National Aeronautics and Space Administration

Transformational Tools and Technologies (T^3) Project

2040 Vision Study: NASA’s T^3 Implementation Activities

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NASA Glenn Research Center

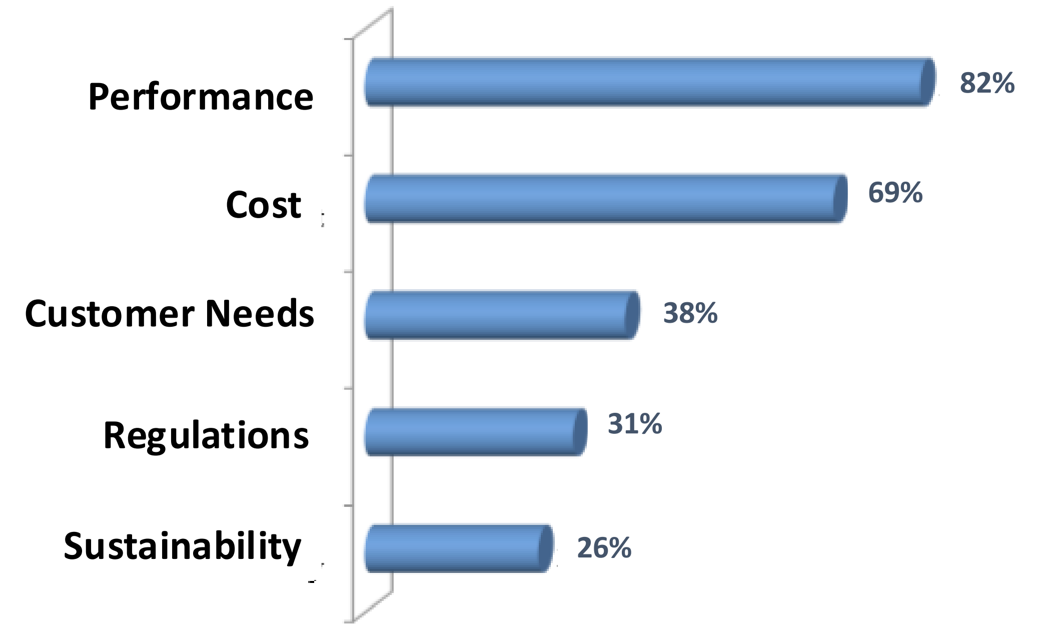
ASSESS Webinar
Feb 19, 2025

Innovative solutions through foundational research and cross-cutting tools

www.nasa.gov

Rapid Material Innovation Essential For Top Performing Organizations

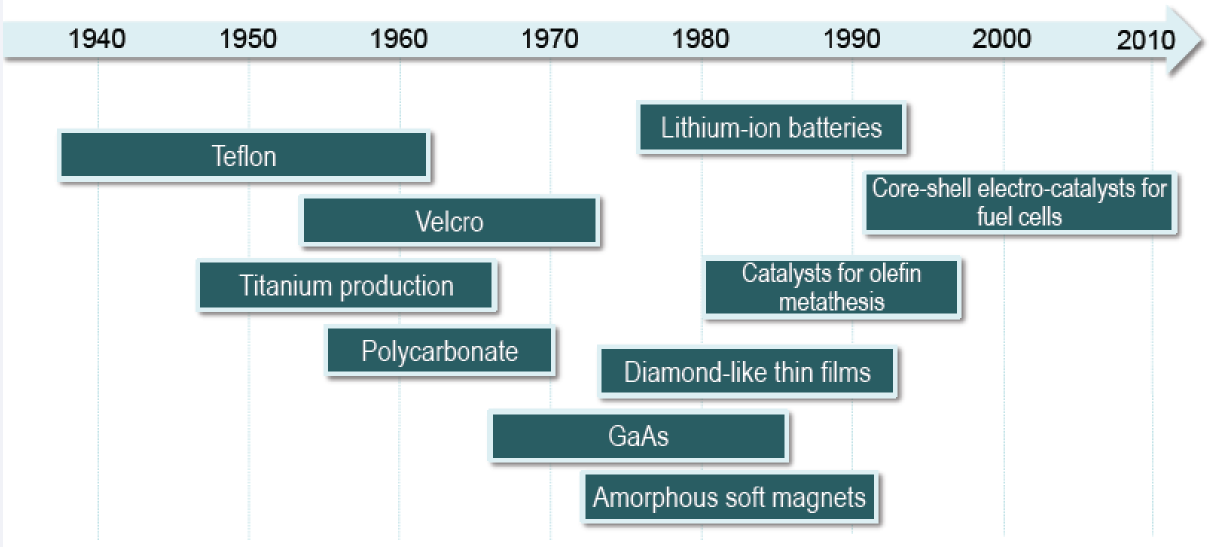
Top Performing Organizations - rated **New Materials** as one of **THE MOST IMPORTANT** factors in meeting their <u>innovation goals</u>.



