Uranium [v1]
 - Vanadium [v1]
 - Plastics (other) [v1]
 - W-11 Materials [v1]
 - Working Folder [v1 Unreleased]
 - Recycle Bin [v1 Unreleased]
 - Isotopic MCNP Cards
 - Documents
 - Subset:Documentation (Default)
 - Aluminum [v1]
 - B61 Stress Cushion [v1]
 - Beryllium [v1]
 - Beryllium Oxide [v1]
 - Boron Carbide [v1]

Ti6Al4V [AMS4928] [v4]

Record Information		
Data Sensitivity	NS - Non Sensitive - No CUI (Controlled Unclassified Info) Present	
Record Create Date	Wednesday, August 5, 2020	
Record Last Modified Date	Wednesday, February 16, 2022	
Data Originator	Laura Tucker (285185)	
Record Review Date	Wednesday, February 16, 2022	
Record Reviewed By	Philip Schembri (151333)	
Name of Modifier	Laura Tucker (285185)	
Project Information		
Project Name	Weapons Engineering Analysis Baseline Material Properties	
Material		
Material Name	Ti6Al4V	
Alternate Material Name	Titanium Alloy	
Material Description	Titanium 6Al-4V alloy per AMS 4928	
Material Specification	AMS 4928	
General		
Density Nominal	4.42878e-9	Mg/mm³
Density Range	4.40664e-9 to 4.45093e-9 Mg/mm³	
Baseline	Y	
Tabular Linking Value	Ti6Al4V (AMS4928) - Baseline	
Mechanical		
Yield Strength (Tension) Nominal	861.845	MPa
Yield Strength (Tension) Range	786 to 910 MPa	
Yield Strength (Compression) Nominal	889.424	MPa
Yield Strength (Compression) Range	848 to 1080 MPa	

Use case 1: Material properties; example record

The screenshot shows a materials database interface. On the left is a navigation tree for 'Weapons Materials' under 'LANL Weapon Systems Engineering Materials Database'. The main area displays the record for 'Ti6Al4V [AMS4928] [v4]'. The record is organized into sections: Record Information, Project Information, Material, General, and Mechanical. A red box highlights the 'Name of Modifier' attribute in the Record Information section, with a red arrow pointing to its definition in the sidebar.

Record Information		
Data Sensitivity	NS - Non Sensitive	
Record Create Date	Wednesday, August 14, 2019	
Record Last Modified Date	Wednesday, February 27, 2020	
Data Originator	Laura Tucker (2851)	
Record Review Date	Wednesday, February 27, 2020	
Record Reviewed By	Philip Schembri (1500)	
Name of Modifier	Laura Tucker (2851)	

Project Information		
Project Name	Weapons Engineering	

Material		
Material Name	Ti6Al4V	
Alternate Material Name	Titanium Alloy	
Material Description	Titanium 6Al-4V alloy per AMS 4928	
Material Specification	AMS 4928	

General		
Density Nominal	4.42878e-9	Mg/mm ³
Density Range	4.40664e-9 to 4.45093e-9	Mg/mm ³
Baseline	Y	
Tabular Linking Value	Ti6Al4V (AMS4928) - Baseline	

Mechanical		
Yield Strength (Tension) Nominal	861.845	MPa
Yield Strength (Tension) Range	786 to 910	MPa
Yield Strength (Compression) Nominal	889.424	MPa
Yield Strength (Compression) Range	848 to 1080	MPa

Name of Modifier

Definition

This attribute contains the name the person who most recently entered or uploaded data to this record.

Standards

This attribute is required.

The format of a name must follow the convention:

- **LANL Employee:** Firstname Lastname (Z number) **Example:** Thom Mason (172327)
 - Note that Firstname and Lastname must appear as they do in the LANL phonebook, except that nicknames (in parentheses in the LANL phonebook) should be used when available.
- **Non-LANL Employee:** Firstname Lastname. **Example:** Sam Smith

Best Practices

Only the most recent modifier needs to be listed since version history can be used to track previous modifiers. If multiple people have worked on a particular version of a record then multiple people may be listed here.

