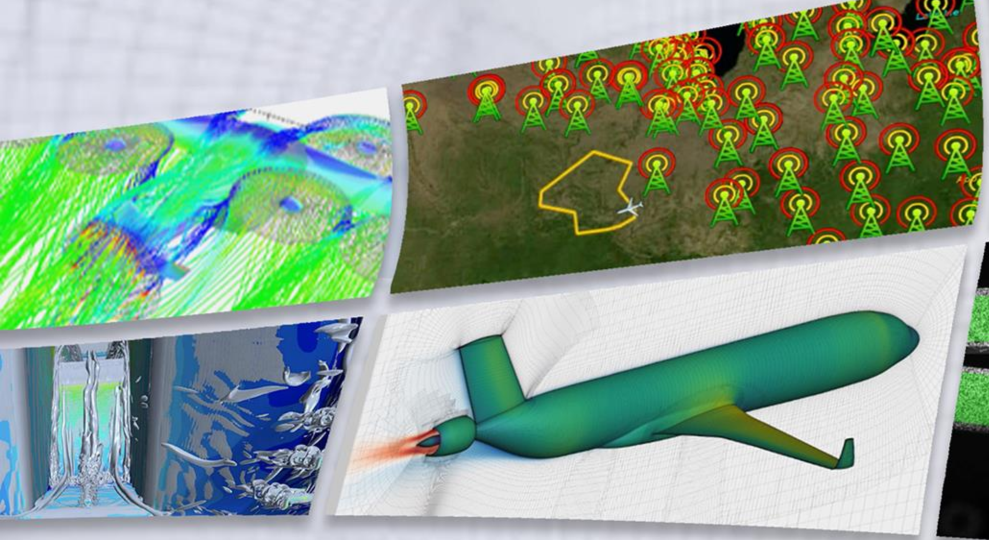
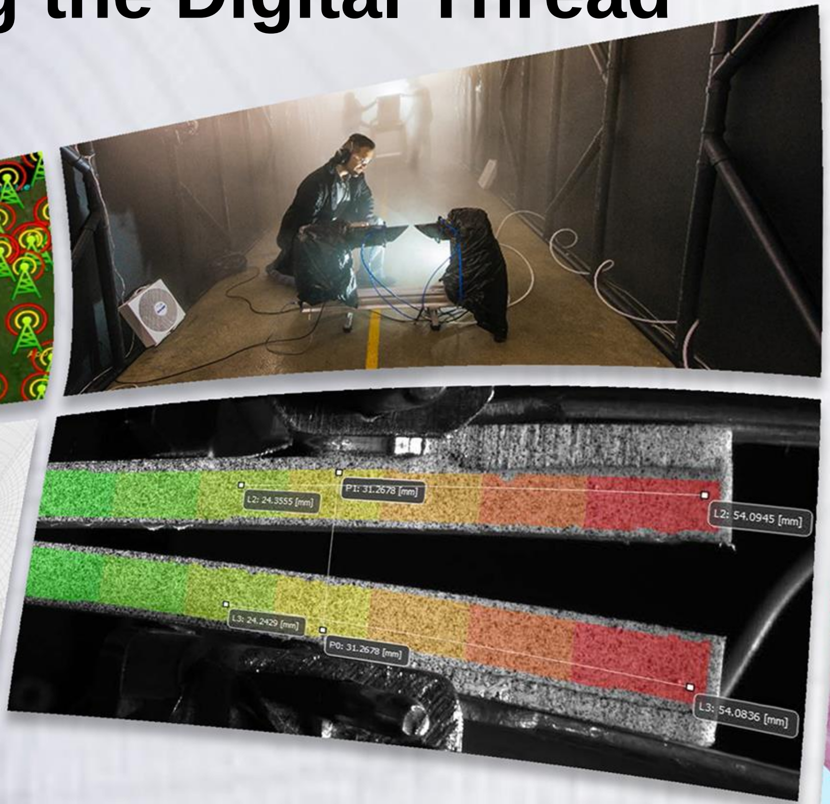
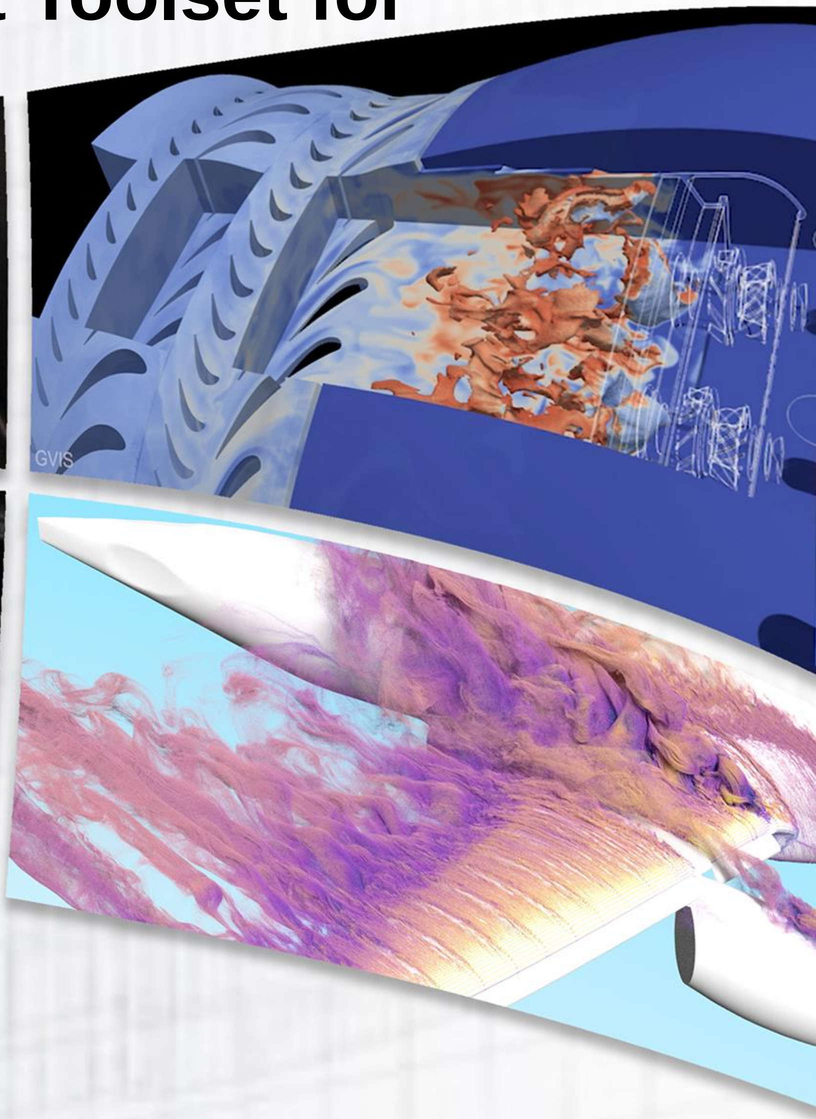
Transformational Tools and Technologies (T^3) Project

Materials Informatics: Information Management Toolset for Establishing/Maintaining the Digital Thread

Brandon Hearley
NASA Glenn Research Center





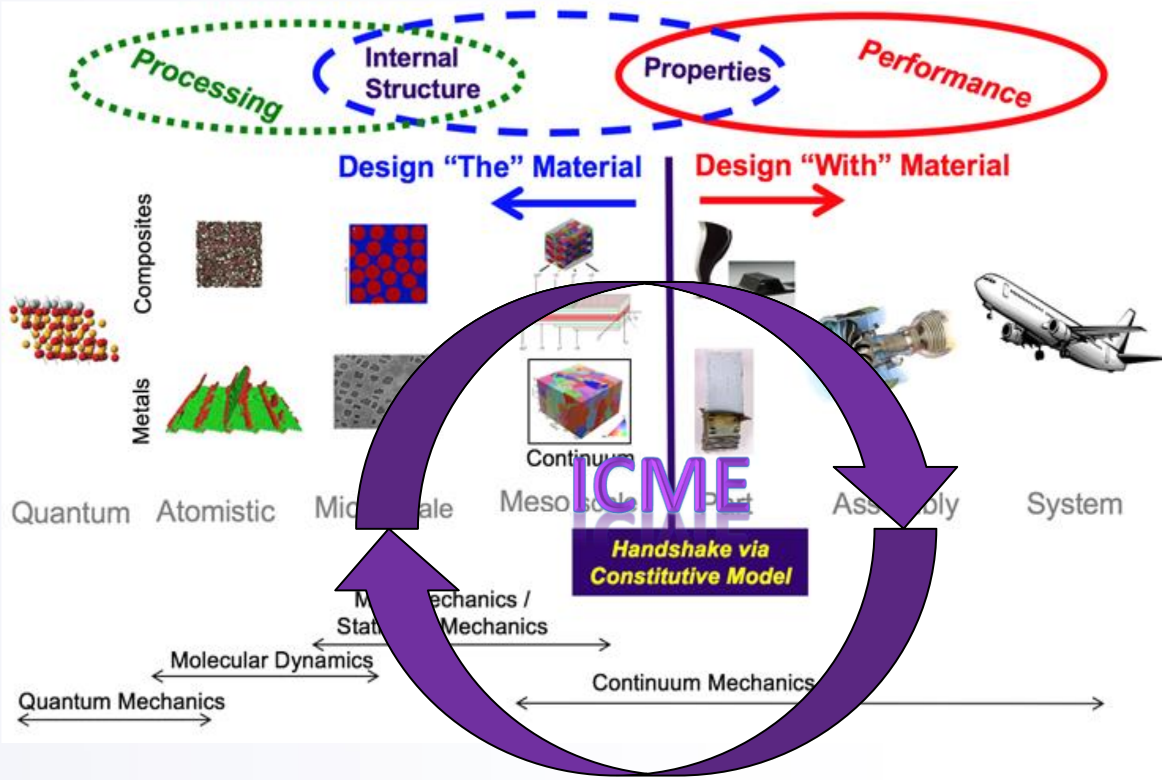


Innovative solutions through foundational research and cross-cutting tools

Dayton Digital Transformation Summit
5/8/2024

Integrated Computational Materials Engineering (ICME) Enables Innovation

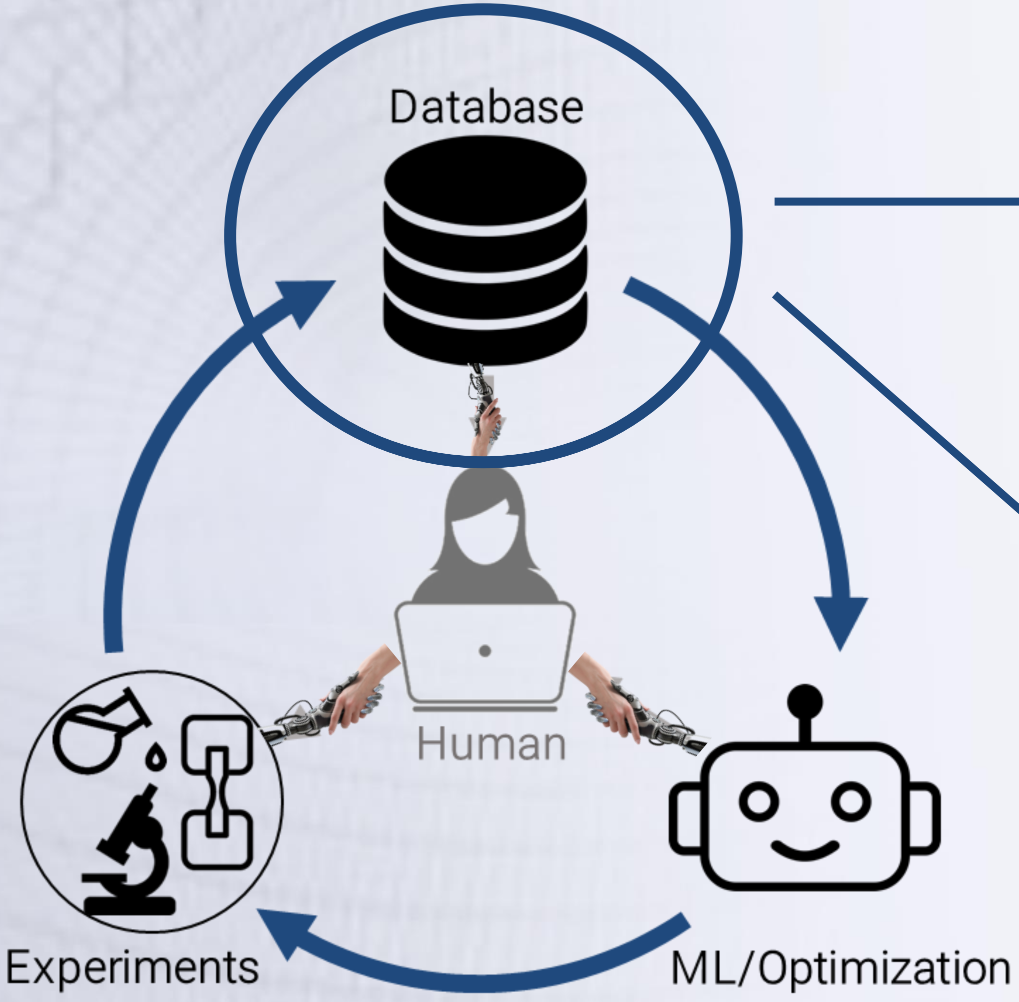
- Top performing organizations rate **New Materials** as one of **THE MOST IMPORTANT** factors in meeting their innovation goals (Historically new materials $\geq$ 20 years)
- Integrated Computation Materials Engineering (ICME) looks to bridge the gap between the "Design-the-Material" (Material Science) 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

