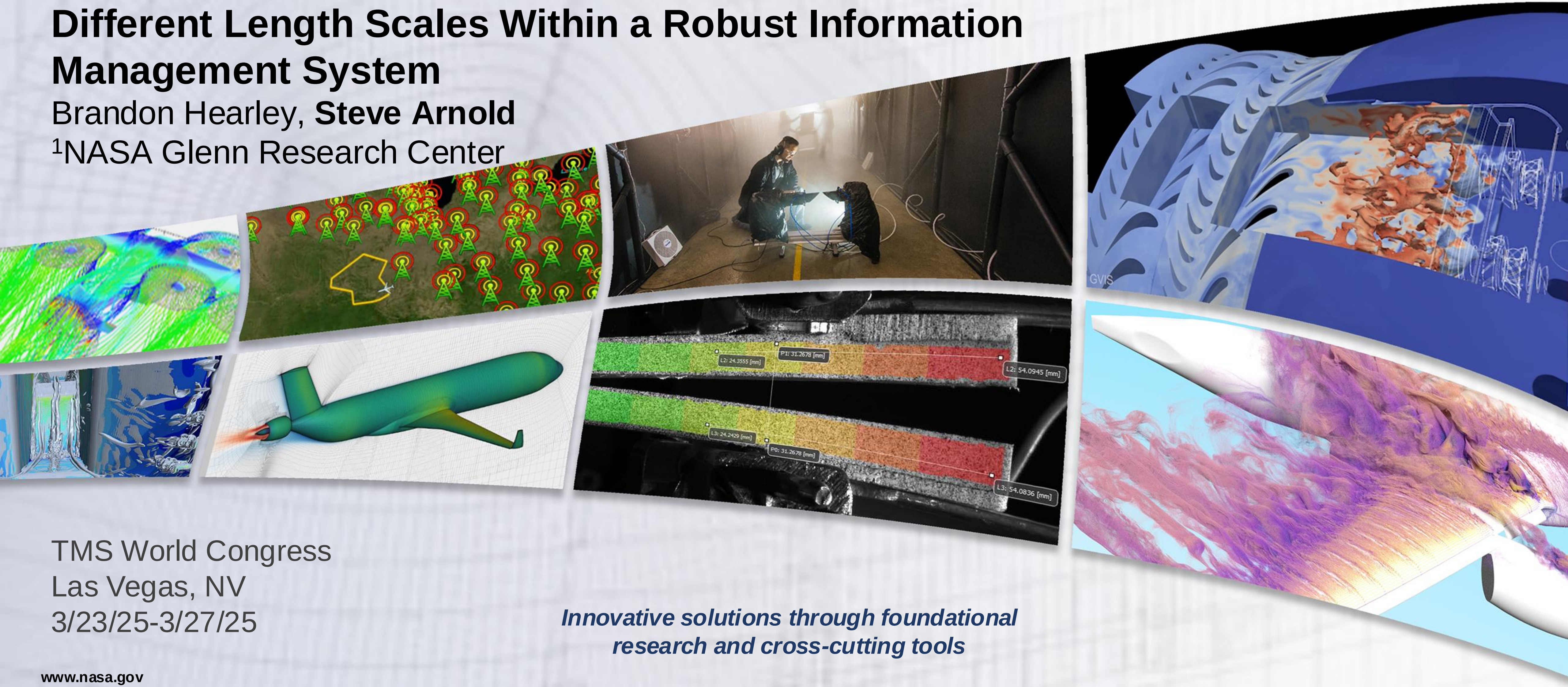
National Aeronautics and Space Administration

Transformational Tools and Technologies (T^3) Project

Automation of the ICME Workflow Incorporating Material Digital Twins at Different Length Scales Within a Robust Information Management System

Brandon Hearley, **Steve Arnold**

[1]NASA Glenn Research Center



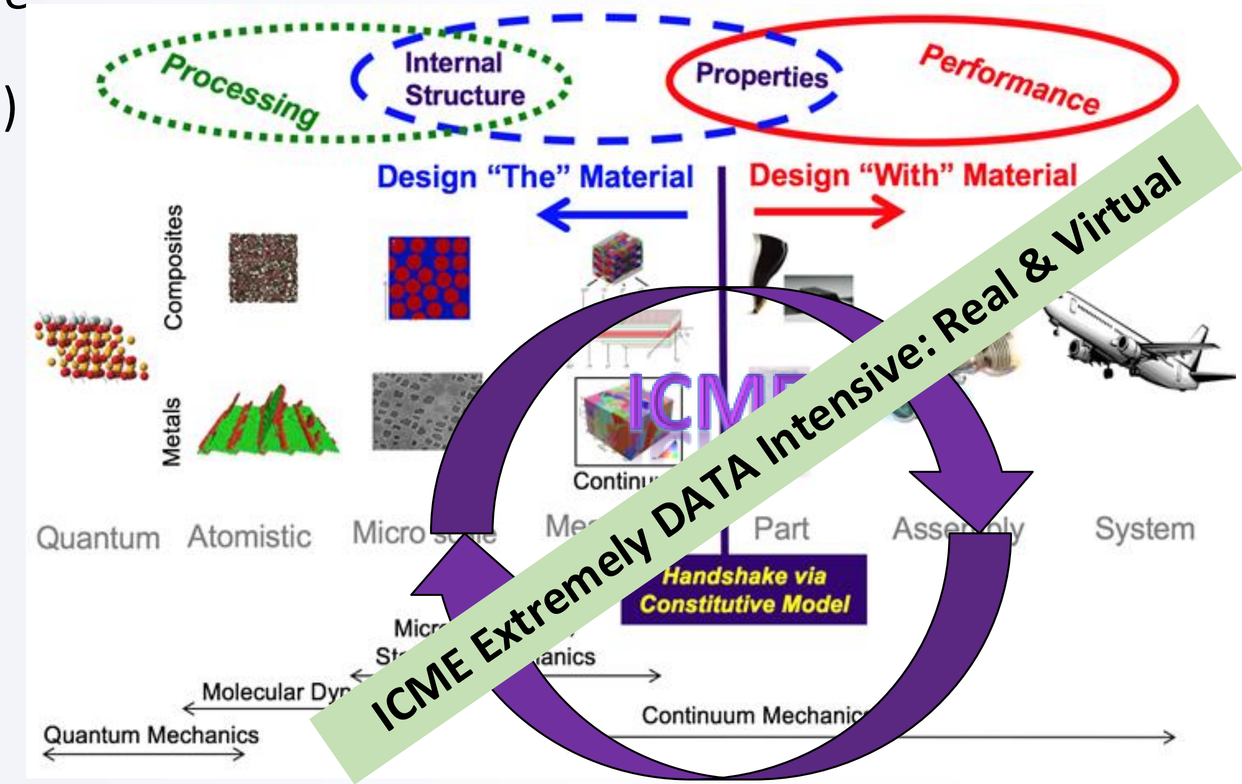
TMS World Congress
Las Vegas, NV
3/23/25-3/27/25

Innovative solutions through foundational research and cross-cutting tools

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)
- **ICME** enables the design of "fit-for-purpose" materials
  - Requires linking experimentally validated materials models at multiple length scales
  - Requires understanding processing-structure-properties-performance relationships
  - Requires fusing of multidisciplinary information (material science vs structural engineering viewpoint)
- Traditional engineering has been split between two paradigms
  - "Design with the Material" – Structural Viewpoint
  - "Design the Material" – Material Viewpoint

2040 goal is to Marry these two paradigms



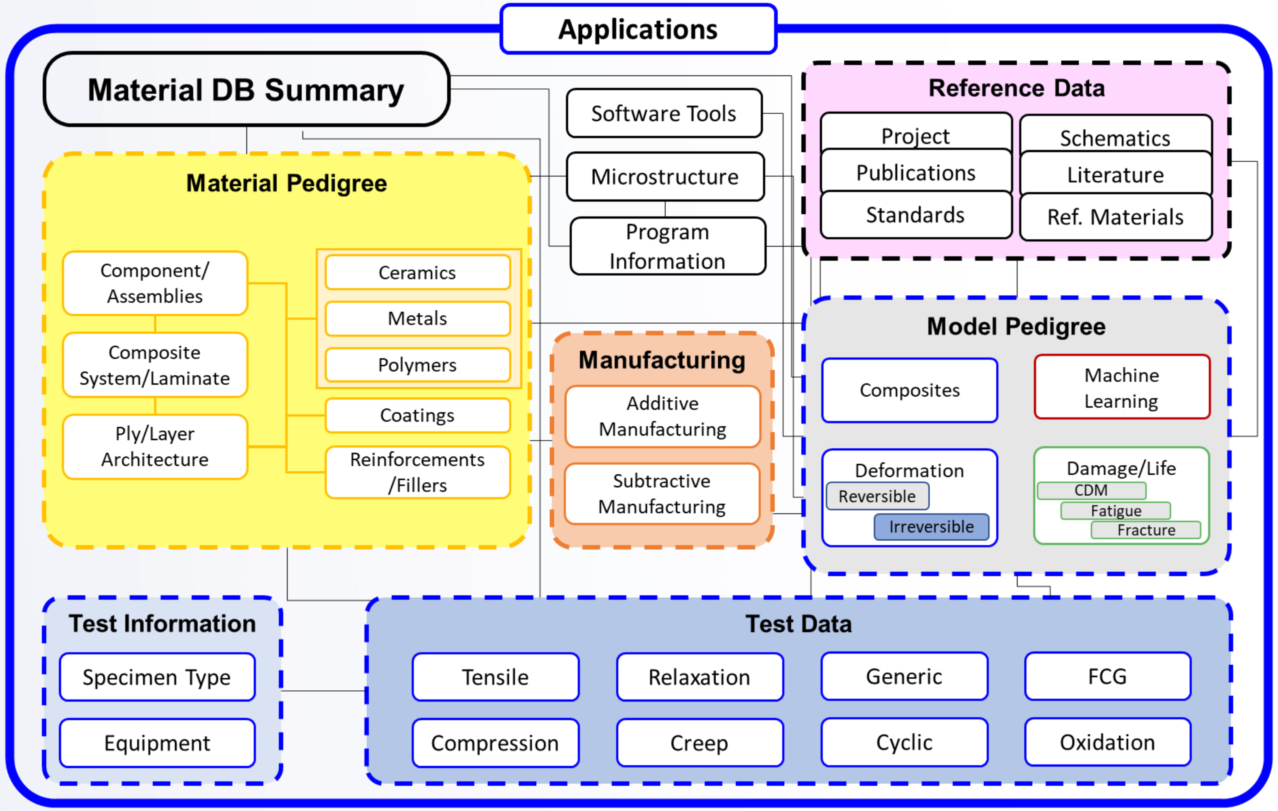
Requires a robust information management system integrated with simulation toolsets