Top Drivers for New Materials

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

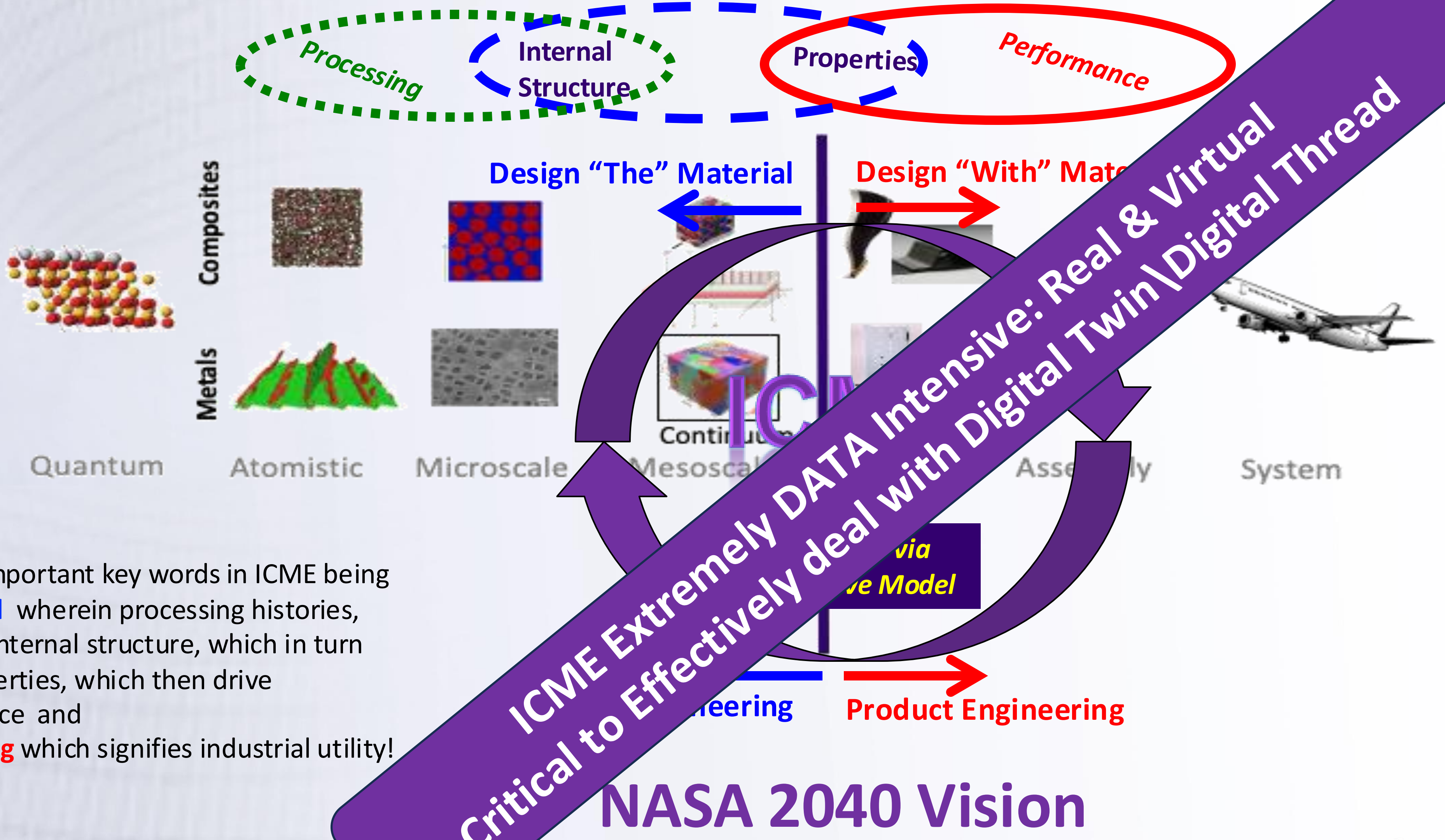


After Gerd Ceder (MIT); materials information from T. W. Eagar and M. King, Technology Review 98 (2), 42 (1995).
Catalysis information from R. Schrock et al. and R. Adzic et al.

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

Recently GRC HT alloy team developed a new ODS alloy – **GRX-810**- in approx. 3 years that betters SOA superalloys by 2.5 UTS, 3.5 Ductility, 2000 creep resistance.

Integrated Computational Materials Engineering (ICME) Enables Innovation & Fit-for-Purpose Materials



ICME Extremely DATA Intensive: Real & Virtual
Critical to Effectively deal with Digital Twin\Digital Thread

NASA 2040 Vision

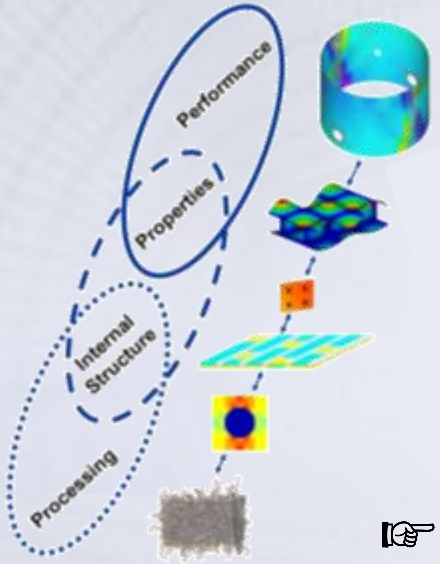
Remember the two important key words in ICME being

1) **Integrated** wherein processing histories, influence internal structure, which in turn drive properties, which then drive performance and