We try to maintain consistent format of 'name' STXT attributes to facilitate 'search' use-cases

- Mistakes are often caught during review
- Discrete lists would be too long
- A table for Personnel would work, but is technically challenging

Use case 1: Material properties; example record

The screenshot shows a materials database interface. On the left is a tree view of the database structure, with 'Weapons Materials' selected. The main area displays the record for 'Ti6Al4V [AMS4928] [v4]'. The record is organized into several sections:

- Record Information:** Data Sensitivity, Record Create Date, Record Last Modified Date, Data Originator, Record Review Date, Record Reviewed By, Name of Modifier.
- Project Information:** Project Name.
- Material:** Material Name (highlighted with a red arrow), Alternate Material Name, Material Description (Titanium 6Al-4V alloy per AMS 4928), Material Specification.
- General:** Density Nominal, Density Range, Baseline, Tabular Linking Value.
- Mechanical:** Yield Strength (Tension) Nominal, Yield Strength (Tension) Range, Yield Strength (Compression) Nominal, Yield Strength (Compression) Range.

Material Name

Definition

This is the commonly-used name of the material.

Standards

This attribute is required.

Best Practices

Naming conventions are not widely documented, and there is no universally accepted taxonomy. Thus, users should not rely on the **Material Name** to find records; instead, the tree-level attributes should be used to find all materials at a specified level. For example, all metals, all aluminum alloys, or all 6061 alloys, etc.

To enter a **Material Name**, consider the following guidance:

- For METALS, the convention is:
 - Element name first, using the elemental symbol such as Ag, W, Cu if the material is an alloy but spelled out (e.g. 'uranium') if it is 'pure'.
 - For alloys, add wt% composition (volume % is unusual for manufacturing use but either can be detailed in the material description internal to the record) of alloying elements: examples are Ta2.5W (i.e tantalum with 2.5wt% tungsten); and Ti6Al4V.
 - Give wt% composition for minor alloying elements only (e.g. "Sn36Pb2Ag" not "Sn62Pb36Ag2")
 - Use just major and minor elements if exact composition is unknown or not specified. E.g. AlBe
 - One exception to this naming rule is for classes of alloys such as Steels. In this case the naming would start with the class name and proceed as follows : Steel Stainless 304L (i.e., not 304L Stainless Steel).
 - As a general rule, we will omit processing information (e.g. 'Cast', 'T6') from the material name. This should be captured in the Pedigree record in the appropriate attributes and/or in an Alternate Material Name attribute.
 - For specific isotopes, the isotope number should be written after the element. For example, 'U238'. Context is expected to make it clear that this is different from an alloy wt%.
 - Examples of metals material names:
 - Steel Stainless 304L
 - Al 6061
 - U6Nb
 - Au15Ag
 - Beryllium
 - U238
- For POLYMERS:
 - If applicable, use a tradename. Examples:
 - SX358
 - Sylgard 184
 - Silastic J
 - If a tradename is not applicable use the chemical name if a single word or acronym if multiple words.
 - Polyurethane Foam
 - Polyethylene
 - Polypropylene
 - PET
 - VCE
- For COMPOSITES:
 - Use the name of one of the components of the composite and the word 'Composite'. Examples:
 - Tungsten Carbide Composite
 - Epoxy Composite
- For CERAMICS, use the spelled-out chemical name (not chemical formula) of the material. Examples:
 - Tungsten Carbide
 - Alumina

Material Name is particularly challenging. It would be really nice to have:

1. Context sensitive discrete types
2. A standard taxonomy

Use case 1: Material properties; example record

Contents

Weapons Materials

LANL Weapon Systems Engineering Materials Database

- Calibrated Material Models
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 - Elastomers [v1 Unreleased]
 - Foams [v1]
 - High Explosives [v1]
 - Metals [v1]
 - Aluminum [v1]
 - Beryllium [v1]
 - Gold [v1]
 - Silver [v1]
 - Steels [v1]
 - Titanium [v1]
 - Ti6Al4V [v1]
 - Ti6Al4V [AMS4928] [v4]**
 - Uranium [v1]
 - Vanadium [v1]
- Plastics (other) [v1]
- W-11 Materials [v1]
- Working Folder [v1 Unreleased]
- Recycle Bin [v1 Unreleased]