NASA GRC's 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
- Recently added the **Application Table**
    - Store material and application performance requirements and criteria
    - Store spatial and temporal information on application microstructure, residuals, damage, etc.
    - Provide unique location to link CAD/PLM/SDM information to materials information
    - Bridges the "Design with the Material" and "Design the Material" paradigms
    - Maintain **Digital Thread and material Digital Twins**

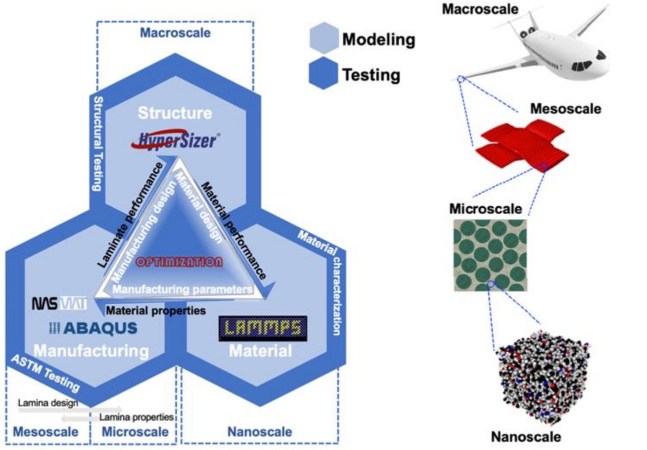
Application Table: Acts as the conductor for the ICME process



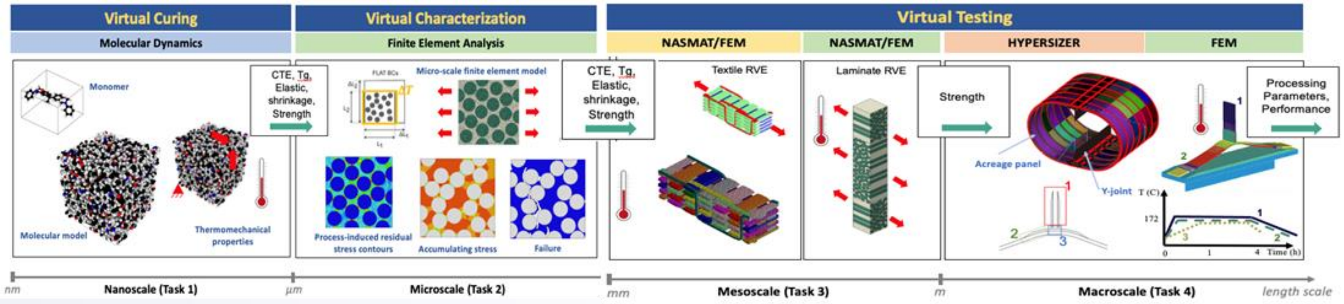
See Arnold S.M, Hearley, B. L., Cebon, D.; "Application Table: A Bridge Connecting the Designing "With-the-Material" and "the-Material" Paradigms", **NASA/TM-20220018403** for more details

AIMAOS: Digital Thread Maintenance Tool

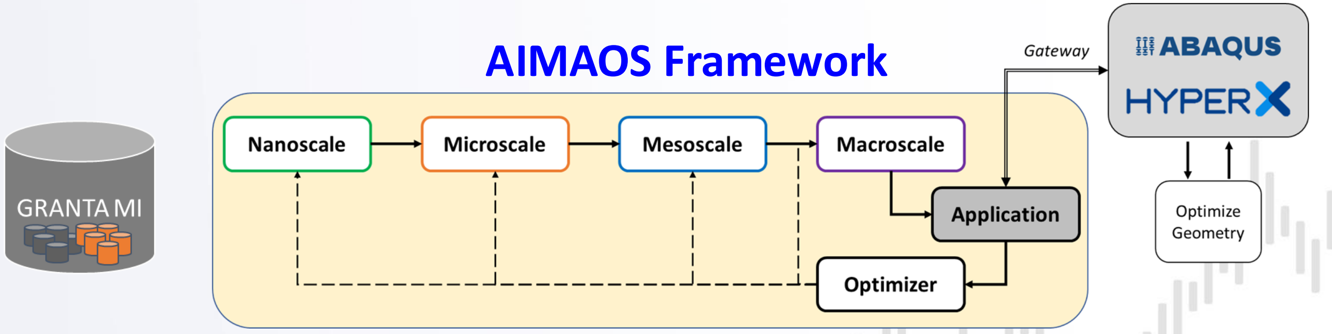
- **AIMAOS** – **A**utomatic **I**nformation **M**anagement **A**cross **O**rganizations and **S**cales
  - Digital thread maintenance tool which orchestrates the ICME process through *judicious automation* across organizations and scales



- 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

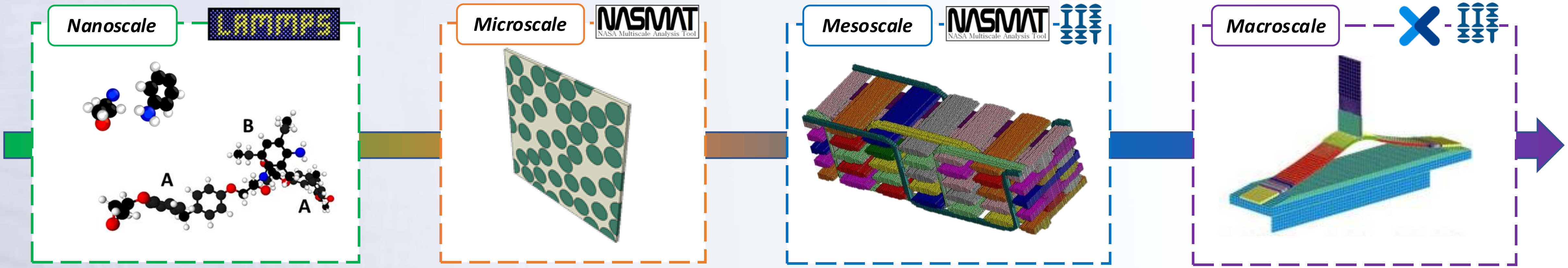


Challenge:
Required ***extensive coordination*** between team members to pass information across scales and relied on users to ***manually track changes*** that occurred in the design



AIMAOS 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

NASA TM 20240010796

Multiscale Analysis Tools

Large-scale Atomic/Molecular Massively Parallel Simulator
- Molecular Dynamics (MD) code for materials modeling
- Simulate curing of the resin to establish thermodynamic properties as a function of the processing
- Characterize resin properties as a function of cure for higher scales

NASA Multiscale Analysis Tool
- Determine homogenized lamina and laminate properties given constituents and microstructure
- Determine macroscale strength allowables by performing various monotonically loaded simulations

Abaqus
- Finite Element Analysis (FEA) software used to analyze the Y-joint at the structural level
- Inherent connections to NASMAT (UMAT) and HyperX (post-processing/optimization)

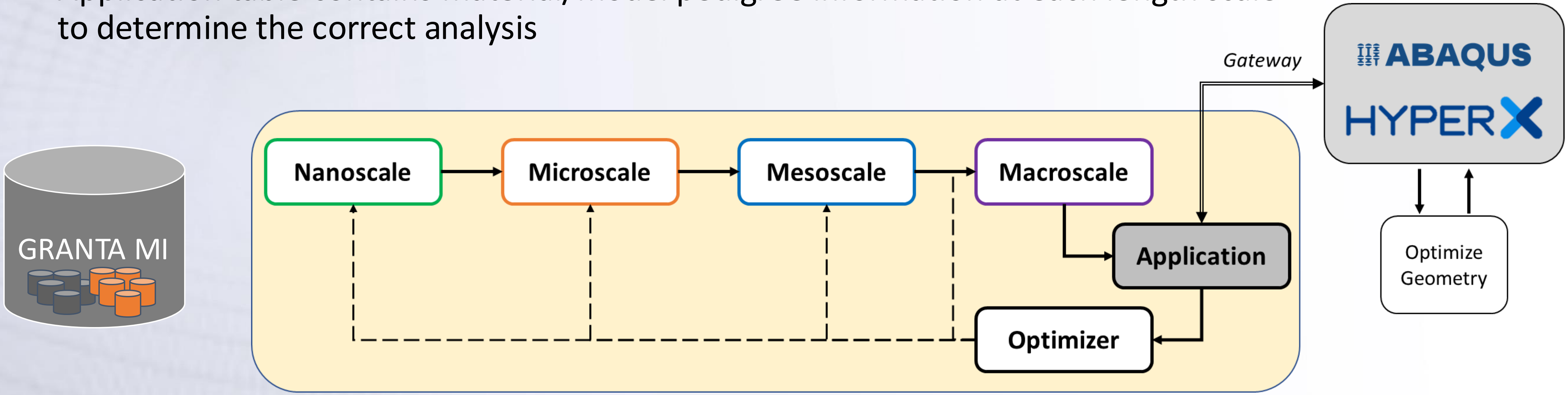
HyperX
- Composite analysis tool for weight reduction/geometry optimization, stacking sequence determination and material selection
- Interfaces with Abaqus to evaluate the Y-joint and determine the optimal weight given the macroscale material properties

Required Infrastructure for Orchestrating ICME

- ICME Design

Fit-for-Purpose Material Design

- Design the material for a specific application from processing through performance (fit-for-purpose)
- Use Multiscale Digital Tools to optimize material design
- Application table contains material/model pedigree information at each length scale to determine the correct analysis



