

Robust Material Information Management System Essential to Enable 2040 Vision

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NASA Glenn Research Center

Innovative solutions through foundational research and cross-cutting tools

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Ansys State of the Art Digital Engineering Capabilities Communication Event

Sept 20-21, 2022

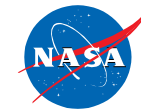


*Innovative solutions through
foundational research and
cross-cutting tools*

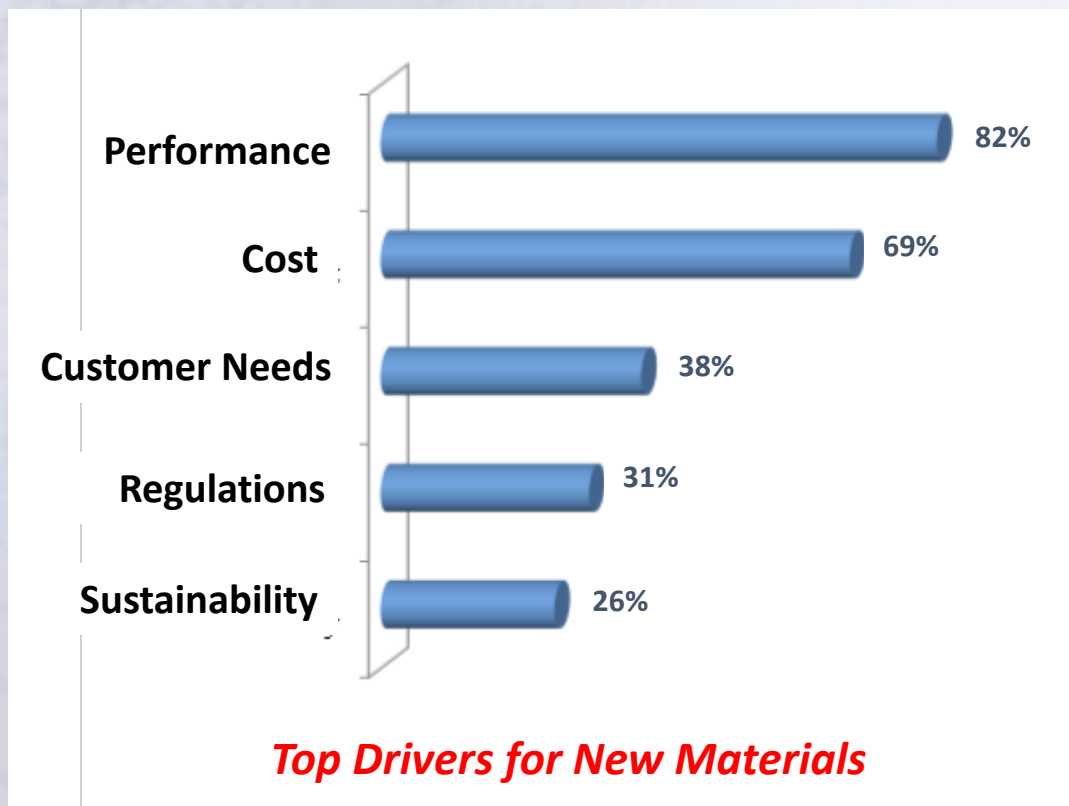
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Rapid Material Innovation Essential For Top Performing Organizations

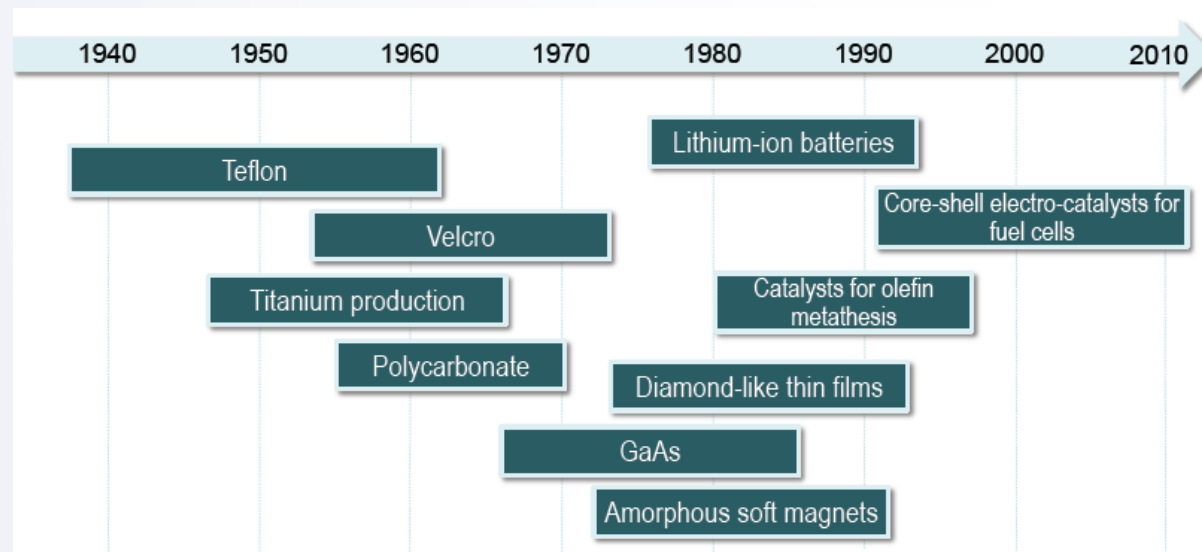


Top Performing Organizations - rate **New Materials** as one of **THE MOST IMPORTANT** factors in meeting their innovation goals.



Data taken from; "How to Empower R&D and Engineering Teams to Innovate with New Materials", Tech Clarity Inc, 2016.

Historical Material Development Time Unfortunately Measured in Decades

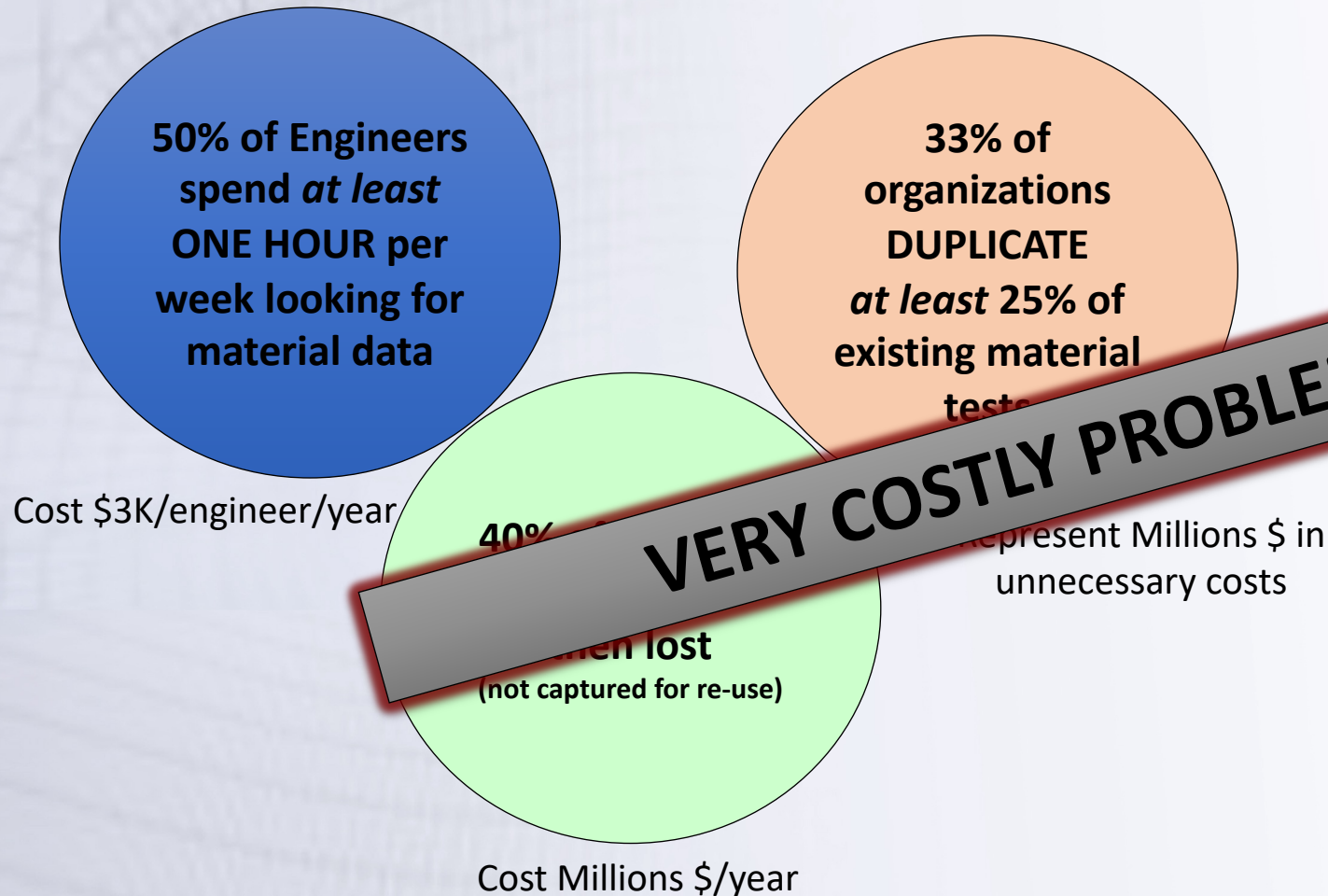


After Gerd Ceder (MIT); materials information from T. W. Eagar and M. King, Technology Review 98 (2), 42 (1995).
Catalysis information from R. Schrock et al. and R. Adzic et al.



Recently, Prof. Olsen demonstrated that if **potentials are known** for material class, material development can be shortened to 3-5 years

Why Does Material Information Management Matter?



