Accelerated Metallurgy
Data Management and Machine Learning

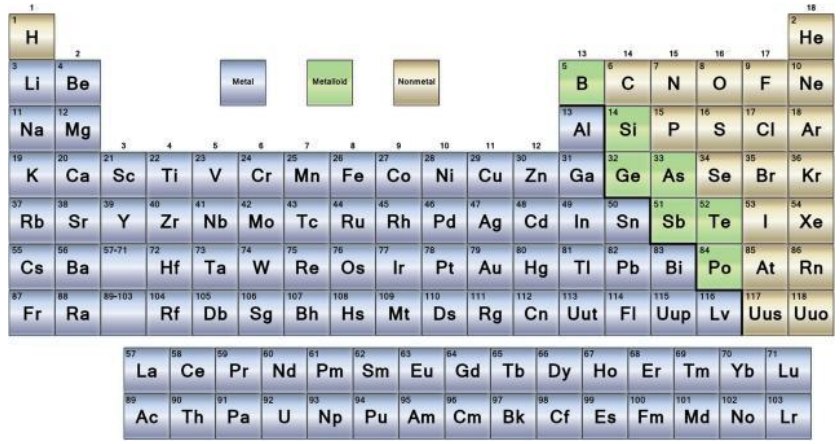
James Goddin

ANSYS GRANTA

www.grantadesign.com

Background

- 87 known metals
- 61 are commercially available.
- Historically alloys developed by trial and error – combined with experience and innovation.
- Typically 3-4 months for one compositional iteration and 5-6 years to identify one promising alloy.

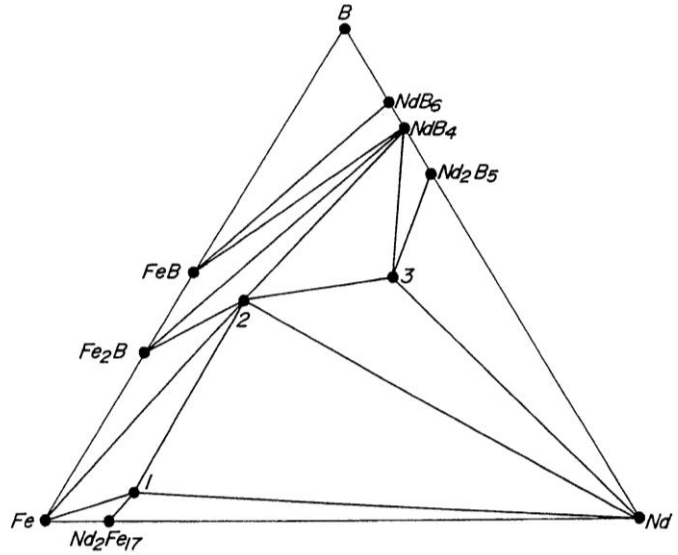


“To create just one isothermal section of a ternary phase diagram requires the effort of one master’s student”.

Of the ~32,000 potential ternary alloy systems, over 90% never explored.

The production and use of alloys accounts for **46% of all EU manufacturing value and 11% of the EU’s total GDP**.

EU added value of over € 1.5 trillion annually, € 4Bn per day (same as total GDP for Spain in 2008)



Accelerated Metallurgy - Consortium

Six Technology Areas

- Lightweight Alloys (Aero & Auto)
- High Temperature Alloys (Rockets, turbines, nuclear fusion)
- High-Tc Superconductors (Electrical applications)
- Thermoelectric alloys (Heat scavenging)
- Magnetic alloys (Motors & refrigeration)
- Phase Change Alloys (Electronics)