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

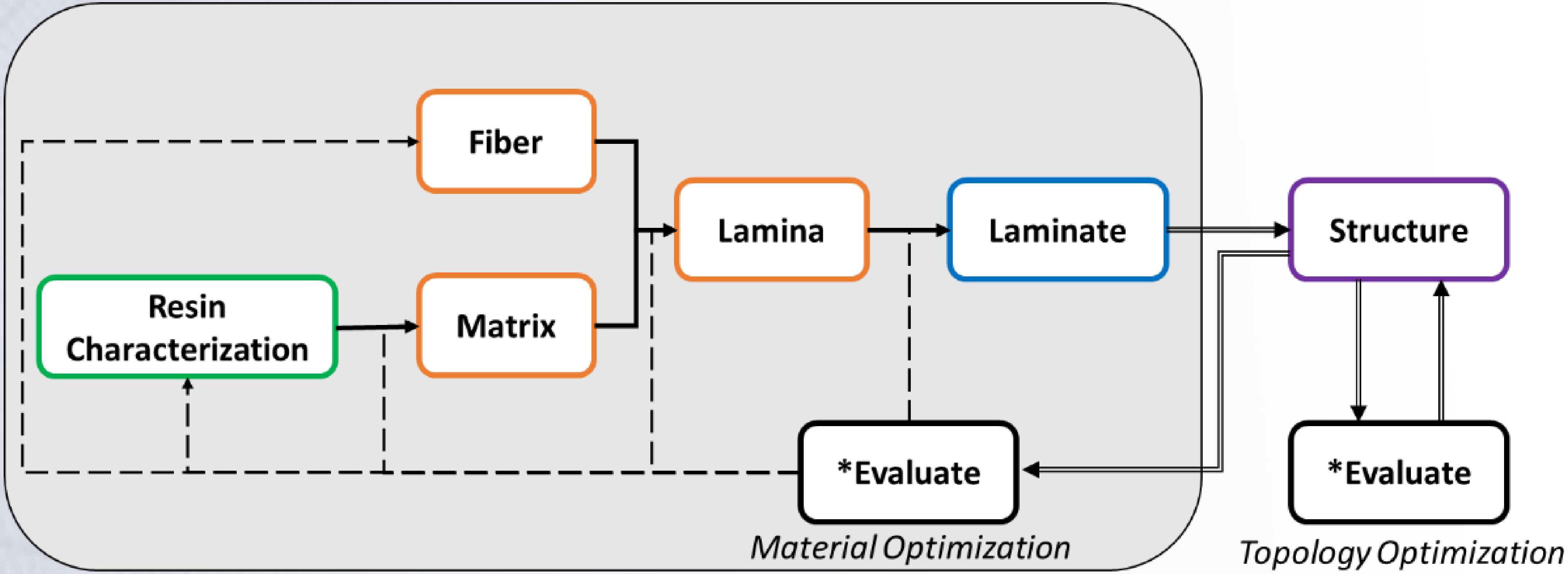
Remember the two important key words in ICME being

1) **Integrated** wherein processing histories, influence internal structure, which in turn drive properties, which then drive performance and
2) **Engineering** which signifies industrial utility!

AIMAOS Is the Enabling Technology for ICME

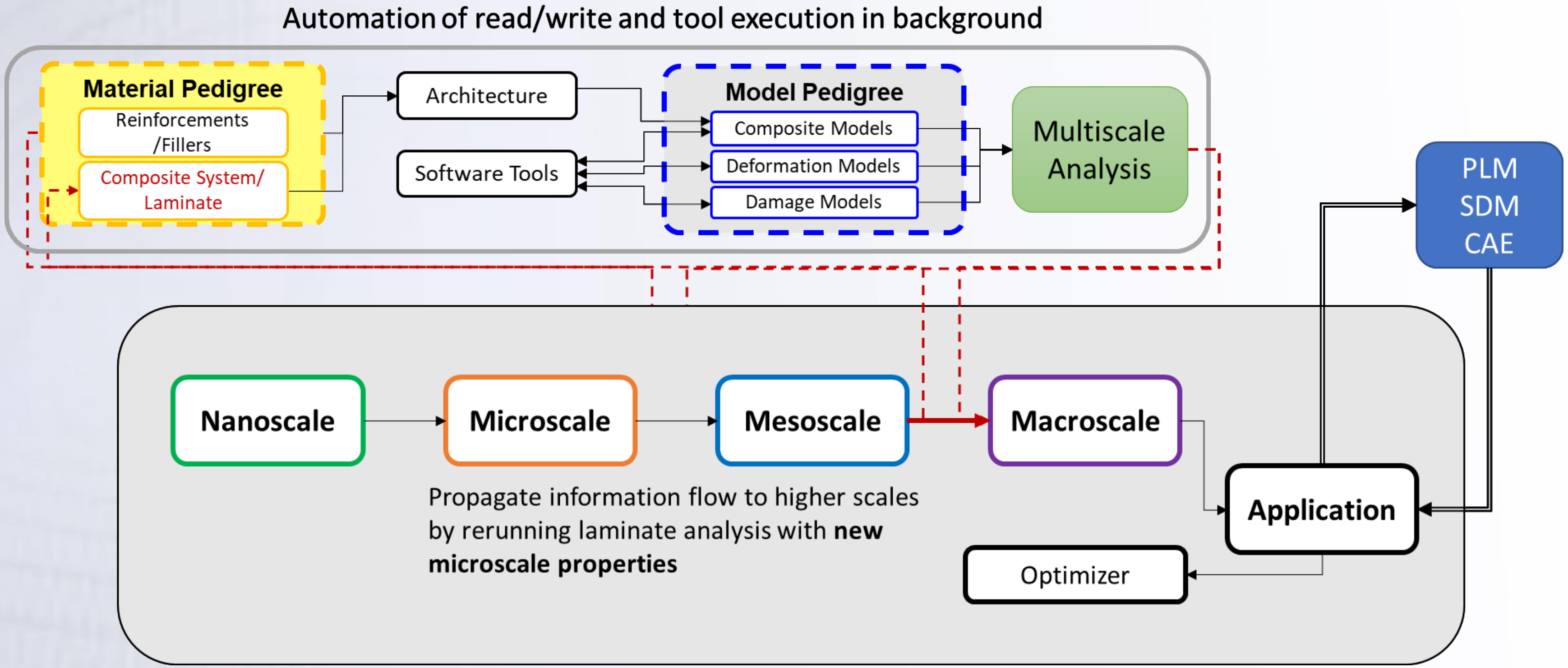
Integrating into Iteration/Optimization Scheme

Composite example workflow



AIMAOS Is the Enabling Technology for ICME

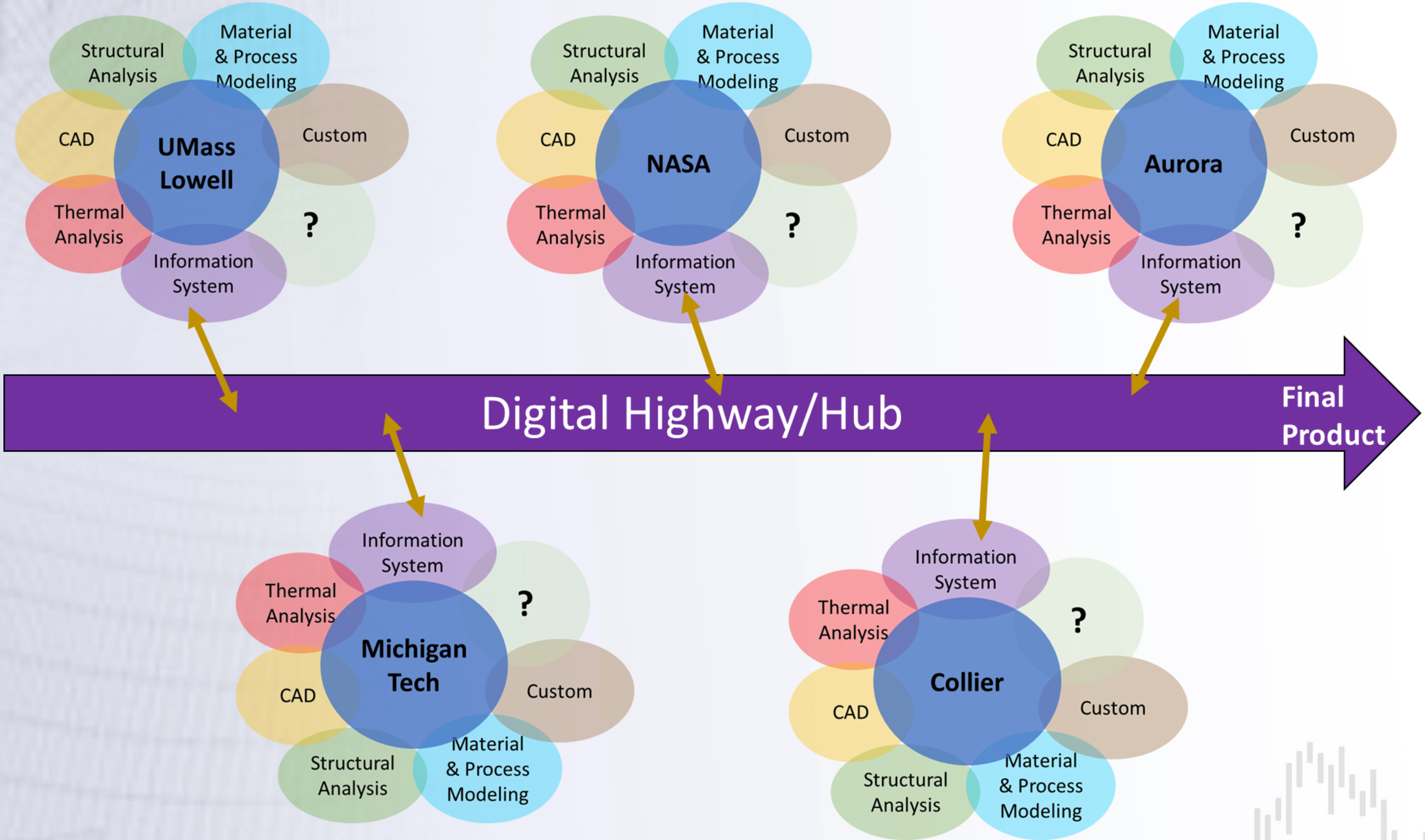
- When a change is made:
  - Propagation of information (data, metadata) is judicially automated



- Changes are automatically tracked with standardized notes
  - We can look at the optimization/iteration history to see what is changing → insight into most influential parameters