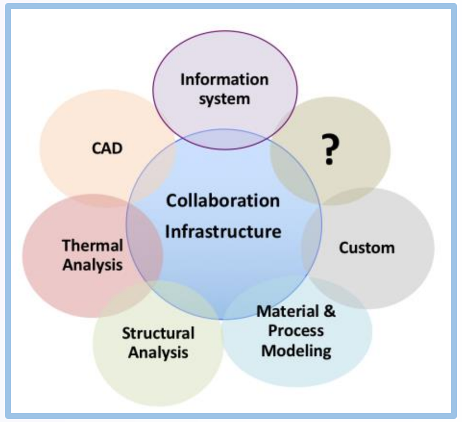
2) **Engineering** which signifies industrial utility!

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

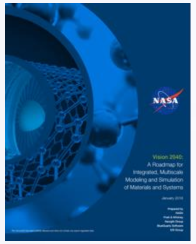


cyber-physical-social ecosystem



NASA CR 2018-219771

https://ntrs.nasa.gov



Nine Identified Key Element Discipline Areas

- ☞ 🟧 1. Models and Methodologies
- ☞ 🟧 2. Multiscale Measurement & Characterization Tools and Methods
- ☞ 🟦 3. Optimization & Optimization Methodologies
- 🟦 4. Decision Making and UQ
- 🟦 5. Verification & Validation
- ☞ 🟥 6. Data, Informatics, & Visualization
- 🟥 7. Workflows & Collaboration Frameworks
- ☞ 🟩 8. Education & Training
- 🟩 9. Computational Infrastructure

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

Major Recommendations: Vision 2040

✓ **#1** Federal agencies and industry both **should fund** sustained R&D programs to address the critical gaps and actions identified in this report.