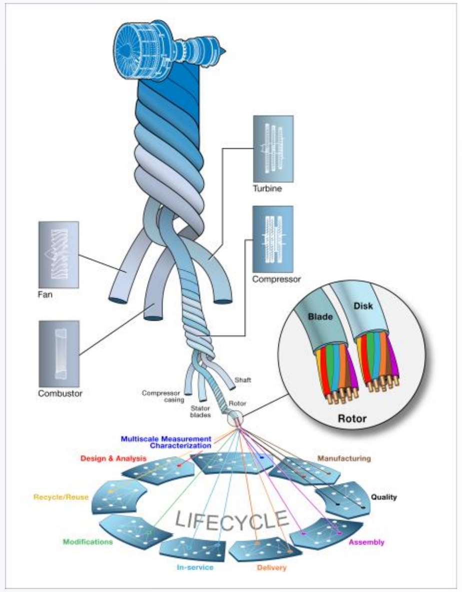


Requires a robust information management system

JARIMIS

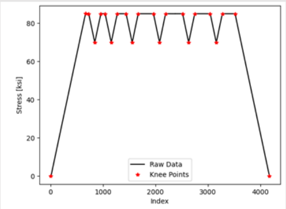
Just a Rather Intelligent Materials Interrogation System



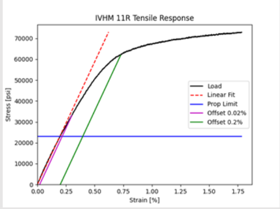


- Establishment of database best practices
- Schema development
- Connecting materials to structures to ***maintain the digital thread***

Python Data Reduction and Analysis Tool



Segment data into load stages



Perform Data Analysis based on Test Type

Determine Granta Record Properties

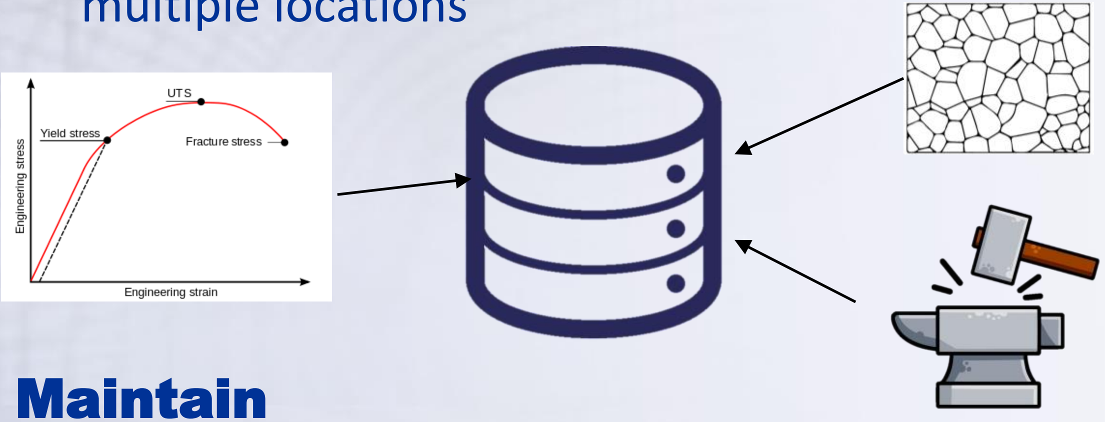
- Table (Tensile, Generic, etc.)
- Folder Placement
- Raw Data (Test Curves)
- Calculated Attributes (E, ν, etc)
- Links to Test Equipment Used
- Links Material Pedigree

- Development of database tools to tackle cultural gaps
- Automatic data analysis is placement
- Digital thread maintenance through automated multiscale workflows

Database Best Practices and Philosophy are Critical to Effective Materials Lifecycle Management

Capture

- Capture data beyond point-wise properties (curves, pedigree information, microstructure, etc.) and from multiple locations



Analyze

- Ensure quality of data reduction or analysis by maintaining full pedigree information
- Easily enable addition of new data through automatic processing and analysis

Maintain

- Ensure traceability between material pedigree, test data, developed models, and application
- Cope with changing data, people, and environments
- Avoid duplication of data to reduce the risk that the digital thread is compromised

Disseminate

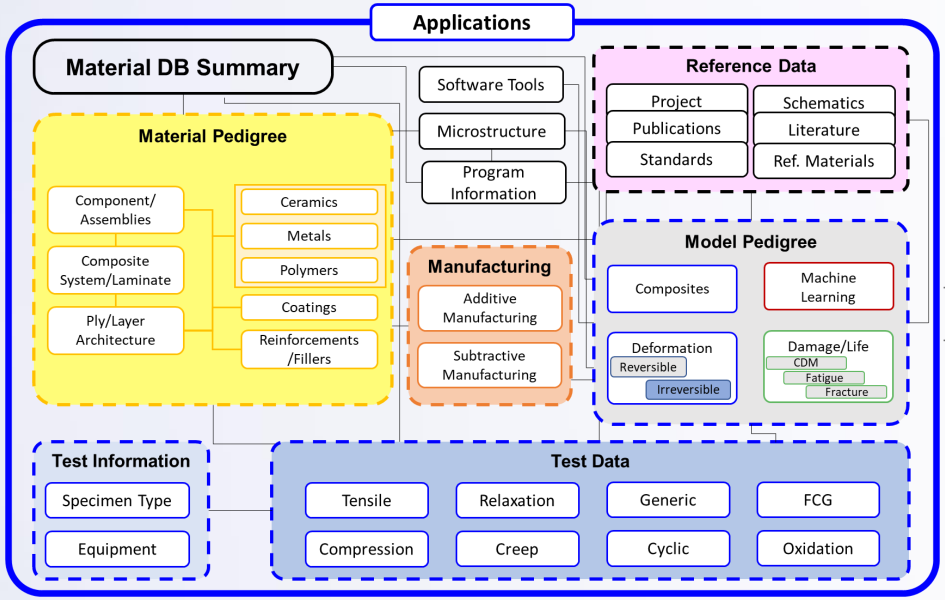
- Ensure data is easily findable and reusable to prevent duplication of data creation
- Scalability, robustness, security across enterprises
- Get data to the right people, at the right time, in the right format, at the right scale

Information Management Essential For Fit-For-Purpose Material Design

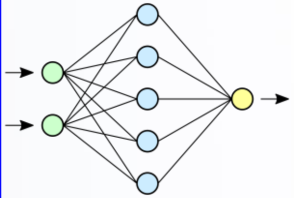
Established Data Schema for ICME that Enables Linkage of Test Data with Simulation Data at Different Length Scales:

- Required establishment of Material Pedigree, Manufacturing, Microstructure, Model Pedigree, and Software Tools Tables within Granta MI
- Digital Thread / Digital Twin
- Six key **accomplishments**

Application Table
NASA TM-2022-00184033



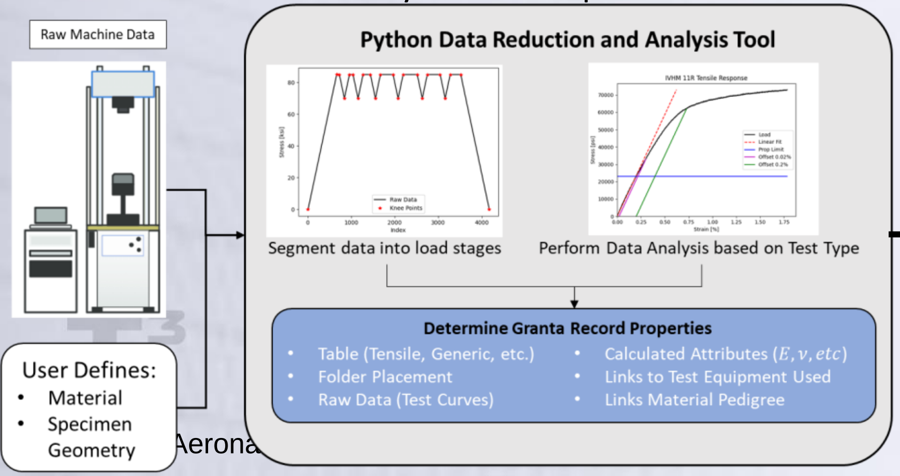
NASA GRC ICME Schema: Executive Summary
NASA TM-2023-0018337



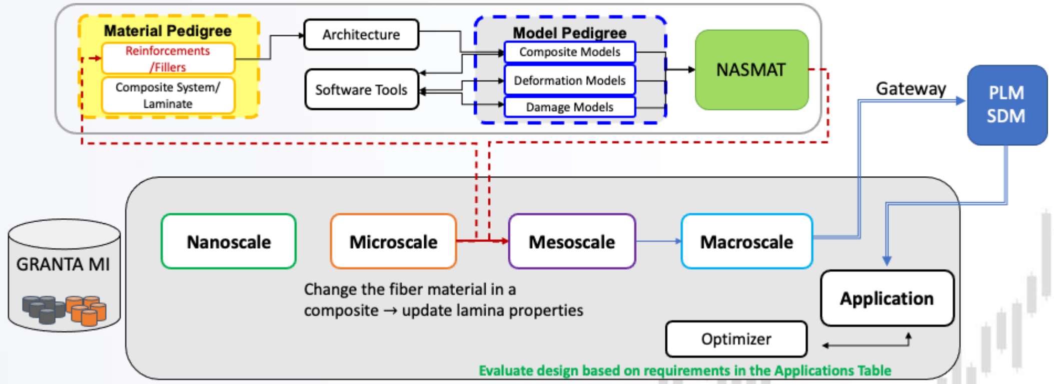
Machine Learning Table
NASA TM-2022-0017137

Additive Manufacturing
ICMAMS 2023, Aug 9, 2023

Py-MILab (ICMAMS 2023, Aug 9, 2023)
Data Analytics and Importer



AIMAOS: Automated Information Management Across Organizations and Scales (TMS ICME, May 21, 2023)

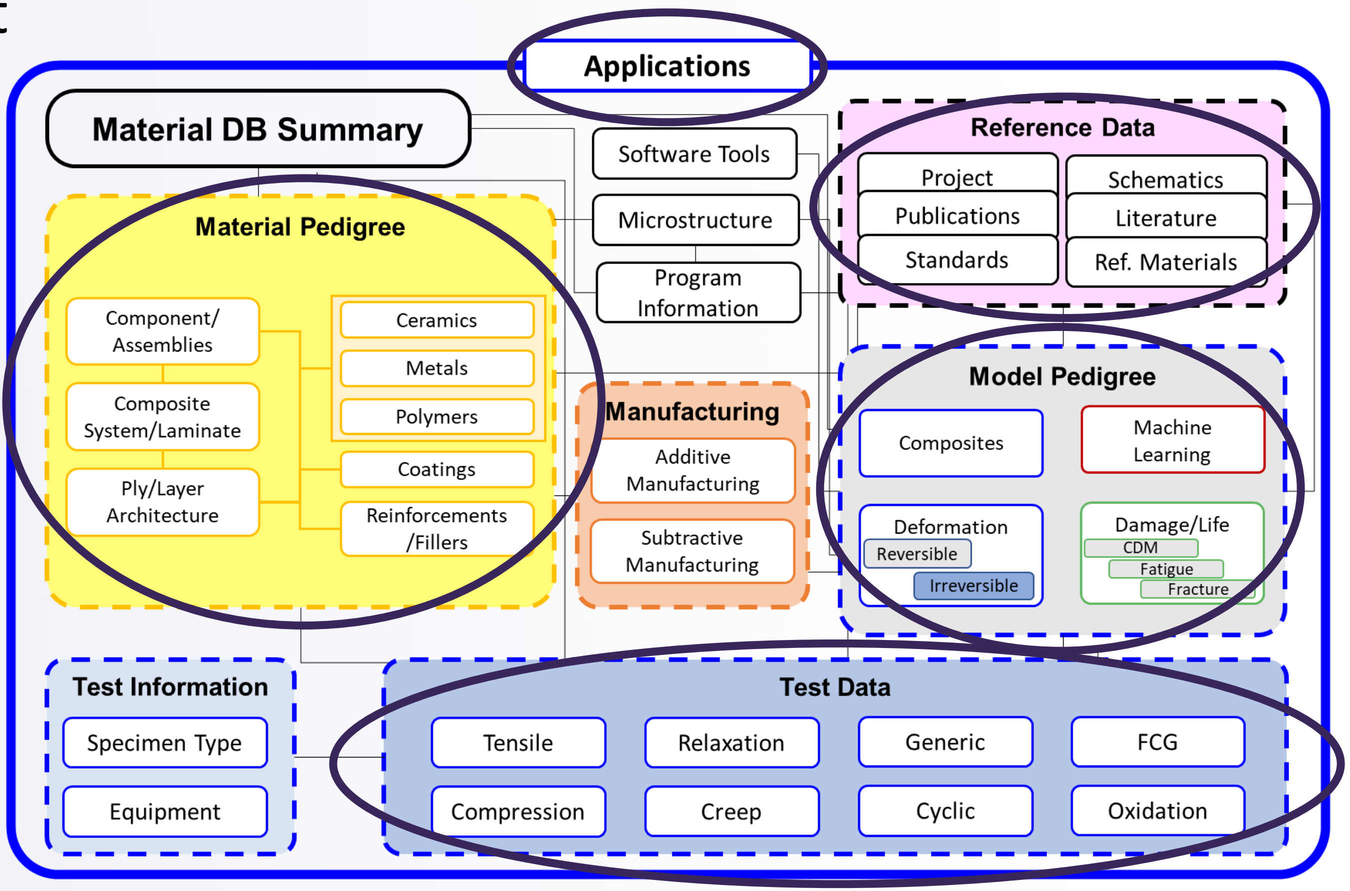


- Re-evaluate the requirements locally with periodic global (structural – PLM/SDM) updates

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
  - Material Pedigree: Store material source information, properties, etc.
  - Test Data/Statistical 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