€21M over 5 years

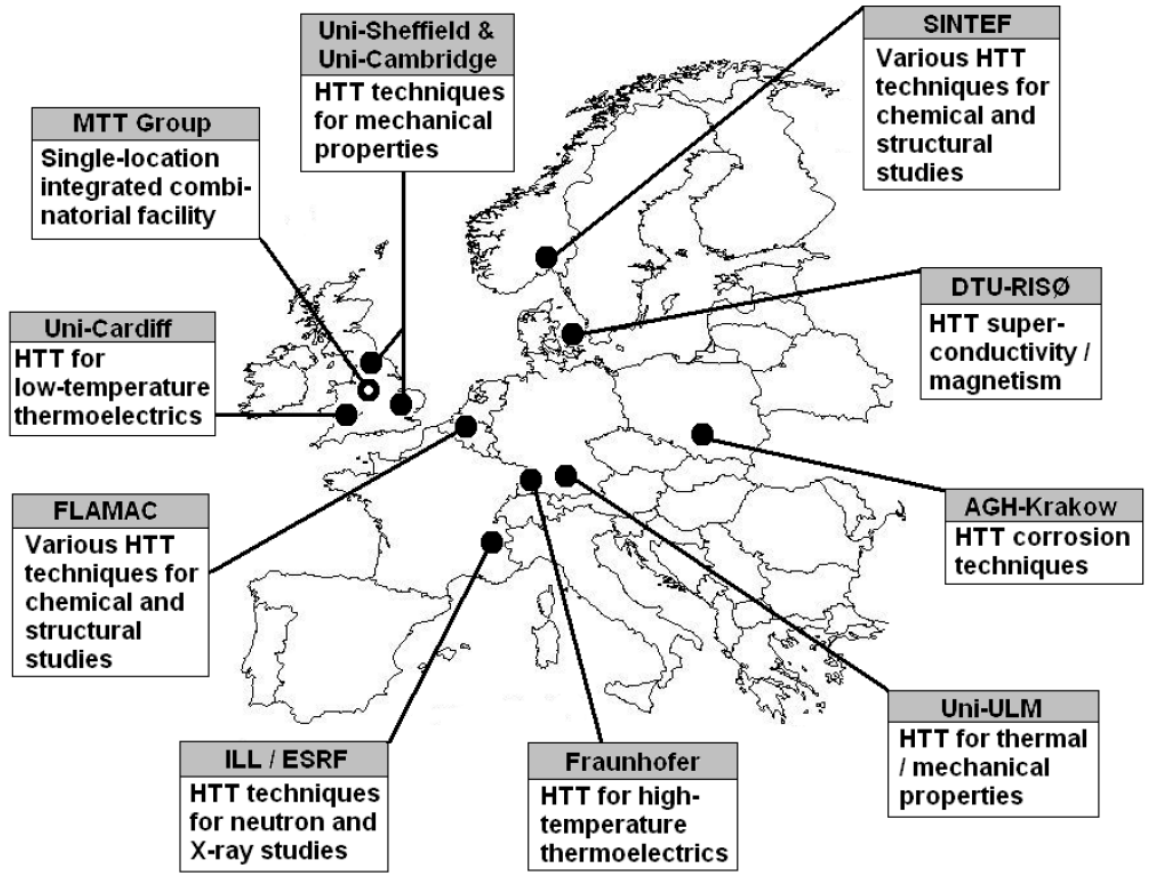
32 Partners

Jun 2011 → Jun 2016

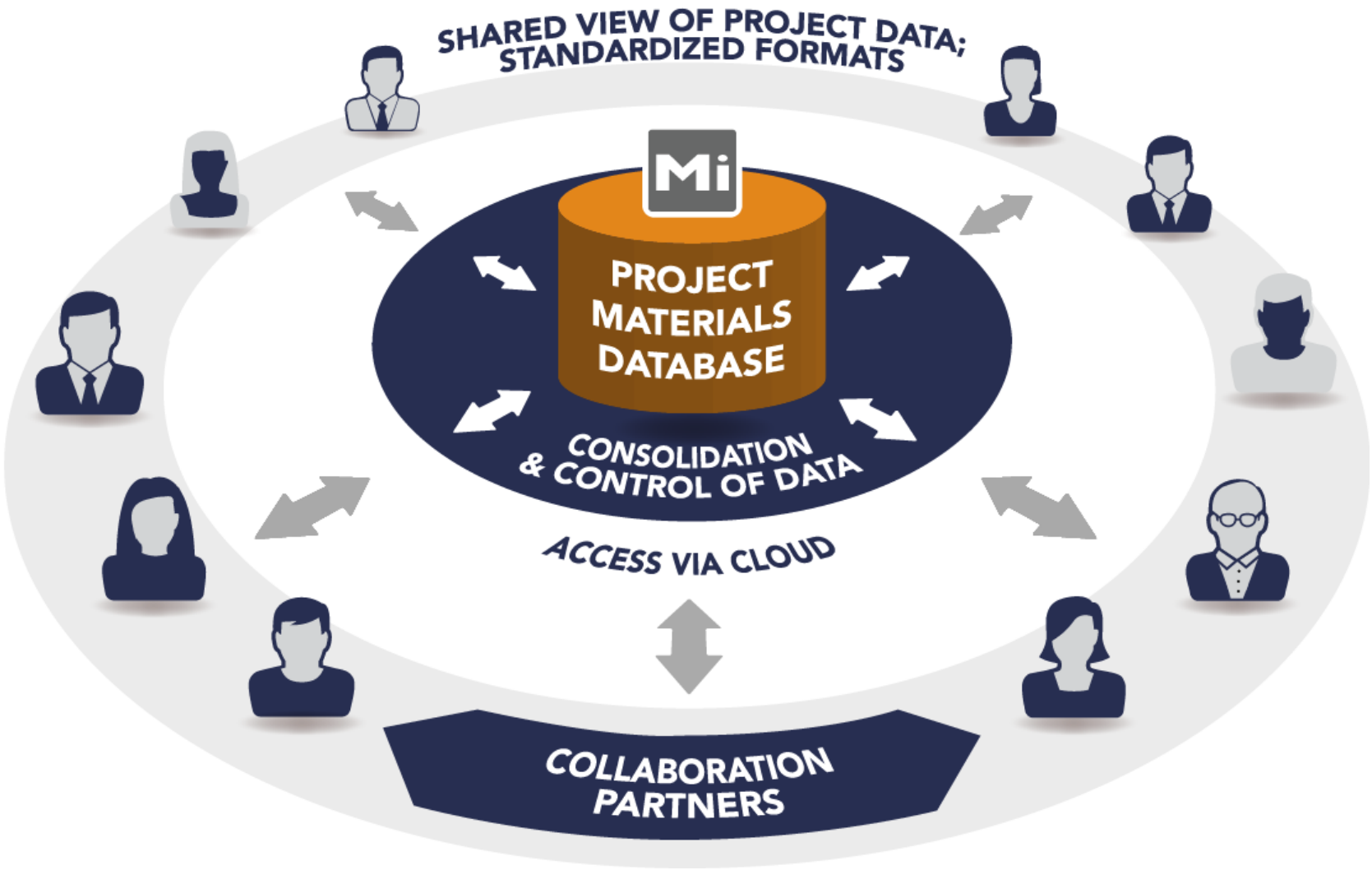
Accelerated Metallurgy - Approach

High Throughput Combinatorial Synthesis & Testing.

- Computational screening & selection of candidates
- Rapid manufacture (using technology adapted from Additive Manufacturing)
- Rapid characterisation – High throughput technique development
- Selective lower throughput testing
- Pooling of Knowledge ➔ Creation of a 'Virtual Alloy Library'



Accelerated Metallurgy – Virtual Alloy Library



All data in a shared Granta MI database, a 'Virtual Alloy Library'

- Strong standardisation
- All data linked appropriately and automatically.
- All data accessible by all partners.
- All compositions screened for risk as part of R&D.
  - Critical Materials
  - Restricted Substances
  - Eco Impacts
  - Cost

GRANTA:MI – Virtual Alloy Library

Viewer | Read Mode | Edit Mode | Home | Optimize | Substitute | Substances | Reports | Quick Search | Advanced Search | Help | Settings | Admin

Contents

MaterialUniverse

- Metals and alloys
  - Ferrous
    - Alloy steels
    - Carbon steels
    - Cast irons
    - Coated steels
    - Iron, commercial purity
    - Microalloy and high strength steels
    - Stainless steels
      - Austenitic
        - Cast
        - Wrought
          - AISI 201 (Low nickel work