✓ **#2:** NASA and other relevant federal agencies should form ***an interagency coordinating body*** •••

#3: NASA should engage with government, industry, and academic stakeholders to develop an **agreed-upon interoperability framework** •••

✓ **#4:** NASA should partner with other government agencies and professional societies to ***identify and pursue benchmark materials, systems, and applications*** •••

✓ **#5:** ••• produce, maintain, and disseminate “***gold-standard” datasets*** with which the community can develop, characterize, verify, validate, and certify datasets, models, tools, and other aspects of the 2040 ecosystem.

✓ **#6:** NASA should lead **demonstration projects** that document and publicize the broad benefits •••

✓ **#7:** ••• should increase fundamental research efforts to ***develop, characterize, and validate improved physics-based and data-driven materials models.***.

Major Recommendations: Vision 2040

✓ **#8** NASA should work with industry, academia, and professional societies to ***update education and training programs**** to reflect the skills needed to achieve the 2040 vision •••

*Collaboration Institutes of Education and Training (CIETs)

✓ **#9** NASA, with support from academia and professional societies, should **stimulate widespread cultural change** by encouraging researchers to meaningfully share and work collaboratively on the data and models needed to increase progress toward the 2040 vision

✓ **#10** NASA and other federal agencies should support the growth of small businesses working in ICME to strengthen U.S. manufacturing competitiveness and establish U.S. leadership in this emerging field.

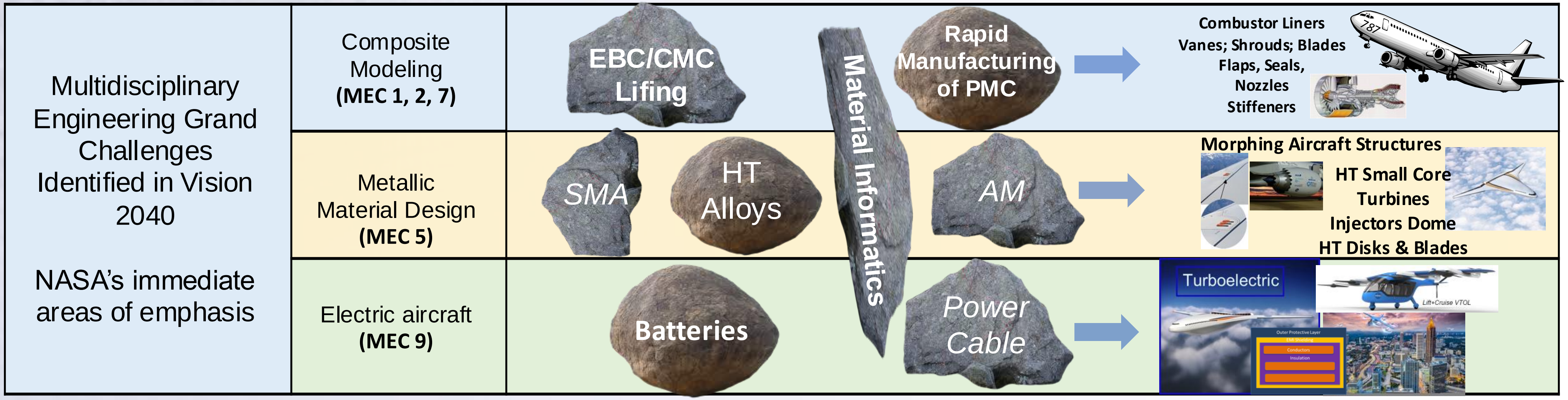
#11 NASA should engage with academia and industry stakeholders to **regularly update** this study and/or conduct follow-up studies •••