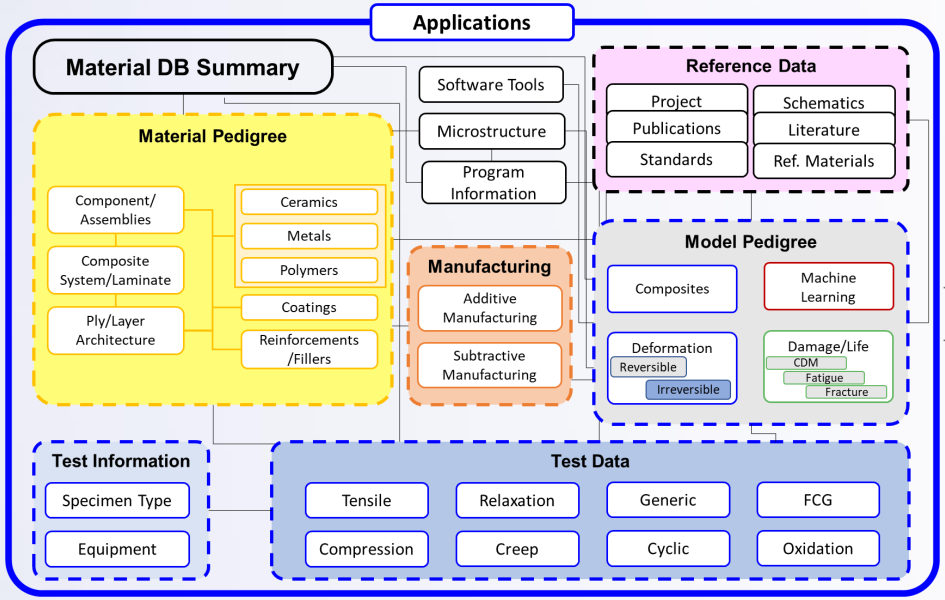
Schema documented in the NASA GRC ICME Schema: An Executive Summary NASA TM-2023-0018337

Information Management Essential For Fit-For-Purpose Material Design

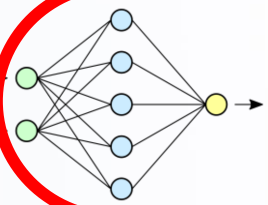
Established Data Schema for ICME that Enables Linkage of Test Data with Simulation Data at Different Length Scales:

- Required establishment of Material Pedigree, Manufacturing, Microstructure, Model Pedigree, and Software Tools Tables within Granta MI
- Digital Thread / Digital Twin
- Six key **accomplishments**

Application Table
NASA TM-2022-00184033



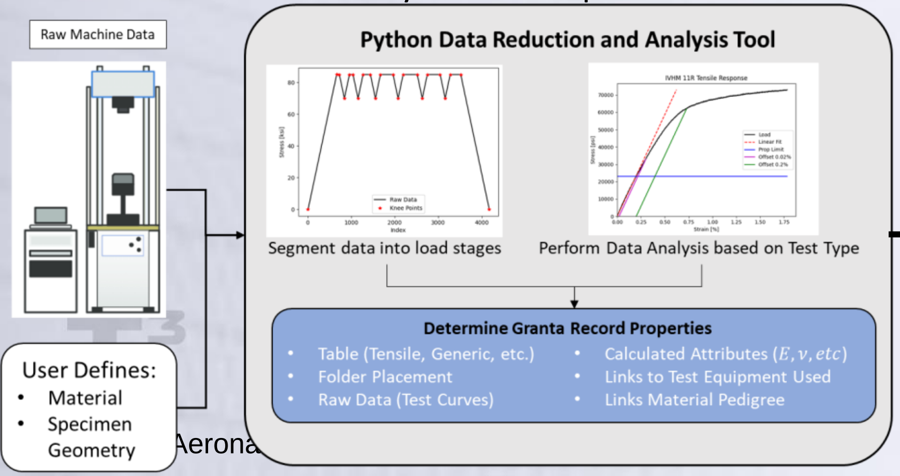
NASA GRC ICME Schema: Executive Summary
NASA TM-2023-0018337



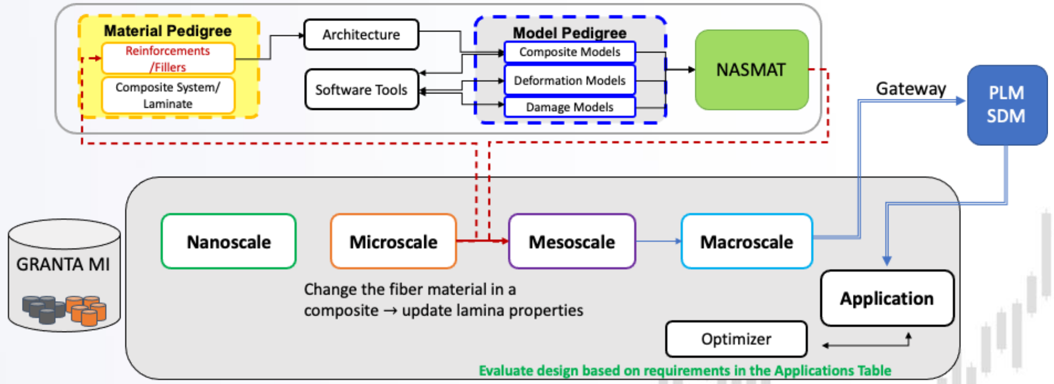
Machine Learning Table
NASA TM-2022-0017137

Additive Manufacturing
ICMAMS 2023, Aug 9, 2023

Py-MILab (ICMAMS 2023, Aug 9, 2023)
Data Analytics and Importer



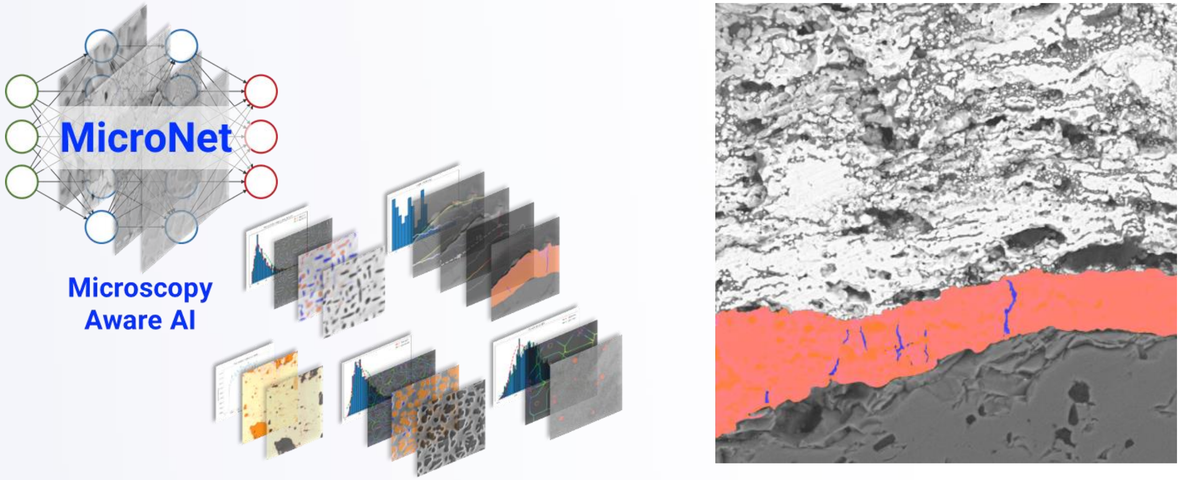
AIMAOS: Automated Information Management Across Organizations and Scales
(TMS ICME, May 21, 2023)



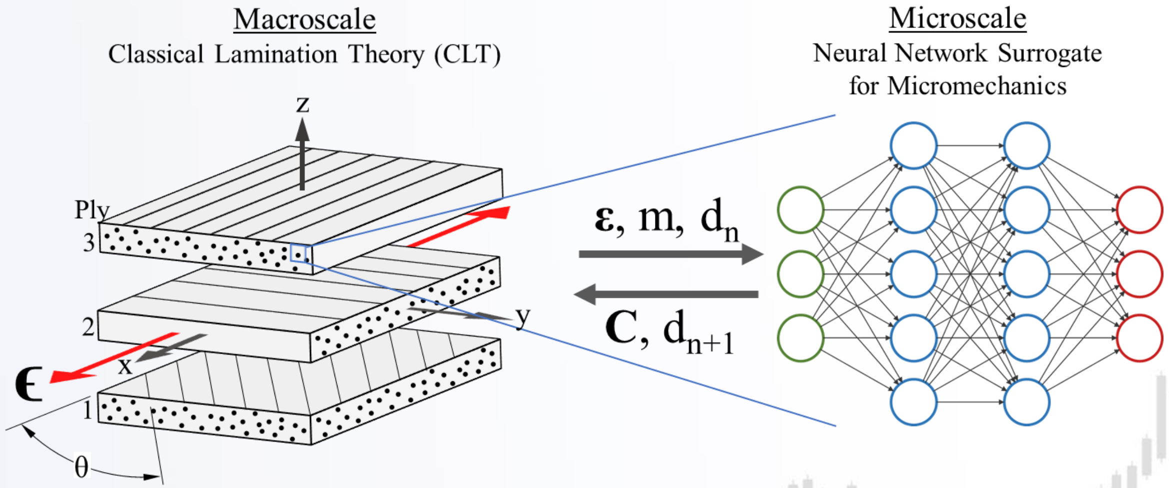
- Re-evaluate the requirements locally with periodic global (structural – PLM/SDM) updates

Machine Learning Is Critical For ICME

- Machine Learning will play a critical role in enabling ICME by providing speed and automation to materials discovery
- Developed image recognition algorithms developed to perform task automation such as micrograph segmentation
  - Reduces time to perform task and removes human bias
- Create surrogate models for physics-based tools
  - Increase computational efficiency, enabling fast and accurate multiscale modeling
- **Data Management is critical for ML → must understand model's full pedigree so that it isn't misused**
  - Lose physics-based relationship between inputs and outputs when using a "black-box" surrogate
  - Incur *intellectual debt*



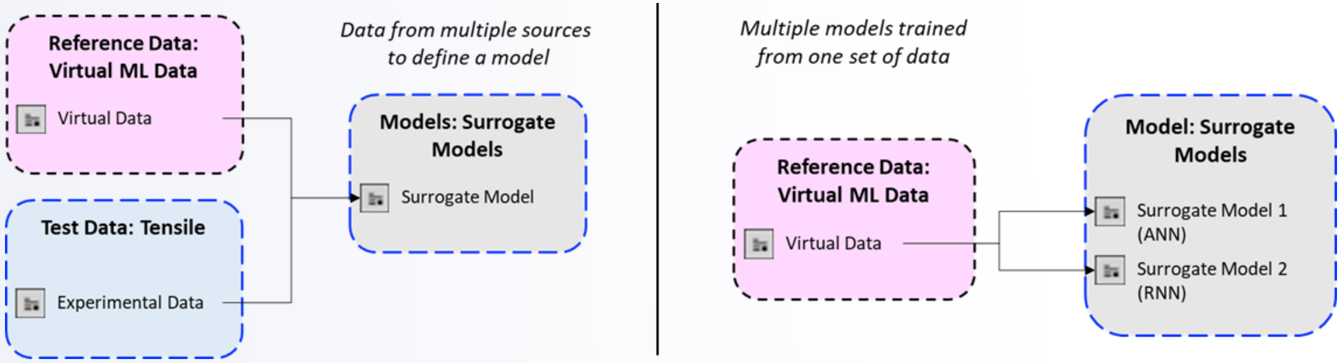
MicroNet: Automatic segmentation of micrographs



ML Surrogates for Physics-based Models

Effective Data Management for Machine Learning Data and Models

- Separate the data from the model in the NASA GRC ICME Schema
  - Flexibility in model definition prevents data from being duplicated multiple places in the database



NASA TM-20220017137

- Developed import tools to facilitate data collection
  - ML Models can have hundreds of thousands of data files → manual import not feasible
  - Importer can ingest ML code and automatically determine an write the neural network architecture
  - Judicious automation of data collection

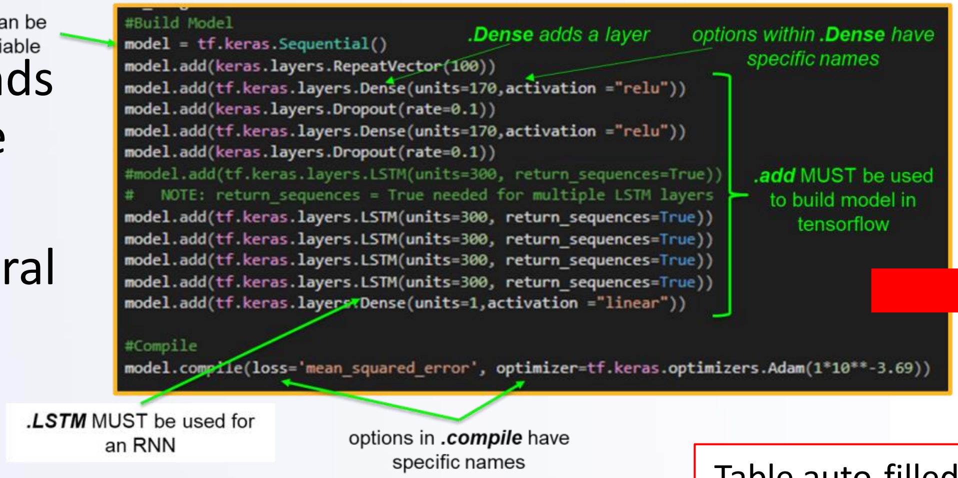
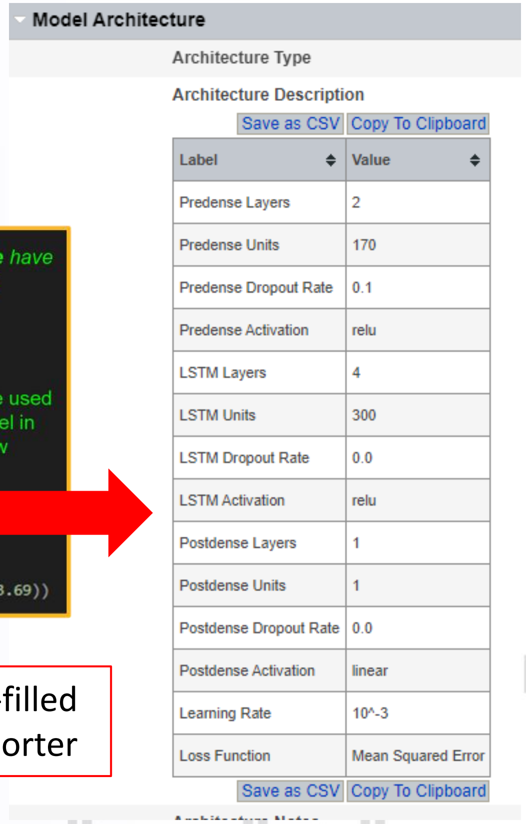