          - AISI 202 (Low nickel gener
          - AISI 204-Cu, annealed
          - AISI 205, annealed
          - AISI 216, annealed
          - AISI 301 (Ductile, high wor
          - AISI 302 (High carbon)
          - AISI 303 (Free machining)
          - AISI 304 (18/8)
          - AISI 305, annealed
          - AISI 308 (Welding filler me
          - AISI 309, annealed
          - AISI 310, annealed
          - AISI 314, annealed
          - AISI 316 (Corrosion resista
            - 316, annealed

Layout: All attributes | View | Tools | Units

Stainless steel, austenitic, AISI 316L, annealed

Composition detail (metals, ceramics and glasses)

C (carbon)	0 to 0.03	%
Cr (chromium)	16 to 18	%
Fe (iron)	61.9 to 72	% (estimate)
Mn (manganese)	0 to 2	%
Mo (molybdenum)	2 to 3	%
Ni (nickel)	10 to 14	%
P (phosphorus)	0 to 0.045	%
S (sulfur)	0 to 0.03	%
Si (silicon)	0 to 1	%

Price

Price	3.63 to 4.07	USD/kg (estimate)
Price per unit volume	28600 to 32800	USD/m^3 (estimate)

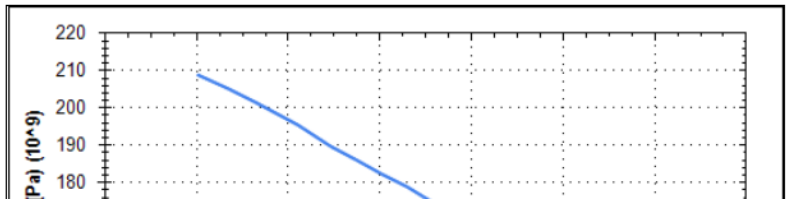
Physical properties

Density	7870 to 8070	kg/m^3

Mechanical properties

Young's modulus	1.9e11 to 2.05e11	Pa

Young's modulus with temperature — Hide Graph



ANSYS GRANTA

Risk Data

Viewer | Read Mode | Edit Mode | Home | Optimize | Substitute | Substances | Reports | Quick Search | Advanced Search | Help | Settings | Admin

