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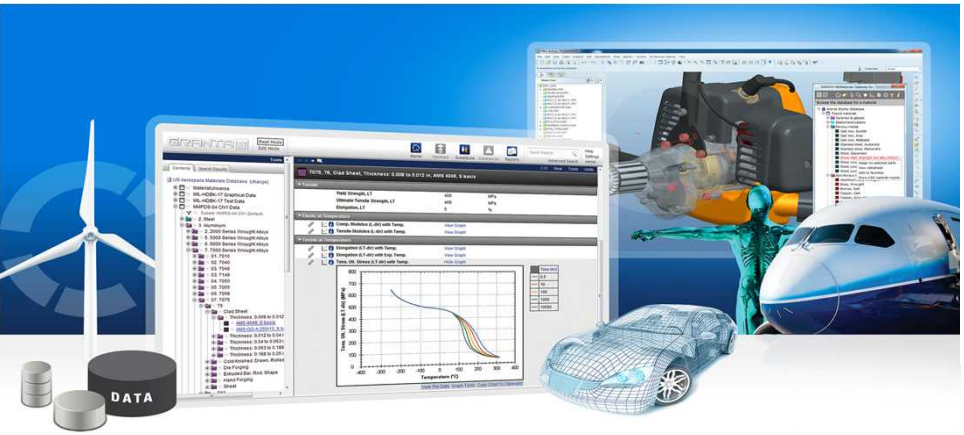

GRANTA MATERIAL INTELLIGENCE

GRANTA MATERIAL DATABASE EFFORTS @ SNL
Interface, Infrastructure & Opportunities

J. Koepke, J. Madison, L. Serna, R. Karnesky, M. Kinnan, A. Baca, D. Hirschfeld

U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

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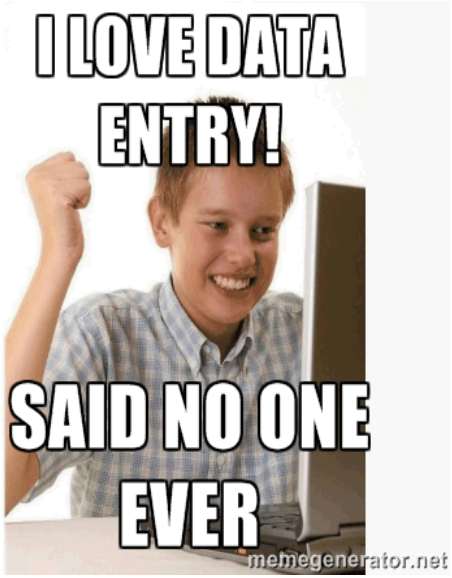
Introduction

- Implementation
  - 5 year milestone and objectives
  - Sandia specific databases
- MDMC Roadmap Projects
  - External collaboration (MI9)
  - Web based database configuration (MI9)
  - Sync schemas (MI9)
- Business case and case studies information
  - Challenges/Solutions at Sandia
  - Collaboration with NSC
  - Sandia Additive Manufacturing Database