Table auto-filled out in importer



Model Architecture

Architecture Type

Architecture Description

Save as CSV | Copy To Clipboard

Label	Value
Predense Layers	2
Predense Units	170
Predense Dropout Rate	0.1
Predense Activation	relu
LSTM Layers	4
LSTM Units	300
LSTM Dropout Rate	0.0
LSTM Activation	relu
Postdense Layers	1
Postdense Units	1
Postdense Dropout Rate	0.0
Postdense Activation	linear
Learning Rate	10^-3
Loss Function	Mean Squared Error

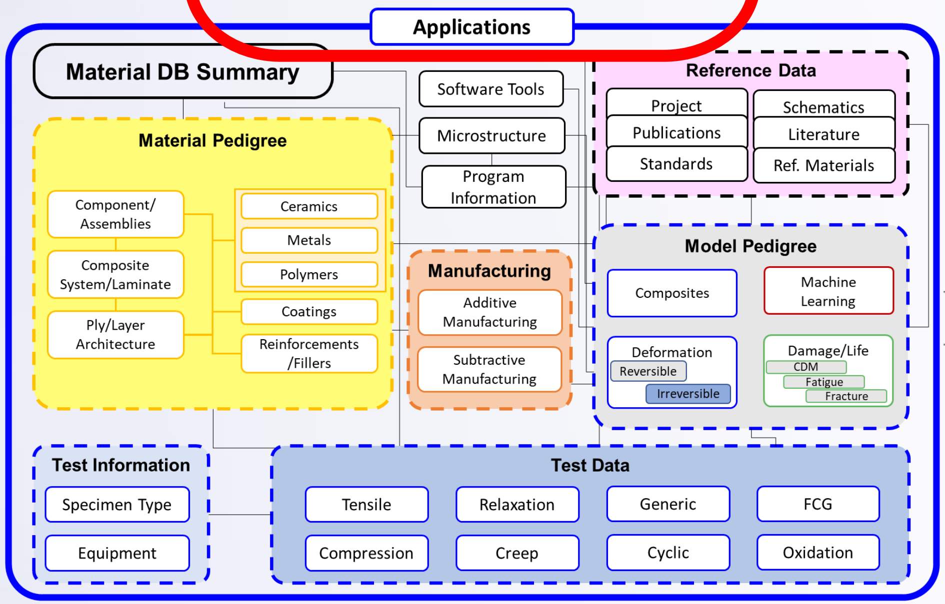
Save as CSV | Copy To Clipboard

Information Management Essential For Fit-For-Purpose Material Design

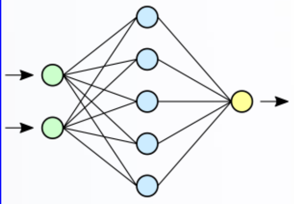
Established Data Schema for ICME that Enables Linkage of Test Data with Simulation Data at Different Length Scales:

- Required establishment of Material Pedigree, Manufacturing, Microstructure, Model Pedigree, and Software Tools Tables within Granta MI
- Digital Thread / Digital Twin
- Six key **accomplishments**

Application Table
NASA TM-2022-00184033



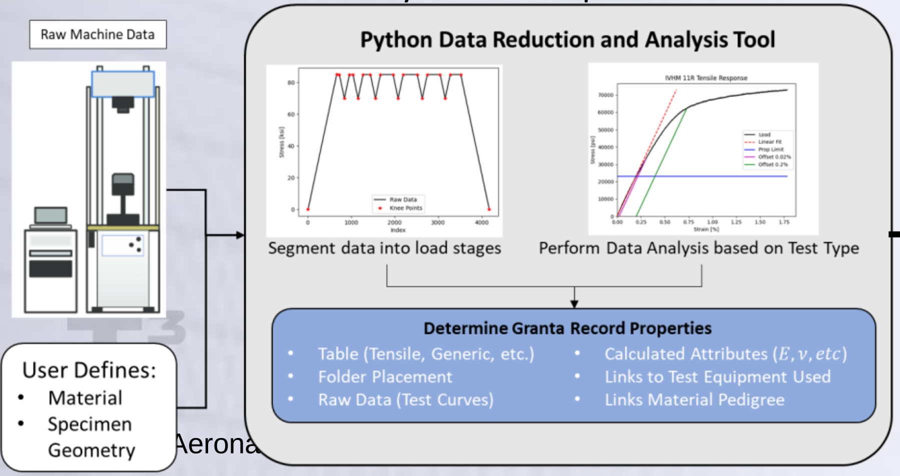
NASA GRC ICME Schema: Executive Summary
NASA TM-2023-0018337



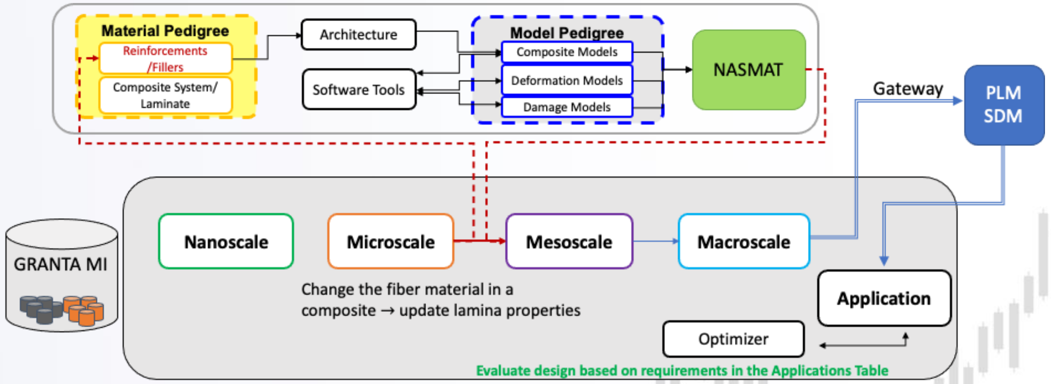
Machine Learning Table
NASA TM-2022-0017137

Additive Manufacturing
ICMAMS 2023, Aug 9, 2023

Py-MILab (ICMAMS 2023, Aug 9, 2023)
Data Analytics and Importer



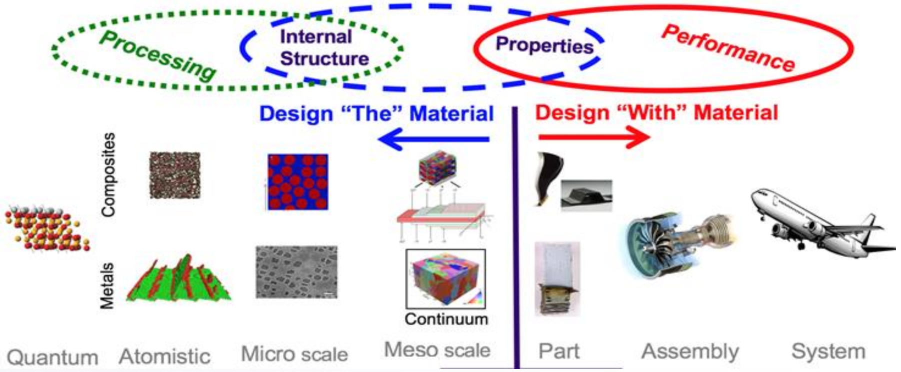
AIMAOS: Automated Information Management Across Organizations and Scales (TMS ICME, May 21, 2023)



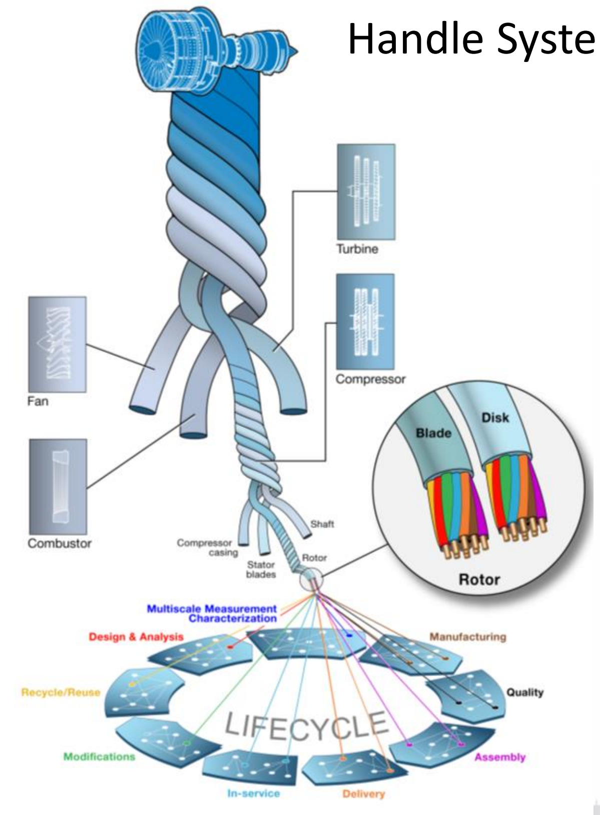
- Re-evaluate the requirements locally with periodic global (structural – PLM/SDM) updates

Application Table: Bridging the Gap Between Material Science and Structural Engineering

- The **Application Table** is the intended "bridge" between "Designing the Material" and "Designing with the Material" and is the **"brains" for ICME**
  - **Orchestrates the ICME Process**
- Enables unique location to link CAD/PLM/SDM 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**



Handle System of Systems



Application Table Orchestrates ICME By Linking Processing, Microstructure, Properties, and Performance

- Attributes and Layout defined to handle any type of application or requirements
  - Nine major categories specified with associated attributes
  - Associated requirements are dispersed throughout three major category (Geometric, Performance, Material)
  - Can be application-based or spatial (allow definition of design points)
  - Contains evaluation criteria (analysis performed and results)
  - Scorecards and Readiness Levels for the requirements
- Granta MI Tabular attribute type used extensively due to its flexibility and generality
  - Significant number of additional attributes associated with each column of a tabular attribute
  - Each row can represent different specifications

Attribute	Type
General Information	
Application Name	STXT
Application Description	LTXT
Data Ownership	DCT
Data Ownership (Other)	STXT
Distribution Category	DCT
Funding Organization	STXT
Performing Oganization	STXT
Project Name	STXT
Project Code	STXT
Project Notes	LTXT
Point of Contact	TABL
Geometric/Manufacturing Requirements	
Owner Information	TABL
Surface Area	RNG
Volume	RNG
Bounding Box Dimmensions	LTXT
CAD/CAE Link	HYP
Manufacturing Process	DCT
Manufacturing Process (Other)	STXT
Geometric Schematic Time History	TABL
Geometric Description	TABL
Coordinate System Definitions	TABL
Design Points / Points of Inerest*	TABL
Geoemtric Notes	LTXT
Manufacturing Requirements*	TABL
Part Yield	RNG
Surface Treatment	DCT
Manufacturing Notes	LTXT
Microstructure Profile	TABL
Performance Requirements	
Weight	RNG
Life	RNG
Cost	RNG
Risk	DCT
Storage Energy	RNG
Ultimate Strength	RNG
Performance Standards*	TABL
Mechanical Requirements*	TABL
Thermal Requirements*	TABL
Environmental Requirements*	TABL
Other Performance Requirements*	TABL
Performance Notes	LTXT
Form/Fit/Function Notes	LTXT

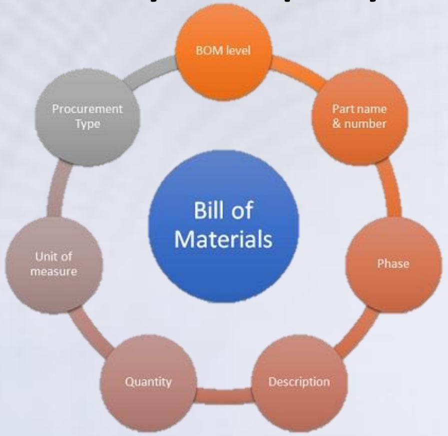
Attribute	Type
Analyses Performed	
Analyses Performed	TABL
Analyses Performed (Subcomponents)	TABL
Analyses Profiles	TABL
Load Profiles	TABL
Analyses Range Definitions	TABL
Failure Mechanism/Modes	
Failure Mode and Effect Analysis	TABL
Material Selection	
Material Requirements*	TABL
Part List	TABL
Bill of Materials*	TABL
Software Tools Used**	TABL
Selection Criteria	FILE
Property File	FILE
Material Selection Assumptions	LTXT
Inspection	
Inspectability Notes	LTXT
Evaluator	TABL
NDE Method	DCT
NDE Geometry	TABL
Equipment	TABL
Examination	TABL
Calibration	TABL
Testing Parameters	TABL
NDE Images	TABL
NDE Comments	LTXT
NDE Information	FILE
Scorecards	
Requirements Scorecard*	TABL
Risk Scorecard*	TABL
Readiness Levels	
Technology Readiness Level (TRL)	DCT
Manufacturing Readiness Level (MRL)	DCT
Integration Readiness Level (IRL)	DCT
System Readiness Level (SRL)	DCT