Contents

Product Risk

- Products and parts
- Coatings
- Electricity mix
- Critical Materials
- End of life
- **Legislations and Lists**
- Materials - in house
- MaterialUniverse
- ProcessUniverse
- Producers
- Reference
- Resources
- **Restricted Substances**
- Shape
- Specifications
- Transport
- Use - mobile mode
- Use - static mode
- Suppliers

Product Risk | Home | Help / Contact

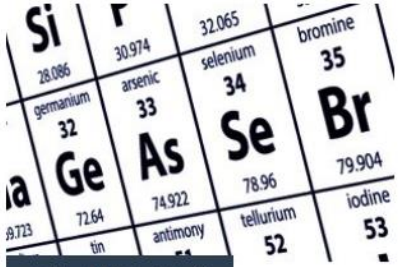
Overview | Map | Restricted Substances | Critical Materials | Engineering & Eco Properties

Product Risk

The Product Risk data module for GRANTA MI is a combined package of Materials, Restricted Substances, Critical Materials, Coatings, and Eco data providing enterprises with a single, integrated view of key engineering, environmental, and regulatory data.

Restricted Substances >

Search, browse and generate reports on legislations and lists, substances, materials, coatings, specifications, and products and parts.



Critical Materials >

Assess supply risks based on factors such as conflict minerals risk (Dodd-Frank Act), geopolitical risk, physical scarcity, and price volatility.

Engineering & Eco >

Find, select and compare materials according to their material properties, restricted substance risk, cost, environmental impact and more.

GRANTA MATERIAL INTELLIGENCE

An integrated source of Materials, Restricted Substances, Critical Materials and Eco data

Find Out More

About Granta's data products here.

Learn

How to get the most from the GRANTA MI software.

Help

For Help and Support.

Search Product Risk

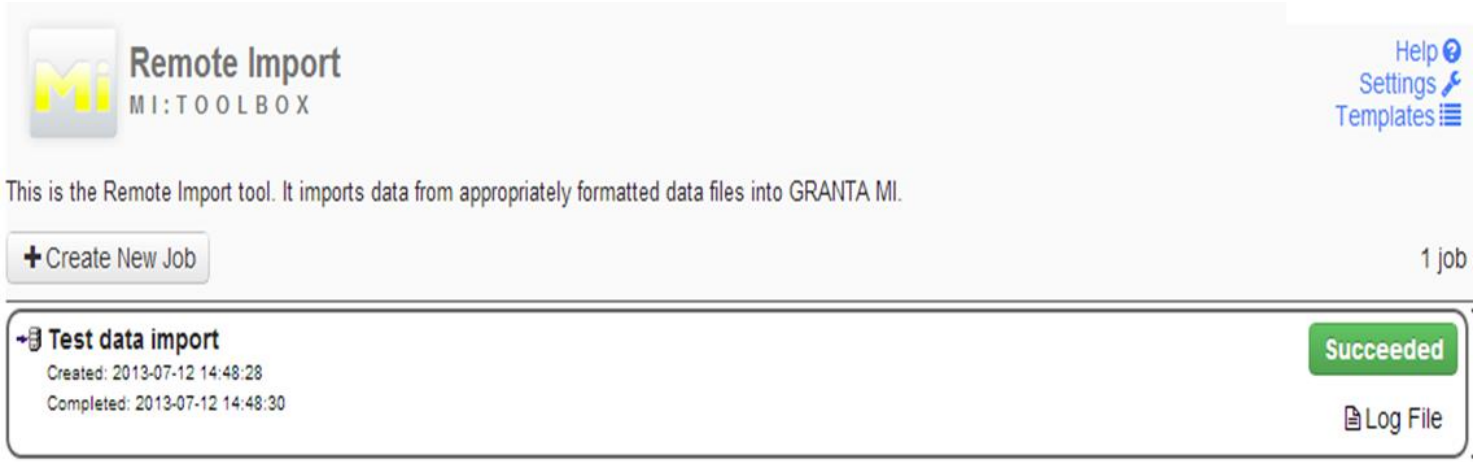
ANSYS GRANTA

Data Capture

- 1,800+ reference alloys (MaterialUniverse)
- 14,629 simulated alloys
- 2,162 physical specimens