Suggested Nine Multidisciplinary Engineering Challenges (MECs)

1. **Mitigation of high-temperature environmental damage, oxidation, and hot corrosion of high-temperature turbine engine components**
2. Development and optimization of **polymeric matrix composites** for aerospace applications
3. Design and lifing of aerospace components with 20 percent weight reduction using location-specific design methodologies, including tailoring of component properties using chemistry or microstructural modifications
4. Optimization of structures and materials for mitigation of thermomechanical fatigue
5. **Design and development of unique materials such as shape memory alloys and high-entropy alloys in aero structures and components**
6. Automated re-adaptation and updating of computer software suites to infrastructure changes (moving away from manual recoding of software to take advantage of new computer architectures such as GPUs or CPU+GPU)
7. Development and optimization of **ceramic matrix composites** for aeronautic applications
8. Application of microstructure definition tools and methods to enable model-based material and probabilistic component definitions
9. **Electrification of aircraft propulsion**

Transformational Tools and Technology (T^3)'s M&S Portfolio Is Tightly Aligned with 2040 Vision

Technologies **Applications**



Multidisciplinary Engineering Grand Challenges Identified in Vision 2040

NASA's immediate areas of emphasis

Composite Modeling **(MEC 1, 2, 7)**

EBC/CMC Lifing

Rapid Manufacturing of PMC

Combustor Liners
Vanes; Shrouds; Blades
Flaps, Seals,
Nozzles
Stiffeners

Metallic Material Design **(MEC 5)**

SMA

HT Alloys

AM

Morphing Aircraft Structures
HT Small Core Turbines
Injectors Dome
HT Disks & Blades

Electric aircraft **(MEC 9)**

Batteries

Power Cable

Turboelectric

Material Informatics

*Development/Validation of toolset for physics-based multiscale life prediction modeling of high temperature materials systems (e.g., CMC/EBC) that **includes environmental effects***

*Development of tools needed to establish a path to **certification of bonded structures** having a reduced reliance on load-path redundancy*

Develop multifunctional materials/toolsets and adaptive structures/concepts for lightweight actuation based on shape memory alloys

Develop high temperature disk alloys and dispersion strengthened alloys (that can be produced through additive manufacturing (AM)) using SOA Material Designer

Develop foundation technologies for next-generation Qualification & Certification (Q&C) of AM to enable widespread use in safety critical applications

Develop toolset (Multiphysics simulator; Interface Designer; Electrolyte Designer) to accelerate the development of safe, high energy, batteries.

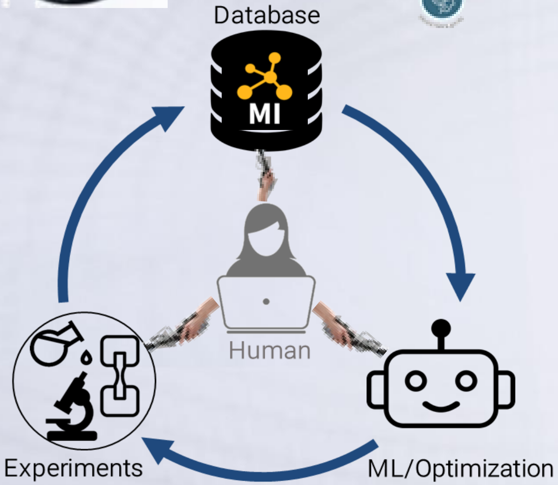
Develop lightweight multifunctional high voltages & high frequency power cables

Develop/Apply transformative tools and principles of informatics to materials science and engineering to improve both speed and accuracy of understanding, use, selection, development, and discovery of materials