* Changed with feature request
** Removed with feature request

DCT	Discrete Text (speificied choices)
FILE	Allows the association of any file type to a given record
HYP	Hyperlink to a web address
IMG	Allows the association of any image format to a given record
LTXT	Long Text Field
PNT	Point Value
RNG	Range Variable
STXT	Short Text Field
TABL	Tabular Attibute

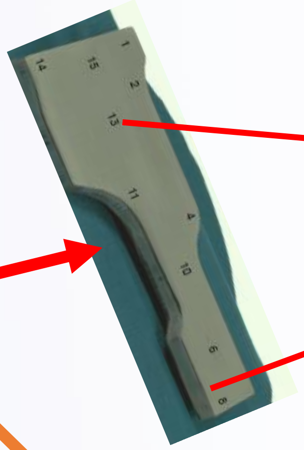
Application Table Orchestrates ICME By Linking Processing, Microstructure, Properties, and Performance

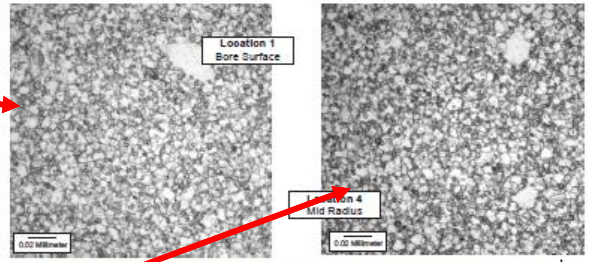
- Application Table links part requirements, microstructure information, material properties, geometry, employed models, relevant analysis, and performance



Summary of material properties

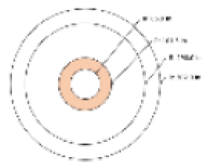
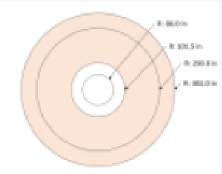
Application



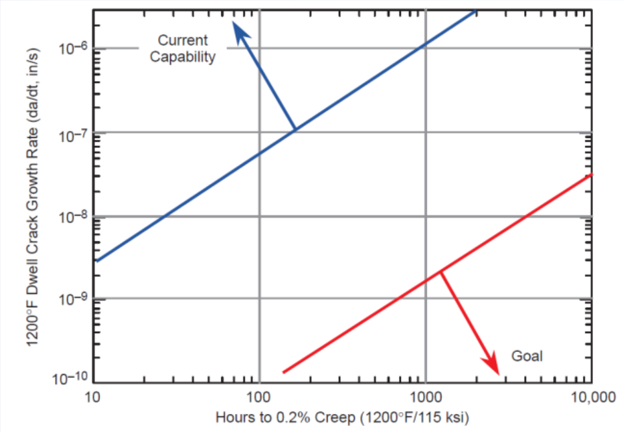


Spatially Microstructure Characterization

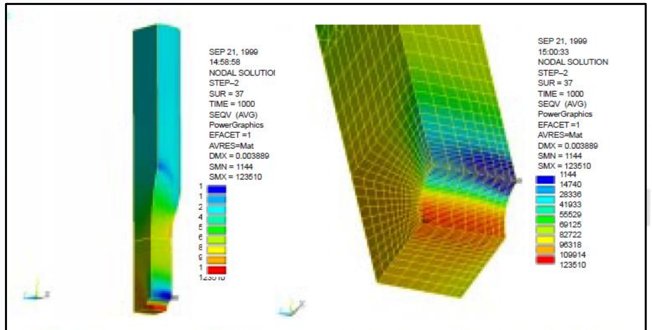
Part Geometry

Assembly	Designed Schematic	Designed Measurements/Tolerances
D1		Inner Radius = 86.0 in +/- 0.005 in Outer Radius = 101.5 in +/- 0.05 in
D1		Inner Radius = 290.0 in +/- 0.05 in Outer Radius = 302.0 in +/- 0.01 in

Performance Requirements



Summary of Relevant Analyses with Links to PLM/SDM



P&W DEN. Supersolvus ME–16/w Creep 1200°F LS = 2 : Hold 125 ksi for 1000 hrs

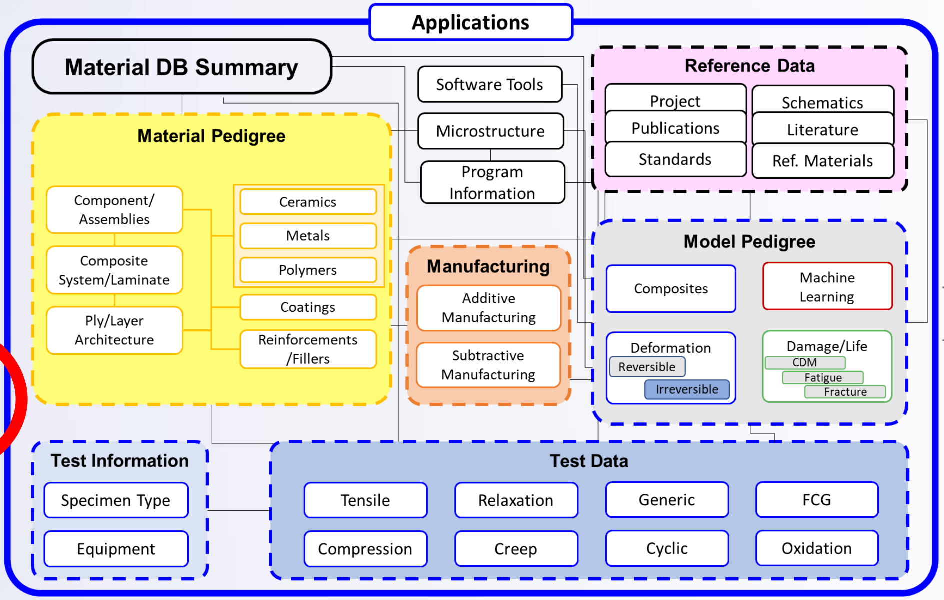
Information Management Essential For Fit-For-Purpose Material Design

Established Data Schema for ICME that Enables Linkage of Test Data with Simulation Data at Different Length Scales:

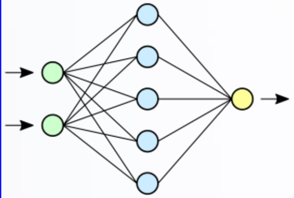
- Required establishment of Material Pedigree, Manufacturing, Microstructure, Model Pedigree, and Software Tools Tables within Granta MI
- Digital Thread / Digital Twin
- Six key **accomplishments**

Additive Manufacturing
ICMAMS 2023, Aug 9, 2023

Application Table
NASA TM-2022-00184033

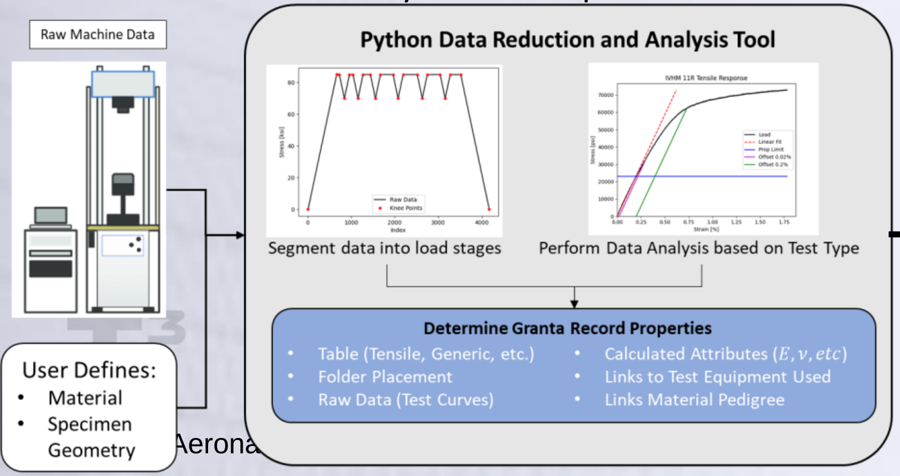


NASA GRC ICME Schema: Executive Summary
NASA TM-2023-0018337

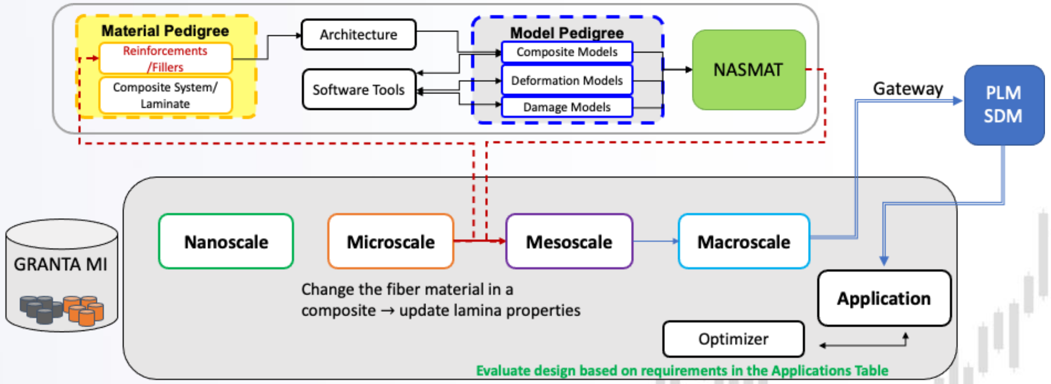


Machine Learning Table
NASA TM-2022-0017137

Py-MILab (ICMAMS 2023, Aug 9, 2023)
Data Analytics and Importer



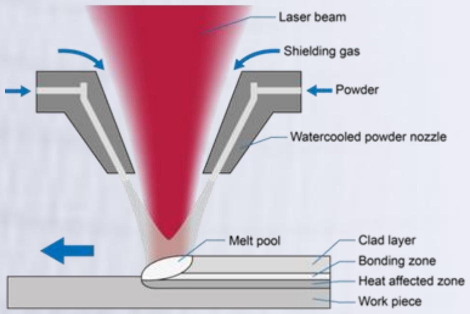
AIMAOS: Automated Information Management Across Organizations and Scales (TMS ICME, May 21, 2023)

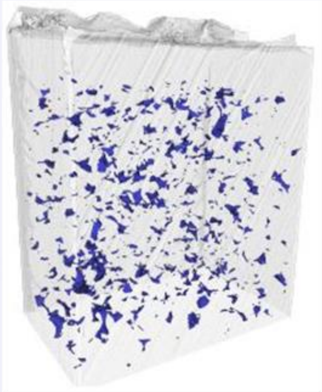


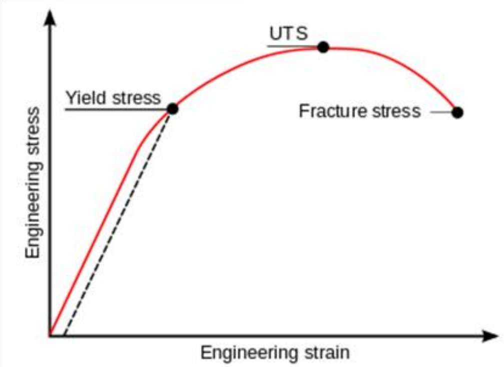
- Re-evaluate the requirements locally with periodic global (structural – PLM/SDM) updates

Extending Pedigree and Application Table to Additive Manufacturing

- Application Table allows for definition of spatially varying properties/microstructure
  - Paired with an optimization tool → design ‘fit-for-purpose” materials with improved properties in critical areas
- Achieve varying microstructure in applications through additive manufacturing
  - Need to understand and link together processing parameters, resultant microstructure, and performance
- Schema was adapted to allow for definition of additive manufacturing processes and applied to the Application Table
  - Designed based on NASA Standard 6030 for Additive Manufactured Materials

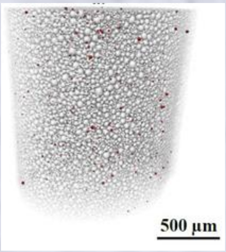






Example Workflow for Additive Manufacturing

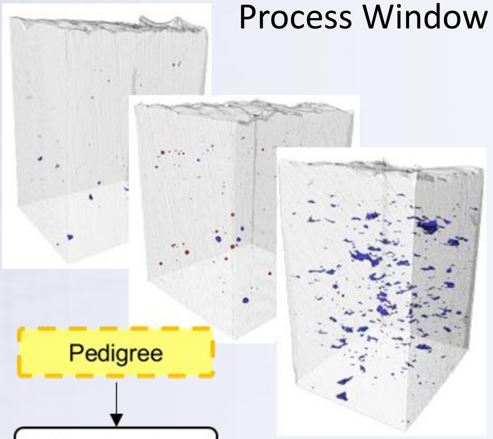
Powder Microstructure Characterization



Pedigree

Microstructure

Perform Multiple Builds to determine Process Window



Pedigree

Microstructure

Define Build Parameters

Manufacturing Process   Hide table

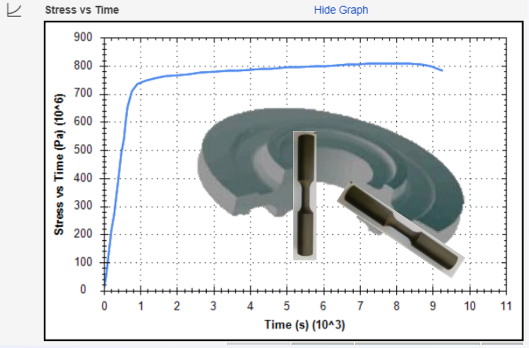
Method Name	Method Type	Feedstock Type	Parameter	Range	Units	Parameters Used
Laser Powder Bed Fusion	Melt-Based	Powder	Deposition Rate	12.5 < x < 33.3	mm^3/s	15
			Power	150 < x < 400	W	280
			Laser Speed	200 < x < 2000	mm/s	1200
			Layer Thickness	25 < x < 65	µm	30
			Hatch Spacing	20 < x < 250	µm	140

