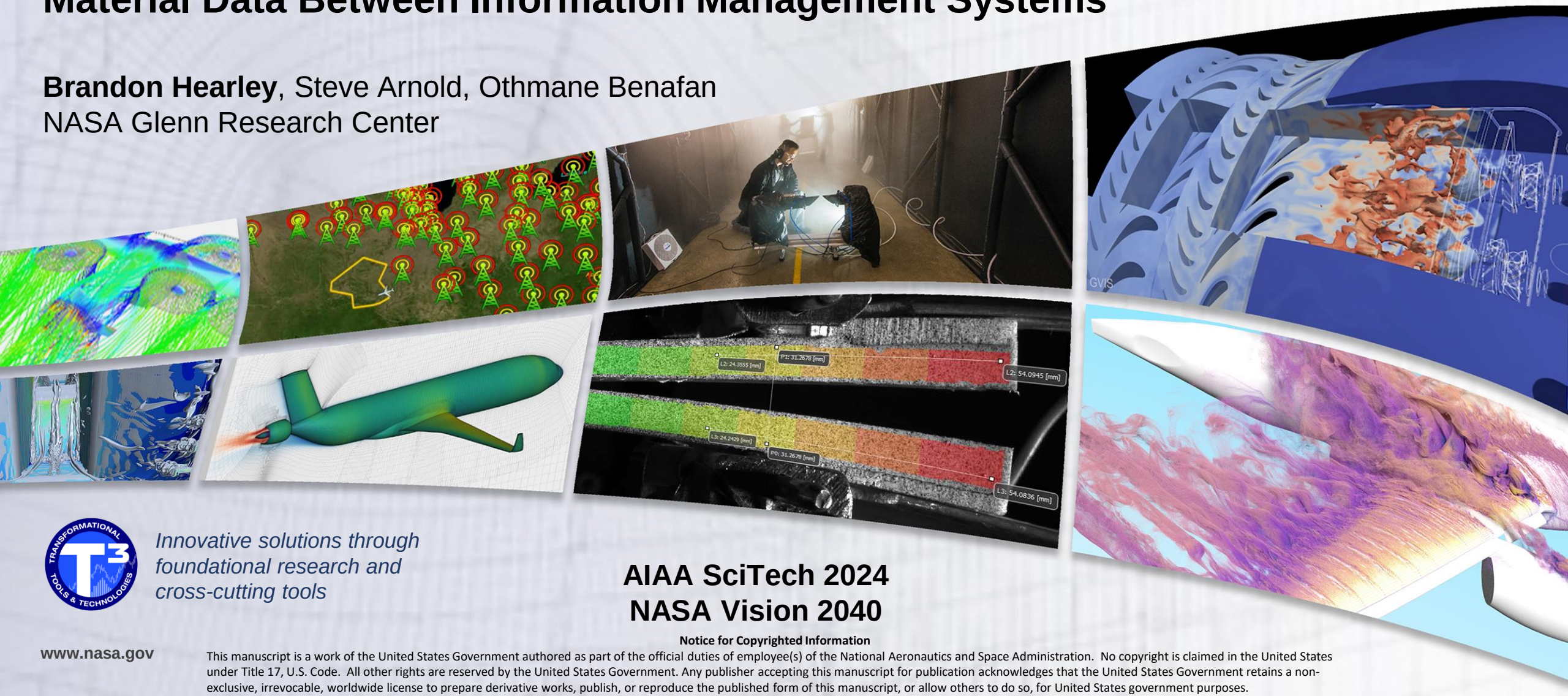
National Aeronautics and Space Administration

Transformational Tools and Technologies (T^3) Project

Capturing, Analyzing, Maintaining, and Disseminating Shape Memory Material Data Between Information Management Systems

Brandon Hearley, Steve Arnold, Othmane Benafan
NASA Glenn Research Center



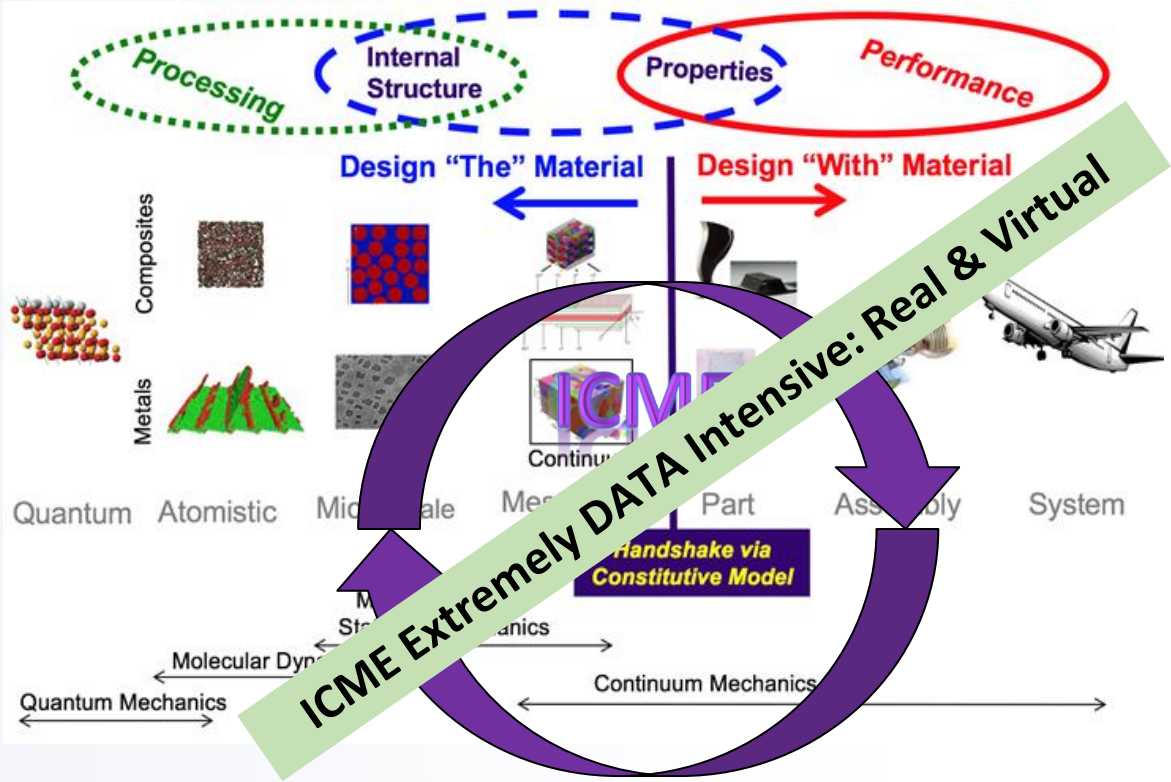
Innovative solutions through foundational research and cross-cutting tools

AIAA SciTech 2024
NASA Vision 2040

www.nasa.gov

Integrated Computational Materials Engineering (ICME) Enables Innovation

- Top performing organizations rate **New Materials** as one of **THE MOST IMPORTANT** factors in meeting their innovation goals (Historically new materials ≥ 20 years)
- Integrated Computation Materials Engineering (ICME) looks to bridge the gap between the "Design-the-Material" (Material Science) and "Design-with-the-Material" (Structural) viewpoints
  - Enables design of 'fit-for-purpose' materials
- Requirements for ICME
  - **Experimentally validated materials models at multiple length scales**
  - Understanding processing-structure-properties-performance relationships
  - Integrated framework that can automatically pass information across scales during design optimization
  - Manufacturing capability to achieve desired microstructure at any location in an application