Isotopic MCNP Cards

Documents

Test Equipment

Pedigree

Projects

Testing Series

Testing - Specimen Measurements

Ti6Al4V [AMS4928] [v4]

Poisson's Ratio Range	0.31 to 0.37	
Young's Modulus Nominal	116521	MPa
Young's Modulus Range	110000 to 119000	MPa
Young's Modulus vs. Temperature	View Graph	
Shear Modulus Nominal	42500	MPa
Shear Modulus Range	40000 to 45000	MPa
Bulk Modulus Nominal	124900	MPa
Bulk Modulus Range	96800 to 153000	MPa
Elongation	10 to 14	%

Thermal

References and Data Basis

Property Attribute Data Basis

All **NOMINAL data** comes from MMPDS-15 (July 1st 2020) and MMPDS-13 (July 1st 2018). The MMPDS-15 Chapter 5 (pp 5-59 to 5-70) is linked below under *Documents*. MMPDS-13 is available in Grant. see link under the *Further Information / MMPDS Data* section. The data can be found in both sources, although the page numbers, table numbers, and /or figure numbers may differ.

All **RANGE/ Min-Max data** comes from Material Universe record *Titanium, alpha-beta alloy, Ti-6Al-4V, annealed*, see link under the *Further Information / Material Universe* section. The range data is for future property sensitivity analysis.

Density Nominal, Young's Modulus Nominal, Poisson's Ratio Nominal, Yield Strength (Tension) Nominal, Yield Strength (Compression) Nominal, and Ultimate Strength (Tension) Nominal comes from MMPDS-15, *Ti-6Al-4V, Annealed, Bar, Thickness: 0.5 to 1.001 in, AMS 4928, A Basis*.

- This data can be found in the linked document, MMPDS-Chapter 5 - 2020, Table5.4.1.0(c1), pp 5-63,
- Note that when MIL-HDBK-5G was updated to MMPDS, the modulus was changed slightly from 16E3ksi to 16.9E3ksi.

Density Range, Yield Strength (Tension) Range, Yield Strength (Compression) Range, Ultimate Strength (Tension) Range, Flexural Strength (bending), Poisson's Ratio Range, and Young's Modulus Range data comes from Material Universe record *Titanium, alpha-beta alloy, Ti-6Al-4V, annealed* available in Granta (link under the *Further Information* section).

Young's Modulus vs. Temperature data comes from Material Universe record *Titanium, alpha-beta alloy, Ti-6Al-4V, annealed* (link under the *Further Information* section)

References and 'data basis' are critical in Properties and CMM records.

Users rarely provide sufficient information in a useful format.

This is caught and corrected during review.

Use case 1: Material properties; Confluence

The screenshot shows a Confluence page within a 'Material Database' space. The page title is 'Guide to Creating Material Property (CMP) and Calibrated Material Model (CMM) Records', created by Philip Edward Schembri on May 12, 2022. The page content includes a 'Prerequisites' section with six numbered steps, a 'Step 1: Create a new CMP record (if necessary)' section, and a 'To create a new CMP record:' section with six numbered steps. The left sidebar shows a page tree with the current page selected.

Confluence Spaces People Calendars Create Search

Material Database

Pages Blog Calendars

PAGE TREE

- > Getting Started with Granta
- ▼ How to Use Granta
 - > I want to get data from Granta
 - ▼ I want to put data in Granta
 - > Guide to Uploading Test Data
 - **Guide to Creating Material Property (CMI)**
 - How to add or edit data using MI:Viewer
 - How to Edit a Version Controlled Record
 - How to create or edit static record links
 - How to create a new document record
 - How to edit a single record using Excel and R
 - How to create multiple records using MI:Tool
 - How to Edit Multiple Records Using MI:Tool
 - How to change the units when importing data
 - How to upload a record using text importers
 - I have some data that should be uploaded, w
 - > How to Make Better Graph Legends Using Pa
 - > I want to modify database schema
 - > I want to integrate Granta with other software
 - > I want even more information about Granta

Pages / ... / I want to put data in Granta

Edit Save for later Watching Share

Guide to Creating Material Property (CMP) and Calibrated Material Model (CMM) Records

Created by Philip Edward Schembri, last modified on May 12, 2022

This page will help you create new CMP and/or CMM records. It's also required reading if you're editing existing CMP or CMM records.