Implementation Summary

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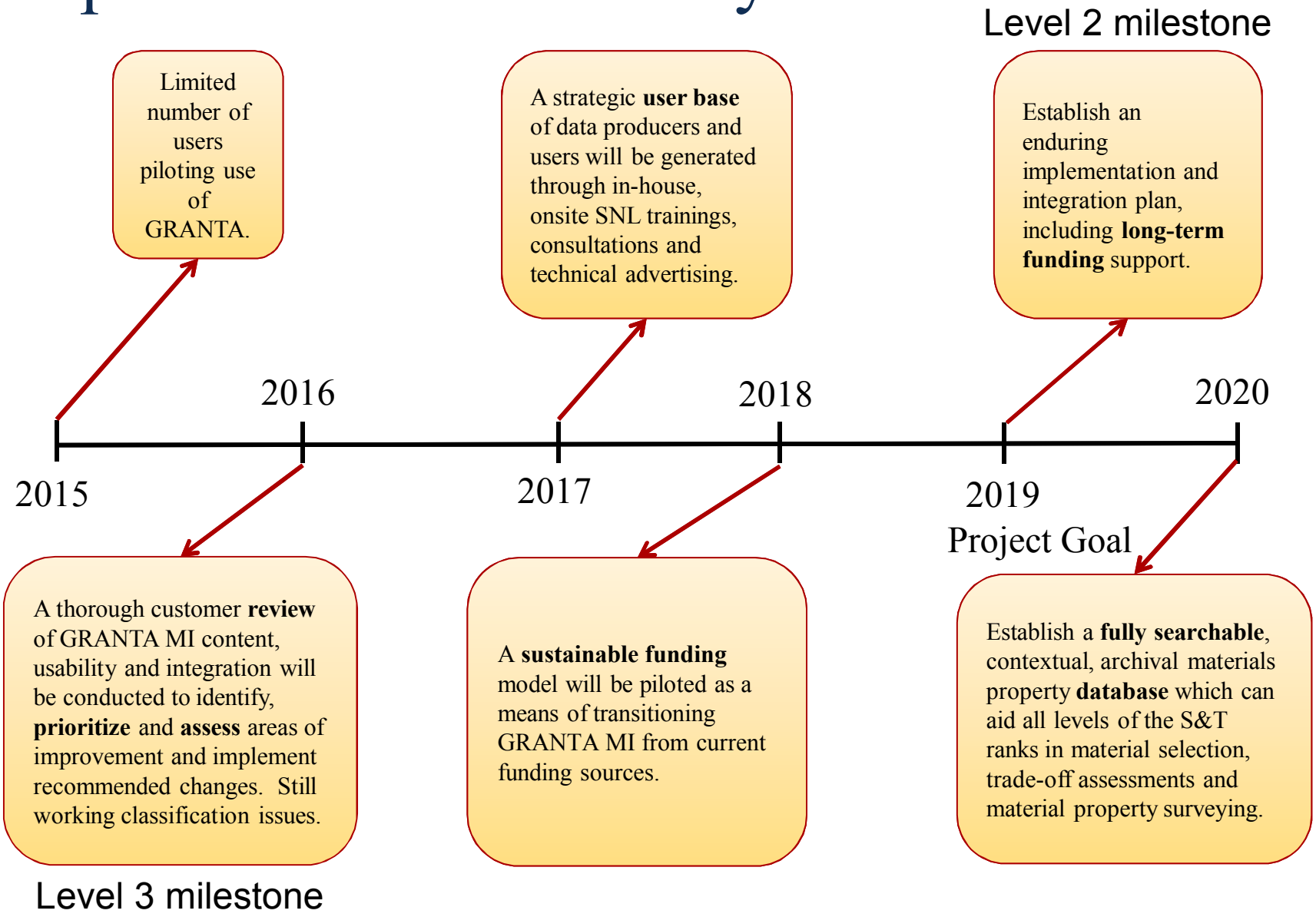
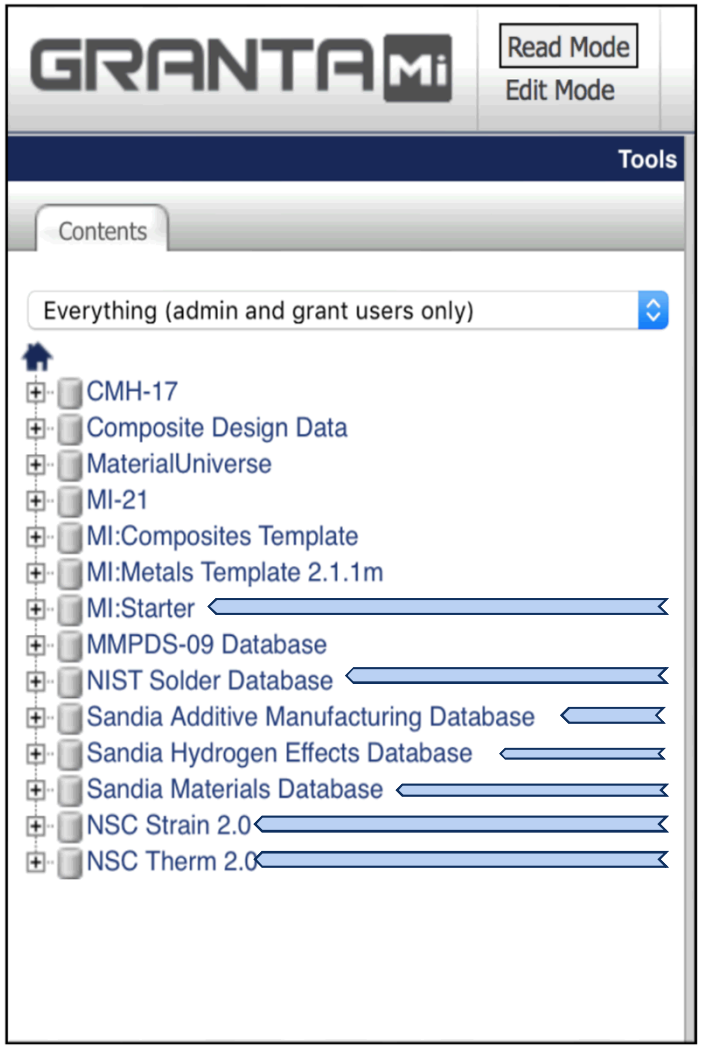