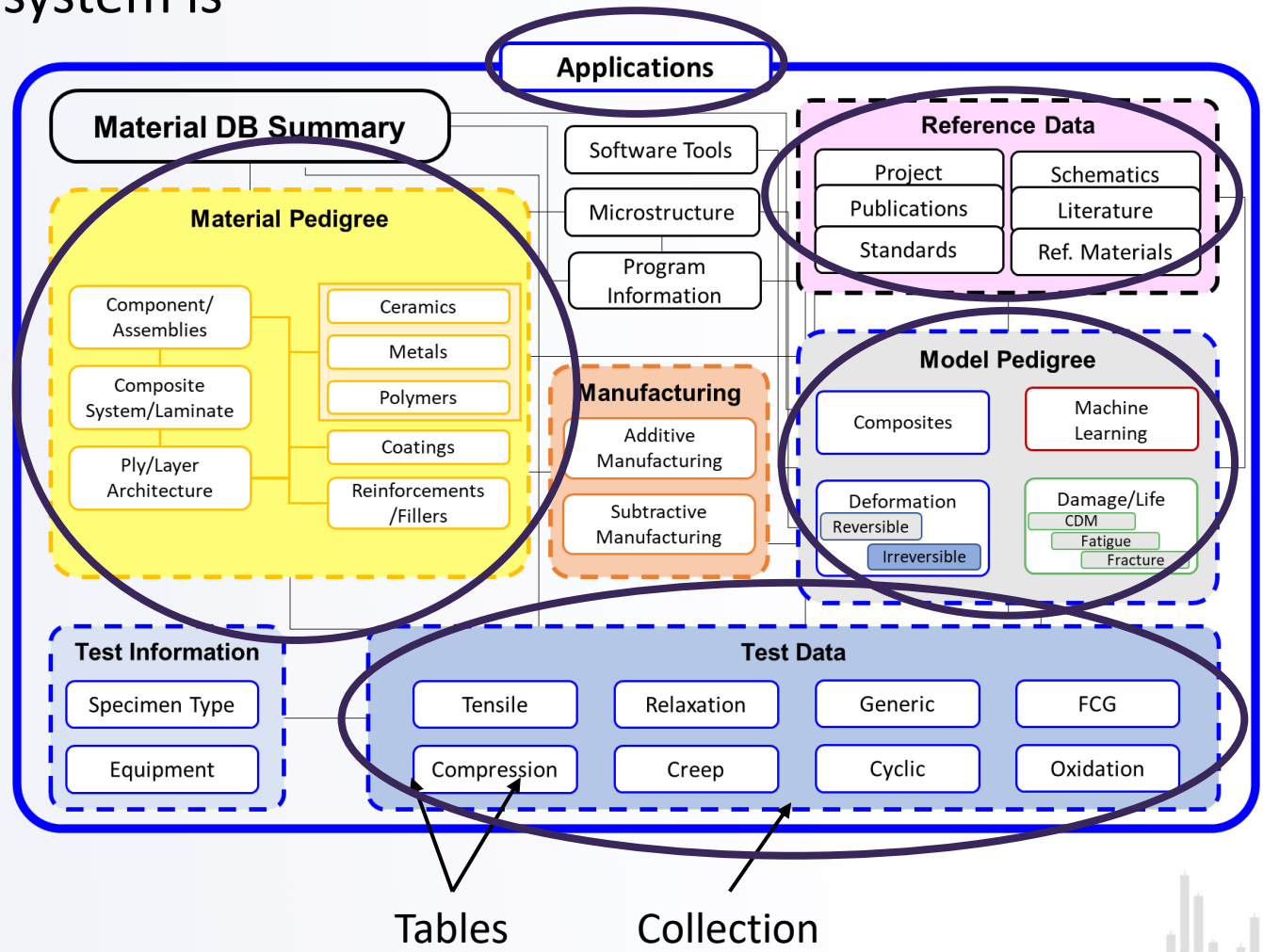
Vision 2040 has identified
Data, Informatics, & Visualization
as a Key Element Discipline Area

NASA GRC ICME Schema

A robust material information management system is **essential** for fit-for-purpose material design

- Developed the NASA GRC ICME Schema within the Granta MI Material Information Management Platform
- Contains *collections* of *tables*, where each table has its own schema (i.e., attributes, layout, linking behavior, security controls, etc.)
  - Material Pedigree: Store material source information, properties, etc.
  - Test Data: Store in-house experimental data and summarize into material properties
  - Model Pedigree: Store material models developed from experimental and virtual data (machine learning)
  - Reference Data: Store references, literature data, virtual data, etc.
  - Application Table: Link material models to parts for digital thread maintenance

NASA/TM-20220018403



NASA/TM-20230018337: NASA GRC ICME Schema for Materials Data Management: An Executive Summary

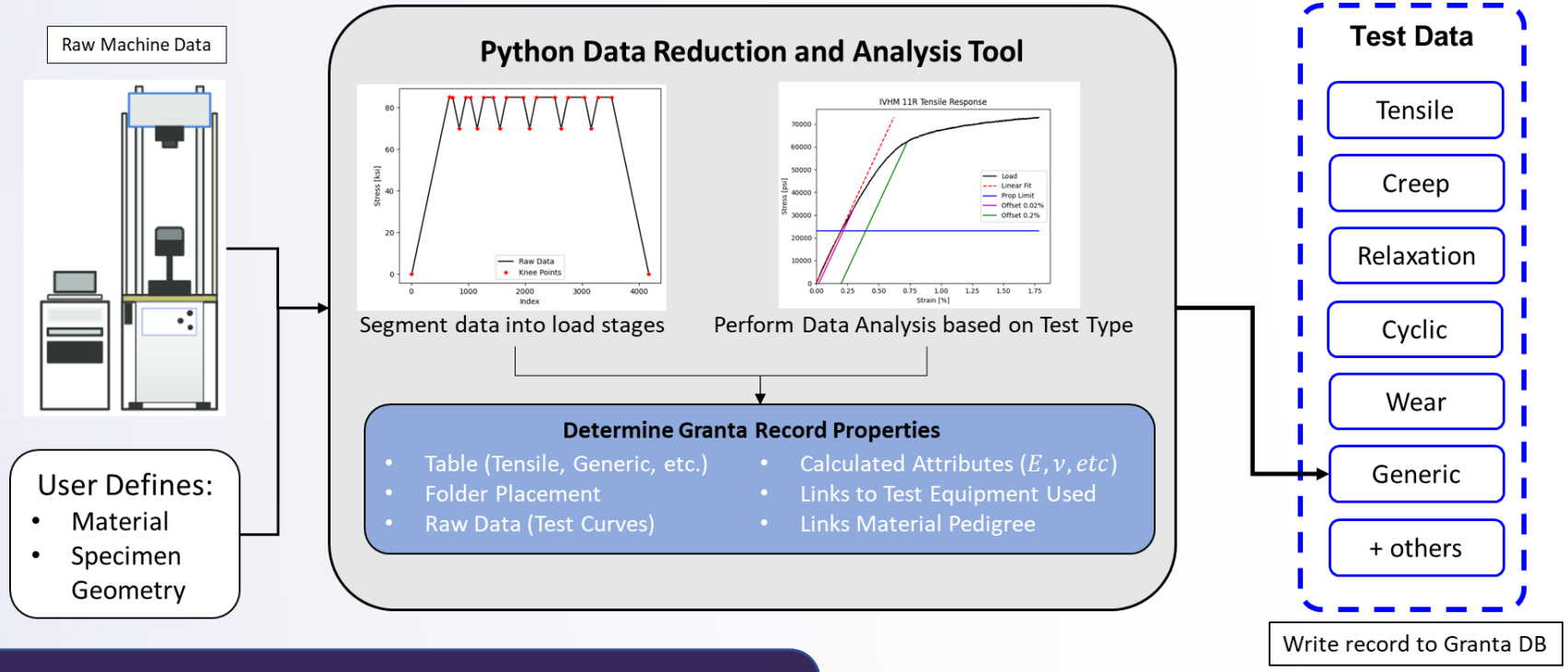
Developing a Cyber-Ecosystem of Validated Tools and Models is Paramount for ICME

- **NASA Vision 2040** envisions a **cyber-physical-social ecosystem** of **experimentally validated** computational models, tools, and techniques, along with the associated digital tapestry, that can enable rapid, optimized, 'fit-for-purpose' design of materials, components, and systems
  - *Unrealistic* to assume one tool will be used by an organization for all data analysis and storage
  - Effective information management tools should be able to interact with other, specialized tool and databases – overcome both **technical** and **cultural** challenges with digital transformation

- Present two different methods for capturing, analyzing, and storing test data within a robust information management system:
  1. User developed analysis tool that directly reads raw data, analyzes it, and stores it in the database
  2. A database tool that interacts with both an existing analysis software and database to capture and link additional information outside of the initial tool's scope

PyMILab: Efficient Data Analysis and Importing is Critical to Effective Data Management

- **Goal:** Develop an automatic framework to capture, analyze, and store **bulk** experimental test data in the NASA GRC ICME Schema
- Benefits
  1. Reduce User Effort for Data Management
  2. Provide traceability between test machine calibration and test performance
  3. Consistency in data analysis and reduction