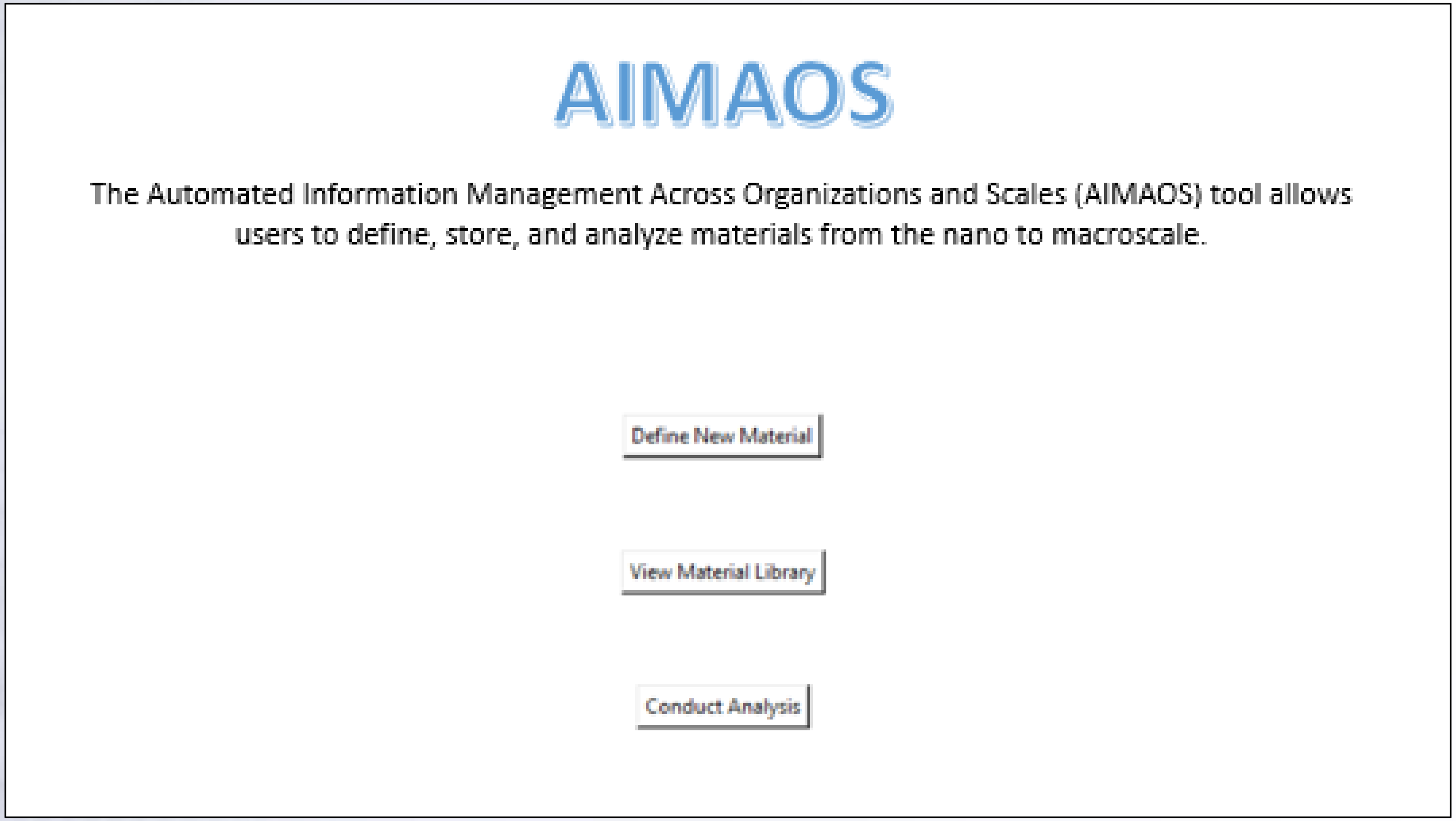
Multi-organizational Collaboration Environment

Vision 2040 Toolset Implemented Throughout Supply Chain



Automatic Information Management Across Organizations and Scales (AIMAOS) GUI

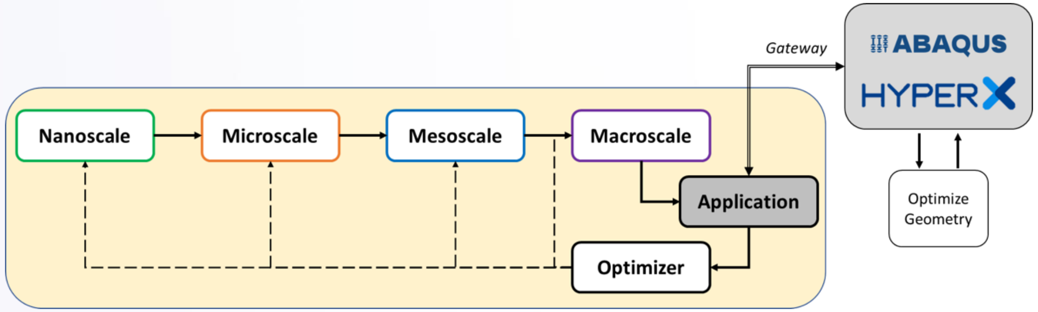
- Developed GUI allows users to navigate across the various scales, create input/output decks to establish digital twins at various length scales, and provides a version-controlled database of defined materials.

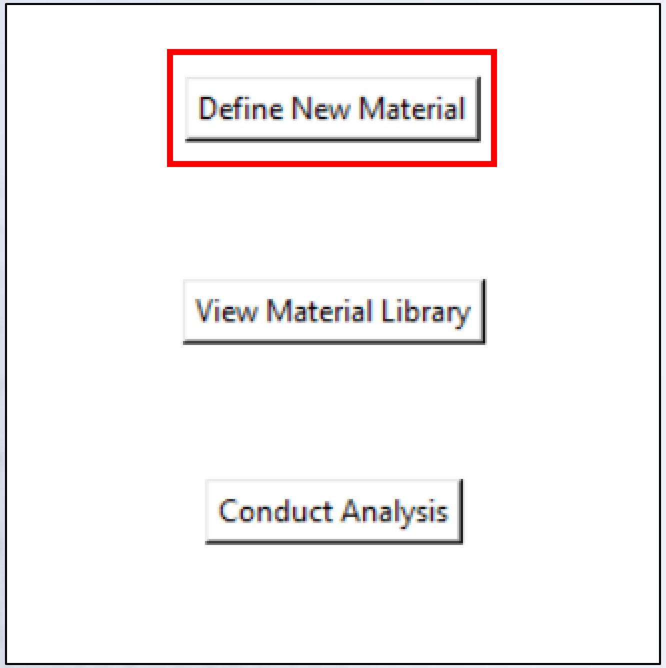


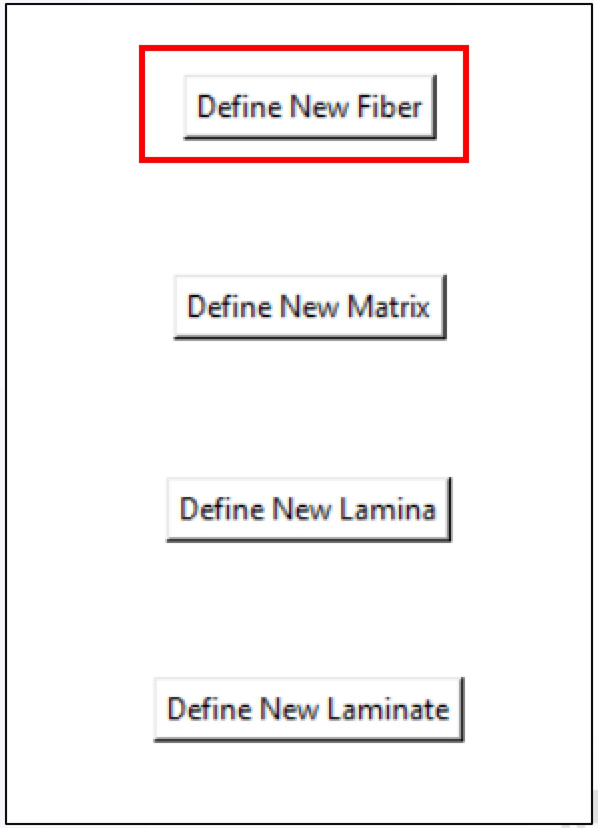
Defining Materials

GUI allows users to create a library of constituents, laminas, or laminates with associated properties to use in any analysis

- Allows an analysis to start from any lower scale (nano, micro, meso)







Micro

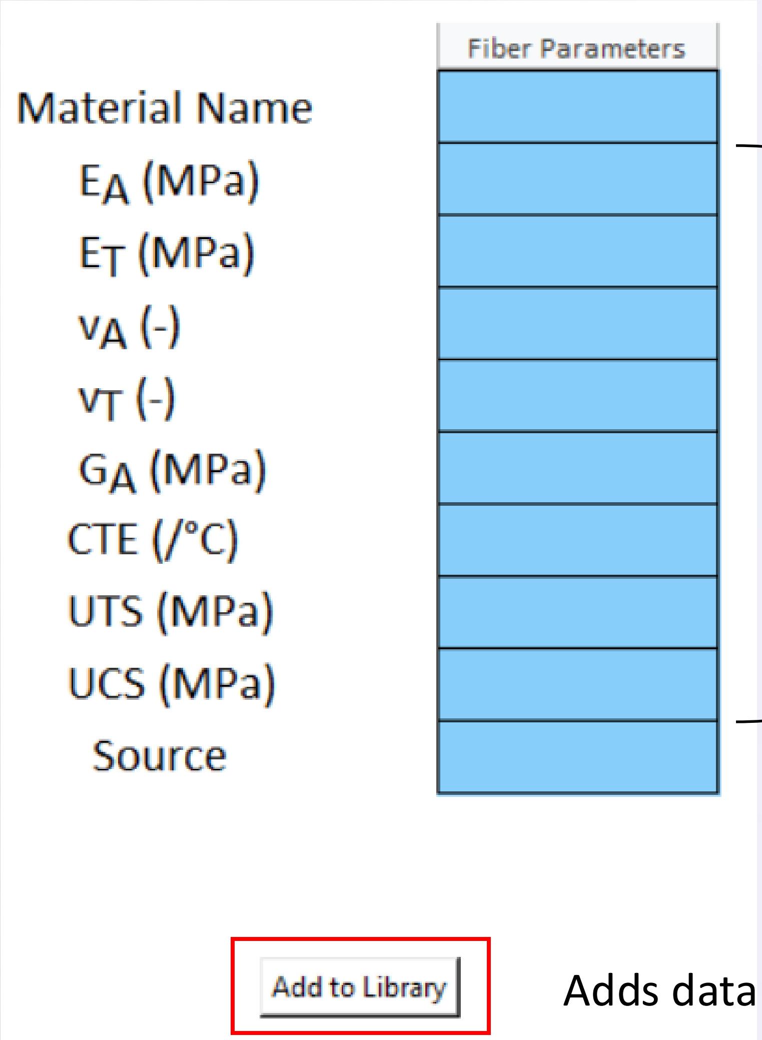
Nano/Micro

Micro

Meso

Defining a Constituent (Fiber/Matrix)