Prerequisites

1. Make sure you have a [Granta account](#) and [read/write access to the LANL Weapon Systems Engineering Materials Database](#) in Granta.
2. Read this page: [How is the LANL Weapons Materials Database \(WMD\) organized?](#) Particularly the sections about the CMP and CMM table. We assume you understand the definitions and conventions described there.
3. Read the [Paradigm of Reproducibility](#).
4. Check to make sure records for the CMP/CMM you want to create don't already exist.
5. Gather all supporting information/references/data about the material properties and material model parameters you are about to create or edit.
6. Consult a DC about the classification of the information. If it is unclassified, create all records on the unclassified Granta instance and later push them to the red side.

Step 1: Create a new CMP record (if necessary)

Note that if you are creating a CMM record then a CMP record must exist for that material.

To create a new CMP record:

1. Create a [working folder](#) for your records in the CMP table if you don't already have one.
2. In your working folder, [create a new CMP record](#).
 - **Important:** Adhere to the CMP record naming convention described here: [Granta Naming Conventions for the Material Database](#).
3. Populate the data
 - a. If necessary ensure that all [attributes are visible](#) in the record you are editing.
 - b. Follow the standards and best practices documented in the [Attribute Help Pages](#) (a.k.a. [Attribute Definitions](#)). Pay particular attention to:
 - **Material Name**
 - **Material Specification**
 - **Other Material Qualifier**
 - c. Most simple attributes can be [edited in MI:Viewer](#) (i.e. in the browser).
 - d. Functional data is best edited/added using a 'round-trip' process of exporting the record into Excel, adding the data in Excel, and importing back into Granta. See: [How to edit a single record using Excel and Remote Import](#).
 - e. Note that the **Tabular Linking Value** attribute will be used to link this CMP record to a CMM record. So if you're planning to create a CMM record, this must be populated. The convention for this attribute is documented in the [help page](#).
 - f. The following properties are necessary for most engineering applications, and thus they are *highly recommended* to be populated for all CMP records. If possible, including these as a function of temperature is desirable in addition to including the nominal value. The reference databases, such as Material