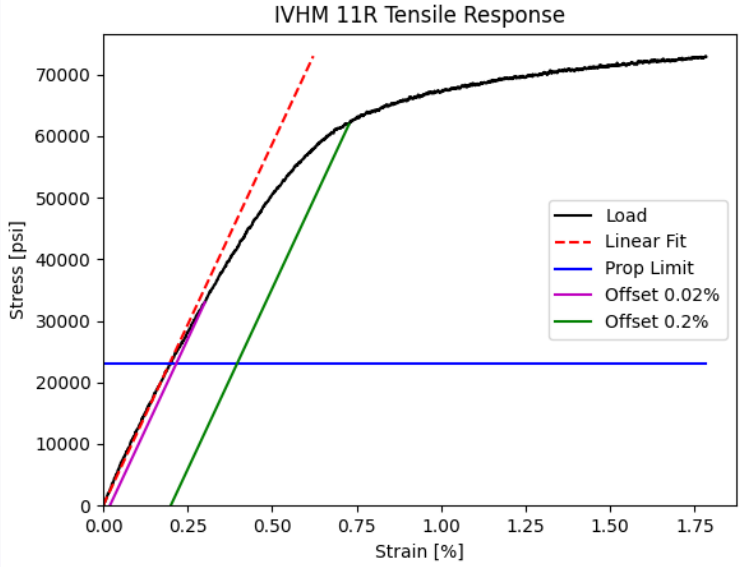


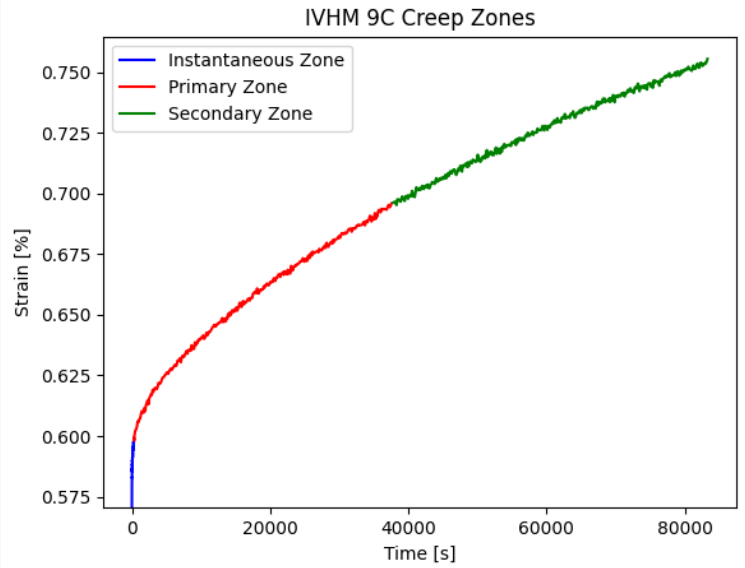
Automatic Placement + Data Analysis → Higher likelihood of organizational adoption

Experimental Data Automatic Import Tool:

Data Analysis for Standard Tests

- Test data is categorized as either Standard or Generic
  - Standard – Tensile, Relaxation, Creep
  - Generic – Combination of various standard test stages
- For each Standard Test, data analysis of raw data performed
  - Tensile – Modulus, Yield
  - Creep – Creep Zones, Creep Stress
  - Relaxation – Relaxation Stress, Loading/Unloading behavior
- Specific subroutines written for each test to perform the data analysis/parameter extraction
  - Store how parameters were calculated and write to each record to maintain material/test pedigree





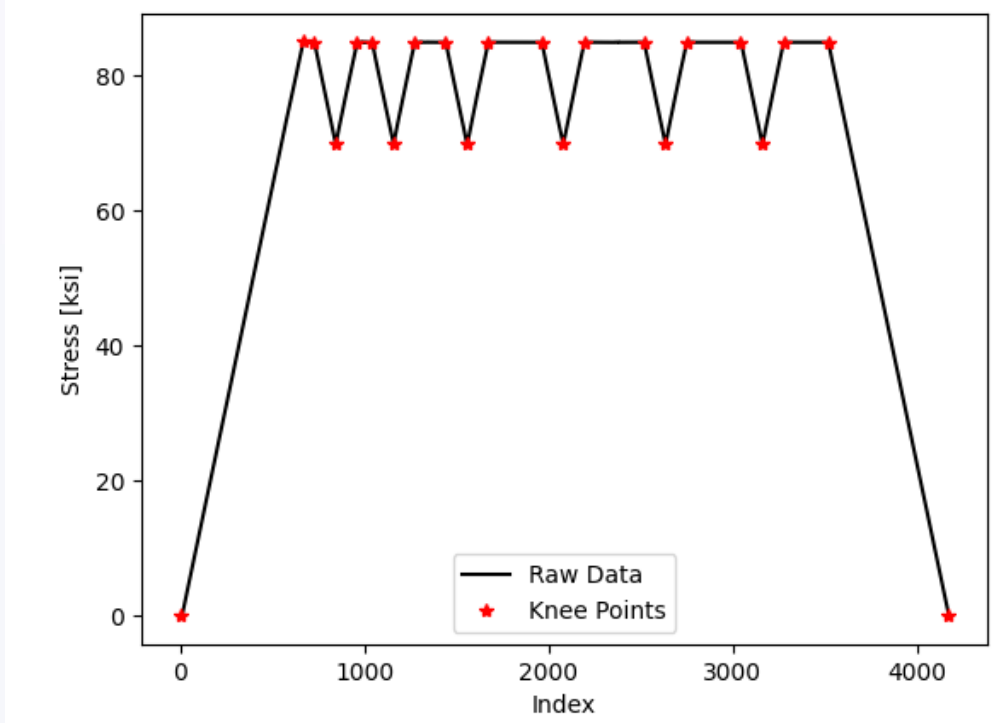
Modulus Calculation Range

- Loading Modulus calculated using datapoints from 5% to 25% of maximum stress, calculated using Linear Fit method (R2 = 1.00)

Experimental Data Automatic Import Tool:

Defining Generic Tests

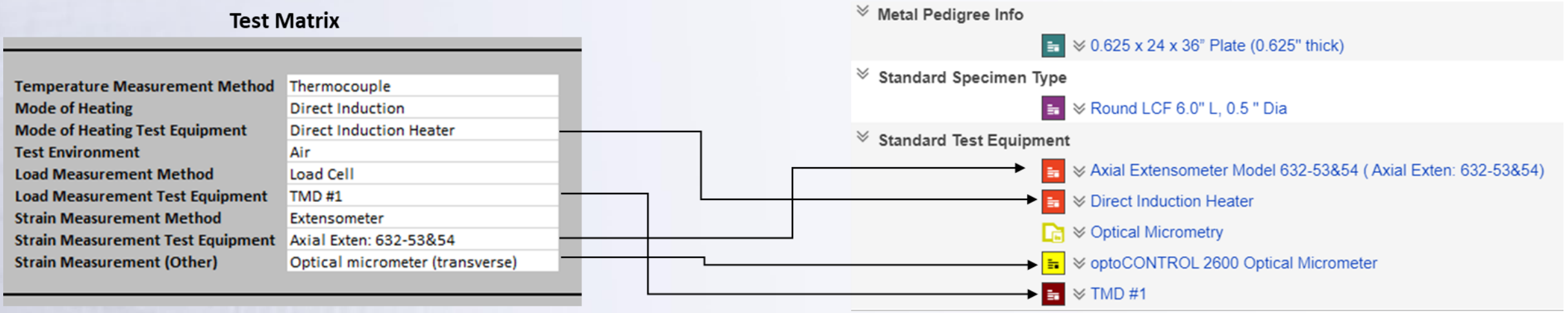
- Generic Tests contain various stages of one of the standard test types
  - Stages endpoints are automatically recognized by implementing a knee-point algorithm
  - Control Modes are determined from analyzing the stress-time and strain-time behavior of each stage
  - Stage Type is determined using the table below



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

Automatic Linking Capability Enables Pedigree Maintenance

- From the information defined in the Excel Test Matrix supplied by the user, links to other records in the database are automatically populated
  - Automatic links to the test equipment and measurement devices ensure that *how* the data was captured is maintained in the database
  - If a test is out of spec. or the machine is found to be out of calibration, automatic linking can provide a list of potentially effected records to ensure that the data in the database is correct