Significant Standardization Effort

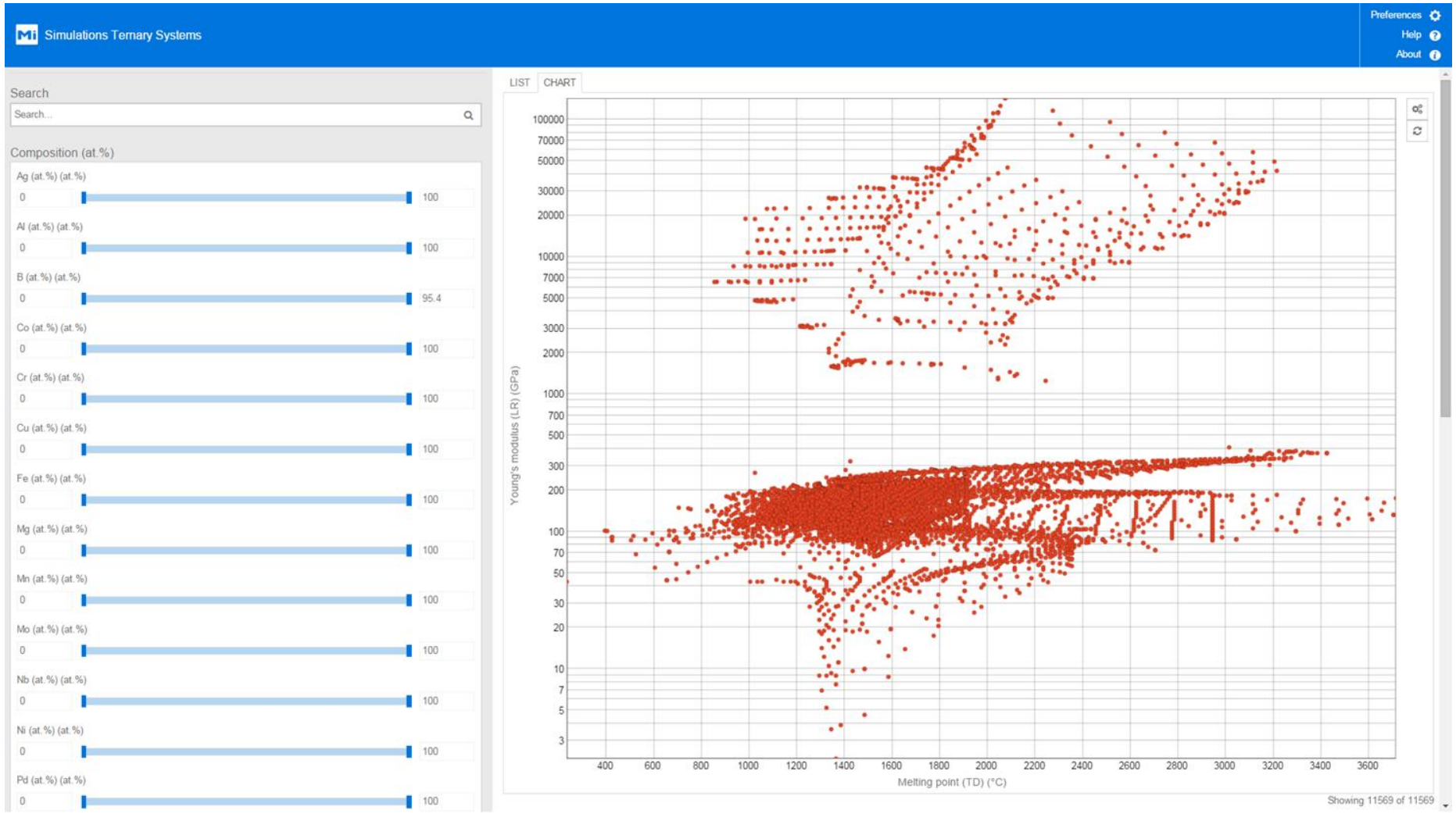
Enabled by Remote Import Tool & Machine Integration (Auto-import) & API's



MI:Explore – Visual Search & Selection

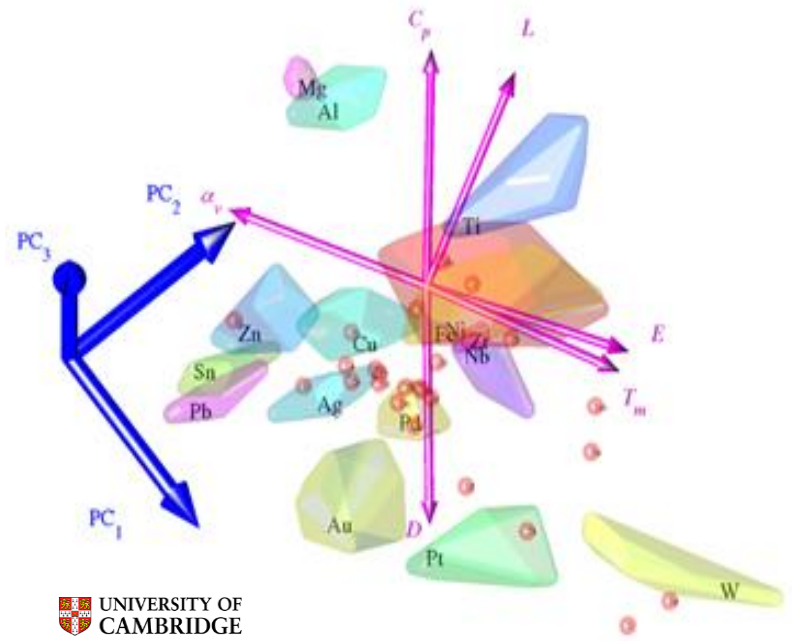
Combined:

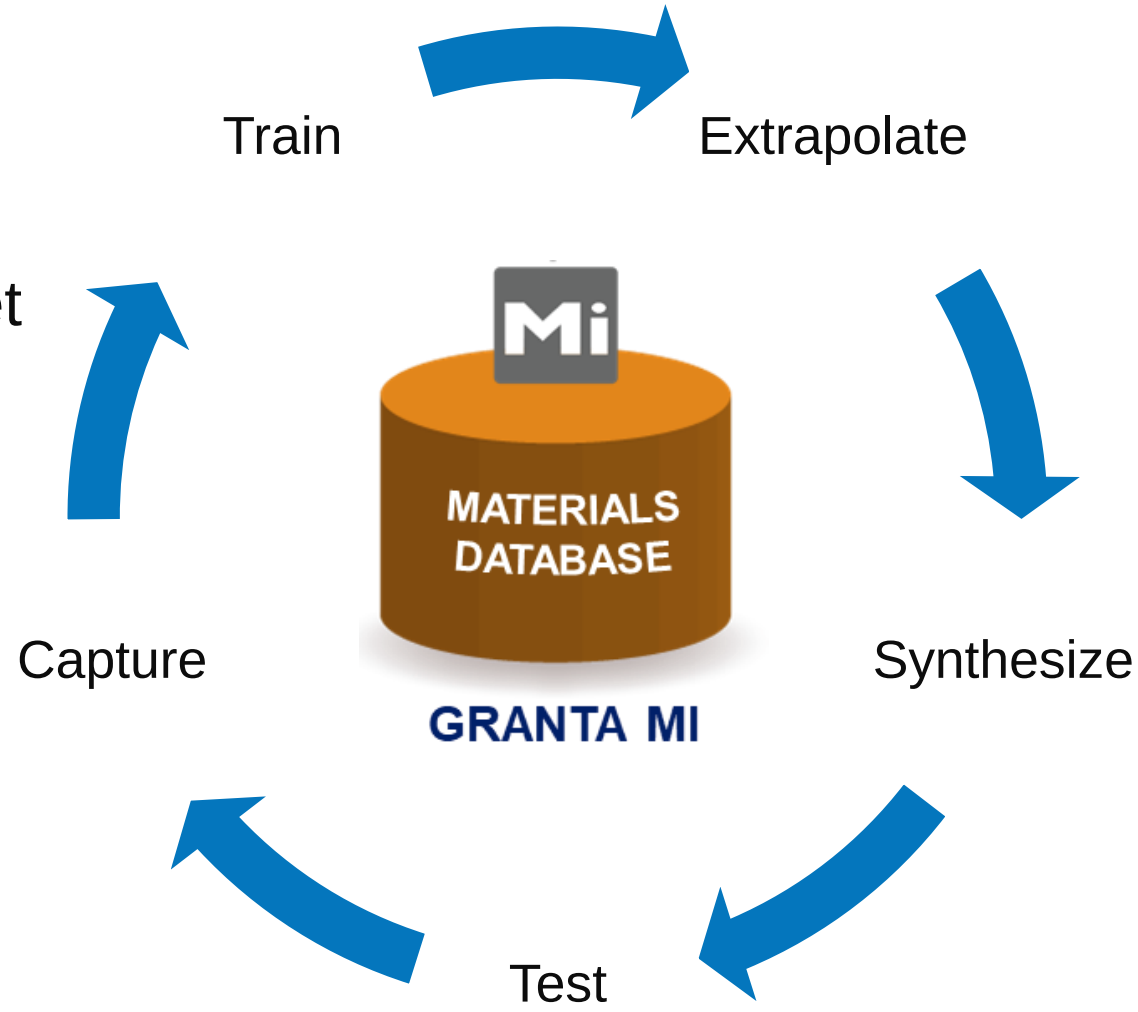
- Experimental data
- Simulation data
- Risk Data
  - Critical Materials
  - Restricted Substances
  - Eco Impacts
  - Costs