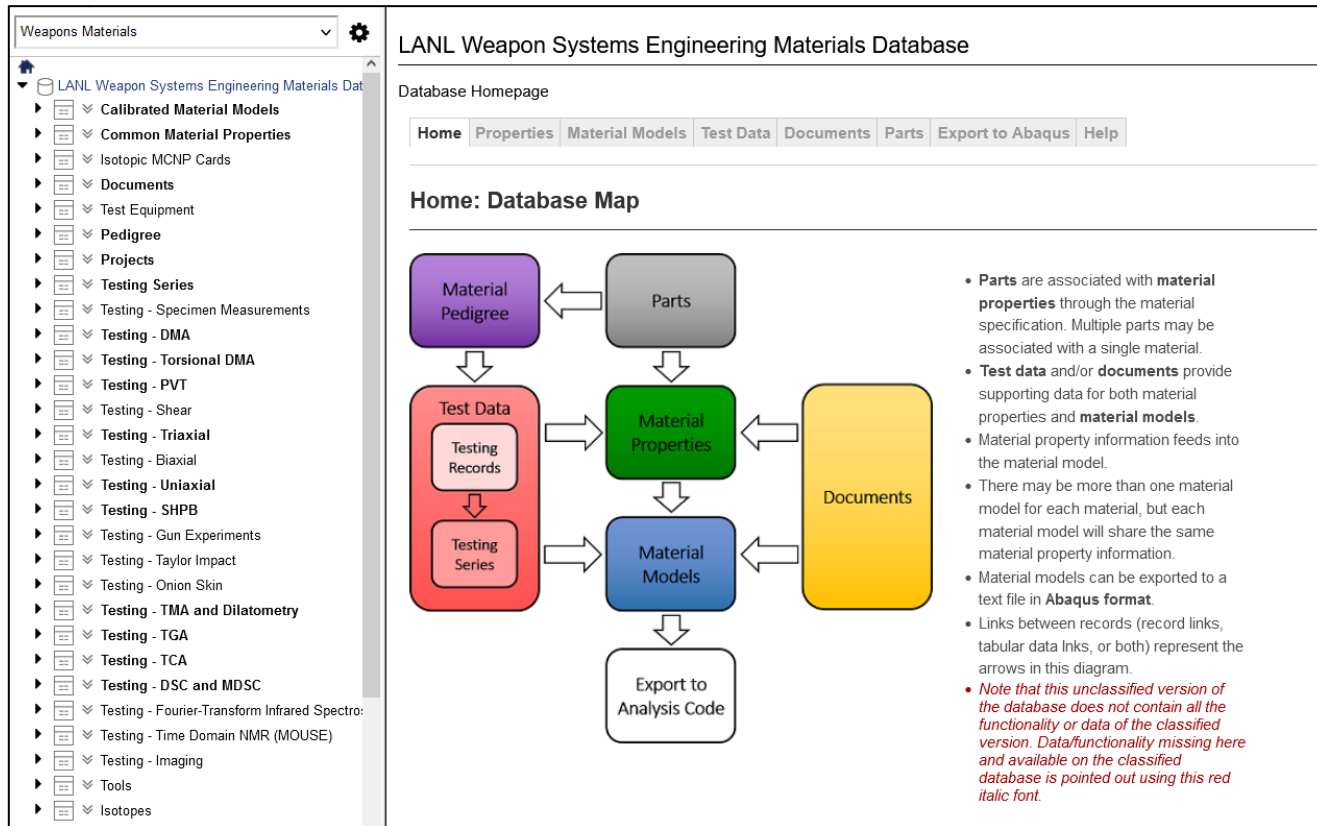
- We use Confluence for:
 - Documentation that cannot be captured in help files
 - Links
 - Record naming conventions
 - General workflow & prerequisites
- It's way too much for users to read in detail. They skip over it and miss important points

Use case 2: Aging & compatibility test records

- Data generated by materials science groups, often for part development and/or qualification
- Large number of records (~4000). Many independent variables including:
 - Material formulation
 - Batch/lot
 - ‘Aging’ temperature
 - ‘Aging’ time
- Multiple test types
 - Differential scanning calorimetry
 - Thermogravimetric analysis
 - Spectroscopy
 - Mechanical compression
 - etc

Use case 2: Aging & compatibility test records

- Data spread across multiple tables:
 - Projects
 - Pedigree
 - Testing Series
 - Test Equipment
 - Documents
 - Testing:
 - DSC
 - Uniaxial
 - TGA
 - Etc...
- Data comes from text files with some metadata
- Organization of data and other metadata added manually



Use case 2: Aging & compatibility test records

Can 31_Center [v1]

Project Information [Hide table](#)

Project Name	Project Code	Project Point of Contact	Funding Organization	Project Notes
18A Compatibility Tests	KNC800-QUALL18A	Paula Crawford (190482), Ronald Parker (094743), Mike Steinzig (118783)	Q-17	This project was performed to determine if there are any agr

Test Plan Document Number: TK5K0276-A-004

Test Report Document Number: TK5K0276-A-010

Test Plan, Test Report, and Other Documents

- LA-CP-19-00857 - (U) 18A Project Report – Part A: Characterization of [redacted] 2019 [v1]
- TK5K0276-A-004 - JTSR-18A Materials Aging and Compatibility Test fo [redacted] 2016 [v1]
- TK5K0276-A-010 - Final Report for JTSR-18A Materials Compatibility Test - 2020 [v1]