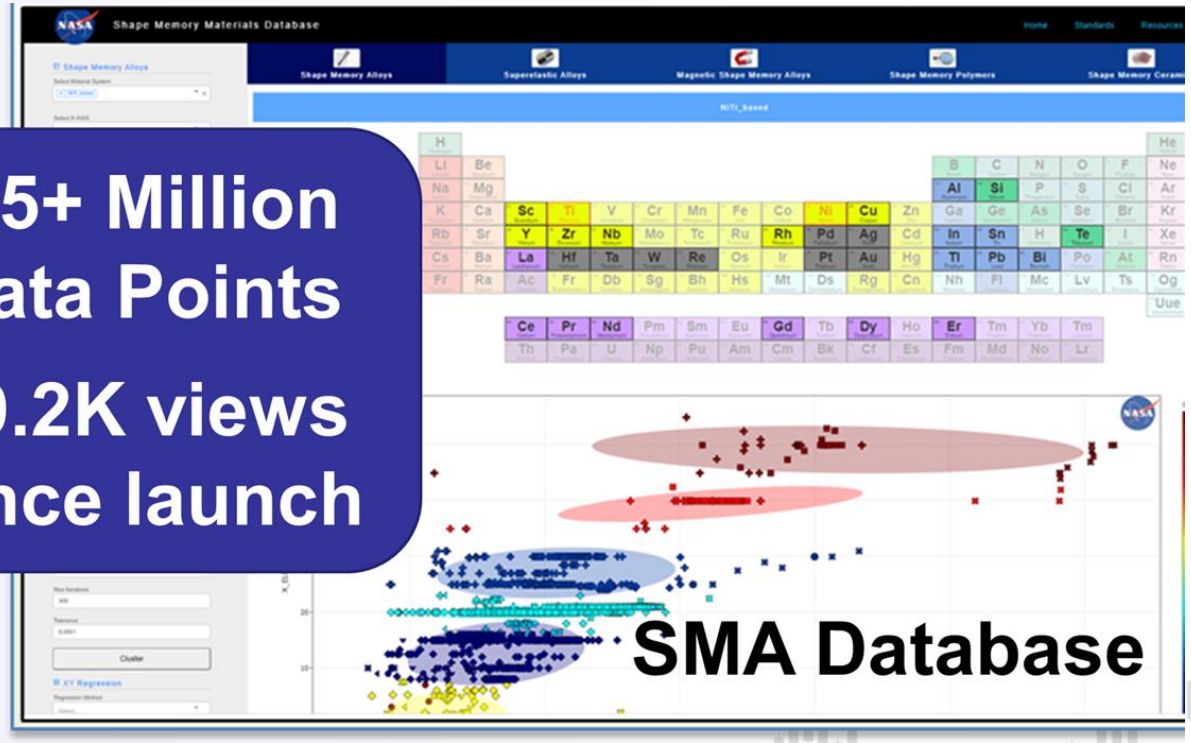
Shape Memory Materials Database

- Shape Memory Alloy (SMA) Materials require additional testing, analysis, and attributes/data collection to properly characterize the material for model development

- The shape memory alloy team at NASA GRC has developed the Shape Memory Materials Database (SMMD) to capture literature and in-house test data on shape memory materials
  https://shapememory.grc.nasa.gov/

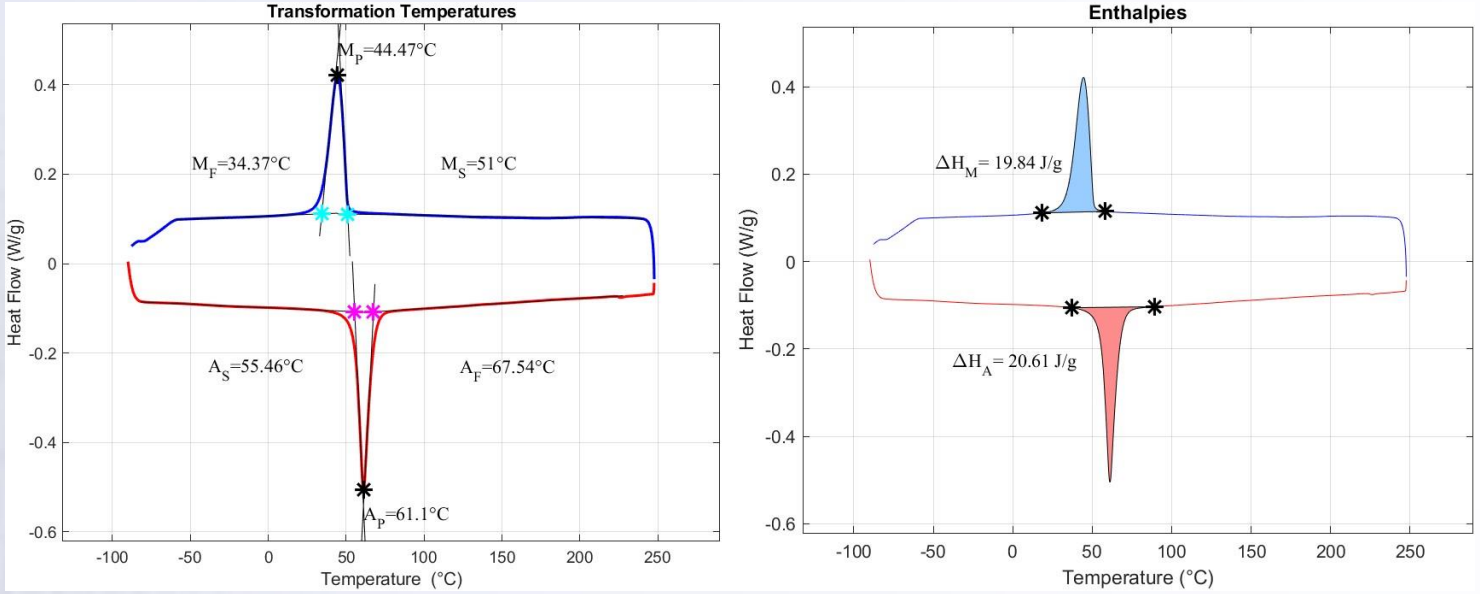
- Offers users an interactive and intuitive way to compare different SMA materials for use in various applications from vetted, published data sources

- **Purpose:** Offer public a single, free location to view and compare literature and government SMM Data



SMAnalytics Tool

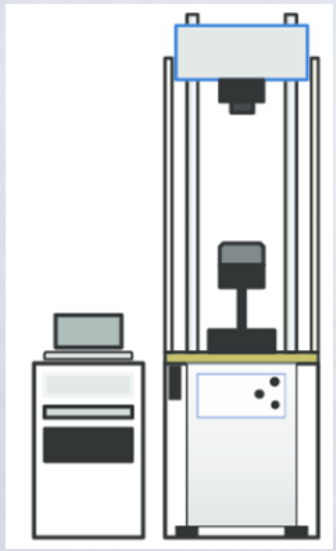
- For in-house test data, the SMAnalytics Tool has also been developed
  - Performs data analysis for SMA Materials for:
    - Uniaxial Constant Force Thermal Cycling (UCFTC)
    - Uniaxial Pre-Strain and Thermal Free Recovery (UPFR)
    - Differential Scanning Calorimetry (DSC)
    - Can be downloaded here: https://software.nasa.gov/software/LEW-20278-1
  - Allows analysis of variants of these methods, such as multi-cycle, multi-stress UCFTC and UPFR.
  - Provides automatic extraction of multiple properties including transformation temperatures, transformation and residual strains, strain recovery, and other related properties.

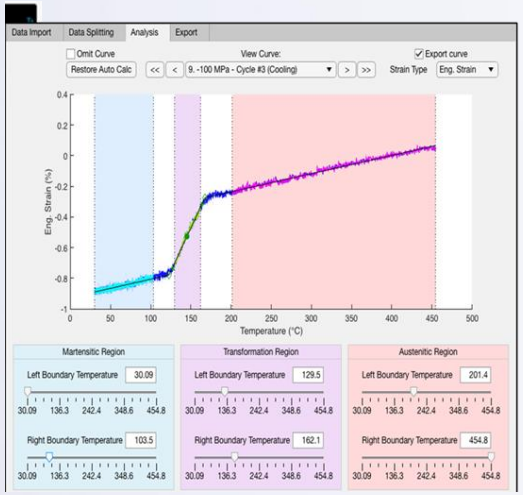


Example output from DSC Analysis using SMA\Analytics

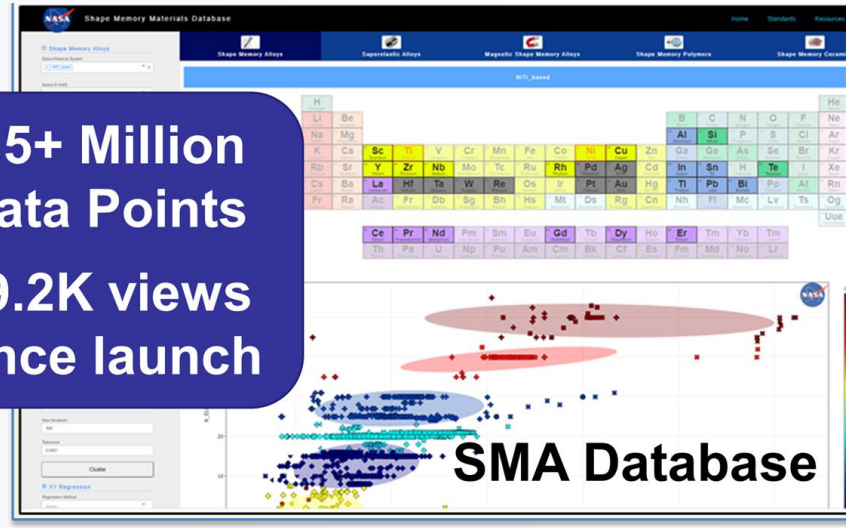
Connecting SMAnalytics and SMMD with Granta MI