David Meza: Head of Knowledge Management at NASA, JSC
Status Quo of Collaboration

- “Most engineers have to look at 13 different sources to find the information they are looking for”
- “46% of workers can’t find the information about half the time”
- “30% of total R&D funds are spent to redo what we’ve already done once before”
- “54% of our decisions are made with inconsistent or incomplete, or inadequate information”

<https://www.youtube.com/watch?v=QEBVoultYJg>

Axel Reichwein, June 5, 2018



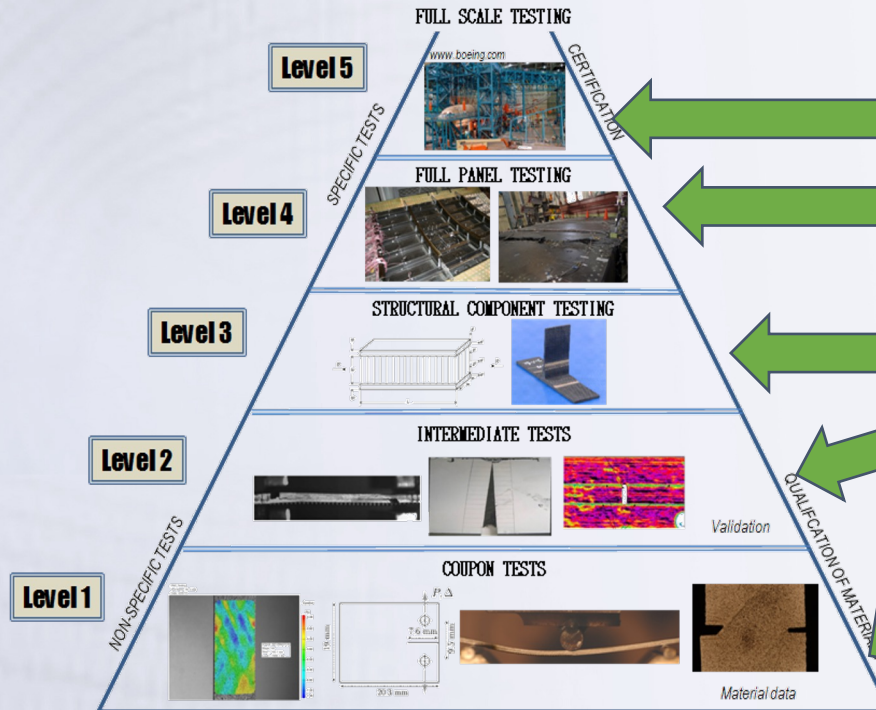
Data from July 2012 survey of 350 Granta customers/contacts; 35% N America, 45% Europe, 20% elsewhere; 25% current customers, 75% not customers

Virtual Testing Can Enable Significant Cost Savings in Certification Process



**Experimental
Building Block
Approach**

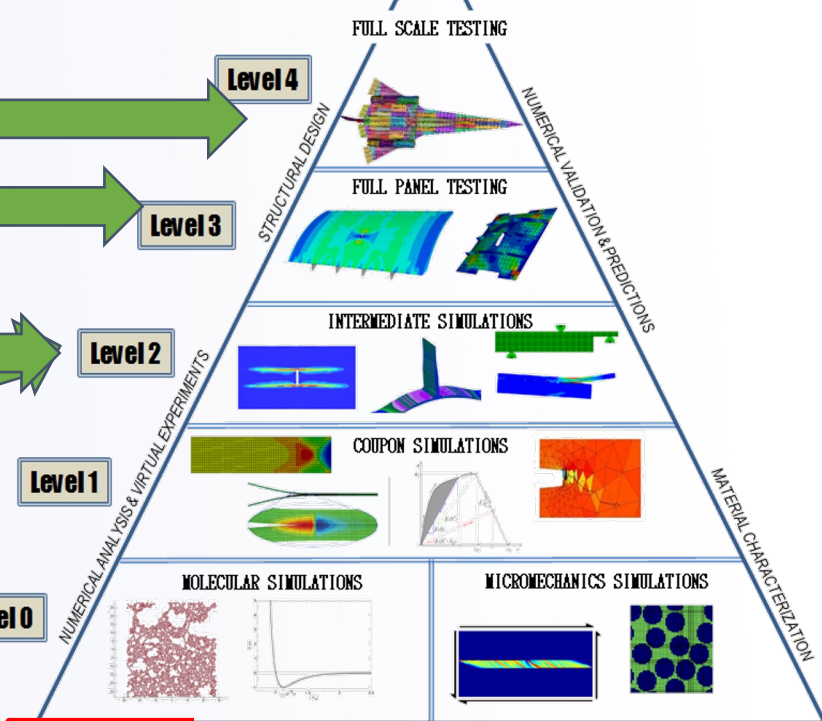
Experimental Test Pyramid



* OEM information

Numerical Simulation Pyramid

**Model
Building Block
Approach**



**Requires Information
Management**

\$\$

Savings!

A robust **validated computational** platform is **essential** for sustainable, cost-effective technology development program
➤ **reduced testing and time to certify!**

T³

MDMC* Organizations Stated Return on Investment (ROI) Arguments (Worth \$Millions)



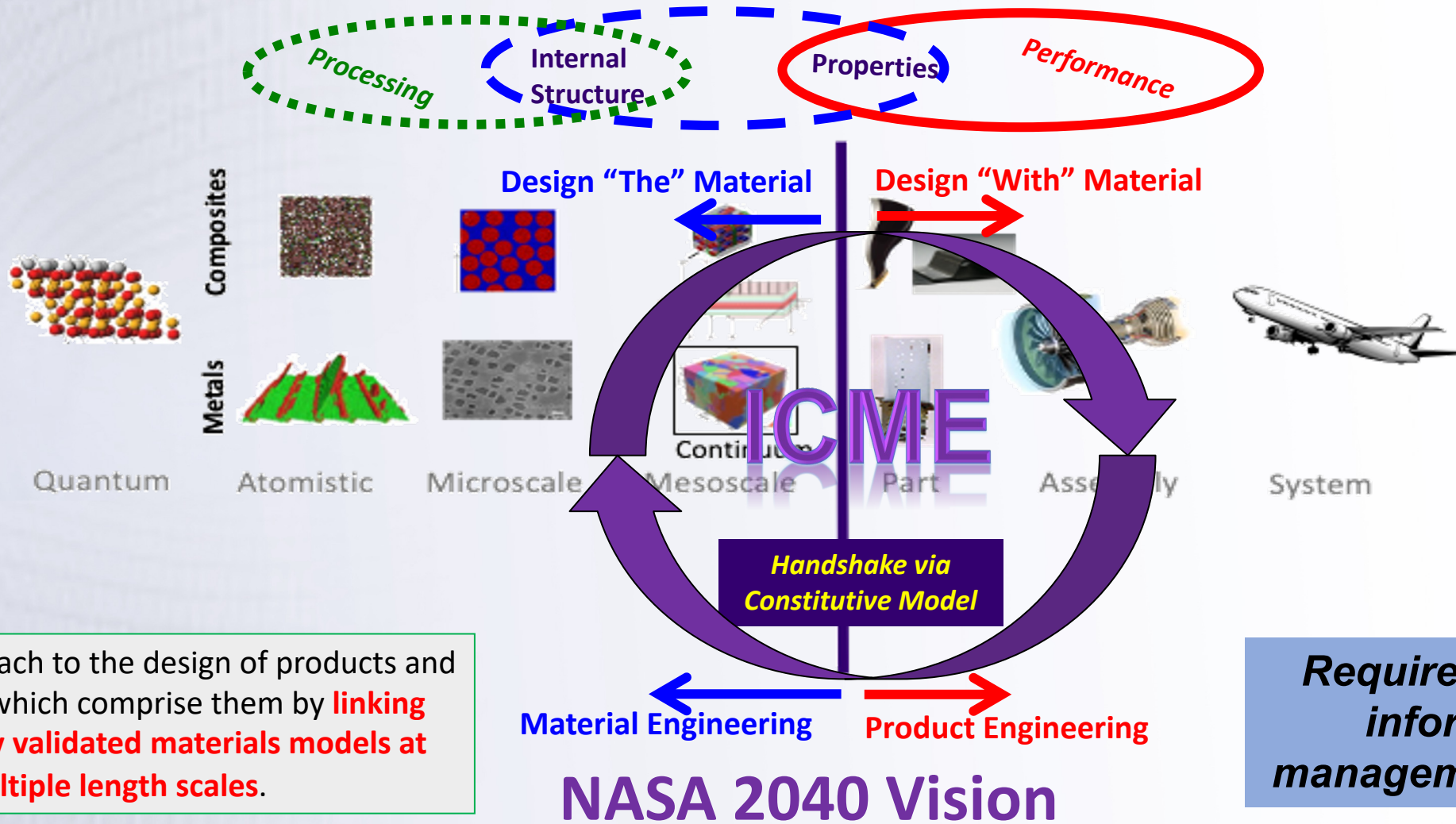
Establishing the case for change			Establishing the value of change		
Problems		Implications		Needs	Value or Payoff
We lose vital materials information (e.g., property data)	→	• Must recreate it • Slow down design cycle • Potential of using uncontrolled information • Appear Unprofessional • Wasted investment (time and money) • Need for redesign • Negative impact on morale		A simple, reliable and easy to GRC Goal: ZERO (Minimal) LOSS of DATA	• Reduce cost/waste • Accelerate design cycle • Increase Confidence from Customers (internal and external) • Better/more innovation • Decrease time to market
I waste a lot of time finding materials data	→	• Inefficient use of time • Waste of money • Miss deadline(s) • Slow Design process • Longer Time to market (Brand image, Customers, Competitive advantage...)		GRC Goal: More Efficient Interaction between experimentalist and Modelers	• Save time and money • Faster market process • Optimize engineering time • Faster Product derivative creation
Problems/issues arise because we use incorrect, inconsistent, or obsolete information/data (e.g., potentially wrong material)	→	• Design and lifing rework • Potential conservative/nonconservative design • In-service failure • Product recalls • Damage to brand image • Loss of internal confidence - lack of buy-in from data customers • Have difficulty getting ISO certification		A simple, reliable, easy to use and error-free way to process, summarize and display/control data GRC Goal: Excellence in Research Improve relationship between materials authority and downstream users - buy-in from customers	• Reduction of rework • Avoid failures • Competitive (efficiently designed) products • Reduction non-recurring engineering • Improve productivity • Help pass ISO certification • Customer confidence • Avoid brand damage through bad publicity • Reduce risk

MDMC Organizations Stated Return on Investment (ROI) Arguments (Worth \$Millions)



Establishing the case for change			Establishing the value of change		
Problems		Implications		Needs	Value or Payoff
The access to my data is not secured enough or controlled	→	• Jail time • Data doesn't go into the system • Severe fines	↔	A simple, reliable, easy to use and error-free way to process, organize and deploy/control my data	→ • Ticket to play • Business continuity
I can't comply with policy or regulations (e.g., ITAR)	→	• Jail or severe fines	↔	A simple, reliable, easy to use and error-free way to process, organize and deploy/control my data	→ • Ticket to play • Business continuity
I don't have appropriate, secure access to mission-critical data throughout my organization.	→	• Don't know what data is available • Restricts ability to work effectively across organization • Reduced productivity • Too much effort to get the data you need - make something up!	↔	A simple, reliable, easy to use and error-free way to process, organize and deploy/control my data	→ • Ability to perform assigned tasks