T^3 Objectives For Fit-for-Purpose Materials And Structures

TRUST-AM

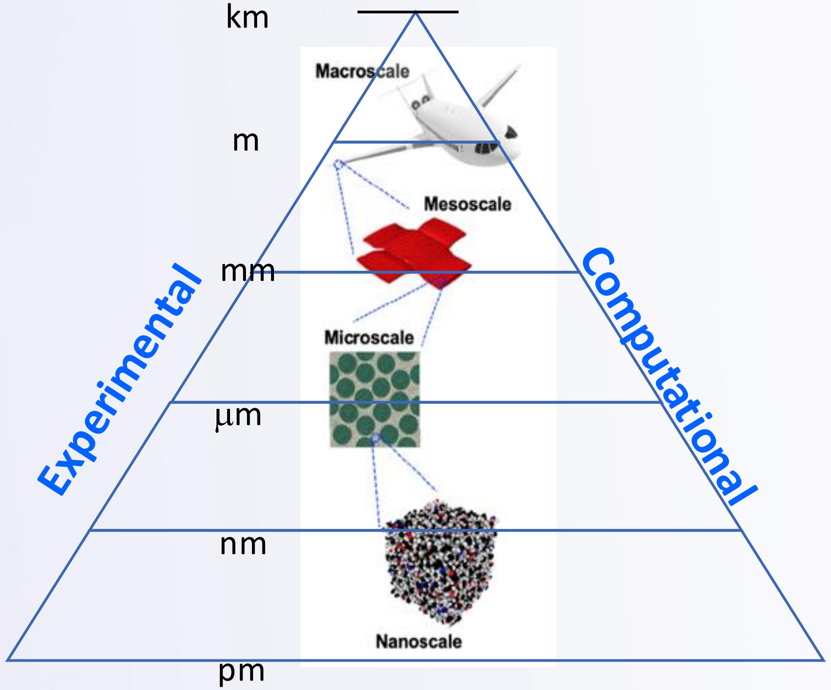
SM^{2}ART



J.A.R.I.M.I.S.

Just A Rather Intelligent Material Interrogation System

All Rocks Possess



Materials Informatics

Material Designer

1) Data Driven Screening
2) High Fidelity Modeling
3) Design of New Materials
4) Multiscale coupling to composites, structures, devices, chemical kinetics models, etc.

Fit-for-purpose materials

- Performance
- Cost
- Sustainability/Maintainability
- Security

Tightly Integrated Modeling Throughout Portfolio To Guide And Identify Sensitivities To Minimize Resources

2040 Vision: NRA Awards Enhances M&S Portfolio Significantly

SwimLane	Subproject	PI Name	Title	Submitting Org	COTR
Electric	FEAP	McDowell, Matthew	Coupling Models and Operando Experiments to Describe Evolution and Degradation of Solid-State Batteries	Georgia Tech Research Corporation	R. Viggiano
	FEAP	Qi, Yue	Predicting Charge Transfer Reactions and Morphology Evolution at Complex Electrode/Electrolyte Interfaces Starting from First-Principles	Brown University	John Lawson
	FEAP	Shao-Horn, Yang	Combined Experimental and First Principles Tool Development of Interface Analysis in An All Solid-State Battery	Massachusetts Institut[illegible]hnology	John Lawson
	FEAP	Wierzbicki, Tomasz	Physics-guided Machine Learning Model of Interfacial Failure Mechanisms of Solid-State Energy Storage Systems Based on a Diagnostic Databank with Advanced Experimenta[illegible] Techniques	[illegible]ology	John Lawson
Composite	ED	Stapleton, Scott	Multi-Scale models based on Machine Learning and a Fi[illegible]	[illegible]assachusetts, Lowell	B. A. Bednarcyk
	ED	Maiaru, Marianna	ICME Optimization of Advanced Composite Compo[illegible]	[illegible]ersity Of Massachusetts, Lowell	S.M. Arnold
	RLCC	Makeev, Andrew	Integrated Structural Methods and Prognos[illegible] Manufacturing Variability [illegible]	University Of Texas, Arlington	James Ratcliffe
	RLCC	Czabaj, Michael	Novel experimenta[illegible]cation and certification of bond[illegible] and manufacturing variability	University of Utah, Salt Lake City	Andrew Bergan
Metallic	ED	Kim, Hyuns[illegible]	[illegible]Down Optimization Crossing Continuum to [illegible] for Nonlinear High-Temperature Applications	University Of California, San Diego	S. M. Arnold
	ED	[illegible]	[illegible]ed, Data-Driven ICME Framework for Shape Memory Materials	Georgia Tech Research Corporation	O. Benafan
	RLCC	[illegible]	[illegible]ntelligence Enabled Descriptions of Fatigue Behavior in Additively Manufactured Titanium Alloys for Aerospace	Johns Hopkins University	Ed Glaessgen
	RLCC	[illegible] Somnath	An Integrated Multi-Scale Modeling and Simulation Platform with Process Design for Improving Performance and Life of Additively Manufactured Components	Johns Hopkins University	Edward Glaessgen
	RLCC	To, Albert	A multiscale process-microstructure simulation tool for predicting defects and microstructure evolution by leveraging GPU acceleration and machine learning	University Of Pittsburgh	Timothy Smith
	RLCC/ED	Wessman, Andrew	Predicting and Classifying Microstructural and Process Defects in Nickel-Based Superalloys Produced by Laser Powder Bed Fusion Using Process Monitoring and Machine Learning	University of Arizona	Timothy Smith