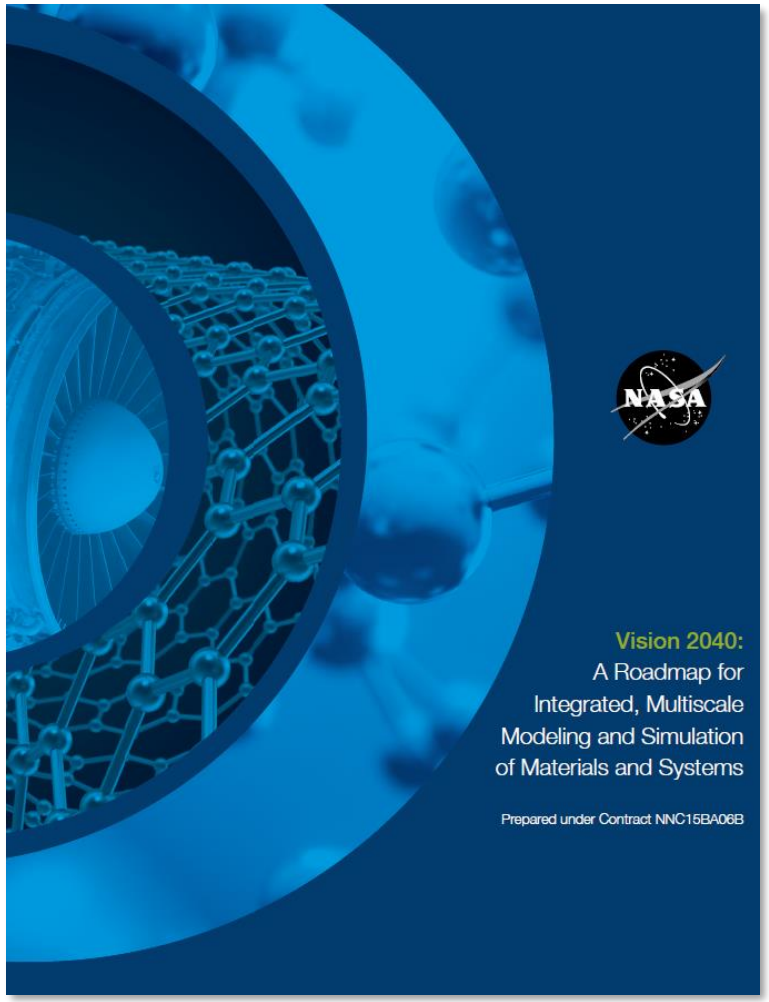
Machine Learning

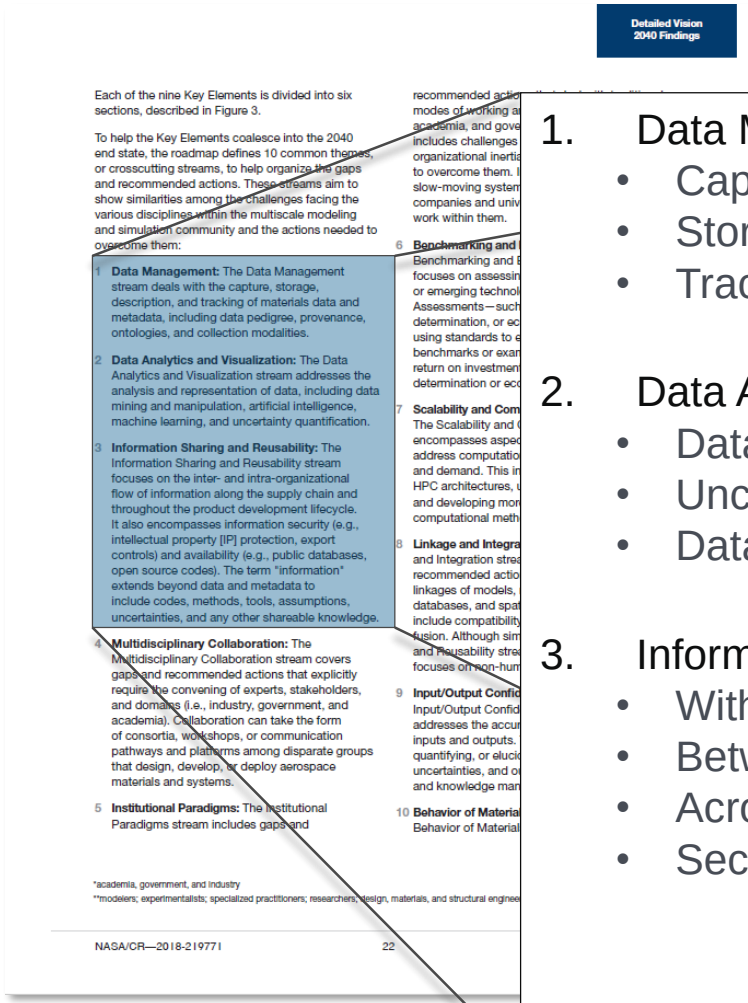
- Used extensively throughout.
- Iterative approach →
- Initially trained on MaterialUniverse dataset