Integrated Computational Materials Engineering (ICME) Enables Innovation

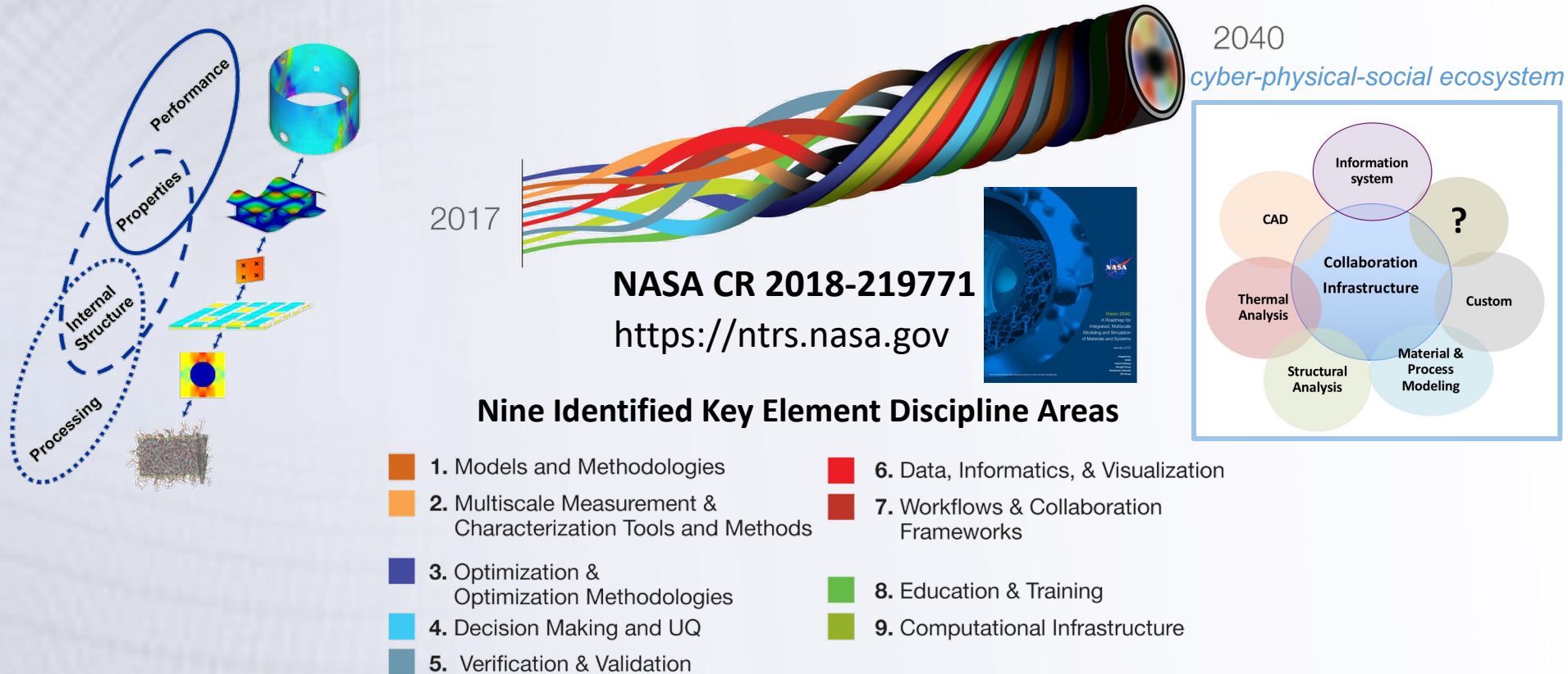


ICME is an approach to the design of products and the **materials** which comprise them by **linking experimentally validated materials models at multiple length scales**.

Requires a robust information management system

Vision 2040: A Roadmap for Integrated, Multiscale Modeling and Simulation of Materials and Systems

Provides a public/private investment strategy for the design of fit-for-purpose materials and structures



2040 Vision State:

*A cyber-physical-social ecosystem that impacts the supply chain to **accelerate** model-based concurrent design, development, and deployment of materials and systems throughout the product lifecycle for **affordable, producible** aerospace applications*

2040 Ecosystem **Revolutionizes** Design Paradigm



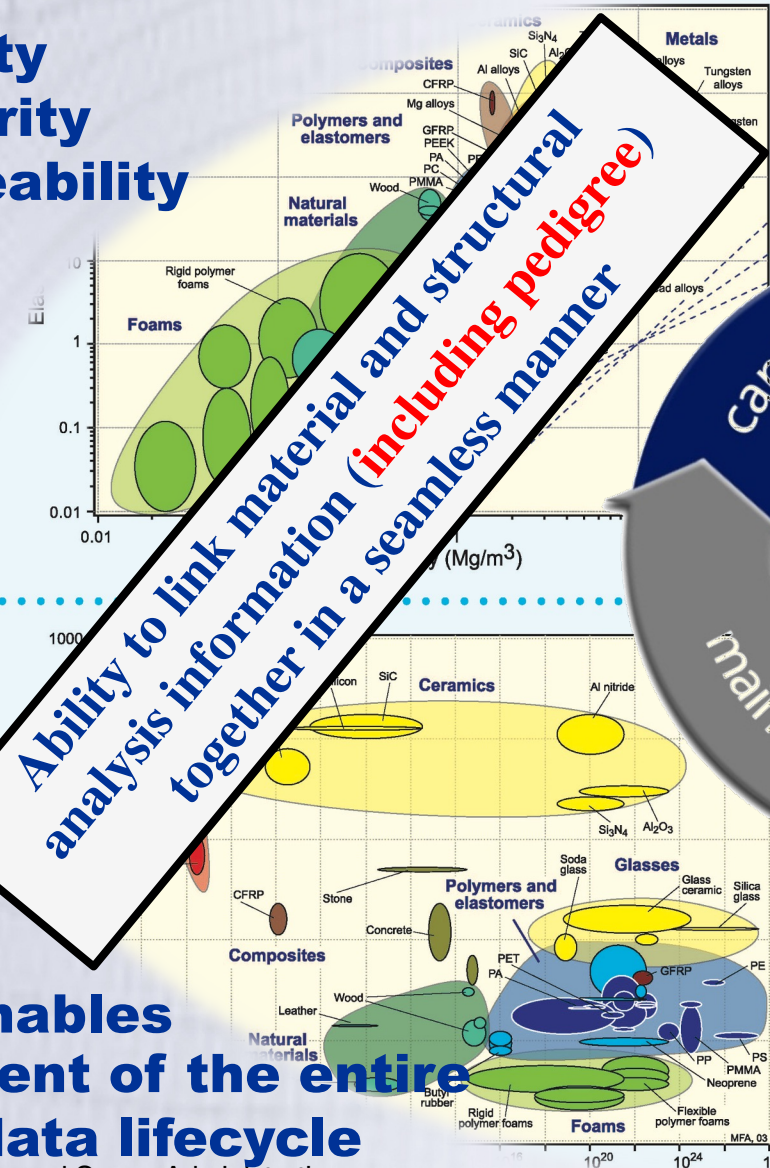
*The cyber-physical-social ecosystem that marries “the design of materials” (material scientist viewpoint) with “the design with materials” (structural analyst viewpoint) approaches into one concurrent **transformational digital paradigm**.*

Today' s Design Paradigm	2040 Design Paradigm
Design Of Materials And Systems Is <i>Disconnected</i>	Design Of Materials And Systems Is <i>Integrated</i>
Stages Of The Product Development Lifecycle Are <i>Segmented</i>	Stages Of The Product Development Lifecycle Are <i>Seamlessly Joined</i>
Tools, Ontologies, And Methodologies Are <i>Domain-specific</i>	Tools, Ontologies, And Methodologies Are <i>Usable Across The Community</i>
Materials Properties Are Based On <i>Empiricism</i>	Materials Properties Are <i>Virtually Determined</i>
Product Certification Relies Heavily On <i>Physical Testing.</i>	Product Certification Relies Heavily On <i>Simulation</i>

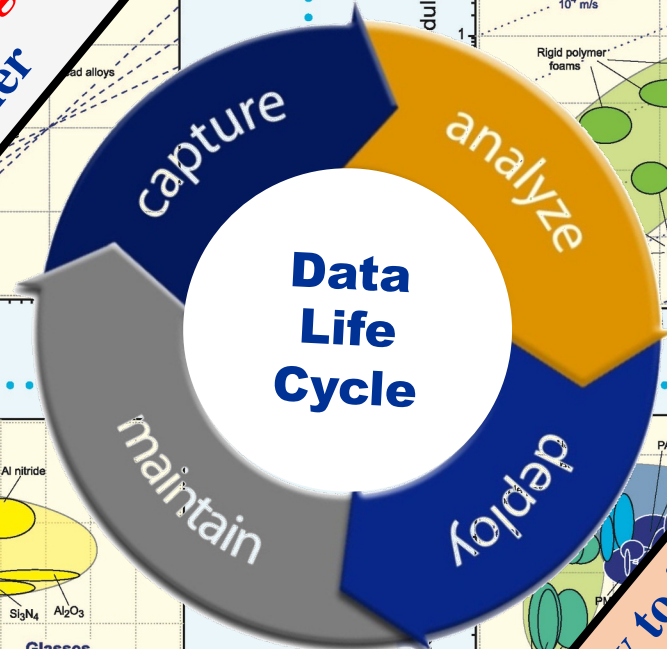
Motivation For Selection of Granta MI As Our Information Management/Collaboration Framework

**Quality
Integrity
Traceability**

**Right Data
Right Time
Right Format**



Ability to link material and structural analysis information (including pedigree) together in a seamless manner

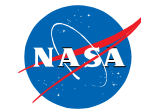


The ability to introduce best practices and preserve corporate knowledge from one generation to the next

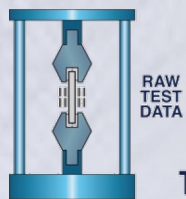
Toolset enables management of the entire material data lifecycle

**Increased Efficiency
Competitiveness**

ANSYS Granta MI Integrated into our Workflow for Design and Analysis at Elevated Temperature



Cradle



RAW TEST DATA

www.mdmc.net

ANSYS GRANTA MI

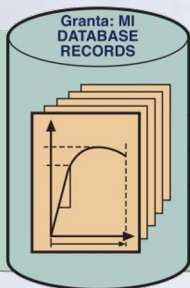
Traceable in-house relational materials database