- Currently, analyzed data can be sent from the SMAnalytics Tool to the SMM Database
  - **Only point-wise values are sent to the database → no information is captured on the raw data curves, test pedigree, material pedigree, etc. that must be captured to maintain the digital thread**
- **Current Work:** Connect SMAnalytics Tool with Granta MI to capture the raw data, data curves (e.g., hysteresis curves) and necessary information not captured by to the SMMD





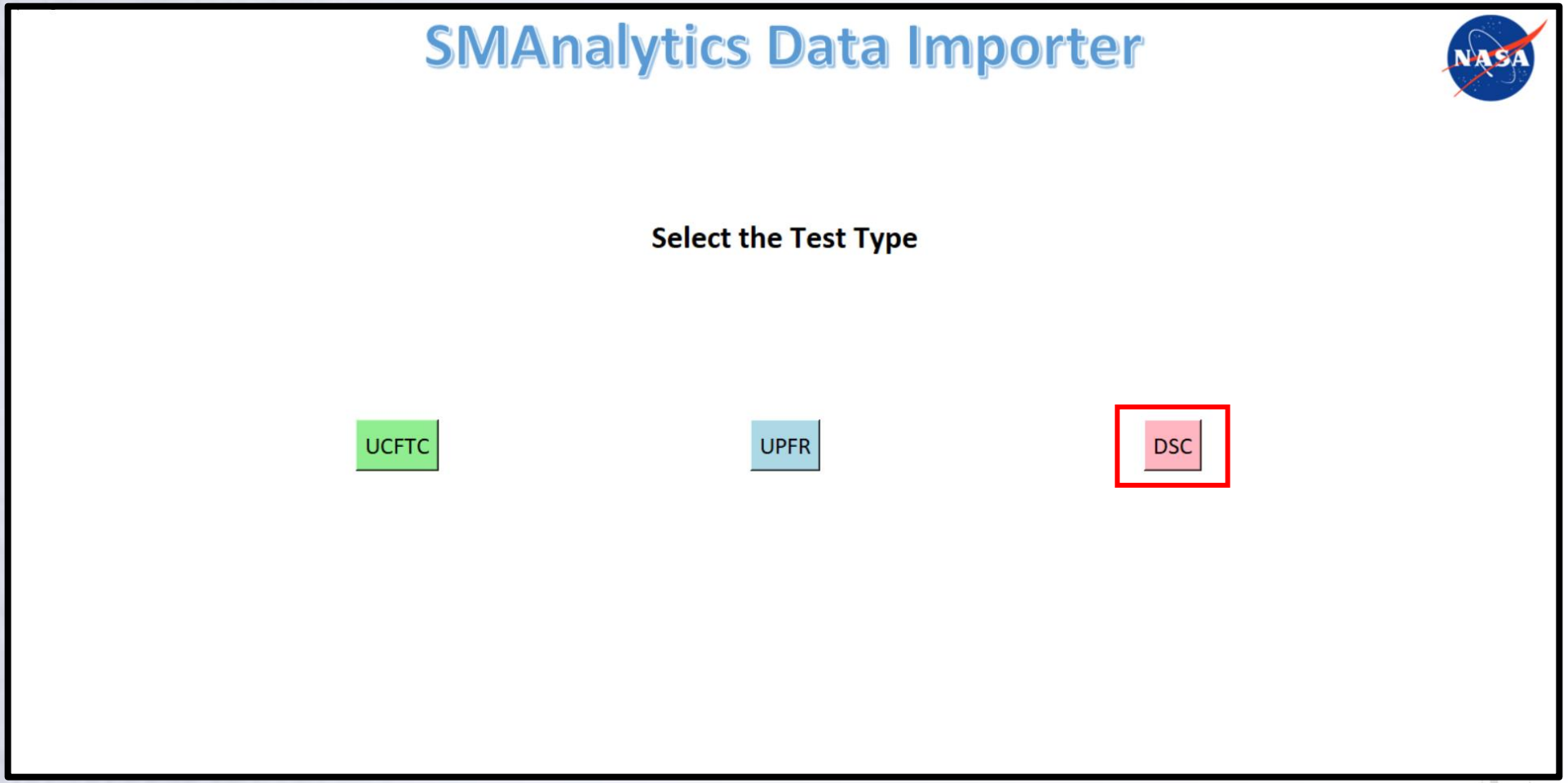
SMAnalytics



GRANTA MI
MATERIAL INTELLIGENCE

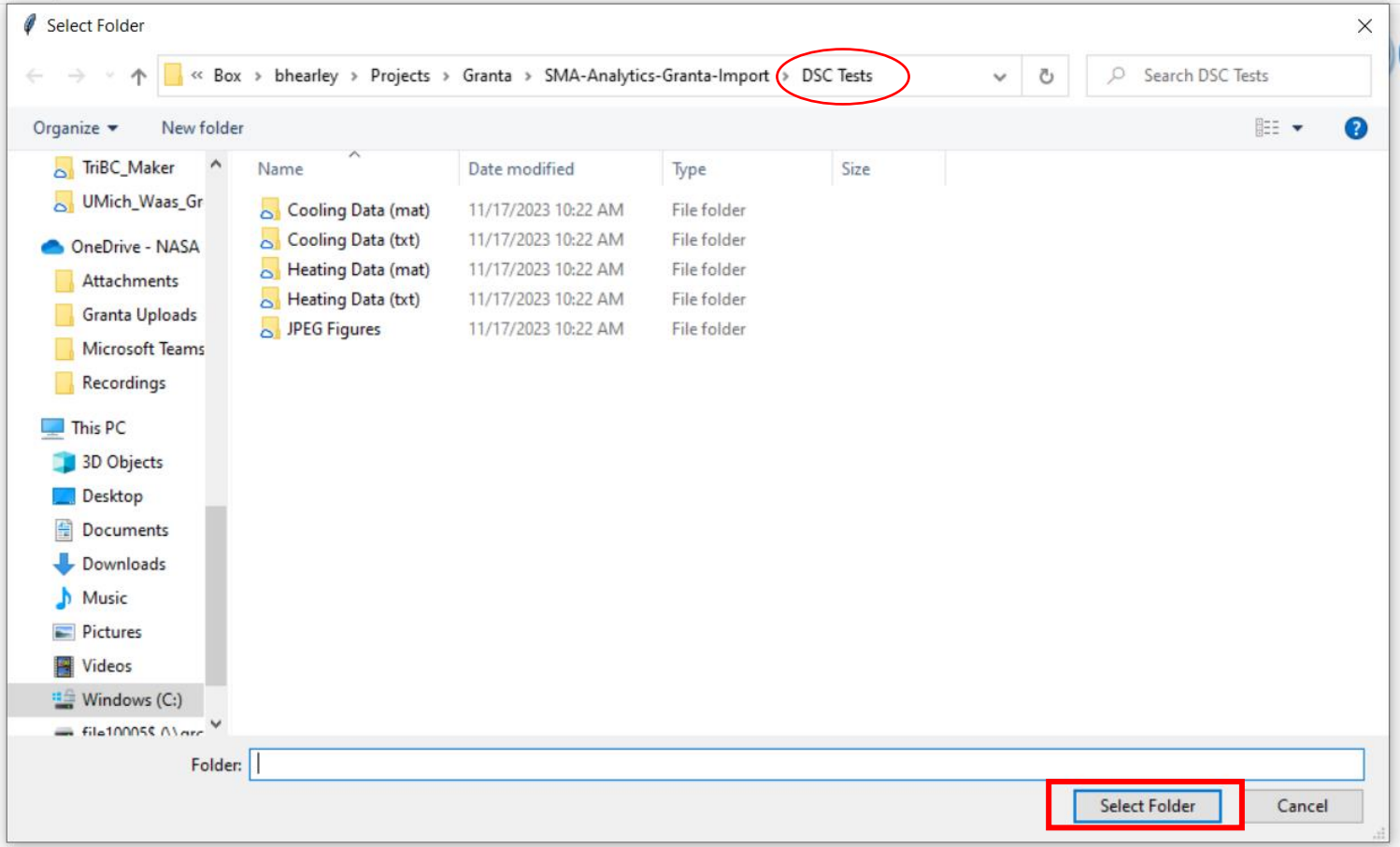
SMAnalytics Data Importer Tool

- Develop the SMAnalytics Data Importer Tool, a Python-based GUI that can read the raw data input and analyzed output from the test machine and SMAnalytics tool