Viewed from Manufacturing Table
Defined for each build record

Manufacturing

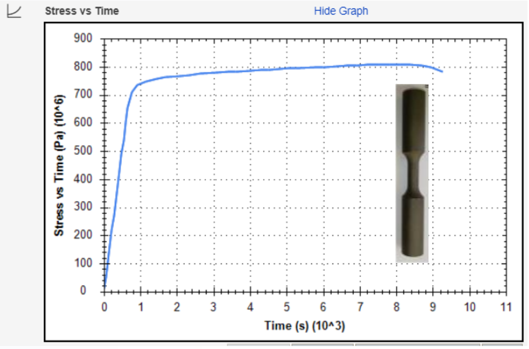
Pedigree

Model Pedigree



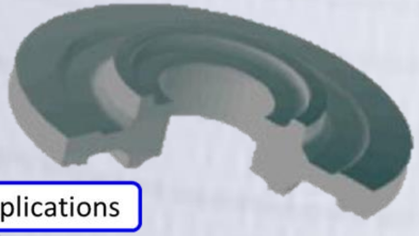
Perform Characterization Tests

Test Data



Design, Build, and Test Witness Articles

Applications → Test Data



Applications

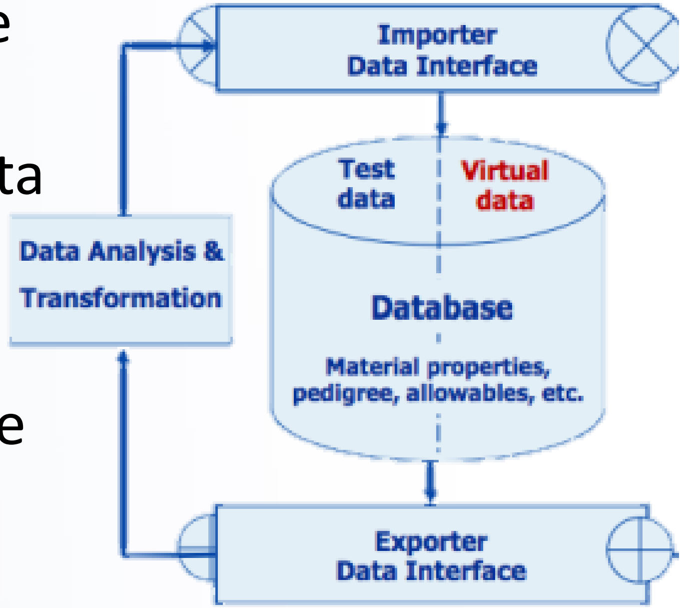
Design Final Part

R. Cunningham, S. P. Narra, C. B. J. Montgomery and A. D. Rollett, "Synchrotron-Based X-ray Microtomography Characterization of the Effect of Processing Variables on Porosity Formation in Laser Powder-Bed Additive Manufacturing of Ti-6Al-4V," JOM,, vol. 69, no. 3, pp. 479-484, 2017.

Tackling Cultural/Workforce Challenges for Digital Transformation

Development of Database Auxiliary Tools

- NASA Vision 2040 outlined both technical and *cultural challenges* for implementing ICME Data Management
  - If data is not findable, accessible, interoperable, and reusable (FAIR principles), it will not be useful
  - People don't like to change how they currently store their data
- The development of import/export tools is critical for cultural adoption of digital transformation
  - Ensure data is uploaded to the right place and exported in the right format
- At NASA GRC, import tools also offer ***additional features*** that facilitate capturing and analyzing data to further promote adoption



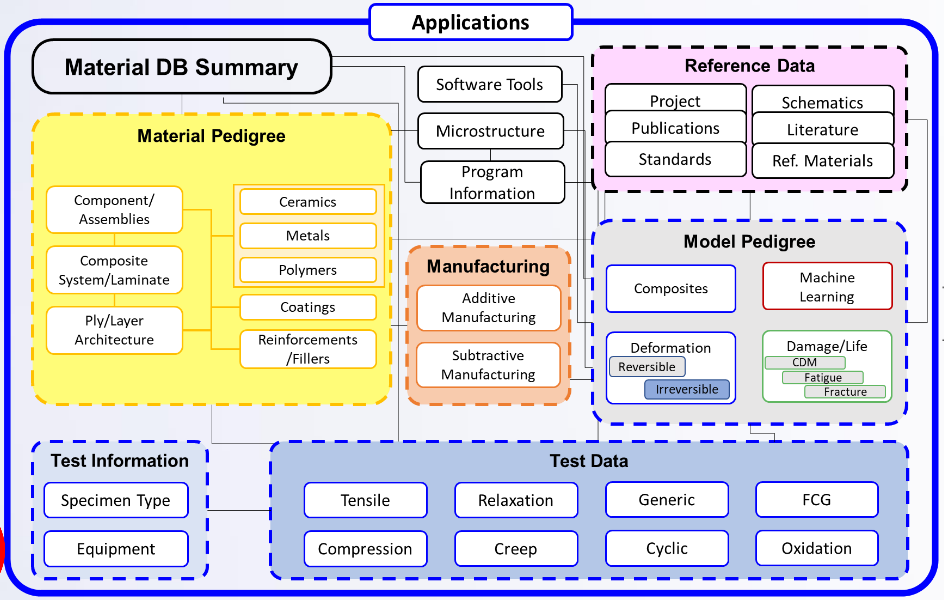
Information Management Essential For Fit-For-Purpose Material Design

Established Data Schema for ICME that Enables Linkage of Test Data with Simulation Data at Different Length Scales:

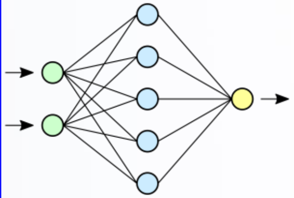
- Required establishment of Material Pedigree, Manufacturing, Microstructure, Model Pedigree, and Software Tools Tables within Granta MI
- Digital Thread / Digital Twin
- Six key **accomplishments**

Additive Manufacturing
ICMAMS 2023, Aug 9, 2023

Application Table
NASA TM-2022-00184033

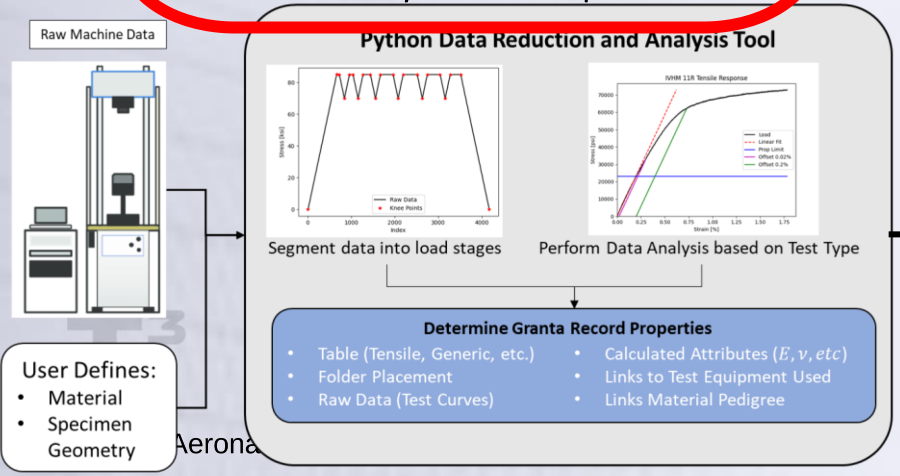


NASA GRC ICME Schema: Executive Summary
NASA TM-2023-0018337

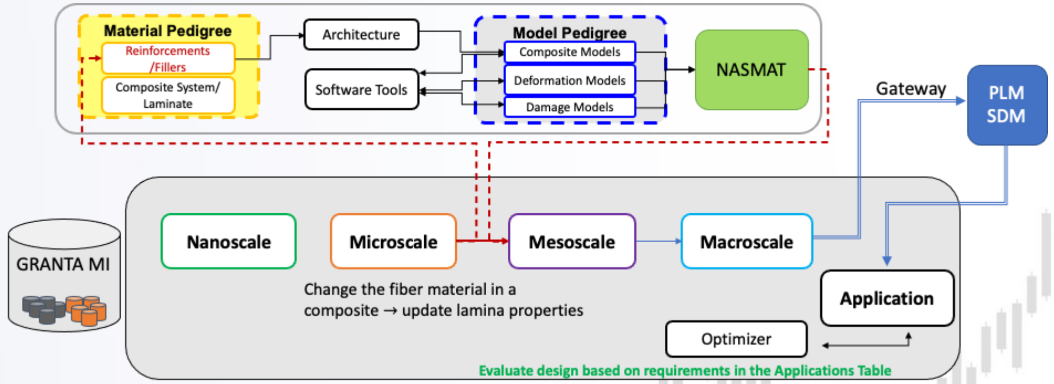


Machine Learning Table
NASA TM-2022-0017137

Py MI Lab (ICMAMS 2023, Aug 9, 2023)
Data Analytics and Importer



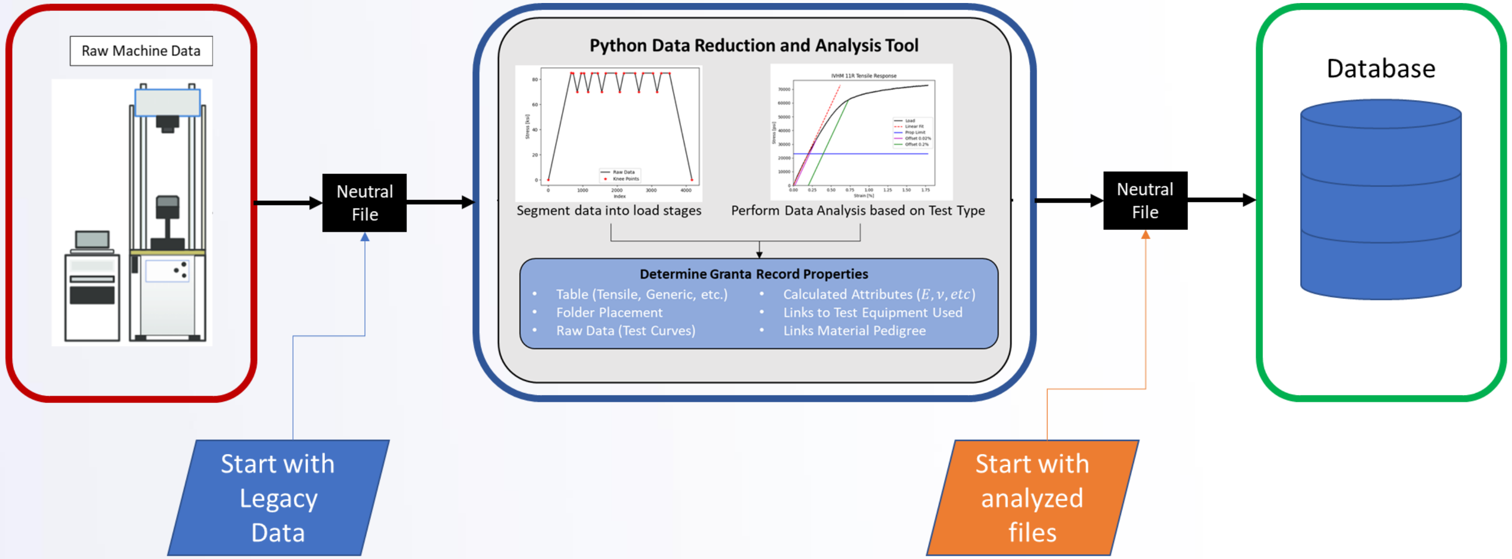
AIMAOS: Automated Information Management Across Organizations and Scales
(TMS ICME, May 21, 2023)

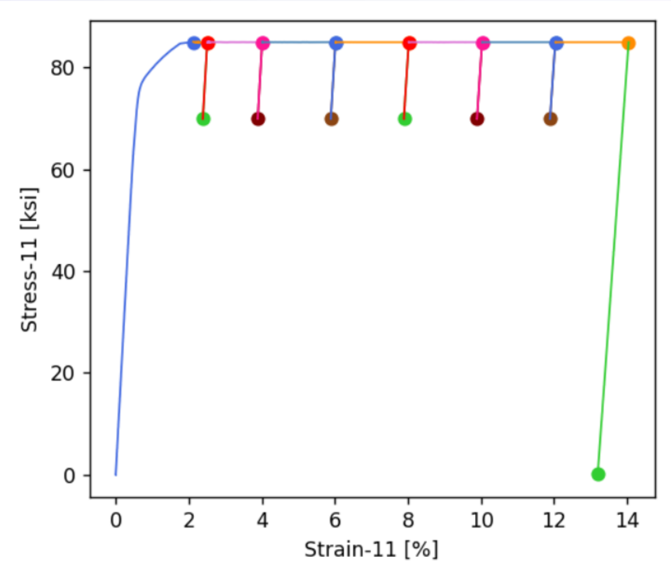


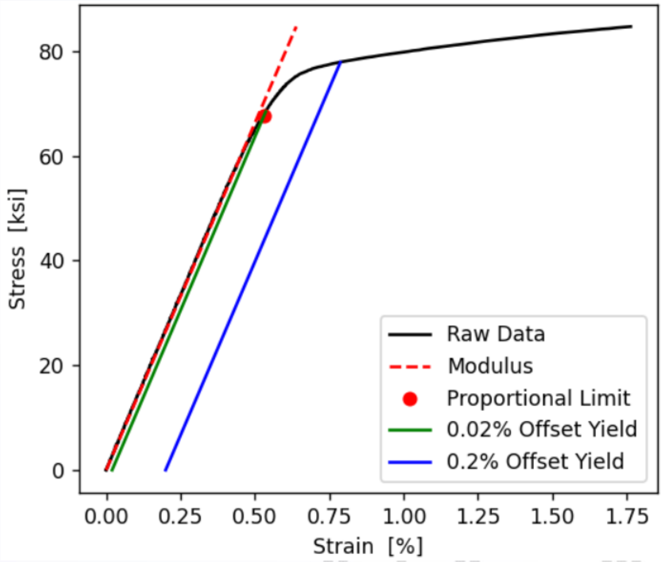
- Re-evaluate the requirements locally with periodic global (structural – PLM/SDM) updates