TENSILE TEST DATA LOG

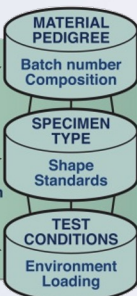
Test date: 04-12-2011
Operator: A. Grant
Test frame: DDC-41-17

Time	Stress	Strain
(s)	(ksi)	(in/in)
0.1	2.0	0.1
0.2	2.2	0.2
0.3	2.4	0.3
0.4	2.6	0.4
0.5	2.8	0.5
0.6	3.0	0.6
0.7	3.2	0.7
0.8	3.4	0.8
0.9	3.6	0.9

CALCULATE key parameters,
ANALYZE multiple files,
STORE original data



LINKS between
database information



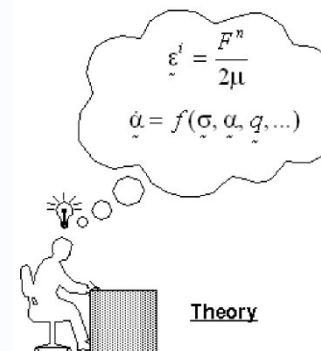
STATISTICAL SUMMARIES OF MULTIPLE TESTS



Mathematical Characterization Of Material Behavior

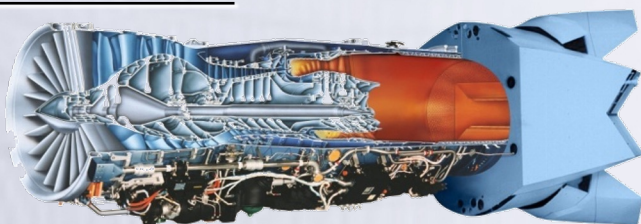
COMPARE

Automatically write required input information

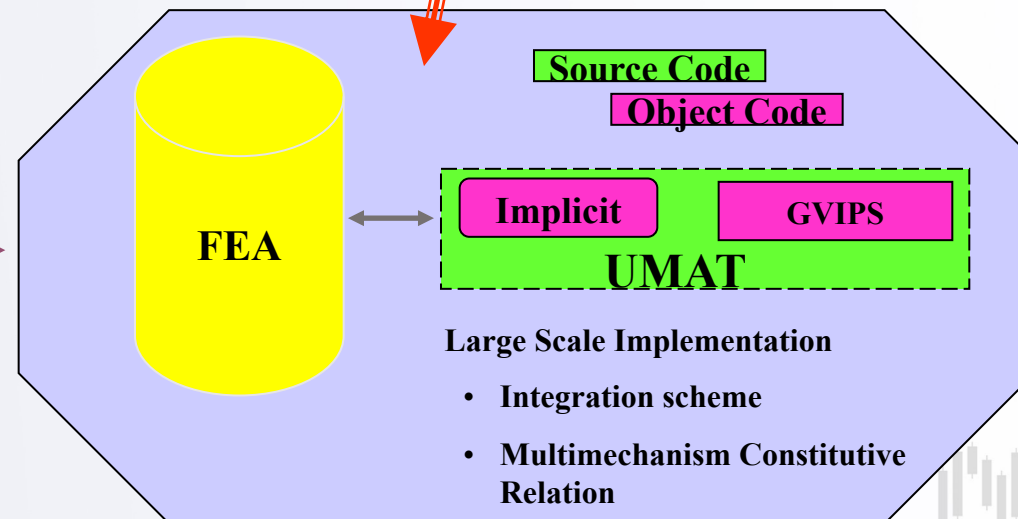


Theory

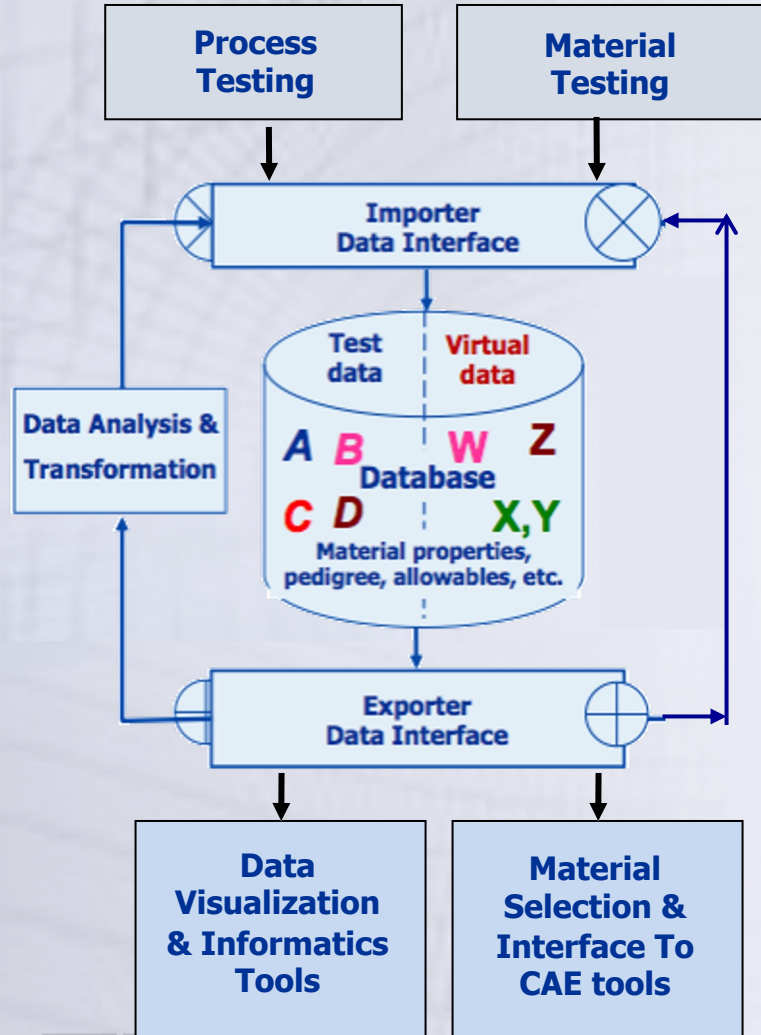
Arm-Chair



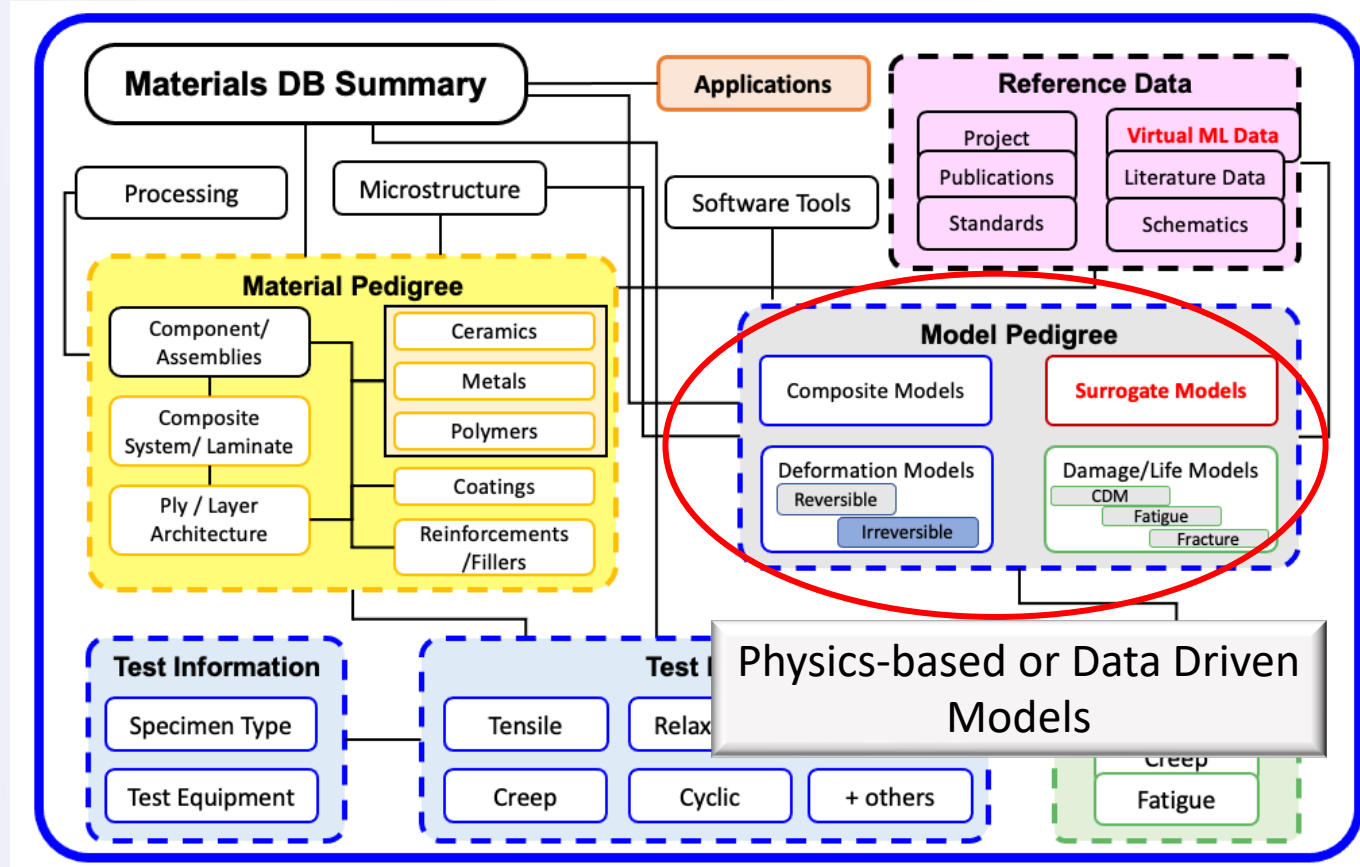
FE Analysis of components



Key To Making ICME & Virtual Testing a Reality Is Coupling Between Testing, Modelling and Application