GRANTA Materials Database Prior Activities



- **Advertised tool internally to grow support & develop collaborations**
  - Nov. 5th, 2014 – Center 1800/8200 Materials Liaisons
  - Dec. 3rd, 2014 – Comp + Sim Leadership Steering Committee
  - Jan. 19th, 2015 – Center 2500 Energetics Materials Working Group
  - Feb. 19th, 2015 – Org. 1526 Comp. Sci & Mechanics Meeting
  - Oct. 28th, 2015 – Comp + Sim Leadership Steering Committee
- **Hosted SNL (NM + CA cross-site) GRANTA seminar and 2-day user-training**
  - March 3 & 4th, 2014
- **Provided 4 cross-lab briefings toward a lab-wide and cross-site complementary deployments of GRANTA**
  - May 5th, 2015
  - July 1st, 2015
  - Feb. 19th, 2016
  - July 19th, 2016
- **Introduced 6 additional databases to the SRN GRANTA deployment**
  - MI : Starter Database
  - NIST Solders Database
  - Sandia Additive Manufacturing Database
  - Sandia Hydrogen Effect Database - http://granta-mi.sandia.gov
  - Sandia Materials Database
  - NSC Therm 2.0
  - NSC Strain 2.0
- **A lot of collaboration, outreach efforts!!**

Ongoing Efforts

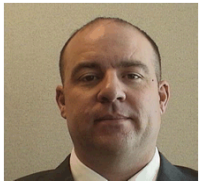
- Actively pursuing the integration framework necessary for SNL's GRANTA MI to operate in tandem with the **Sandia Analysis Workbench** (SAW)
  - **SAW** enables Sandia's simulation code suite (aka DART)

- The SNL GRANTA team (led by D. Hirschfeld) are also active contributors & facilitators for the ongoing dialogue regarding data management & sharing across the **NNSA** (National Nuclear Safety Association) complex and beyond
  - Using a commercial trusted software tool that allows for access controls

- On going:
  - Pursuing internal collaborators
  - Actively interfacing with data producers
  - Iterating on data definition
  - Uploading data
  - Developing databases for increased usability