Most nearing completion of Third Year
Many will have No Cost Extensions

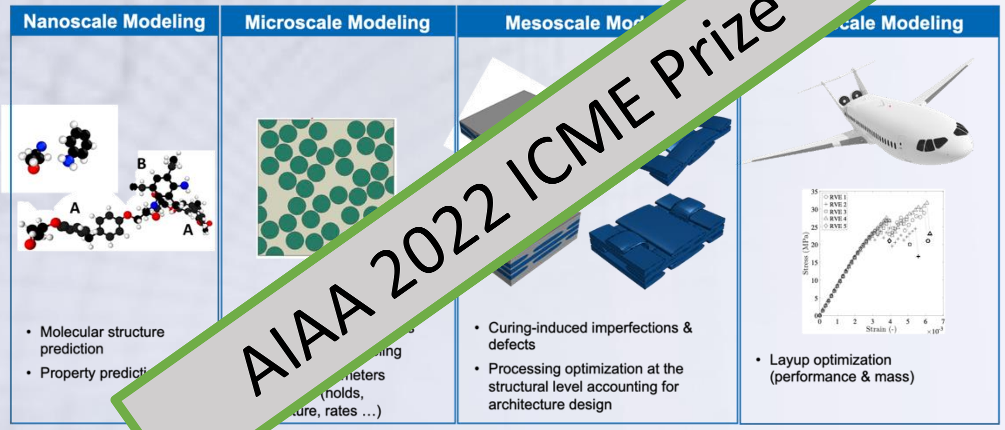
- **14 Awards approx. $3.5M/year**
- Balance between experimental and computational work
- 43% proposals have significant ML/AI activities