SMAnalytics Data Importer Demo

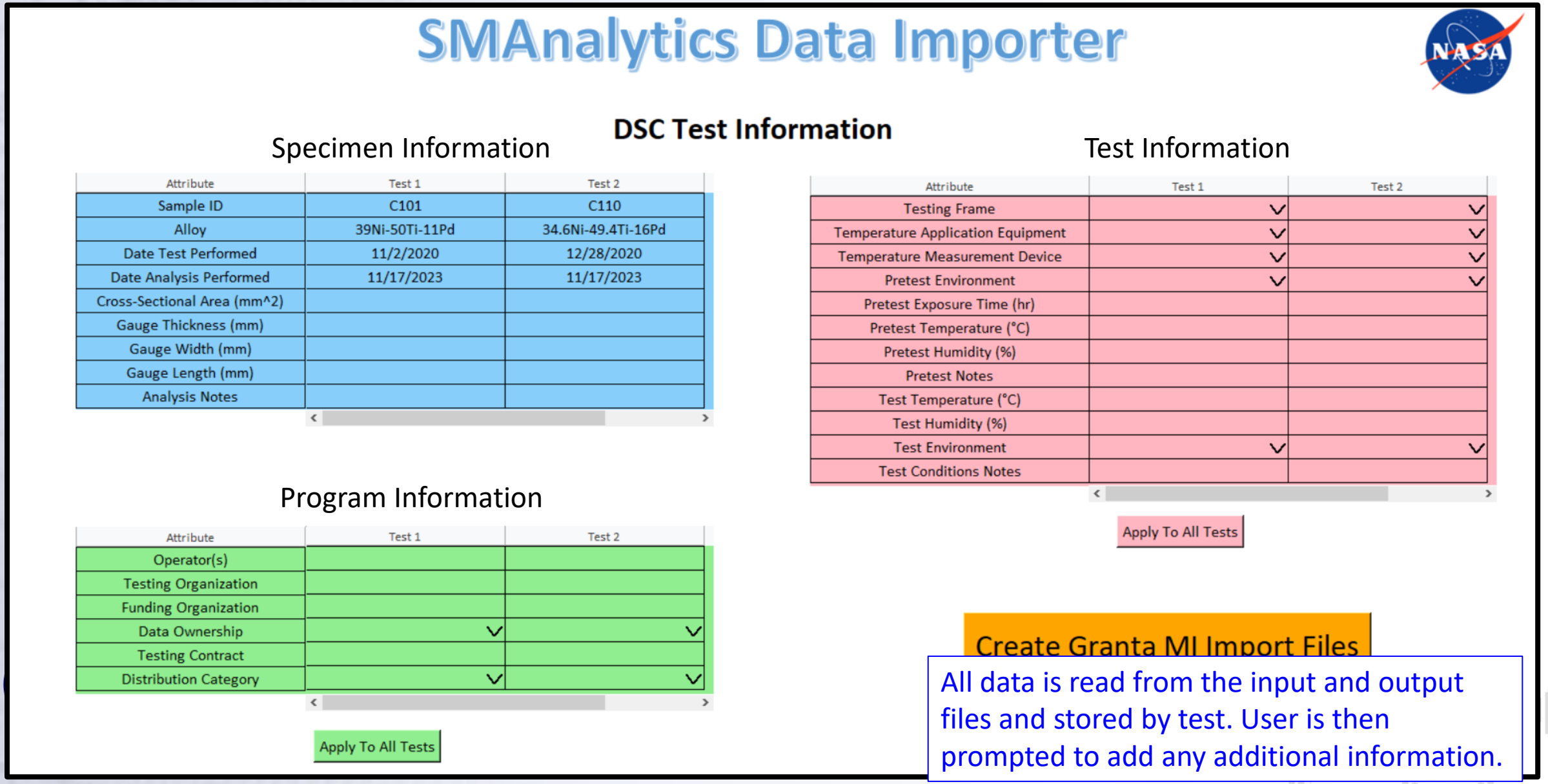
File Selection



User is prompted to select the **folder** containing the raw data input files, analyzed output files, curves, and images

SMAnalytics Data Importer Demo

Adding Additional Information



All data is read from the input and output files and stored by test. User is then prompted to add any additional information.

SMAnalytics Data Importer Demo

Additional Features/Capabilities

Specimen Information

Attribute	Test 1	Test 2
Sample ID	C101	C110
Alloy	39Ni-50Ti-11Pd	34.6Ni-49.4Ti-16Pd
Date Test Performed	11/2/2020	12/28/2020
Date Analysis Performed	11/17/2023	11/17/2023
Cross-Sectional Area (mm^2)		
Gauge Thickness (mm)		
Gauge Width (mm)		
Gauge Length (mm)		
Analysis Notes		

Scroll bar allows arbitrary number of tests to be uploaded at once

Test Information

Attribute	Test 1	Test 2
Testing Frame		
Temperature Application Equipment		
Temperature Measurement Device		
Pretest Environment		
Pretest Exposure Time (hr)		
Pretest Temperature (°C)		
Pretest Humidity (%)		
Pretest Notes		
Test Temperature (°C)		
Test Humidity (%)		
Test Environment		
Test Conditions Notes		

Air
Inert: Argon
Inter: Helium
Inert: Oil
Vacuum

Drop Downs used for Discrete Attribute Types to ensure no upload errors

Program Information

Attribute	Test 1	Test 2
Operator(s)	Brandon Hearley	Brandon Hearley
Testing Organization	NASA GRC	NASA GRC
Funding Organization		
Data Ownership	Government/NASA	Government/NASA
Testing Contract		
Distribution Category	Publicly Available	Publicly Available

Apply To All Tests

"Apply to All Tests" Button takes the values in the first column and applies to all columns to save time

Additional Information

SMAnalytics Data Importer

DSC Test Information

Specimen Information

Attribute	Test 1	Test 2
Sample ID	C101	C110
Alloy	39Ni-50Ti-11Pd	34.6Ni-49.4Ti-16Pd
Date Test Performed	11/2/2020	12/28/2020
Date Analysis Performed	11/17/2023	11/17/2023
Cross-Sectional Area (mm^2)		
Gauge Thickness (mm)		
Gauge Width (mm)		
Gauge Length (mm)		
Analysis Notes		

Program Information

Attribute	Test 1	Test 2
Operator(s)		
Testing Organization		
Funding Organization		
Data Ownership		
Testing Contract		
Distribution Category		

Apply To All Tests

Test Information

Attribute	Test 1	Test 2
Testing Frame		
Temperature Application Equipment		
Temperature Measurement Device		
Pretest Environment		
Pretest Exposure Time (hr)		
Pretest Temperature (°C)		
Test Humidity (%)		
Test Environment		
Test Conditions Notes		