GRANTA @ SNL – Team Members

Deidre Hirschfeld, Ph.D.
Manager (1832) – Coatings & Additive Manufacturing



Joshua Koepke
Year Round Intern (1832)
Coatings & Additive Manufacturing

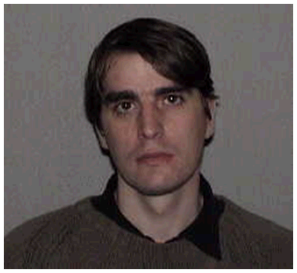
- *Data Entry*
- *Importer Creator*

Ana Baca
Technologist (1819)
Materials Characterization & Performance

- *Data Entry*
- *Importer Implementation Testing*

Mark H. Baumgardner
PO Contractor (9324)
Infrastructure Computing Systems

- *Application Maintenance*
- *Server Management*

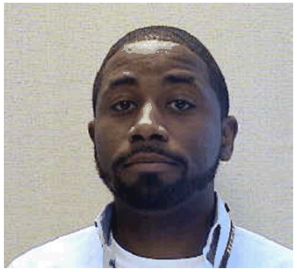


Rick Karnesky, Ph.D.
Staff Member (8367)
Hydrogen & Combustion Technologies

- *Granta Application Admin*
- *Customer Development & Technical Partnerships*
- *Hydrogen Compatibility Database*
- *Hydrogen Effects **

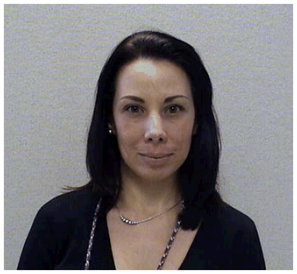
Mark Kinnan, Ph.D.
Staff Member (6632)
Chemical & Biological Systems

- *Importer & Schema Development*
- *Decontamination Foams **



Jonathan D. Madison, Ph.D.
Staff Member (1851)
Materials Mechanics & Tribology

- *Granta Application Admin*
- *Customer Development & Technical Partnerships*
- *Sandia Materials Database*
- *Additive Manufacturing Database*
- *Metallurgy **

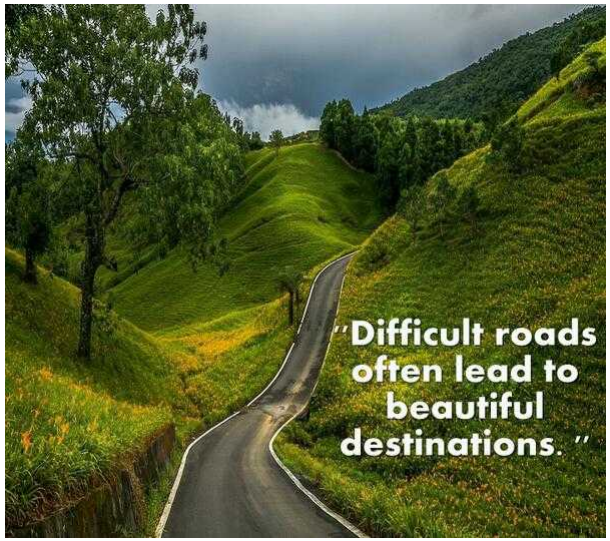


Lysle Serna, M.S.
Staff Member (1852)

- *Customer Development & Technical Partnerships*
- *Material Listings Nomenclature*
- *Material Compatibility **
- *Corrosion **

MDMC Roadmap Projects

- We Support
  - External collaboration (MI9) - Sharing data between MI installations at separate organizations
  - Web based database configuration (MI9) - A way to add, remove and update databases (MI:Server Config) without needing client software / IT help
  - Sync schemas (MI9) - A way to synchronize schemas without sending any data, e.g. to support database development
- We would like to see
  - Ability to more easily track user usage
  - An easier way to make edits on multiple records



Why do we use Granta MI?

Survey Data, Granta Business Case White Paper (2012)
www.grantadesign.com/papers

- Engineers spend an average of one hour per week looking for materials data
- Typically 20% of materials tests duplicate existing work
- 50% of acquired data is used once and never re-used