Py MI LAB: Analyzing and Storing Test Data

- Py MI LAB performs automatic reduction, analysis, and placement of thermomechanical test data
- Benefits:
  1. Reduce user effort for data management and increases throughput
  2. Provide traceability between machine, material, and test data
  3. Consistency in data analysis and reduction
- Able to perform automatic segmentation for complex load histories
  - User has ability to edit within the GUI
- Individual analysis subroutines for each load type (tension, compression, creep, relaxation)
  - Applied to each stage







Py MI Lab GUI Combines Automation with User Input for Efficient and Accurate Analysis

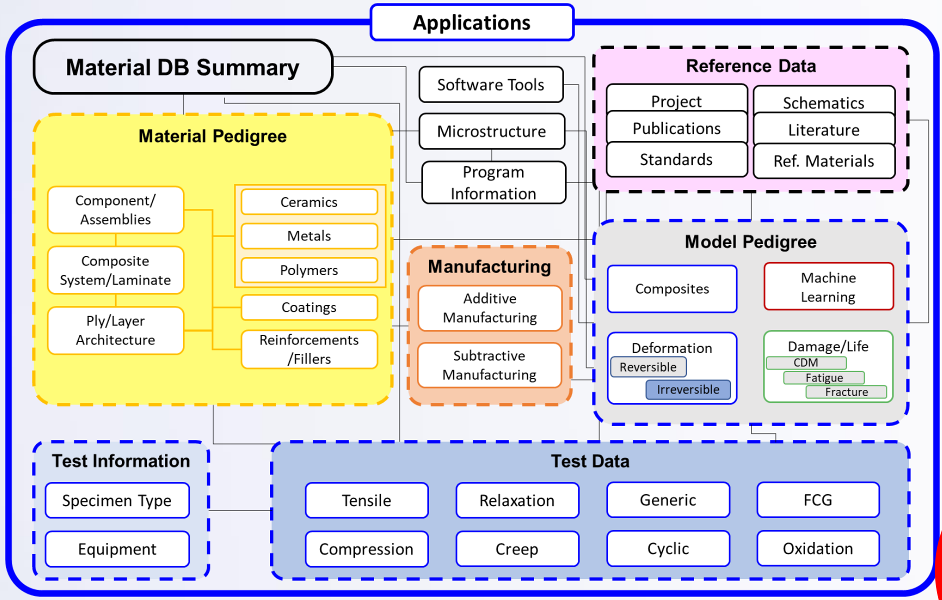
Information Management Essential For Fit-For-Purpose Material Design

Established Data Schema for ICME that Enables Linkage of Test Data with Simulation Data at Different Length Scales:

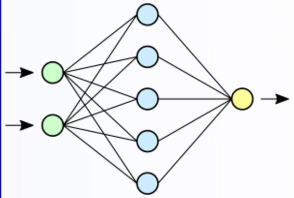
- Required establishment of Material Pedigree, Manufacturing, Microstructure, Model Pedigree, and Software Tools Tables within Granta MI
- Digital Thread / Digital Twin
- Six key **accomplishments**

Additive Manufacturing
ICMAMS 2023, Aug 9, 2023

Application Table
NASA TM-2022-00184033



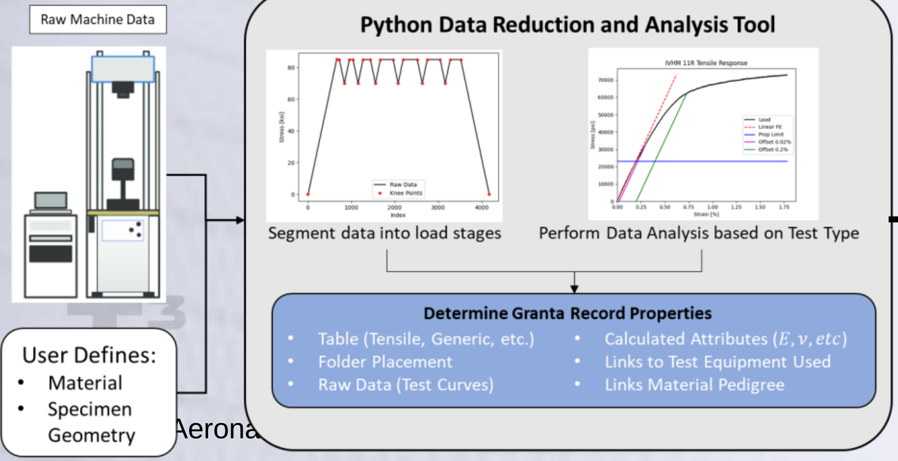
NASA GRC ICME Schema: Executive Summary
NASA TM-2023-0018337

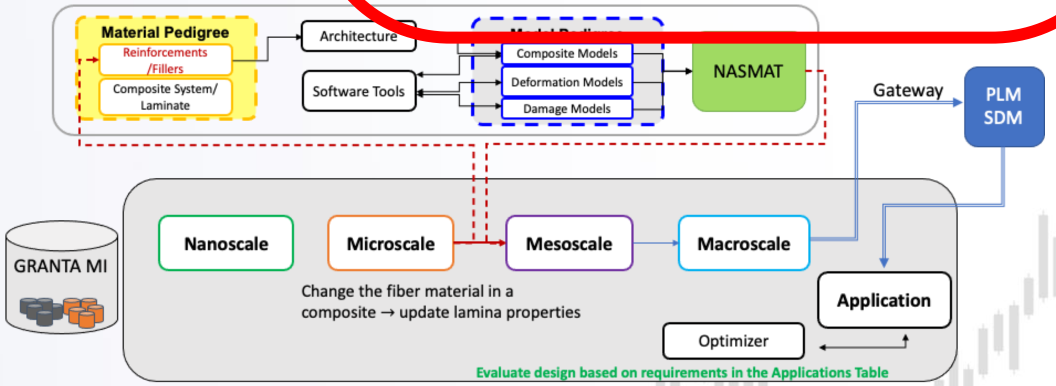


Machine Learning Table
NASA TM-2022-0017137

AIMAOS: Automated Information Management Across Organizations and Scales (TMS ICME, May 21, 2023)

Py-MILab (ICMAMS 2023, Aug 9, 2023)
Data Analytics and Importer



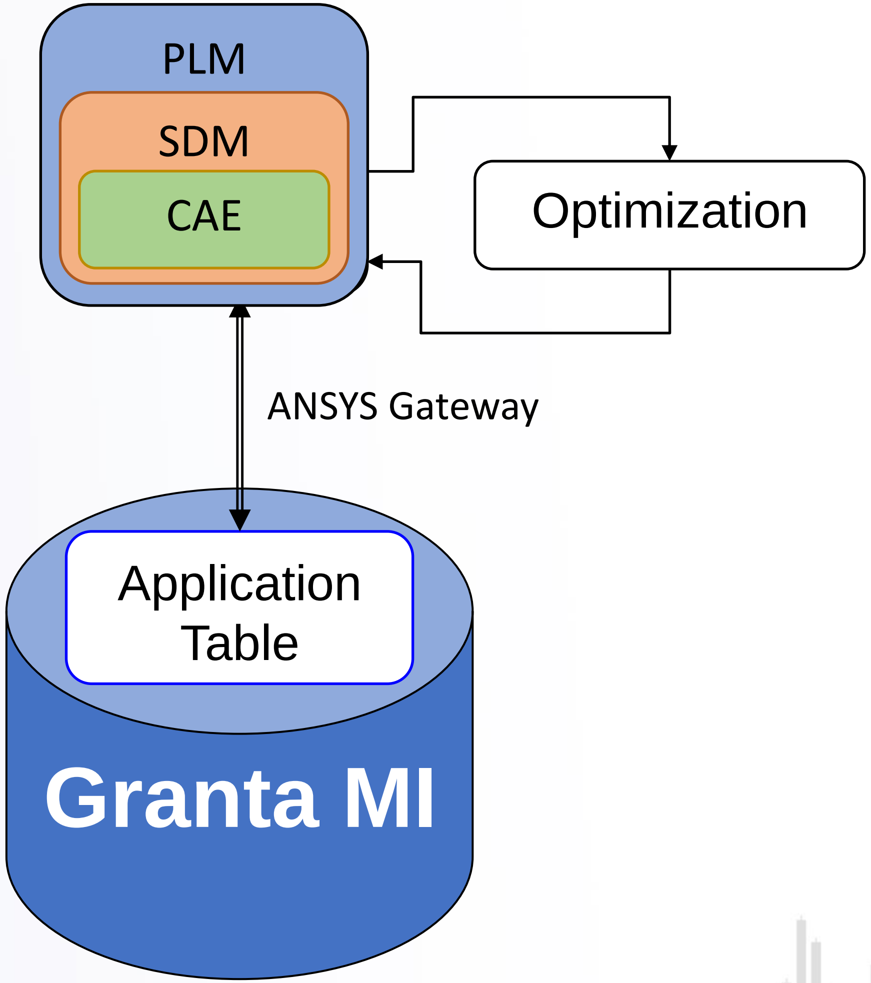


- Re-evaluate the requirements locally with periodic global (structural – PLM/SDM) updates

Traditional Database/Simulation Management Only Deals with a Single Scale

- Select a known material based on application requirements
  - Use macroscale material properties (which incorporate all lower length scales effects)

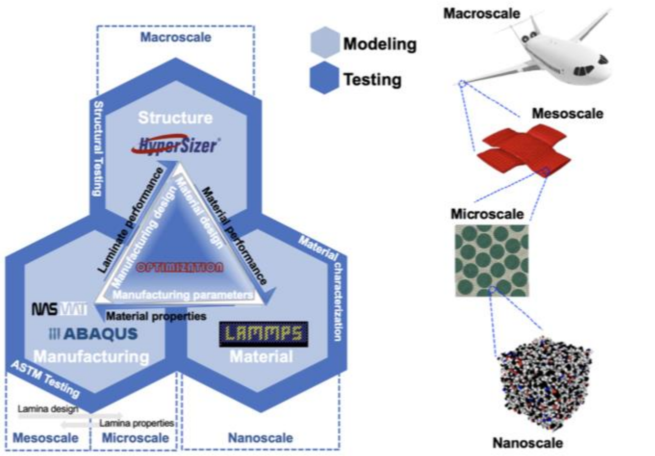
- Iterate on the structural design until requirements in the PLM/SDM are met
  - If requirements cannot be met, select a new material



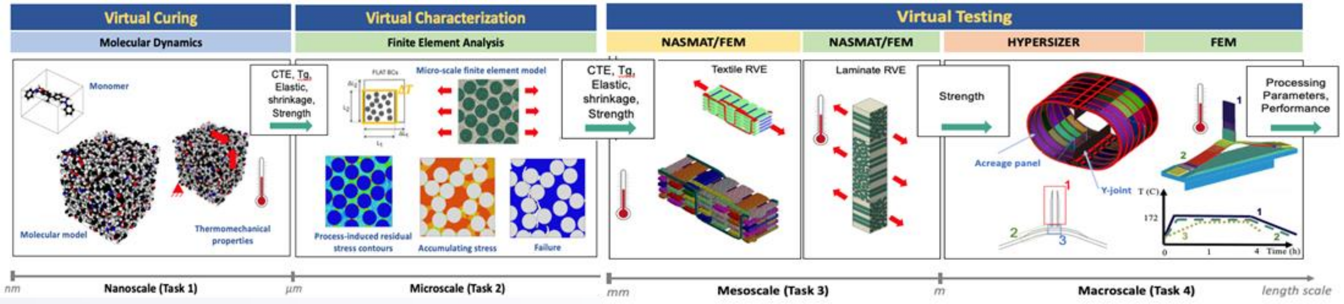
Material and Structure viewpoints are non-concurrent!