Users can add properties and strengths for a constituent (e.g., fiber) that will be used in subsequent analyses

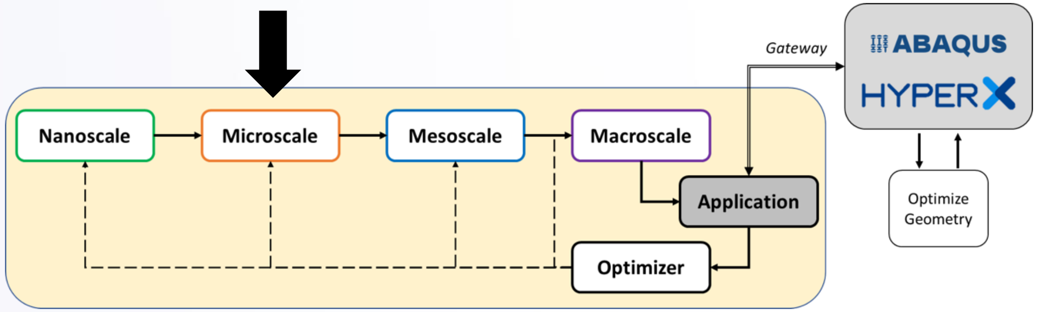


Reference Name

Properties for the NASMAT input deck

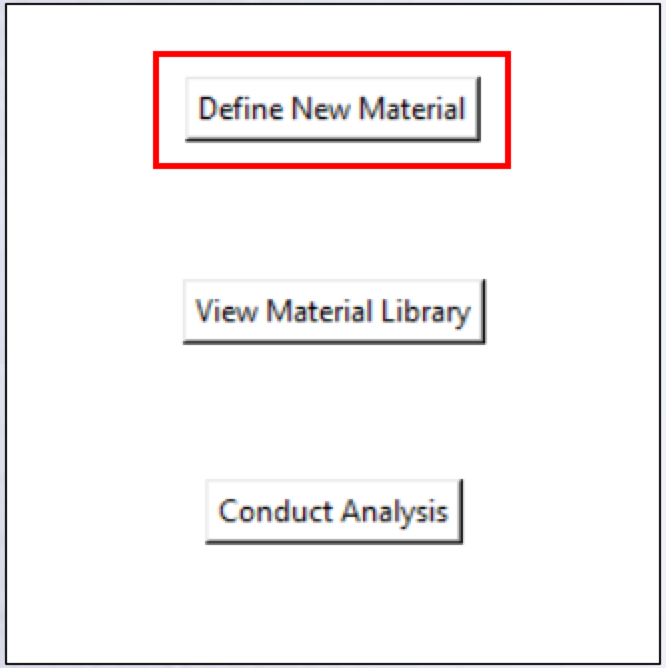
Notes on source (file path, website, reference, etc.)

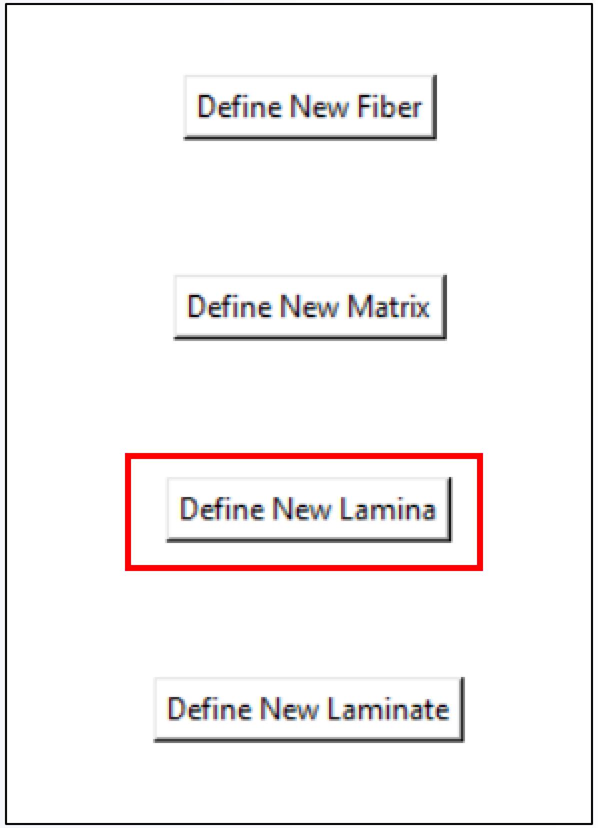
Adds data to the fiber library



When a new material is added, a unique ID number is generated for that material – used to link up the scales