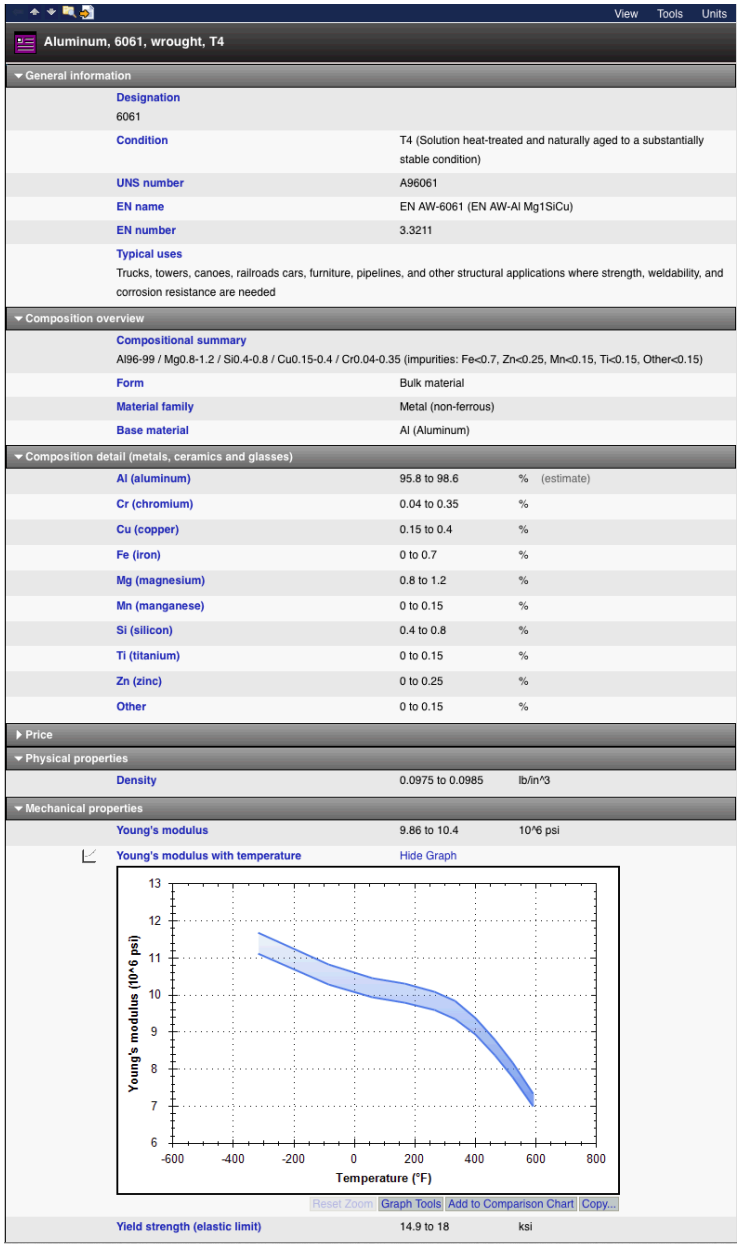
THE CHALLENGE AT SANDIA

- All levels of S&T ranks import/access materials properties from various sources
- No verifiable means to ensure consistency or accuracy of data across SNL
- When data in unavailable, testing can be duplicated to derive needed info
- S&T turnover leads to lost knowledge, expertise & material selection rationales
- Existing SNL databases are not widely employed nor easily accessible

PROPOSED SOLUTION

- Leading, commercially-available materials information management system
- Well-established, archival, highly customizable & scalable
- Single resource for publicly available & private SNL materials information
- Enables in-house comparisons across private and public domains
- Information traceability beyond material properties
  - (*e.g.* data producer(s), instrumentation, date, supplier, etc.)
- Data pedigree & context are an integral part of framework

Organization and Retention of Data



Business Case Information

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- What we get from being part of the MDMC
  - Practical help
  - Use of models from other institutions
  - Tips on access controls for data
  - See latest advances with Granta MI software

- ROI arguments we rely on
  - We have not established ROI metrics for Granta MI but items of focus are:
    - Amount of data populated
    - Storage of internally generated data
    - Success on our current network to encourage use on multiple networks

Looking Ahead

- What we would like to see changed
  - 6 months
    - tools or guidance on how to easily share data with other sites
      - To make NNSA cross site data sharing quick and easy
  - 2 years (or sooner)
    - flexibility in pricing structure per seat

How we use Granta

- **Collaboration between SNL and NSC**
  - Sandia National Labs (SNL) is a science laboratory (NNSA)
  - National Security Campus (NSC) is a production facility (NNSA)

- **NSC provided SNL the following datasets:**
  - **Strain2.0 database** acquired from National Security Campus (NSC), containing Basic Mechanical Property Data