Data Management for ICME

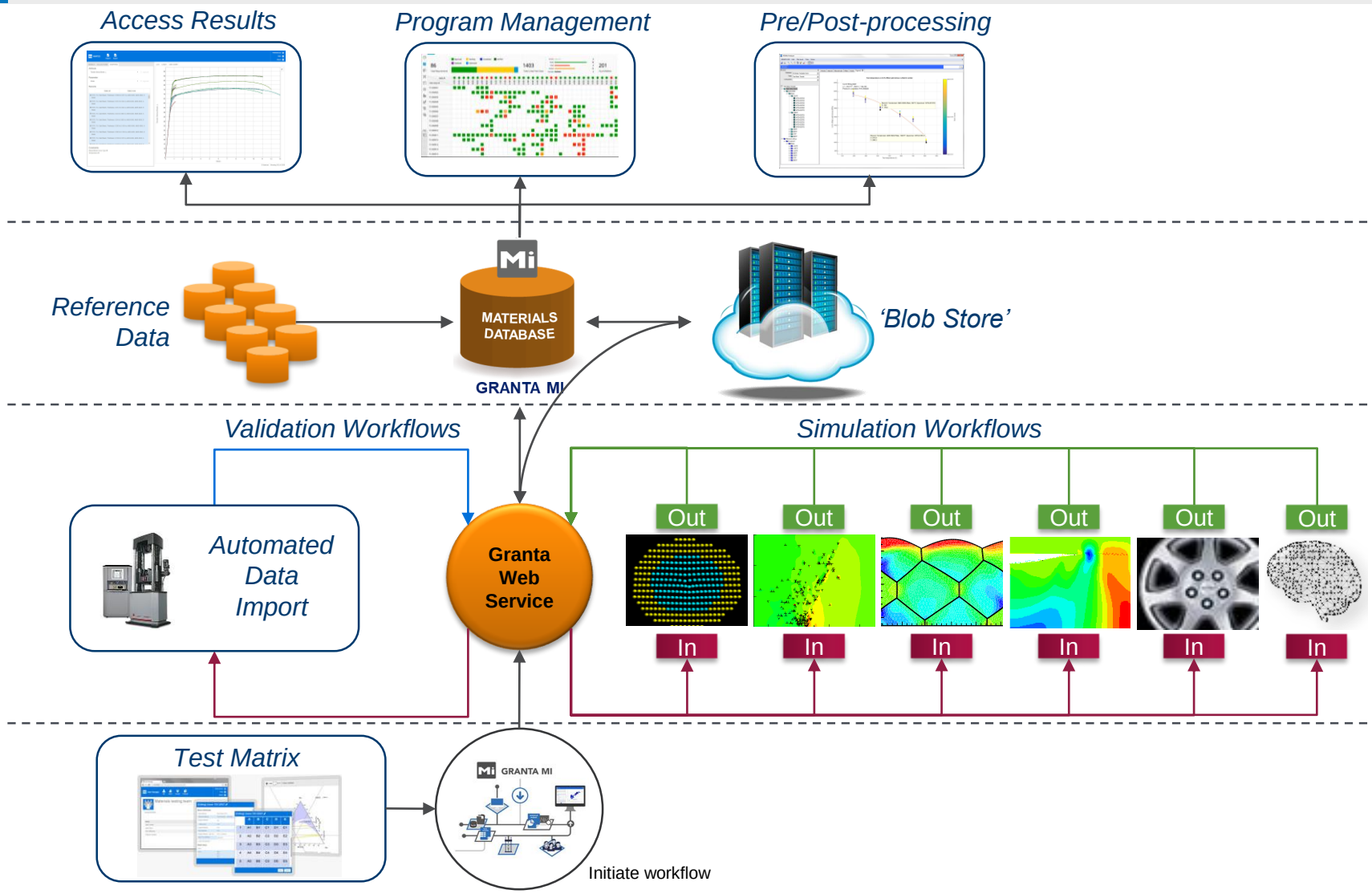




Crosscutting themes

1. Data Management
   - Capture
   - Storage
   - Traceability
2. Data Analytics & Visualisation
   - Data mining
   - Uncertainty quantification
   - Data representation
3. Information Sharing & Reusability
   - Within organisations
   - Between organisations
   - Across product development
   - Security and access control

Granta Vision for ICME



Data Visualisation & Processing
(Experiment & simulation in one place)

Data Management
(Big Data, Secure, Traceable & Consistent)

Integration
(Automated import, equipment & codes)

Workflows
(Experiment and Simulation management)

Questions

James.Goddin@ansys.com