AIMAOS: Digital Thread Maintenance Tool

- **AIMAOS** – **A**utomatic **I**nformation **M**anagement **A**cross **O**rganizations and **S**cales
  - Digital thread maintenance tool which orchestrates the ICME process through *judicious automation* across organizations and scales

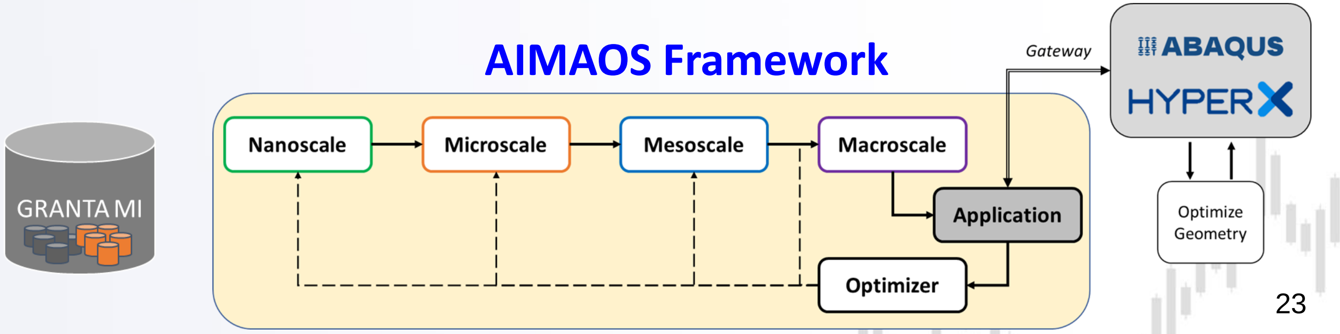


- Motivation
  - Benchmark problem will serve to demonstrate the benefits of the ICME)
    - **Digital Twins** at each scale
    - Input/output from each scale will constitute the **digital thread**
  - Won the 2022 AIAA ICME Prize
    - 17% manufacturing cost savings for the Y-joint
    - 30% weight reduction for the part
    - Fuel cost savings of $1204 per aircraft per year
    - Manufacturing cost savings to investment of additional material cost (GNP reinforcement) can produce a ROI 200:1



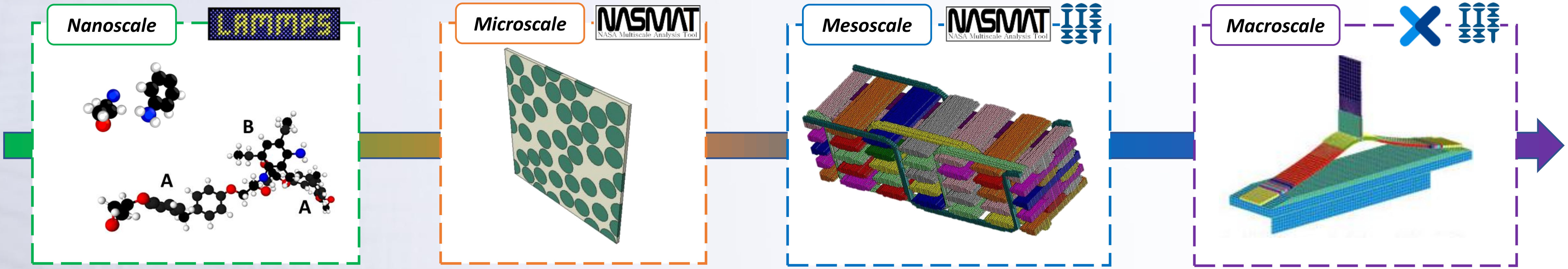
Challenge:
Required ***extensive coordination*** between team members to pass information across scales and relied on users to ***manually track changes*** that occurred in the design

AIMAOS Framework



AIMAOS Methodology

- Create a Python-based tool that can store information, write input decks, and read output decks across the various scales
- Develop a GUI so users can easily navigate through the different scales as changes occur and
- Store **digital twins** at each scale as input/output decks between tool sets
- Establish minimum metadata to describe a **digital twin** and distinguish from a **digital representation** as time evolves



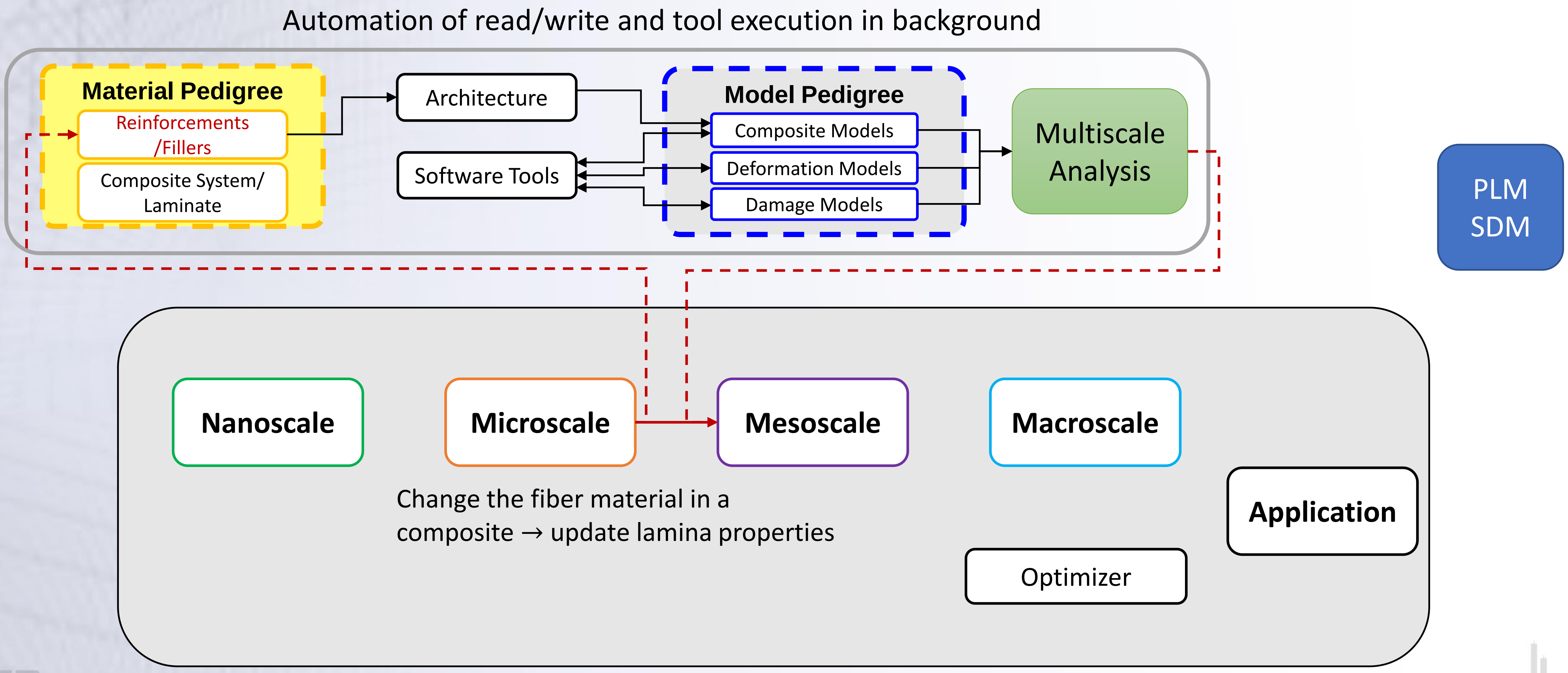
- Resin chemistry as a function of cure

- Define fiber and resin properties
- Determine lamina effective properties

- Determine laminate effective properties and allowables

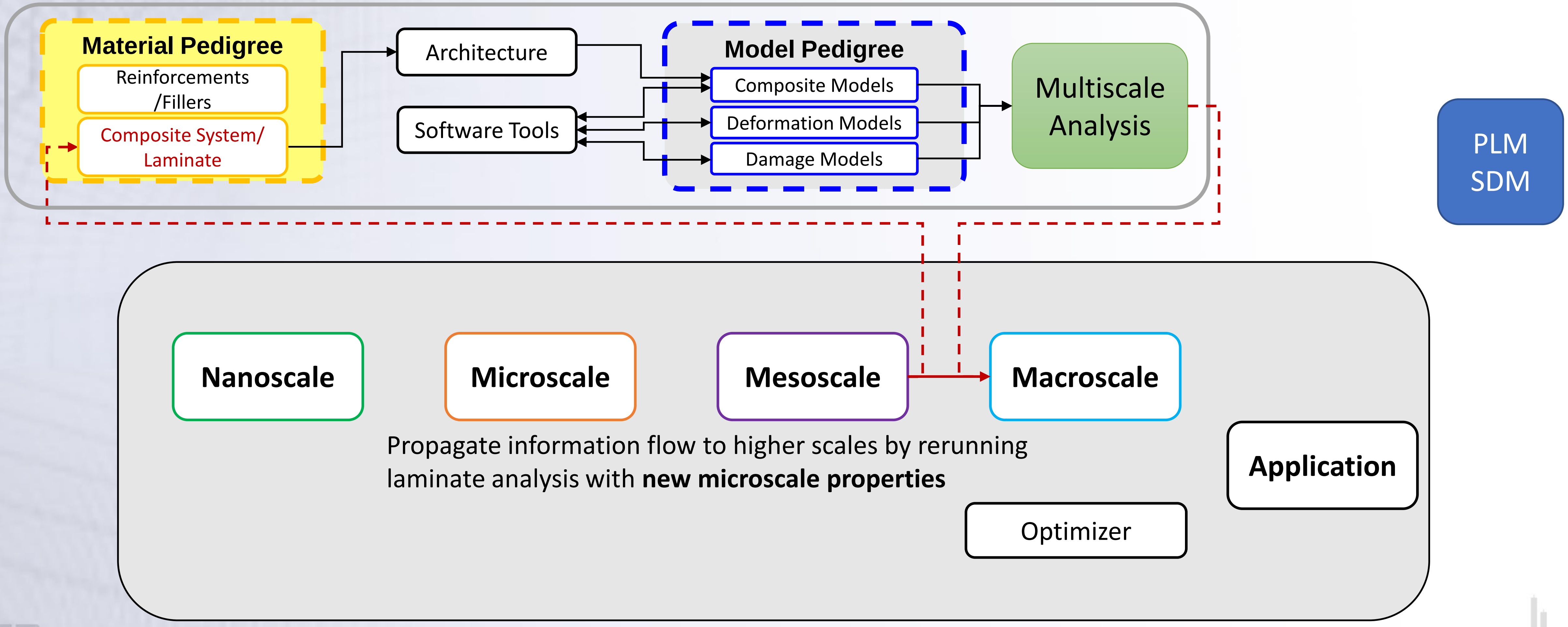
- Apply structural loads
- Optimize geometry
- Evaluate the design

AIMAOS assists Digital Thread Management in ICME

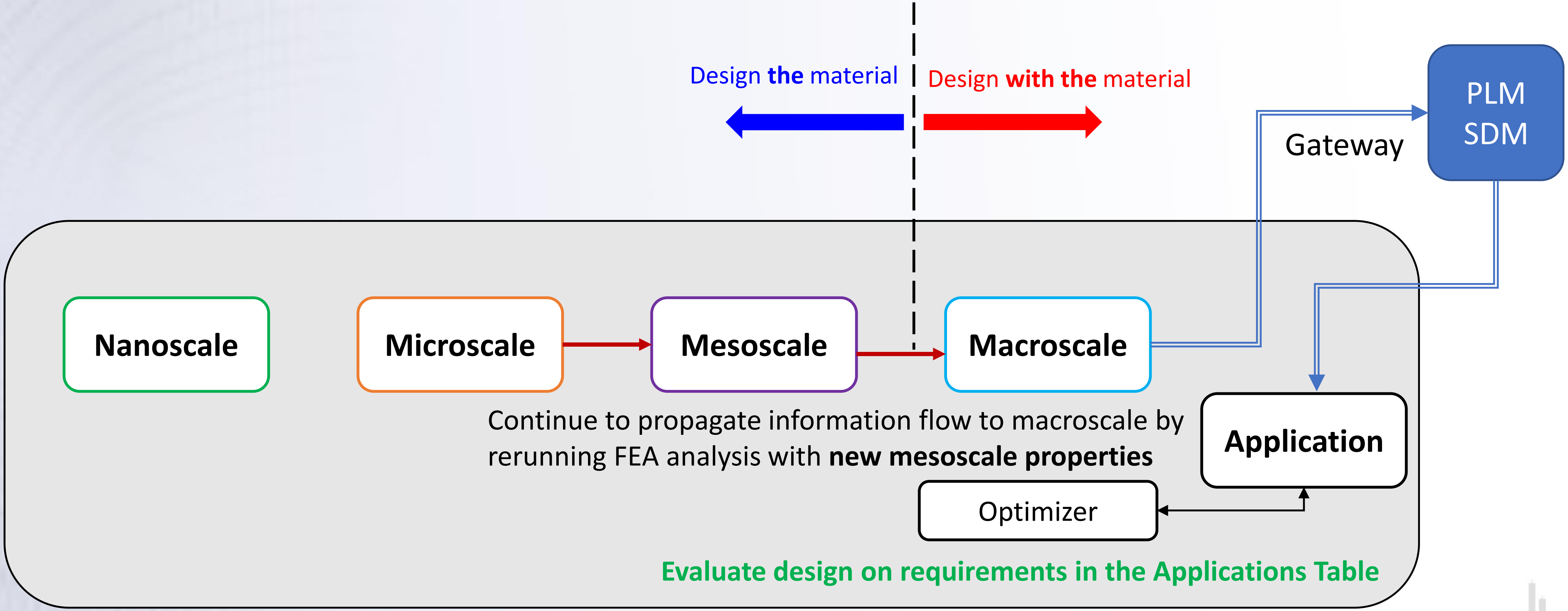


AIMAOS assists Digital Thread Management in ICME

Automation of read/write and tool execution in background



AIMAOS assists Digital Thread Management in ICME



Closing Comments

- Effective Material ***Information Management*** is essential for efficient and cost-effective design of new materials
  - Data management is a critical element of the NASA Vision 2040

- Granta MI offers a platform for importing, storing, and disseminating data to the right people, in the right format, at the right scale, and at the right time
  - Commercial database platforms remove the burden from end users of maintaining a database system and allow focus to be placed on schema design and development of auxiliary tools

- NASA GRC has developed a robust schema to handle both real (test) and virtual (simulation) data, physics-based and data driven models, and applications to facilitate capturing and *maintaining institutional knowledge*

- The toolsets developed at NASA GRC interact with the database to enable automatic capture, analysis, maintenance, and dissemination of data to realize ‘fit-for-purpose’ materials

Available Publications

- NASA TM-20230018337 : NASA GRC ICME Schema for Materials Information Management: An Executive Summary
- NASA TM-20220018403 : Application Table: A Bridge Connecting the Designing "With-The-Material" and "The-Material" Paradigms
- NASA TM-20220017137 : A Robust Machine Learning Schema for Developing, Maintaining, and Disseminating Machine Learning Models

Thank You for Your Attention

Integrate Don't Duplicate

Steve Arnold
NASA Glenn Research Center
Multiscale and Multiphysics Modeling Branch
steven.m.arnold@nasa.gov

Brandon Hearley (Digital Transformation Specialist)
NASA Glenn Research Center
Multiscale and Multiphysics Modeling Branch
Brandon.L.Hearley@nasa.gov

Joshua Stuckner(Informatics focus lead)
NASA Glenn Research Center
Multiscale and Multiphysics Modeling Branch
joshua.stuckner@nasa.gov

NASA