    *(e.g. Modulus, Poisson Ratio, Yield Stress, etc.) for some **1000 + basic materials of interest to NNSA)***
  - **Therm2.0 database** acquired from National Security Campus (NSC), containing Basic Thermal Property Data

    *(e.g. Thermal Conductivity, Specific Heat, etc.) for some **1000 + basic materials of interest to NNSA)***

- **The datasets were provided in an Excel file that was exported from databases from their Granta MI that we had to match to be able to upload it on our end**
  - Not an easy or quick process

Case Study

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Data from NSC

- Data received from Mike McNary at NSC

Good luck

Create new database

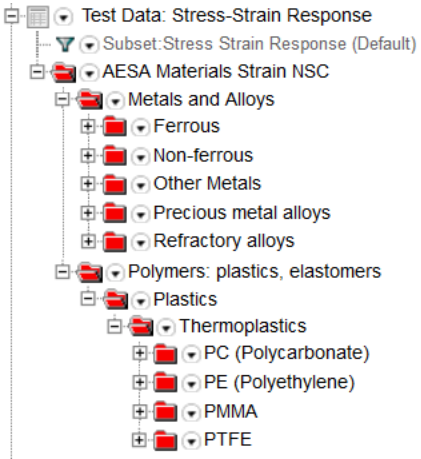
- Originally datasets were loaded into MI: Starter
- 2 databases were developed to store data once import was accomplished

Match attributes

- Attributes created had to match exactly for import to work
- Discrete types and units also had to be created to match

Test importer

- Attempt import
- Fix errors
- Attempt import until there's no more errors



Much easier to find what Your looking for

Hierarchy

- Since each dataset included over **1000** records a hierarchy needed to be created

Final Import

- !!!!!!!!!

Sandia Additive Manufacturing Database

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- Sandia Additive Manufacturing Database
  - Projects
  - Reports
  - Part Design
  - Machines
  - Machine Calibration
  - Materials
  - Material Batches
  - AM Builds
  - Parts
  - Post Processing
  - Testing Series
  - Design Data
  - Tools
  - Statistical Data: Creep
  - Statistical Data: Fatigue
  - Statistical Data: Hopkinson bar
  - Statistical Data: Tensile
  - Test Data: Charpy
  - Test Data: Compression
  - Test Data: Corrosion
  - Test Data: Creep
  - Test Data: Fatigue
  - Test Data: FCG
  - Test Data: Hopkinson bar
  - Test Data: Residual Stress
  - Test Data: Tensile
  - Test Data: Torsion
  - Test Data: Ultrasonic

Projects, Reports, Machines, Materials, AM Builds, Statistical data, and Test data records are linked

Material System	Test Types	Material Properties	Amount
AlSi10Mg	Charpy	Charpy impact vs Angle	1
		Charpy impact vs distance	
	Corrosion	Electrochemical impedance	1
		Open circuit potential	1
		Polarization test	1
	Creep	Strain	4
	Residual Stress	Residual stress bulk	1
		Residual stress corner	
	Tensile	Ductility	112
		Yield Stress	112
		Young's modulus	112
		Ultimate tensile strength	93
		Tensile response	29
	Torsion	Torsion	1
	Ultrasonic	Poisson's ratio	1
		Young's modulus	
304L	Hopkinson bar	Stress vs strain	83
	Tensile	Strain rate	91
		Proportion limit	60
		Ultimate tensile strength	60
		Tensile failure stress	60
		Load vs displacement	31
Ti6Al4V	Tensile	Yield stress	74
		Ultimate tensile strength	74
		Ductility	74

Data from various mechanical tests – organized and tracked

Summary of Issues

- **Key Issue: Pricing and per seat cost**
  - **SNL has a large number of exploratory users**
  - **Quantity of users is very difficult to predict while trying to increasing the amount of users**

- Other Issues
  - Implementation of existing SNL computer resources
  - Ability to create/edit databases without needing IT
  - Ability to hide attributes in layout but still able to upload the data (auto-linking)
- Smaller Issues
  - When exporting data any files, pictures, links, etc are included in excel file
  - Tables should be auto-linked to all other tables in database

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Questions