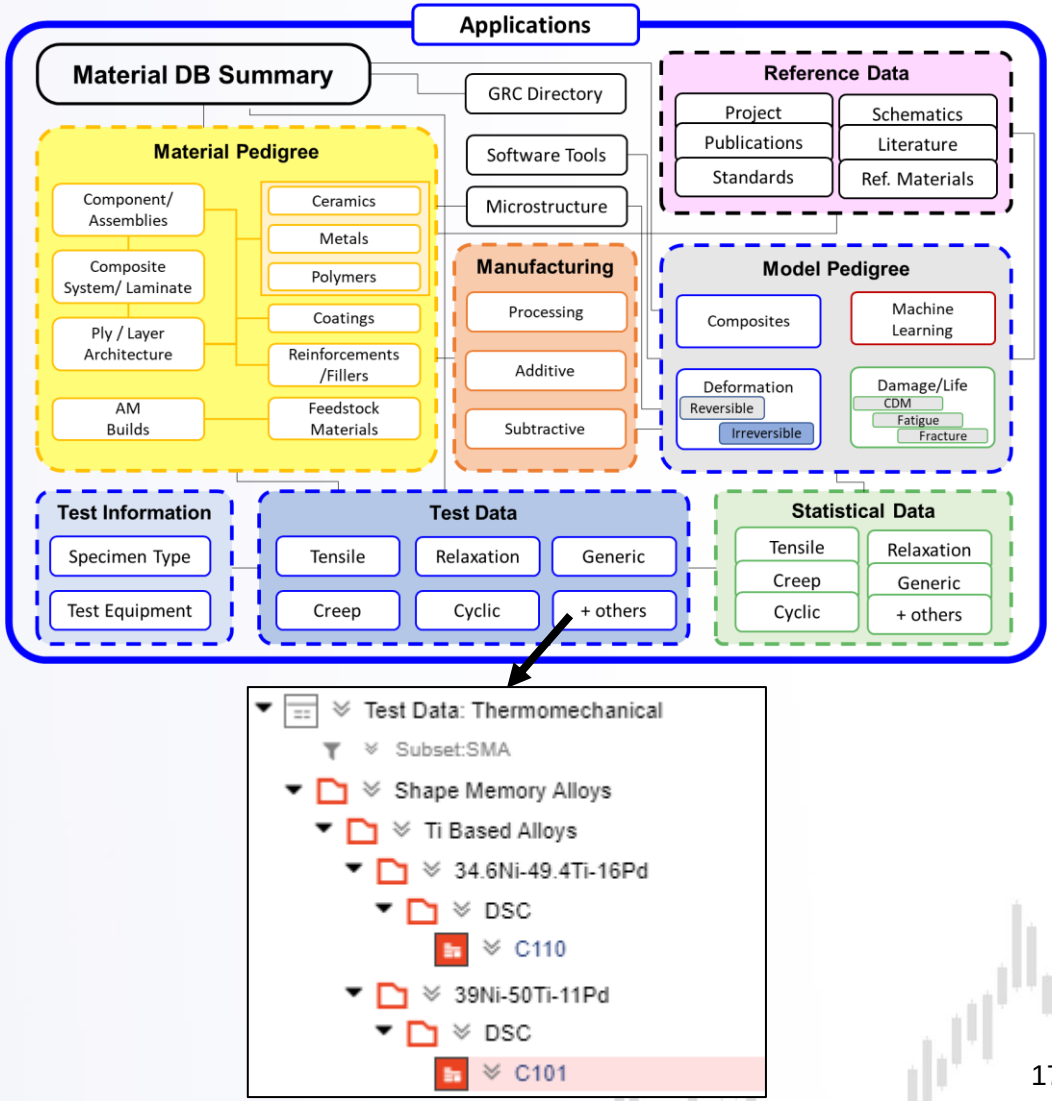
Create Granta MI Import Files creates the import files used by the Remote Import Tool.

Apply To All Tests

Create Granta MI Import Files

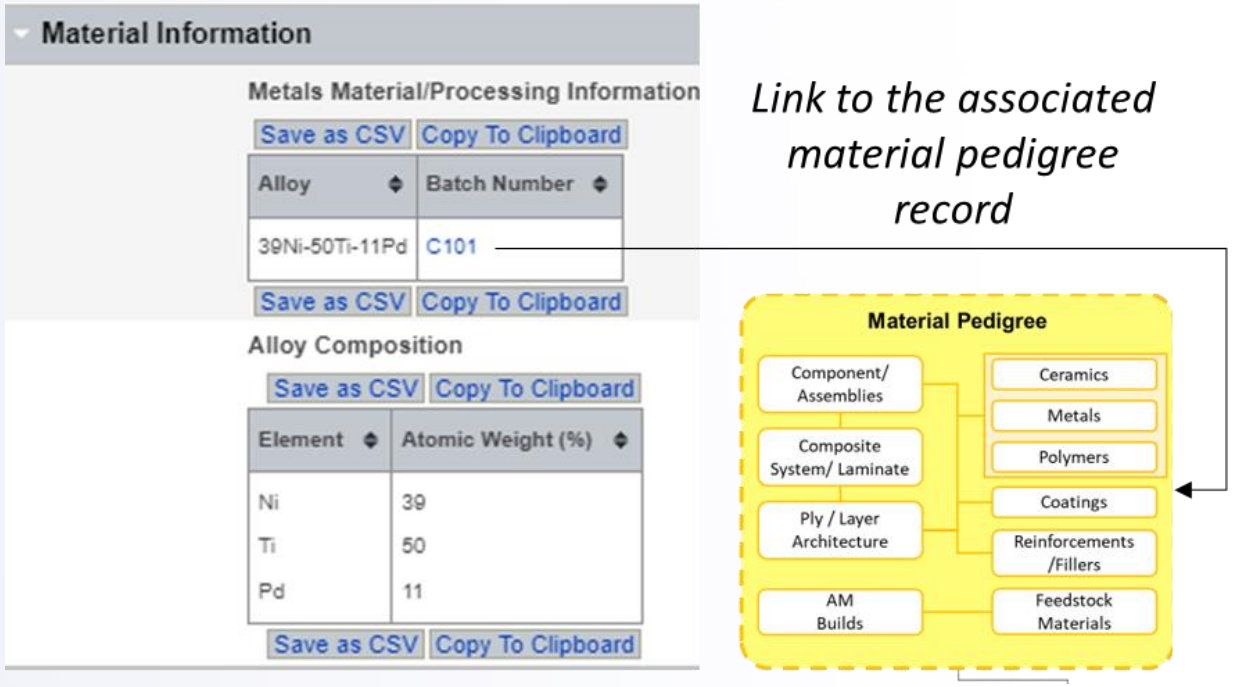
Automatic Placement of Data into Granta MI

- Records are automatically written to the Test Data: Thermomechanical Table in Granta MI from the SMAnalytics Data Importer
  - A SMA **subset** was created to store additional attributes unique to SMA Materials (e.g., Transformation Temperatures, Peak Heat, etc. for Austenite and Martensite Phases)
  - **Subsets** are used in Granta MI to group records in a Table with common properties together, making it easier for MI users to work with **smaller, targeted collections of data** of interest for a **specific purpose**
  - Records are organized in the database by:
    - Alloy Base
    - Alloy
    - Test Type
    - Individual Specimen



Additional Data Captured in Granta MI

- In addition to the information displayed in the SMMD, the Granta Records also provide:
  - Links to the Material Pedigree
  - Links to the Test Frame/Equipment
  - Test Information
  - Raw Data Curves
  - Additional Analysis not captured in the SMMD



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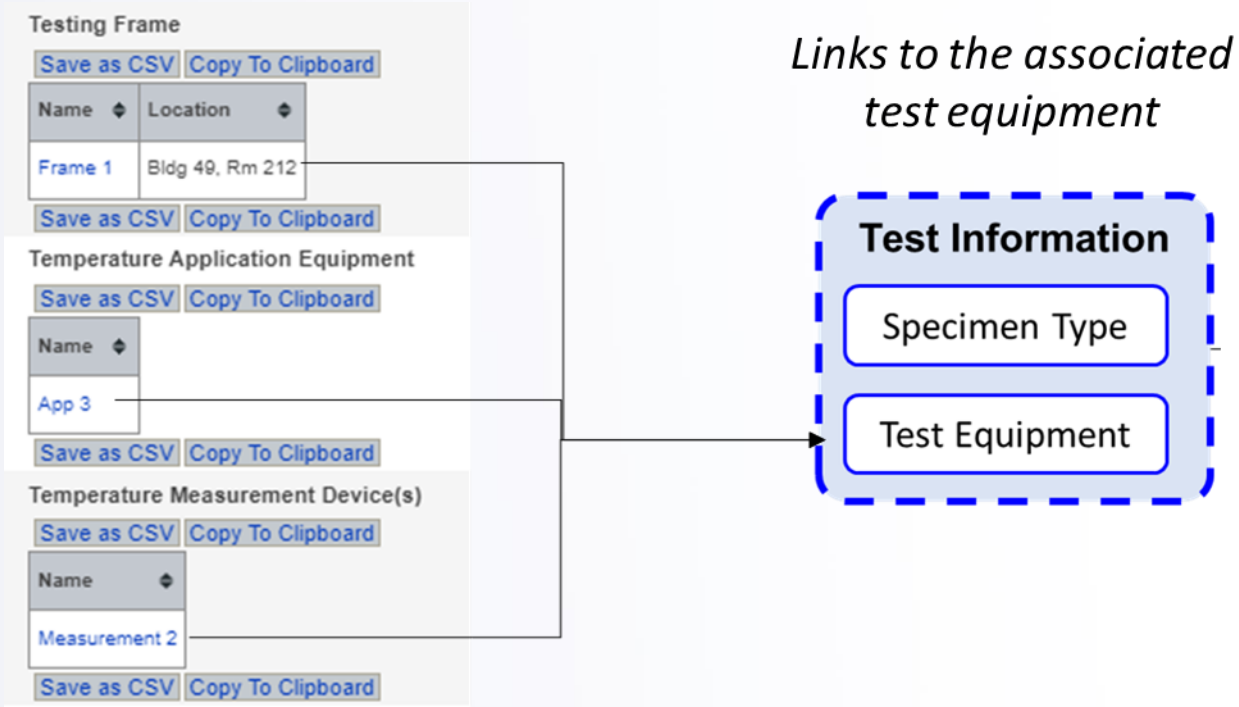
  - Additional Analysis not captured in the SMMD