Defining a Lamina





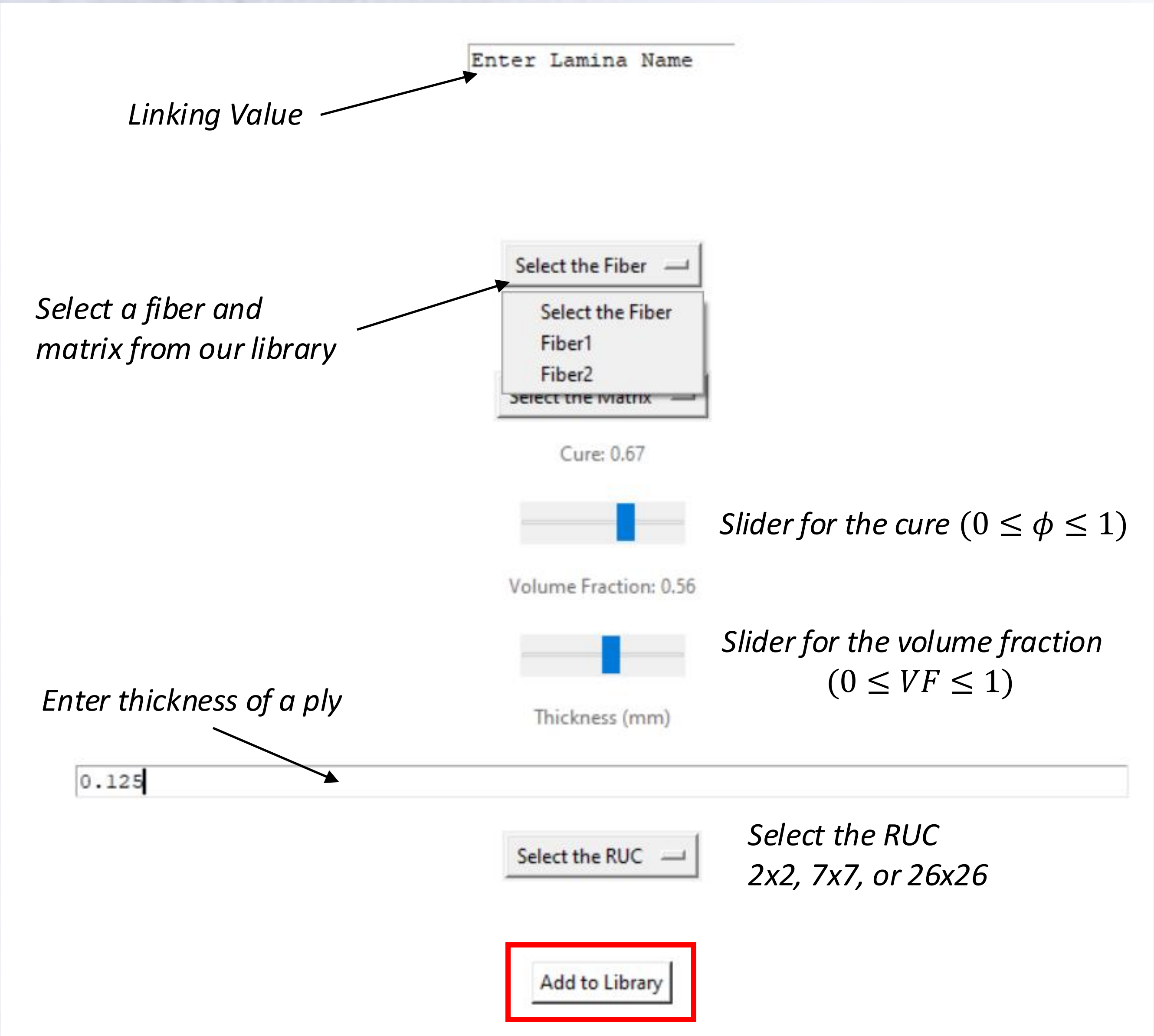
Micro

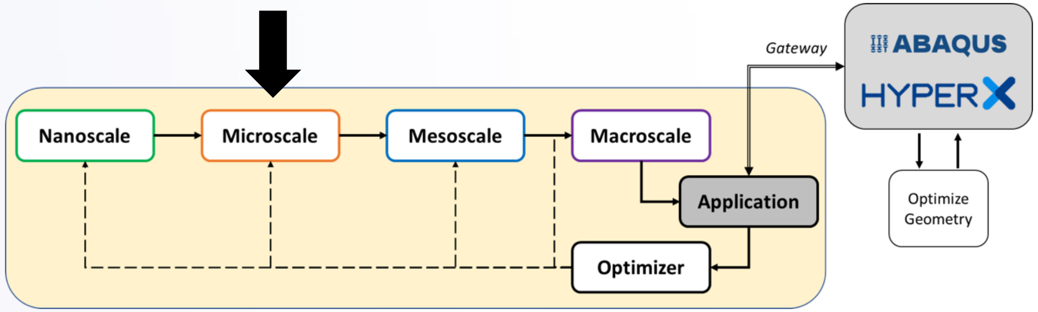
Nano/Micro

Micro

Meso

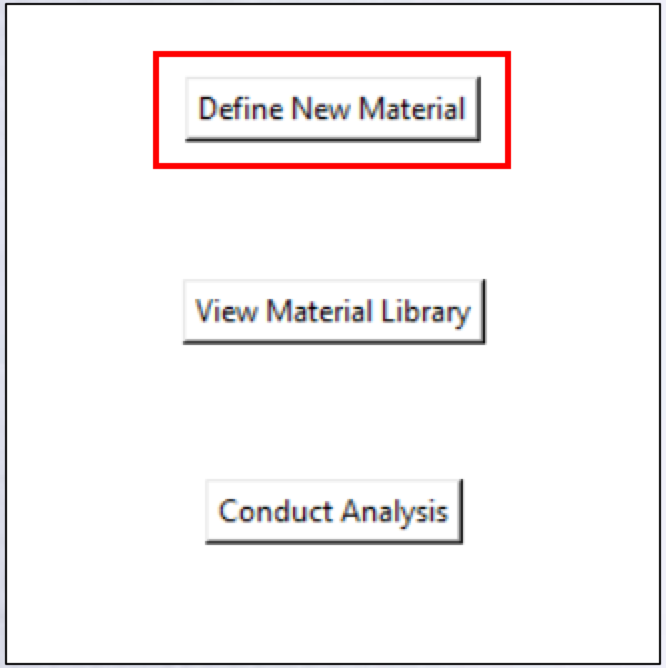
Defining a Lamina

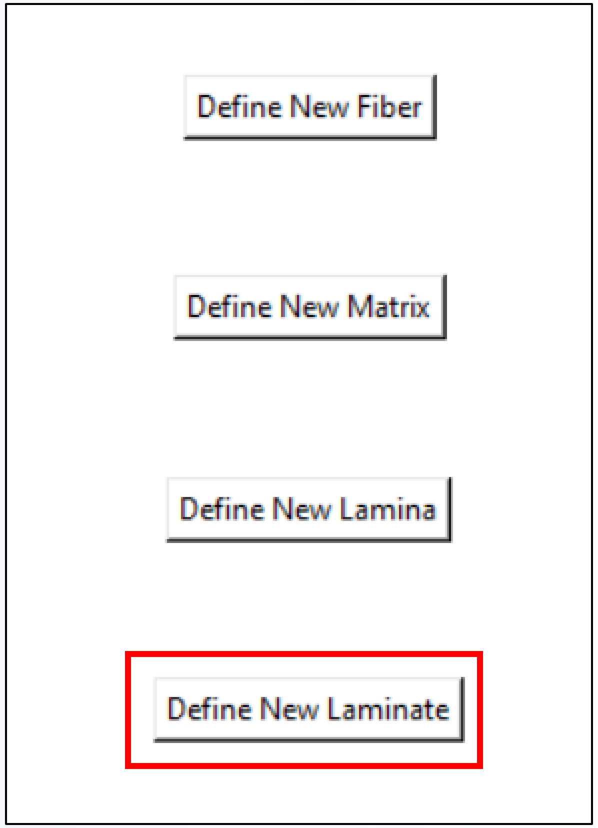




1. Calls characterization code to solve for microscale properties of the matrix as $f(\phi)$
2. Write a NASMAT input deck and run
3. Reads the output (effective properties, Q matrix)
4. Saves all inputs and outputs to the lamina library
5. Lamina library also has the input/output full file paths stored for traceability

Defining a Laminate





Micro

Nano/Micro

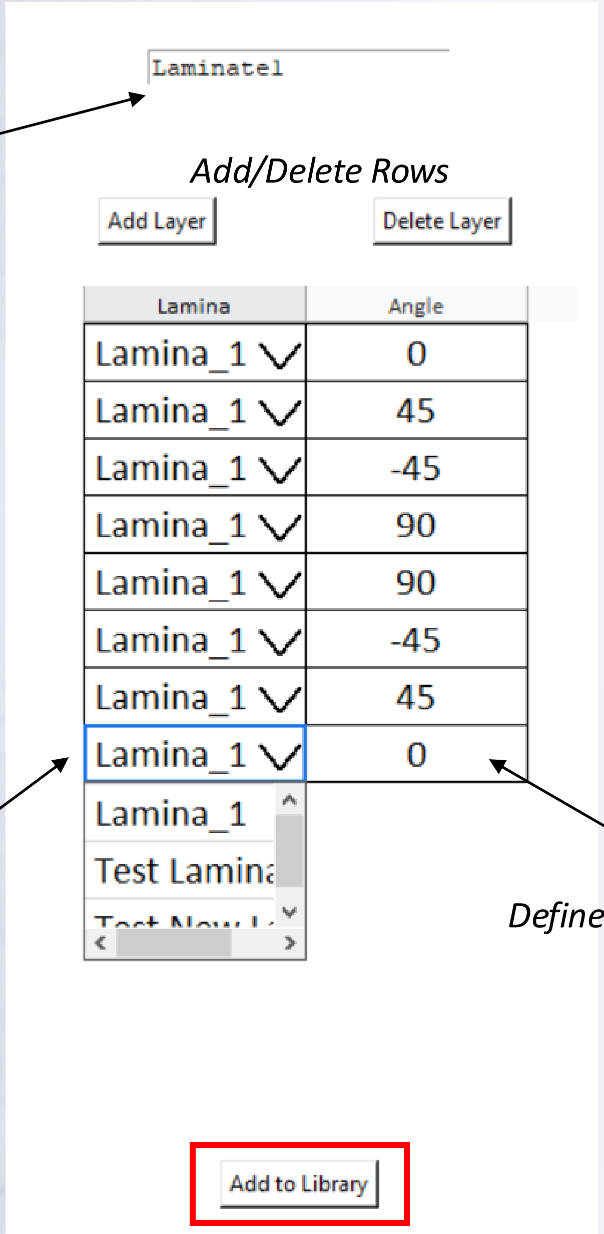
Micro

Meso

Defining a Laminate

Linking Value

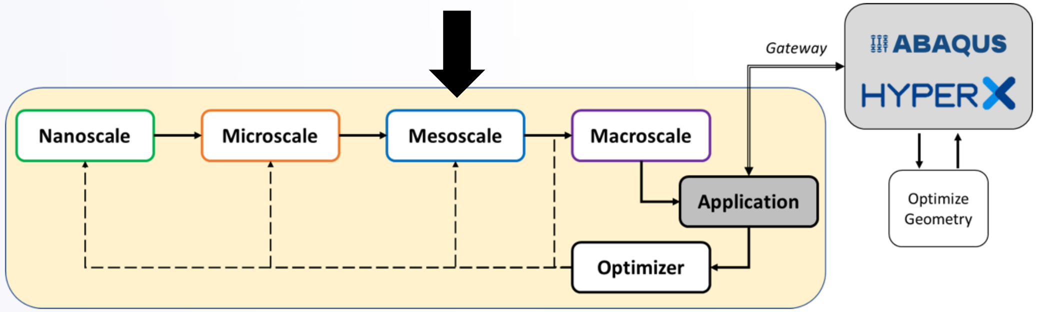
Add/Delete Rows



***Lamina has an associated microstructure and volume fraction*

Select a lamina from the library

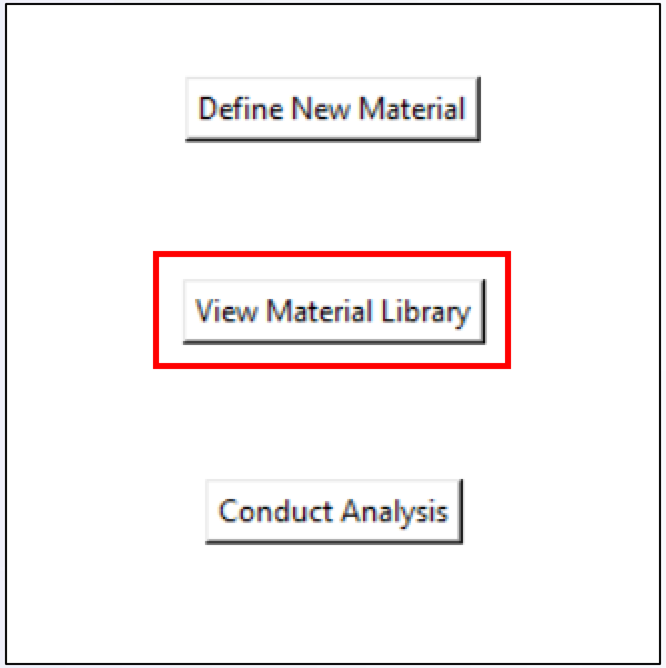
Define the ply orientation



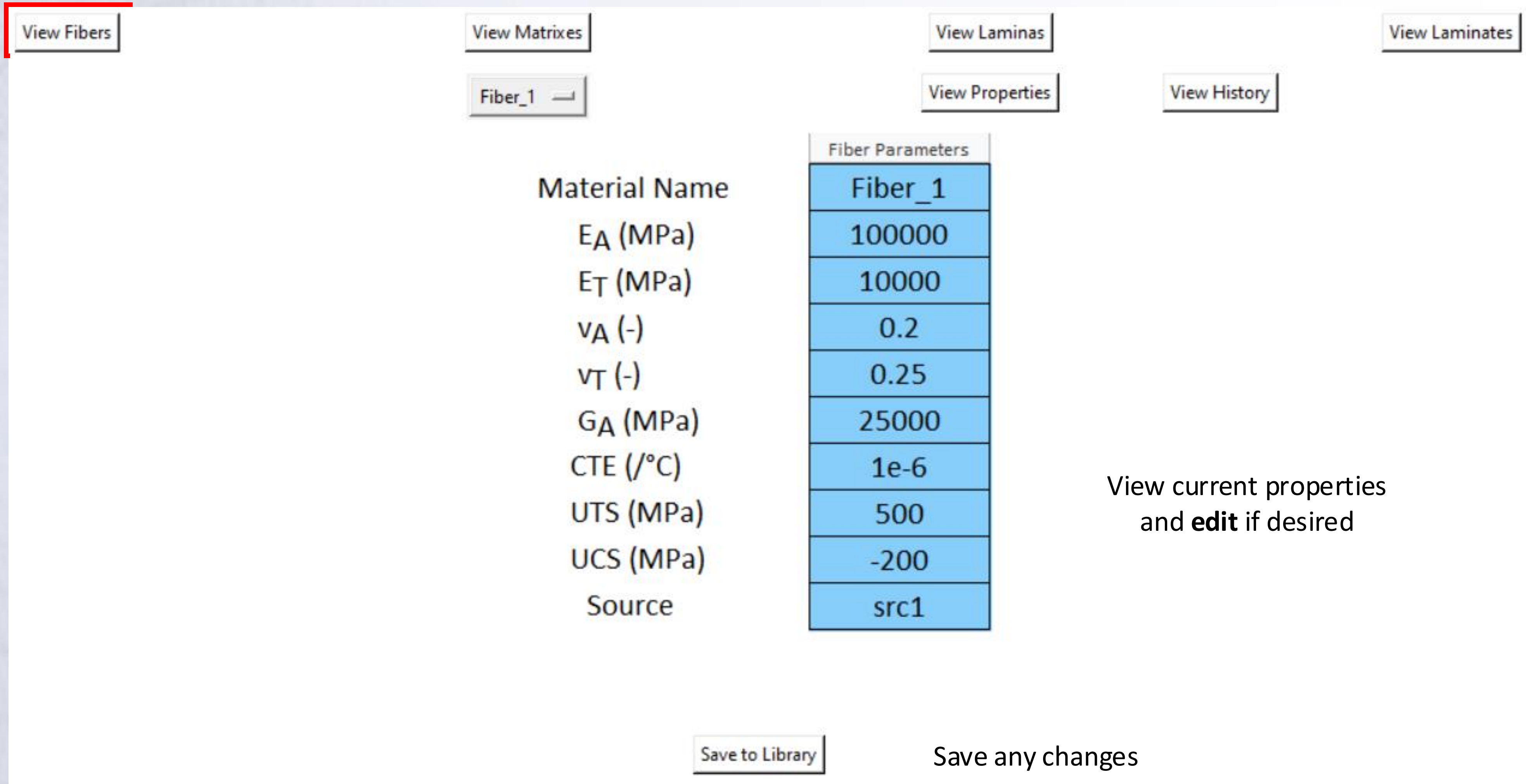
1. Write a NASMAT input deck and run
2. Reads the output (effective properties)
3. Saves all inputs and outputs to the lamina library
4. Laminate library also has the input/output full file paths stored for traceability