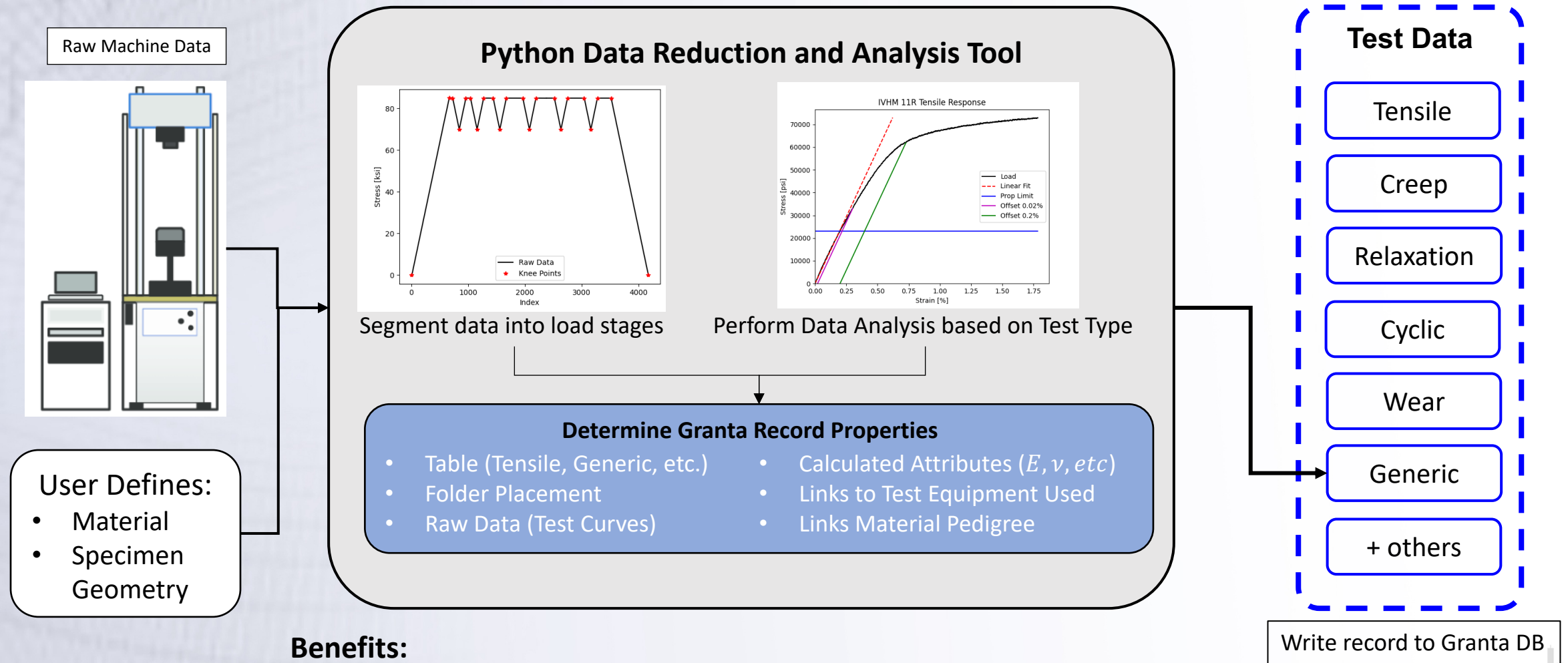
To accomplish this introduced Model, Microstructure, Software Tools and Application Tables



Arnold, S.M., Holland, F. and Bednarczyk, B.A.; (2014). Robust Informatics Infrastructure Required For ICME: Combining Virtual and Experimental Data, **55th AIAA/ASME/ASCE/AHS/SC Structures, Structural Dynamics, and Materials Conference**, National Harbor, Maryland, 13 - 17 January **2014, AIAA-2014-0460**

Arnold, S. M., et. al (2015). ; "Microstructural Influence on Deformation and Fatigue Life of Composites Using the Generalized Method of Cells", **56th AIAA/ASME/ASCE/AHS/SC Structure AIAA SciTech 2015, ICME Special Session**, Kissimmee, FL, **2015; AIAA 2015-0202**

Automatic Data Analysis and Database Placement Via APIs



Benefits:

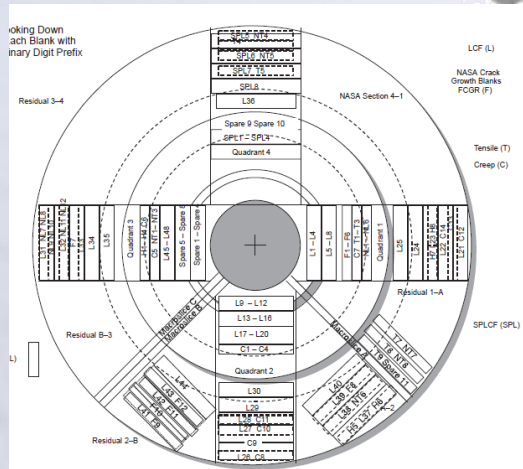
- Consistent and significant data analysis/reduction
- Ease of importation of data with maximum automation included

ICME Data Schema Enables Data Mining of Microstructure / Property/ Performance Relationships

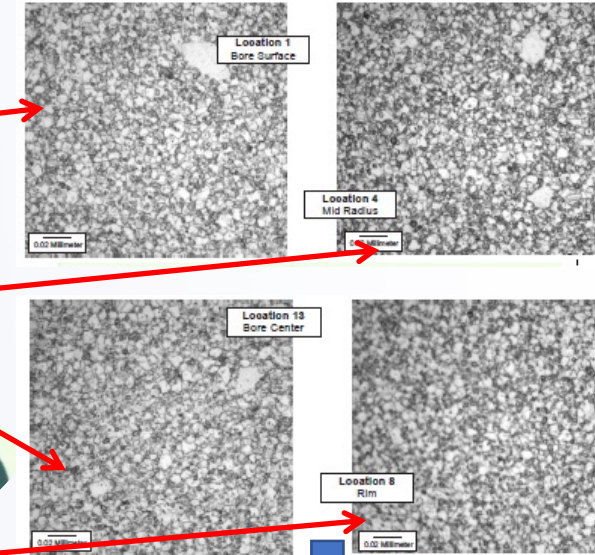
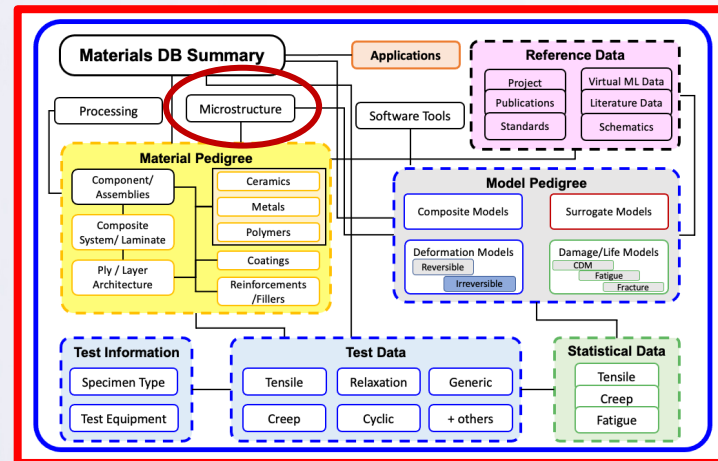
Established data scheme for capturing and analyzing Nickel based superalloy, e.g., **ME3**, turbine disk material information necessary to enable **microstructure/property/failure** relationships.

Location Pedigree: Requires tracking of specimen location and microstructure

Processing

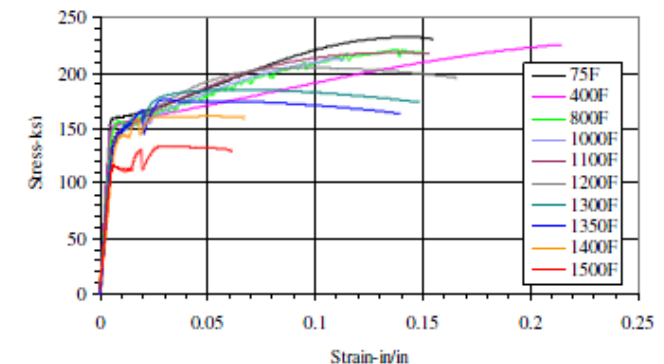


Microstructure Table



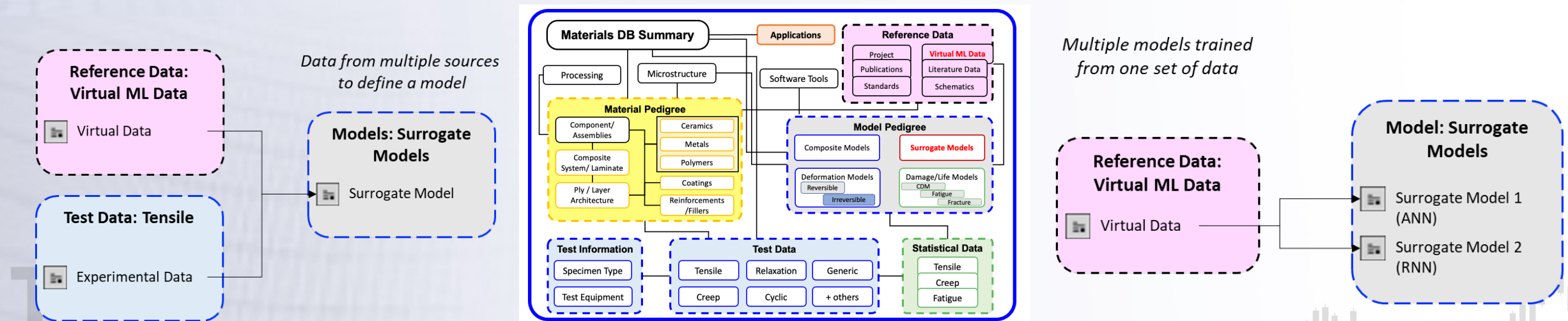
Supersolvus Tensile Stress-Strain Curves

Performance



Model Table Enables Machine Learning

- Created two new tables in the NASA GRC Database
 - Reference Data: Machine Learning
 - Contains all reference and virtual data created specifically for training machine learning models
 - Models: Machine Learning
 - Contains records for developed machine learning / surrogate models
 - Links to the associated data used for training/validation/testing
- Flexibility in model definition prevents data from being repeated multiple places in the database



Examples of data storage flexibility for ML models

Attributes Defining Machine Learning



Reference Data: Machine Learning

Attribute	Type
Data Series Information	
Standard Test Description	LTXT
Data Ownership	DCT
Data Ownership (Other)	STXT
Distribution Category	DCT
Funding Organization	STXT
Software Tools	STXT
Project Code	STXT
Project Name	STXT
Project Notes	LTXT
Point of Contact	TABL
Testing Organization	STXT
Original Data Filename	FILE
Data Series Information	
Data ID	STXT
Data Labels	TABL
Attribute 1	LTXT
Attribute 2	LTXT
Attribute 200	LTXT
Data Series Information	
Model Records	LINK