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  - Links to the Test Frame/Equipment
  - Test Information
  - Raw Data Curves
  - Additional Analysis not captured in the SMMD

Test Information

Standard Test Description

DSC is a thermal analysis apparatus measuring how physical properties of a sample change, along with temperature against time

Operator(s) Hide table

Save as CSV | Copy To Clipboard

Name	Email	Office	Phone	Mail Stop	Current Employment Status	Additional Information
Brandon Hearley	brandon.l.hearley@nasa.gov	B 49 Rm 210	216-433-3215	49-7	Civil Servant	Cell Phone: 518-577-0509

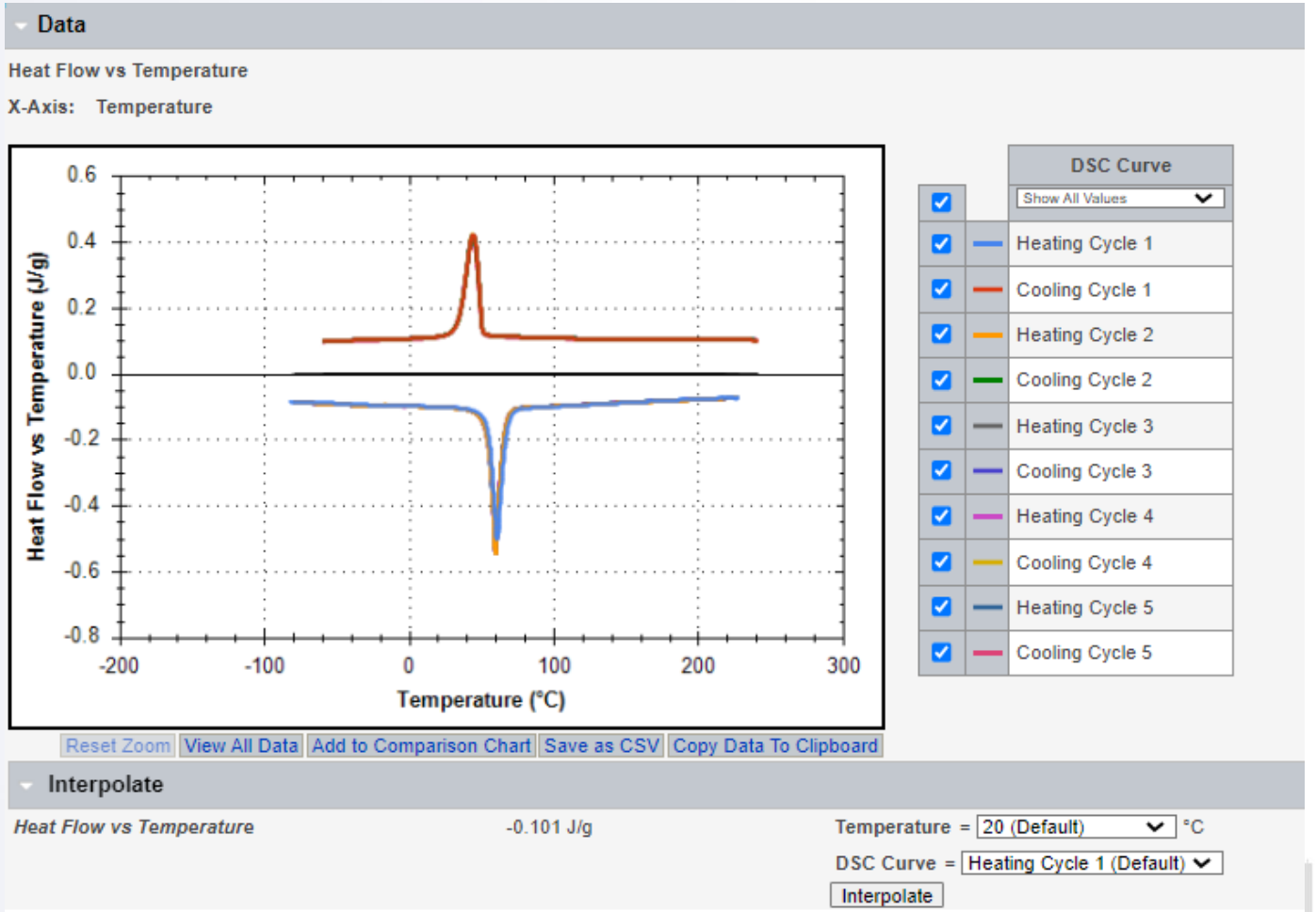
Save as CSV | Copy To Clipboard

Date Test Performed Monday, November 2, 2020

Date of Analysis Friday, November 17, 2023

Additional Data Captured in Granta MI

- In addition to the information displayed in the SMMD, the Granta Records also provide:
  - Links to the Material Pedigree
  - Links to the Test Frame/Equipment
  - Test Information
  - Raw Data Curves
  - Additional Analysis not captured in the SMMD



Additional Data Captured in Granta MI

- In addition to the information displayed in the SMMD, the Granta Records also provide:
  - Links to the Material Pedigree
  - Links to the Test Frame/Equipment
  - Test Information
  - Raw Data Curves
  - Additional Analysis not captured in the SMMD

Differential Scanning Calorimetry Analysis Hide table

Save as CSV Copy To Clipboard

Cycle Number	Austenite Start Temperature (°C)	Austenite Start Heat Flow (J/g)	Austenite Peak Temperature (°C)	Austenite Peak Heat Flow (J/g)	Austenite Finish Temperature (°C)	Austenite Finish Heat Flow (J/g)	Austenite Enthalpy (J)	Martensite Start Temperature (°C)	Martensite Start Heat Flow (J/g)	Martensite Peak Temperature (°C)	Martensite Peak Heat Flow (J/g)	Martensite Finish Temperature (°C)	Martensite Finish Heat Flow (J/g)	Martensite Enthalpy (J)	Analysis Image
1	55.5	-0.107	61.1	-0.505	67.5	-0.108	20.6	51	0.111	44.5	0.421	34.4	0.111	19.8	
2	55.5	-0.11	60.2	-0.548	65.9	-0.107	17.8	51	0.111	44.4	0.422	34.3	0.111	19.9	
3	55.4	-0.107	60.2	-0.548	65.8	-0.106	20.8	51	0.111	44.4	0.422	34.3	0.111	19.8	
4	55.3	-0.107	60.1	-0.547	65.7	-0.106	20.8	50.9	0.111	44.3	0.422	34.3	0.111	19.9	
5	55.3	-0.107	60	-0.547	65.7	-0.106	20.7	50.9	0.109	44.1	0.412	33.9	0.109	19.7	

Summary

- Data Informatics and Effective Data Management are critical to enabling ICME and achieving the NASA Vision 2040
  - Ensure the integrity of our data, prevent loss of institutional knowledge, and trust that our data is protected
- Unrealistic to assume one tool/database will be used to capture all material information
  - Information Management systems must be able to communicate with specialized databases to establish a “digital ecosystem” for materials information
- At NASA GRC, the recently developed Shape Memory Material Database and SMAnalytics Tools are being connected with the NASA GRC ICME Schema to provide traceability between test data, analysis, and design data for shape memory alloys

Future Work

- Currently, the SMAnalytics Import Tool requires the user to run the SMAnalytics tool first and then upload the data to both the Granta MI Database and SMMD
  - The SMAnalytics tool has been recently converted to a Windows Executable that can be called by Python → allow users to call the SMAnalytics tool within the Python Importer to perform analysis and automatically write records to Granta

- When data is added to the SMMD, a link between the data presented there and the additional data and metadata stored in Granta MI needs to be established
  - Currently linking the two through a manually entered hyperlink between databases, but need to automate to remove potential human error/breaking of the digital thread

Thank You for Your Attention

Integrate Don't Duplicate