Editing Materials

Users can edit material properties with automatic tracking of the changes that have occurred during from one instance to the next



Editing a Constituent



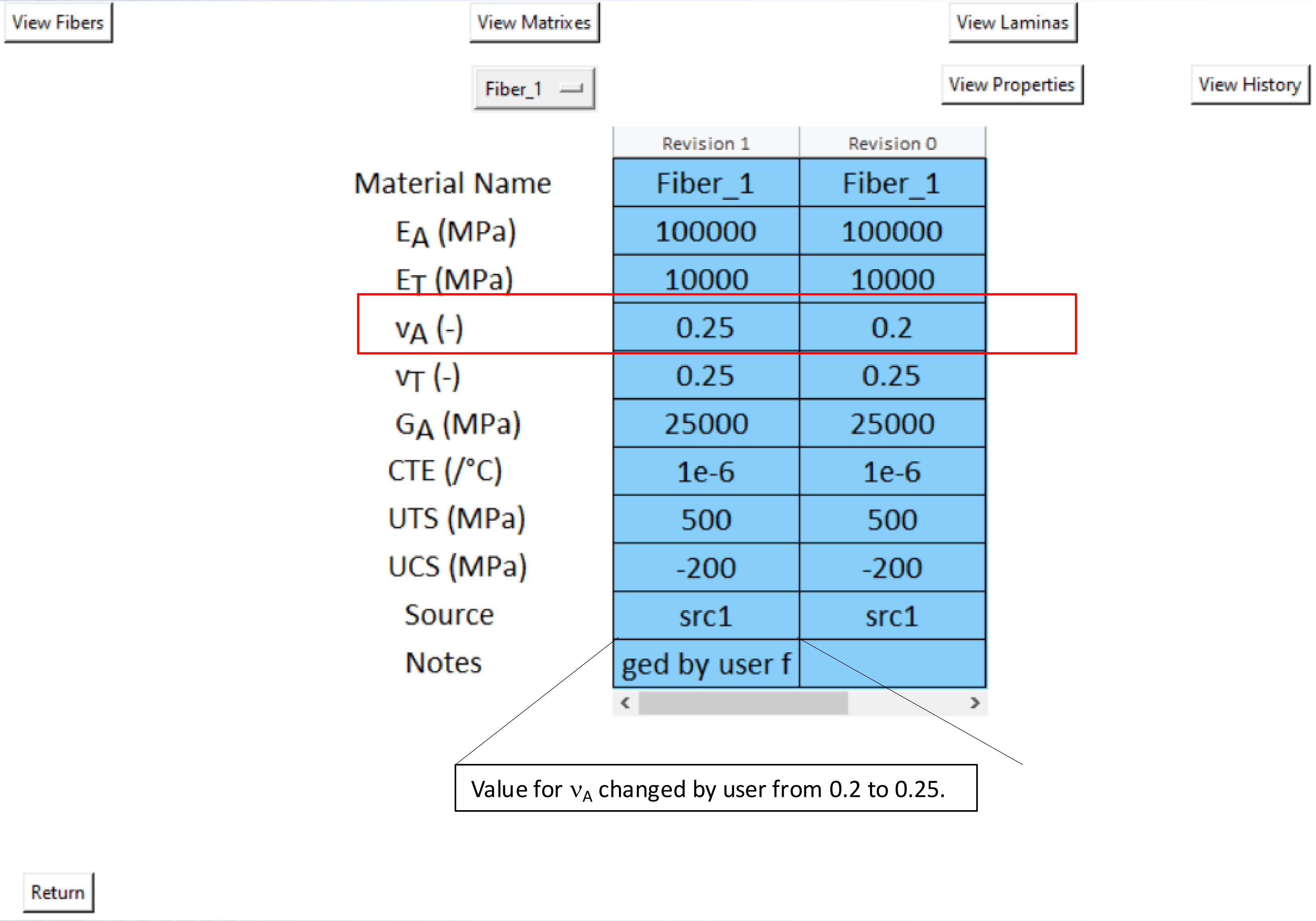
View current properties and **edit** if desired

Save any changes

Automatic Information Propagation

- If Changes are made, information must be propagated upstream
  - Example: Fiber Poisson ν_A changed from 0.2 to 0.25
  - Result:
    - New GUID is generated for the fiber with the new properties (original GUID added to its version history)
      - Revision notes automatically generated
    - All Lamina and Laminates that contain the original fiber GUID are updated:
      - Determine the Revision Number
      - Copy all input/output files with the edited revision number
      - Rerun the analysis: Tool writes a new input deck with the updated properties, run the multiscale analysis tool, reads the output, and stores the information in the database
      - Update the libraries with revision notes

Updating Information at the Current Scale



Updating Information at Higher Scales

View Fibers | View Matrixes | View Laminas | View Laminates

Lamina_1 | View Properties | View History

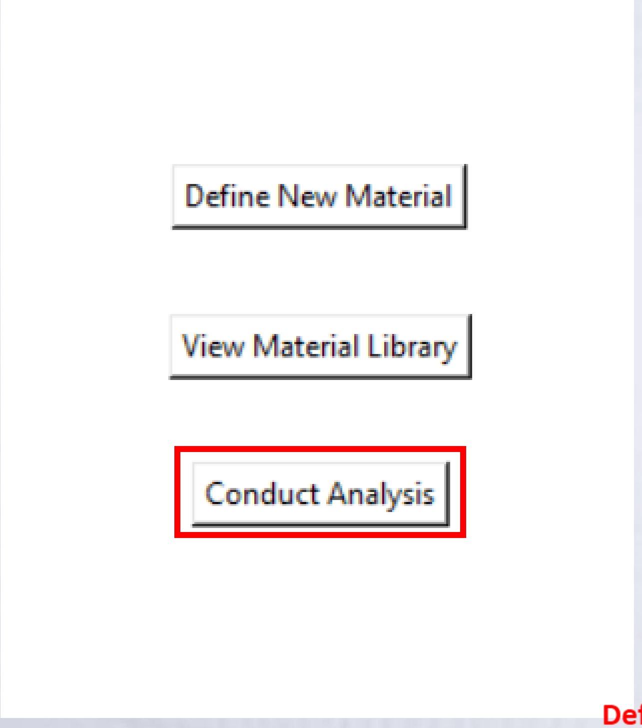
	Revision 1	Revision 0
Material Name	Lamina_1	Lamina_1
Fiber	Fiber_1	Fiber_1
Matrix	Matrix 1	Matrix 1
Cure %	0.7	0.7
VF	0.59	0.59
Thickness (mm)	0.125	0.125
RUC	2 x 2	2 x 2
Input File	Lamina_1.mac	Lamina_1_Rev0.mac
Output File	Lamina_1.out	Lamina_1_Rev0.out
Notes	ged. See Revision No	

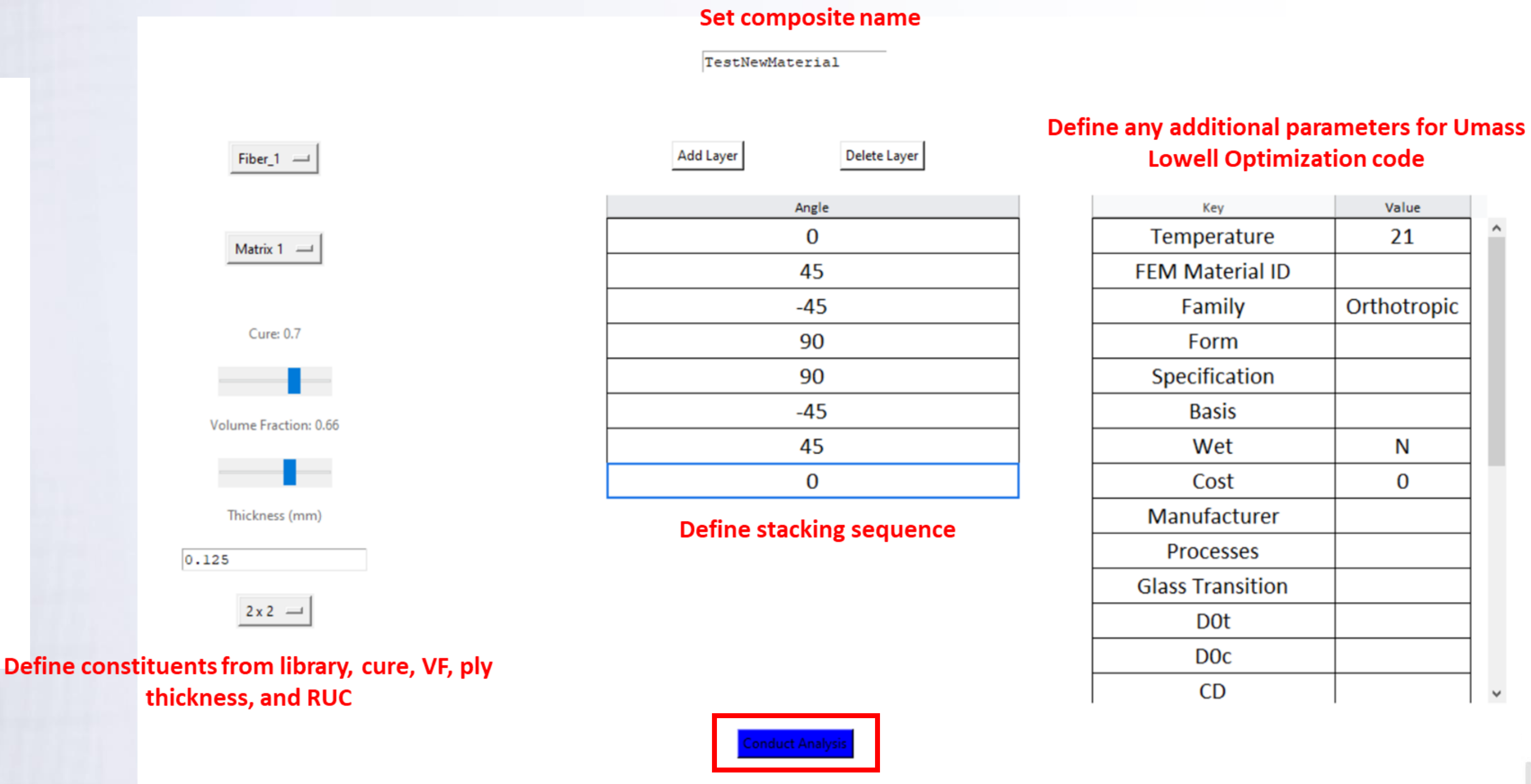
Fiber Properties were changed. See Revision Notes for Fiber_1: Revision 1