Models: Machine Learning

Attribute	Type	Attribute	Type
Project Information		Data Definition	
Performing Organization	STXT	Data Variables Summary	TABL
Data Ownership	DCT	Data Assembly	TABL
Data Ownership (Other)	STXT	Training Data Set (View)	TABL
Distribution Category	DCT	Validation Data Set (View)	TABL
Funding Organization	STXT	Test Data Set (View)	TABL
Project Code	STXT	Model Validation	
Project Name	STXT	Training Loss	FUNC
Project Notes	LTXT	Validation Loss	FUNC
General Model Information		Validation Predictions (Define)	TABL
Model Name	STXT	Test Predictions (Define)	TABL
Model Description	LTXT	Accuracy	PNT
Source Code Locaiton	HYP	Accuracy Metric	DCT
Point of Contact	TABL	Validation Notes	LTXT
Version	STXT	Further Information	
Date	DATE	References	LINK
Libraries/Modules	TABL	Data Information	LINK
Model Notes	LTXT	Software Information	LINK
Model Architecture			
Architecture Type	STXT		
Architecture Description	TABL		
Architecture Notes	LTXT		



Application Table Orchestrates ICME



- Required to enable Integrated Computational Materials Engineering (ICME)
 - Marrying of Design “the” Material and Design “with” Material paradigms
 - Application Table provides an intimate link to **Performance Requirements**
- Enables unique location to link CAD/PLM/SLM information to materials information as well as **BOM**
- Provide information (application requirements) that can be used to drive the design and manufacture of “fit-for-purpose” materials
- Provides spatial and temporal information on application microstructure, residuals, damage, etc.
 - Maintenance of the **Digital Thread**

Attribute	Type	Attribute	Type
General Information		Inspection	
Performing Organization	STXT	Inspectability Notes	LTXT
Project Name/Funding Source	STXT	Evaluator	TABL
Point of Contact	TABL	NDE Method	DCT
Application Name	STXT	NDE Comments	LTXT
Manufacturing Process	DCT	NDE Information	FILE
Manufacturing Process (Other)	STXT	NDE Images	TABL
Readiness Levels		Standards	
Technology Readiness Level	DCT	ASTM Standards	LINK
Manufacturing Readiness Level	DCT	MMPDS Standards	LINK
Integration Readiness Level	DCT	NASA Standards	LINK
System Readiness Level	DCT	Load Definition/Operating Conditions	
Regulatory Readiness Level	DCT	Analyst Information	TABL
Performance Requirements		Stress Analysis Performed	DCT
Weight	RNG	Stress Analysis Performed (Other)	STXT
Cost	RNG	PLM/SLM ID	STXT
Life	RNG	PLM/SLM Link	HYP
Risk	DCT	Design Profile	TABL
Storage Energy	RNG	Analyzed Profile	TABL
Safety Factor	RNG	Stress Range	RNG
Ultimate Strength	RNG	Strain Range	RNG
Images	TABL	Temperature Range	RNG
Performance Notes	LTXT	Failure Mechanism/Modes	
Material Selection		Failure Mode	DCT
Part List	TABL	Failure Mechanism	DCT
Bill of Materials (BOM)	TABL	Failure Mode and Effect Analysis	TABL
Material Links	LINK	Failure History	LTXT
Selection Criteria	FILE	Failure Report	LINK
Software Tool Used	LINK	Failure Analysis Case Number	STXT
Software Tool Used (Other)	STXT	Failure Analysis Case Study	LINK
Property File	FILE	Uncertainty	
Material Selection Assumptions	FILE	Nominal Load	PNT
Geometric/Manufacturing Requirements		Nominal Load Unit	STXT
Owner Information	TABL	Measurement Uncertainty Analysis - Component	TABL
Surface Area	PNT	Uncertainty Analysis - Total Measurement System	TABL
Volume	PNT	Total Measurement System Uncertainty	PNT
Boudning Box Dimensions	LTXT	Total Measurement System Uncertainty Unit	STXT
CAD/CAE Link	LINK	Measurement Uncertainty Calculation File	FILE
Geometric Schematic: Target	IMG	DCT Discrete Text (specified choices) FDA Functional Data Attribute (with associated parameters) FIL Allows the association of any file type to a given record INT Integer Value LOG Logical LTXT Long Text Field PIC Allows association of any image format to a given record PNT Point value RNG Range variable STXT Short Text Field TABL Tabular Attribute (multiple columns of data - PNT, STXT, DCT, INT, link)	
Geometric Schematic: Actual	IMG		
Tolerances	STXT		
Geometric Notes	LTXT		
Coordinate System Definition	IMG		
Microstructure Profile Location Definition	TABL		
Microstructure Profile Time History Definition	TABL		
Microstructure Profile History	TABL		
Residual Profile Location Definition	TABL		
Residual Profile Time History Definition	TABL		
Residual Profile History	TABL		
Part Yield	PNT		
Surface Treatment	DCT		
Manufacturing Notes	LTXT		



Illustration of Multiscale Database Management in ICME



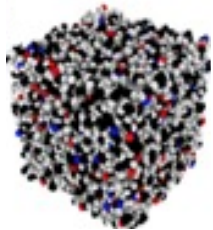
Design **the** material

Design **with the** material



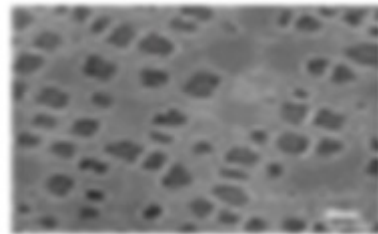
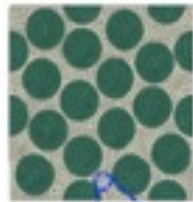
Nanoscale

- Nanoparticles /fillers
- Resin chemistry characterization
- Molecular Dynamics simulations



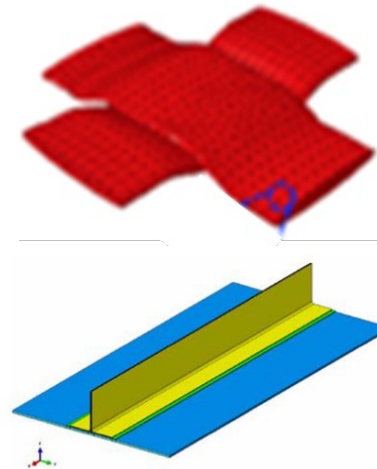
Microscale

- Composite constitutive properties
 - Fibers
 - Matrixes
- Lamina Properties



Mesoscale

- Laminate/Ply Sequences
- Subcomponents
 - T-stiffened panel



Macroscale

- Applications and Assemblies
- Structural components/system

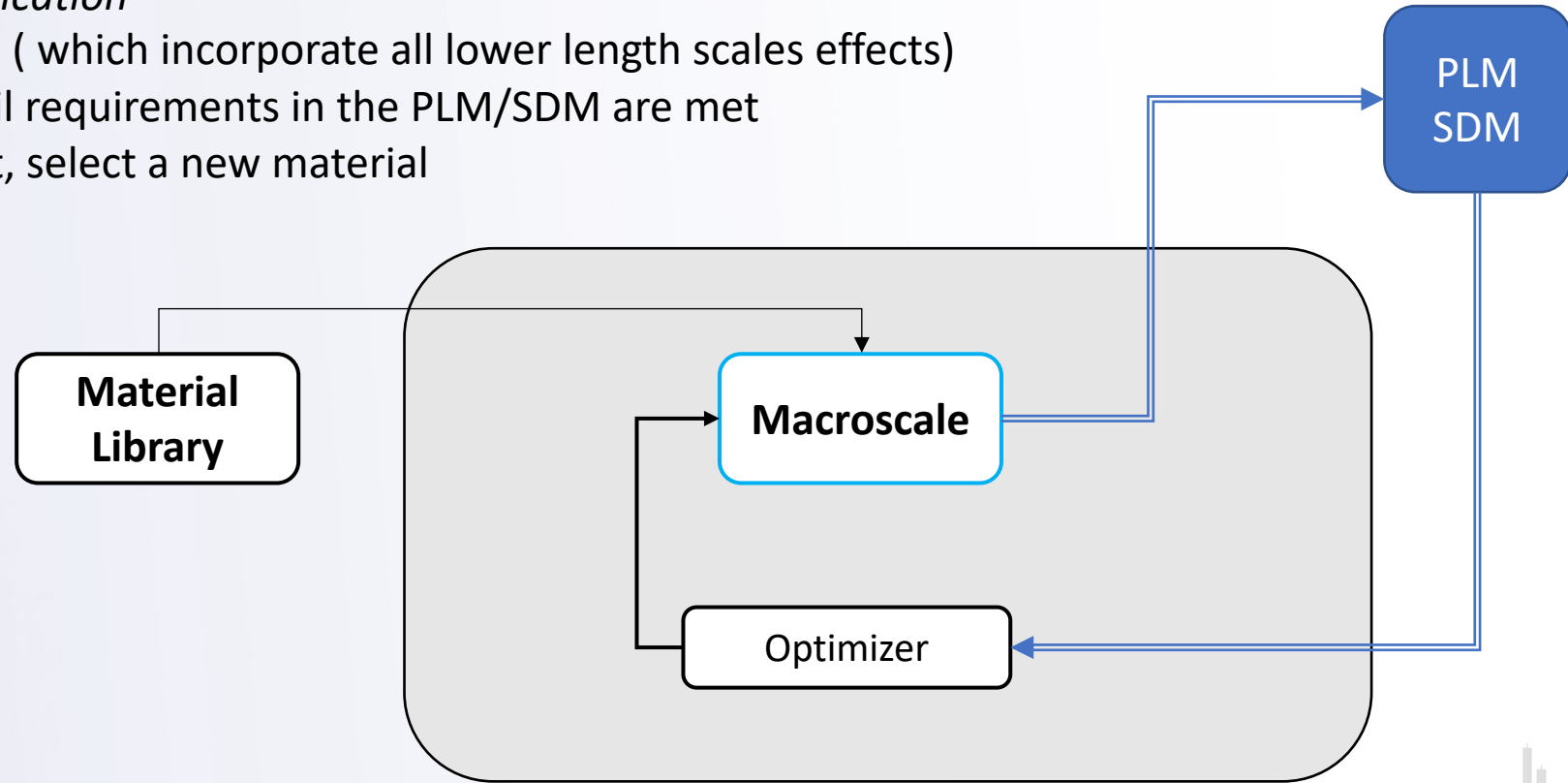


Traditional Database/Simulation Management Only Deals with a Single Scale



Traditional Design

- *Select a known material for an application*
- Use macroscale material properties (which incorporate all lower length scales effects)
- Iterate on the structural design until requirements in the PLM/SDM are met
 - If requirements cannot be met, select a new material