Data Information

Source of Testing

Calibration Information

Test information

Specimen Information

Specimen ID: Can 31_Center

Number of Replicates in this Record: 1

Replicate Number: 1

Specimen Location: Center

Material Name: [redacted]

Pedigree ID: Can 31 - 16 Months Cycle [redacted]

Material Pedigree Information [Hide table](#)

Pedigree ID	Material Name	Part Name	Part Number	Barcode Number	Linking value (Pedigree ID)	Linked records found
Can 31 - 16 Months Cycl	[redacted]	FLAT SHEETS (U)	4	[redacted]	Can 31 - 16 Months Cycl	Can 31 - 16 Months Cycl [redacted] [v1]

Material Pedigree

- Can 31 - 16 Months Cycl [redacted] [v1]

Workflow for uploading

- Gather files, reports, and any other information
- Upload test records using text import templates
- Create Pedigree records using Excel
 - These contain the ‘aging’ metadata
- Round-trip test records (per table) Toolbox & Excel
 - Export to Excel
 - Add metadata, links
 - Some is tabular, so VBA tools are needed to move data between sheets
 - Import
- Create additional records (Testing Series, Project, etc) manually
- Review (exporting to Excel...)

Use case 2: Aging & compatibility test records

The screenshot shows a Confluence page with a green header bar containing navigation options like 'Spaces', 'People', and 'Calendars'. The page title is 'Reviewing records before releasing them' under the path 'Pages / ... / Reference Information (Administration)'. The content is organized into three parts:

- Part one - using Viewer to look at a single record**

Sometimes looking at a record in Viewer helps you spot potential issues. So although it's not practical to look at every testing record, I usually spot-check one or two. Look at a record both with 'empty attributes' turned on and also turned off.

 - Make sure there aren't empty attributes that could/should be populated
 - Look for units errors in numerical attributes
 - Look for typos or stuff that doesn't make sense in text attributes
 - Click the data file to make sure it matches the record
 - Make sure any tabular attribute show up and show the correct information
- Part two - using Viewer to compare functional data**

For comparing functional data, I add all records I'm reviewing to a list and create a comparison chart for each functional data attribute.

 1. Check to make sure there aren't any curves much higher or lower than others
 2. Check to make sure the order of magnitude of the data makes sense, assuming it's data you have some intuition about (e.g. if it's an aluminum stress-strain curve, does it roughly agree with what you know about the strength of aluminum).
 3. Check that they all pass through the origin if they're supposed to.
 4. Select or unselect specific series (like 'cycles') to make the plot cleaner and easier to spot issues

This is mainly a high-level sanity-check (e.g. for units issues)
- Part three - using Toolbox to export to Excel**

Exporting records to Toolbox is very useful because it's easy to look down each column and see if any records stand out in any way. It's also handy in case there's anything obvious you want to correct.

 1. Open Toolbox, Select 'Export', and select all the records you want to review
 2. Use 'Automatically generated template' to export *almost* all attributes. I usually omit:
 - a. Tabular data - unless I know I want to edit it
 - b. Functional data - there's no useful way to review it in Excel
 3. Update the data file on your laptop. I usually include them and use check to make sure they are returned correctly and

- Review process can take as long as upload process.
- Confluence or reports document upload & review process.
- Because review often performed by technical SME, the 'Granta review' and 'technical review' overlap.
 - It becomes a very big job

Tools that might be useful

- In Viewer/Explore:
 - Walk user through workflow of uploading
 - Provide help file text in edit window
 - Check consistency of record name and attribute data
 - Check the format of STXT and LTXT attributes
 - Provide example text in the correct format
 - Disallow any incorrect format
 - Check whether linking values are valid
- For existing records:
 - Find data in a set of records that is *almost* identical (or is in an almost identical format)
 - Find records in a set of records that a missing attribute data that most other records have
 - Check validity of linking values
 - Identify records that are missing from a test matrix
- Automatic bulk record/data creation
 - Based on a test matrix (set of attribute values that are independent variables), e.g. for Pedigree records
 - Automatic creation of linking ('ID') values, which can then be tweaked