Return

Connecting Nanoscale to Macroscale

- Conduct analysis across from nano to macro





Connecting Nanoscale to Macroscale

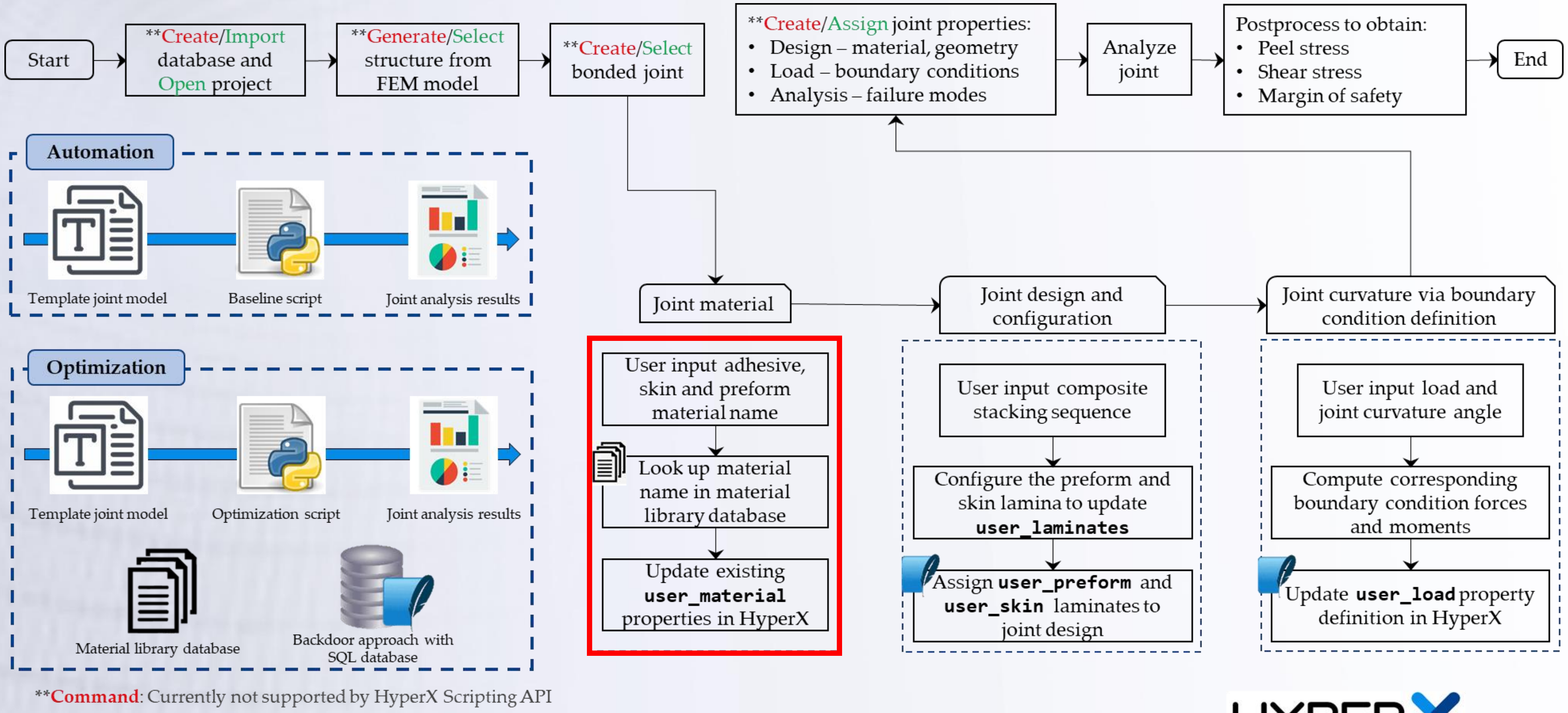
- Conduct analysis button:
  - Write input decks, calls NASMAT, reads the output, stores in the information in the database, and tracks all changes that have been made for that composite
  - Writes the material to the user_material JSON library used by the macroscale optimization code such that HyperX can perform macroscale geometry optimization
  - Not only allows connection across scales/tool sets, but also across organizations (NASA GRC, UMass Lowell)

HyperX Input Format


```
"TechScout2x2": {
    "Name": "TechScout2x2",
    "FEM Material ID": "Null",
    "Family": "Null",
    "Form": "Null",
    "Specification": "Null",
    "Basis": "Null",
    "Thickness": 0.375e-3,
    "Density": "Null",
    "Wet": "Null",
    "Buckling Kd": "Null",
    "Bending Factor": "Null",
    "Fiber Volume": 0.4,
    "Glass Transition": "Null",
    "Cost": "Null",
    "Manufacturer": "Null",
    "Processes": "Null",
    "Temperature": "0",
    "Et1": 112844.906403149,
    "Et2": 6081.74922733345,
    "vt12": 0.3044170096,
    "Ec1": 112844.906403149,
    "Ec2": 6081.74922733345,
    "vc12": 0.3044170096,
    "G12": 2529.64206109671,
    "G13": 2529.64206109671,
    "G23": 1925.69169960474,
```

Structural Level Analysis

- University of Massachusetts Lowell has developed a structural optimization scheme for the Y-Joint assuming some known macroscale (laminate) properties/strengths



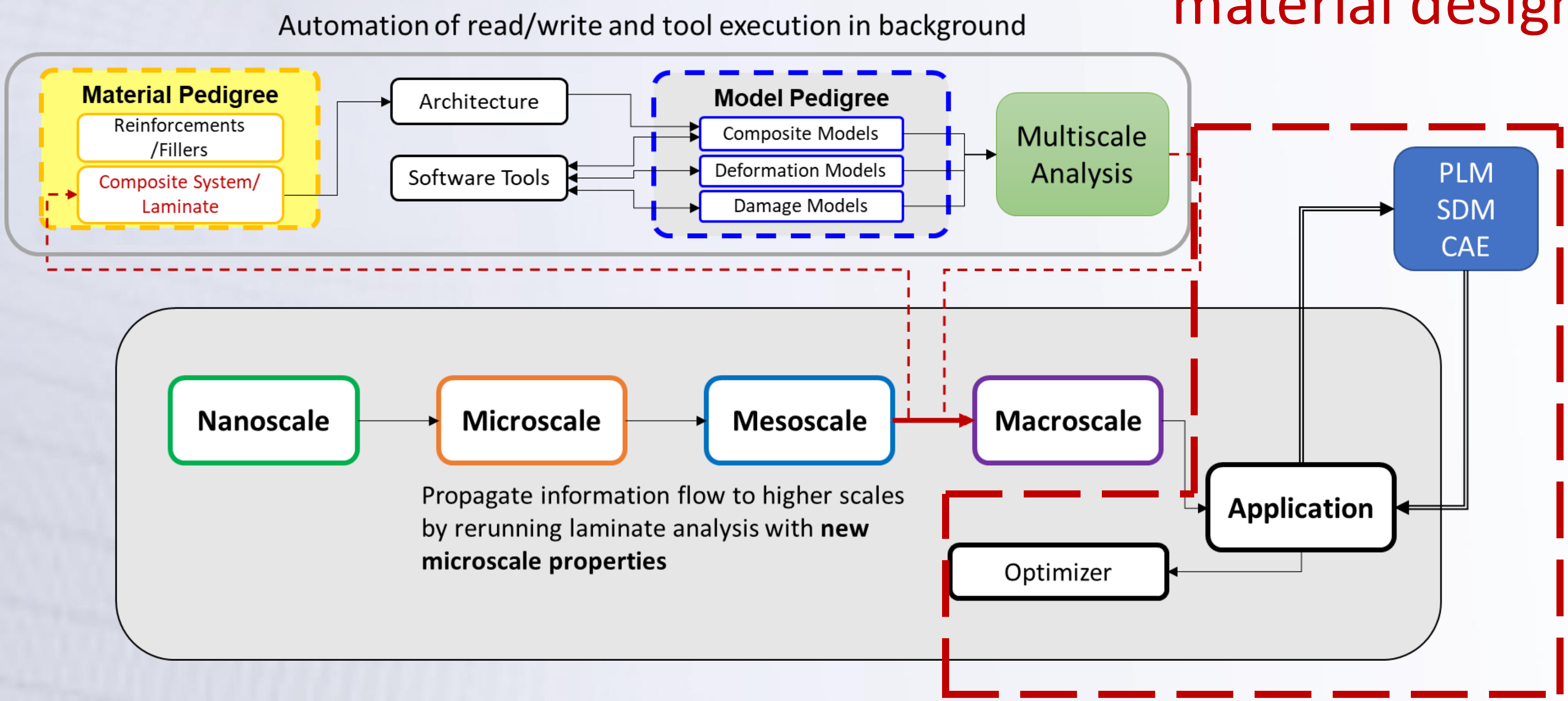
HYPERX

Summary

- Integrated Computation Materials Engineering requires a robust infrastructure to create, store, and maintain digital twins across various length scales
- 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*
- Developed a Python-based framework that allows users to automatically pass information across length scales and track changes that occur during design to significantly reduce human error/time
- Framework can be further integrated into an iteration/optimization for the design of fit-for-purpose materials, and can gather metadata on the changes made during the optimization process for future design

Future Work: AIMAOS 2.0

Connect Macro to Application Table and/or PLM/SDM along with optimization within material design and topology



Thank You for Your Attention

Integrate Don't Duplicate

NASA