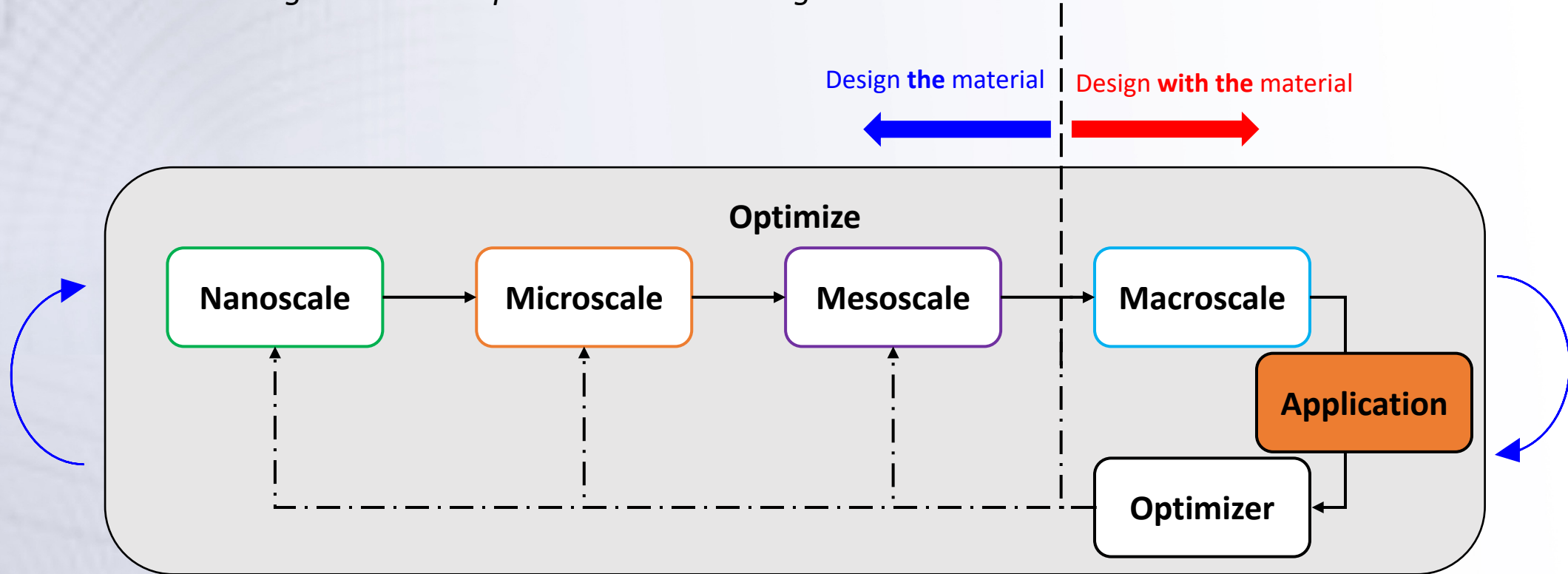


Database Management in ICME



ICME Design

- Design the material for a specific application from processing through performance (fit-for-purpose)
- Use Multiscale Digital Tools to optimize material design



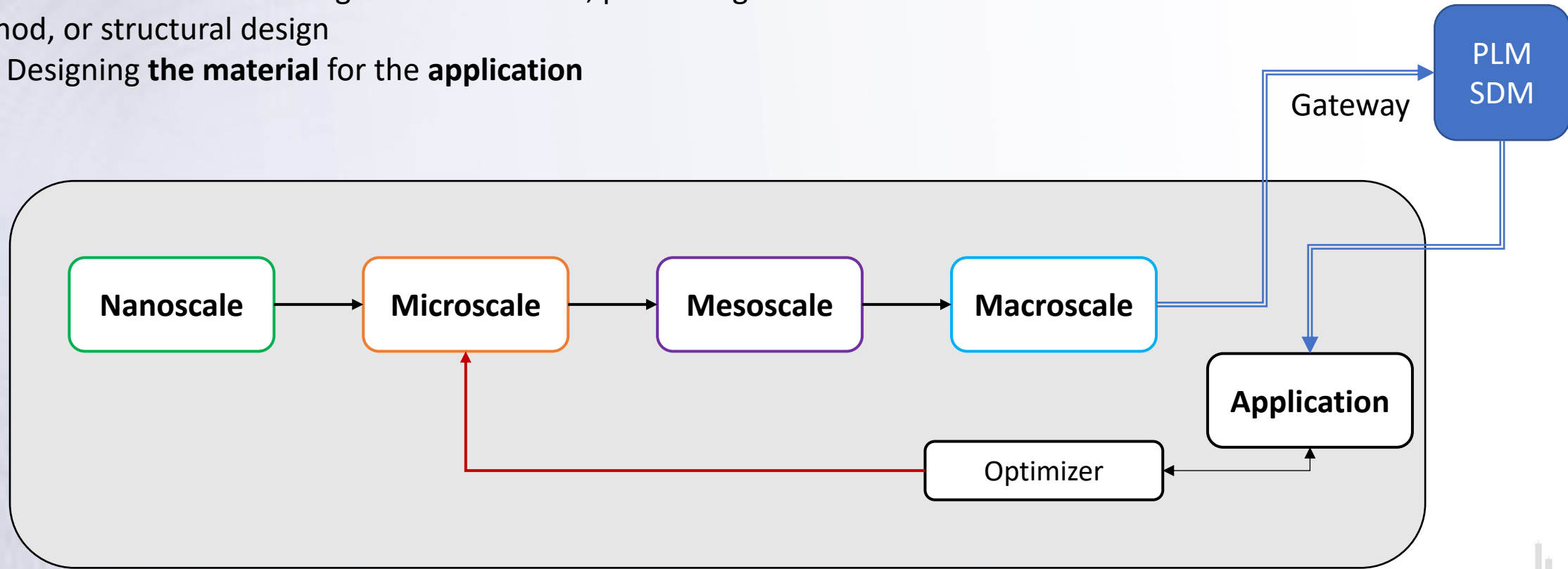
Remember the two important key words in ICME being 1) **Integrated** wherein processing histories, influence internal structure, which in turn drive properties, which then drive performance and 2) **Engineering** which signifies industrial utility!

Database/Simulation Management in ICME



Illustrate with Example in which the fiber reinforcement of a composite material used for a structural component is varied

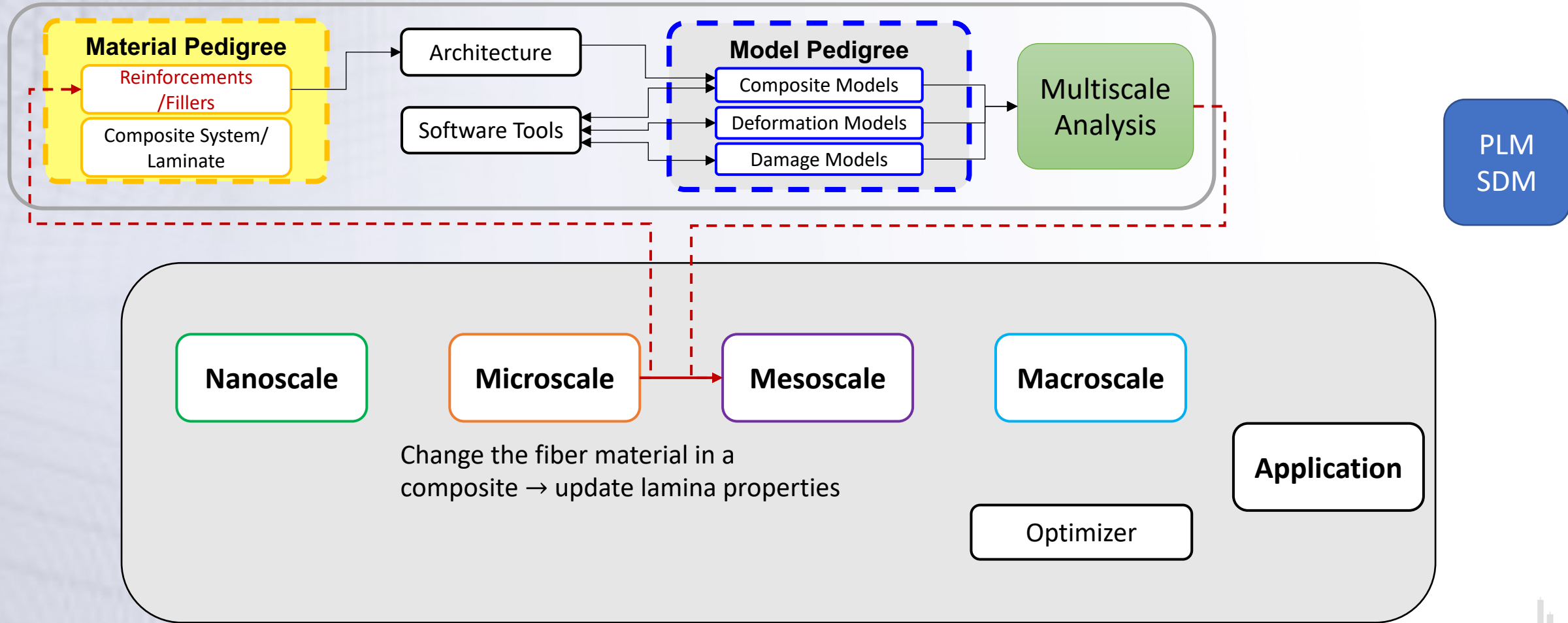
- Consider changing the material characteristics at lower scales
- Optimization can either change material choice, processing method, or structural design
 - Designing **the material** for the **application**



Database/Simulation Management in ICME



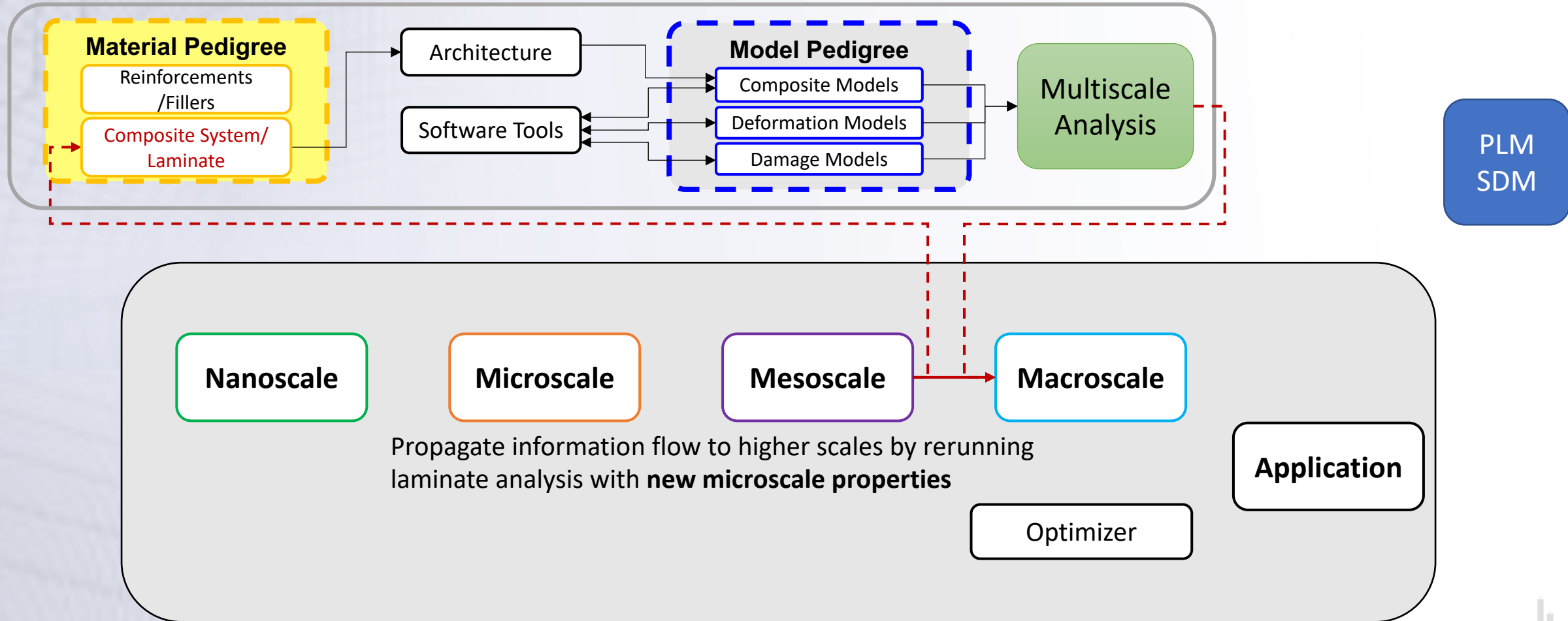
Automation of read/write and tool execution in background



Database/Simulation Management in ICME



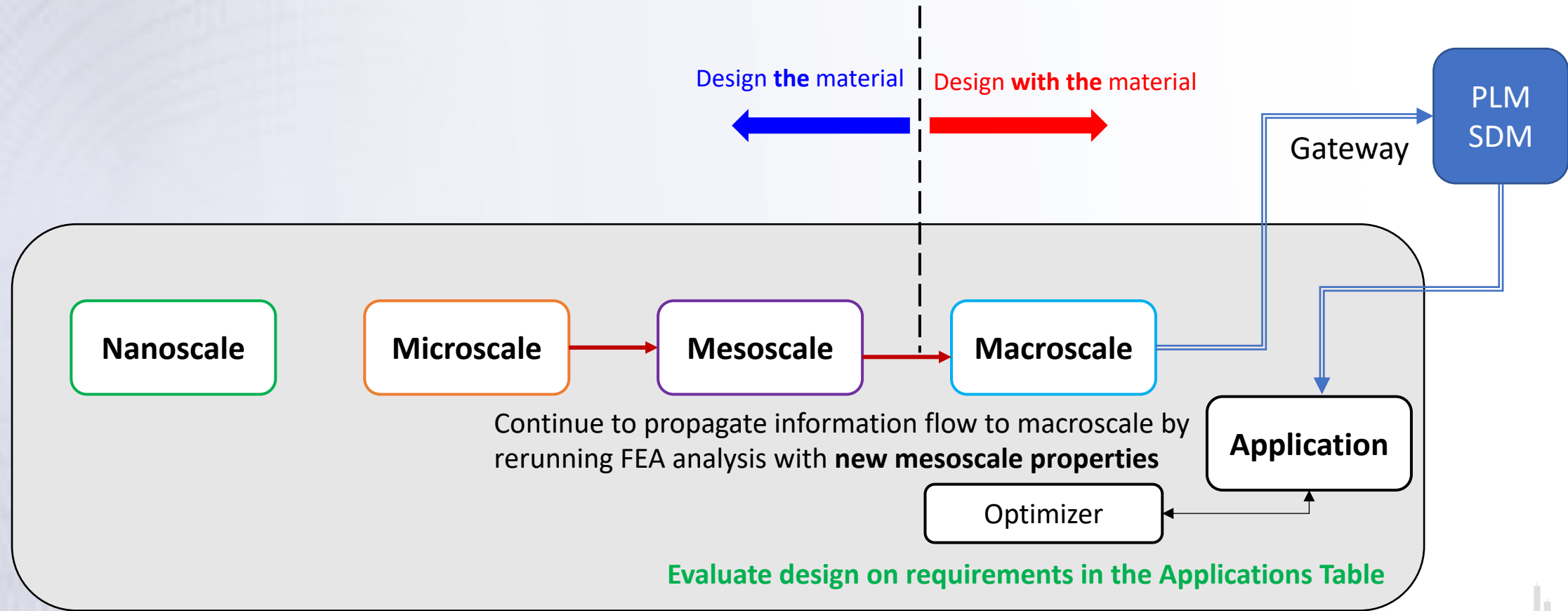
Automation of read/write and tool execution in background



Database/Simulation Management in ICME



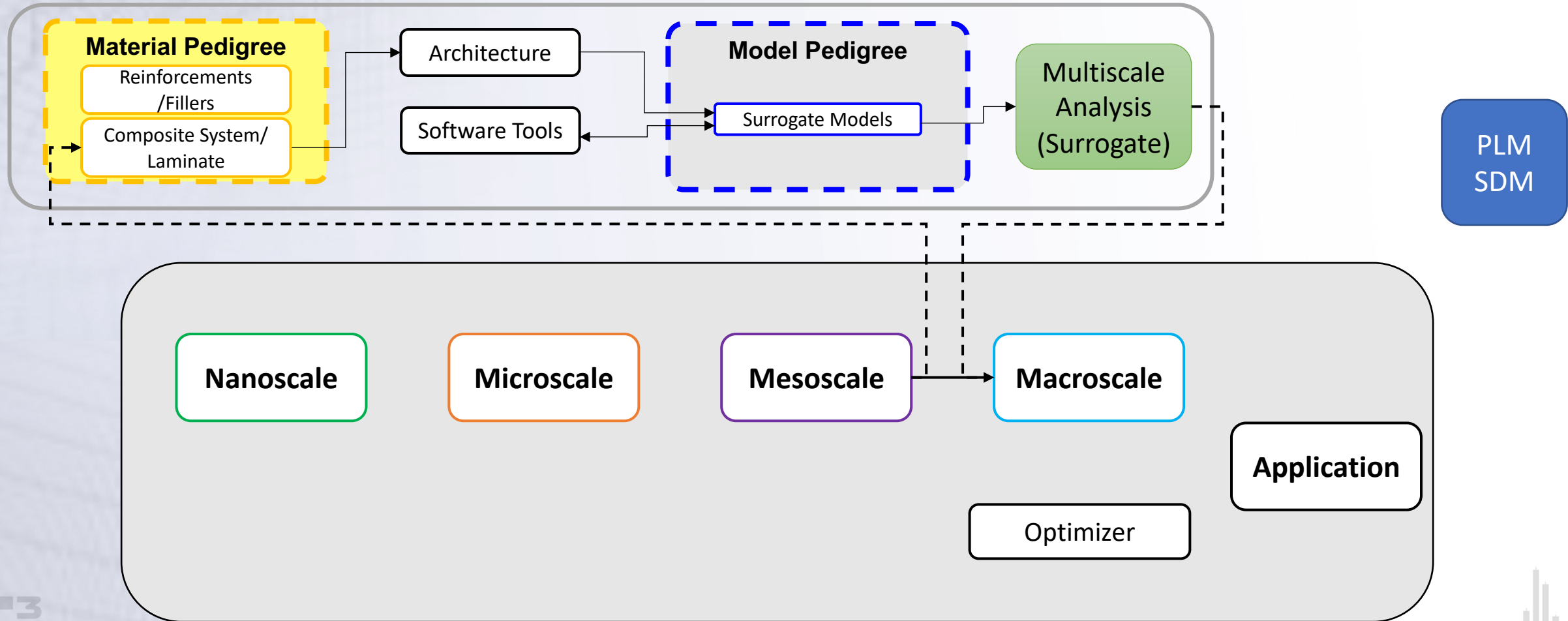
Illustrate with Example in which the fiber reinforcement of a composite material used for a structural component is varied



Database/Simulation Management in ICME



Enhancing optimization and design speed by replacing physics-based models with **surrogate models** developed using **machine learning** at **any scale**



Closing Comments



Foundational to **ICME** and thus **material innovation** is the linkage of real and virtual data in which materials processing, microstructure, properties, and performance are coupled to enable application-driven design and optimization of materials and structures!

Herein we have Demonstrated

- A robust information management schema – based on the ANSYS GRANTA MI system - that can be utilized as an ICME Platform
 - Enables the capture, analysis, dissemination and maintenance of various types of data for all materials.
 - New additions – Microstructure, Model Pedigree Tables (physics-based or data driven), Software Tools Table and Application Table
 - Facilitates the characterization and uncertainty quantifications of model input parameters, verification and validation of model output, and certification of toolsets at multiple length scales
 - Accepted and being implemented/tested by MDMC members
- GRANTA MI can handle the demands of integrating **both** *virtual* and *experimental* data
 - Achieved linkage of virtual and experimental data at two length scales (micro and macroscale)
- Seamless integration of in-house simulation toolsets (e.g., MAC/GMC) and workflow engines (e.g., Matlab) with GRANTA MI via newly created Python GUI and API functions as well as third party tools

Moving forward, NASA GRC is working on

- Establishment of the final link -- an **Application Table**
 - Enables linkage of structural application (performance) requirements with the “design of material” problem
 - Provides location for BOM and summary information for application requirements
 - Enables unique location to link CAD/PLM/SLM information to material information
- Integration of optimization algorithm(s) to provide final linkage of processing to performance criteria; thus, making ICME a reality.

Thank You for Your Attention



Integrate Don't Duplicate

Acknowledge colleagues: Drs. Brandon Hearley and Joshua Stuckner