Integration of Multiscale Modeling within Three T^3 NRAs

ICME Optimization of Advanced Composite Co s of the Aurora D8 Aircraft

PI: Marianna Maiaru, U. Mass. Lowell; Co-PI: Greg O Tech

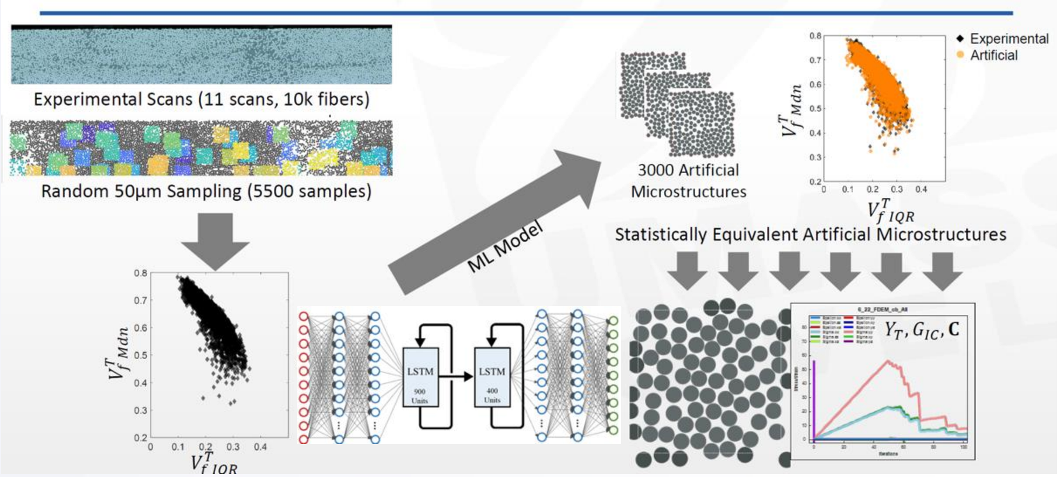
AIAA 2022 ICME Prize Winner



Integration with **AIMAOS** Digital Thread management

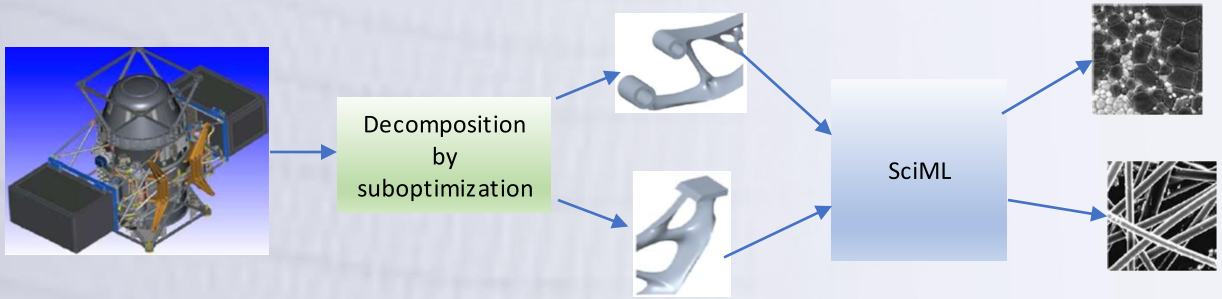
Multi-Scale Models based on Machine Learning and a Fiber Network Model

PI: Scott E. Stapleton, Co-PI: Farhad Pourkamali Anaraki, U. Mass. Lowell



Ultra Efficient Multiscale Top-Down Optimization Crossing Continuum to Micromechanics for Nonlinear High-Temperature Applications

PI: Alicia Kim, University of California, San Diego
Co PI: Karen Wilcox, University of Texas, Austin



Decomposition by suboptimization

SciML

- T^3 multiscale modeling tools are *essential* to success of these NRAs
- Innovative application of tools
  - ICME
    - 17% mfg. savings/\$1204 fuel savings/aircraft/ year
    - 30% weight reduction for the part
  - Topology + morphology optimization
  - Machine learning

Synergistic SBIR Activities

Vision 2040 Focused Activities

MI - ED

SBIR 2023 Phase I (Completed)

Contract 80NSSC23PB480
Title: SBIR Phase I: Materials Modeling Hub: Interoperable and Collaborative Multi-Scale Modeling Ecosystem for Data Analysis, Visualization, and Management
Materials Data Management, Inc.

HT Alloy - ED

SBIR 2019 Phase I; Phase II and Phase II E funded (Completed)

Contract #: 80NSSC19C0409; Additive Manufacturing Innovations; Title: A Multiscale Model for Material Systems with Hierarchical Microstructure using Generalized Method of Cells (GMC)

Crystal Plasticity – FEAMAC/GMC – Experimental Characterization/Validation – Additive Manufacturing

EBC/CMC- ED

SBIR 2017 Phase I , Phase II, and Phase IIE (Completed)

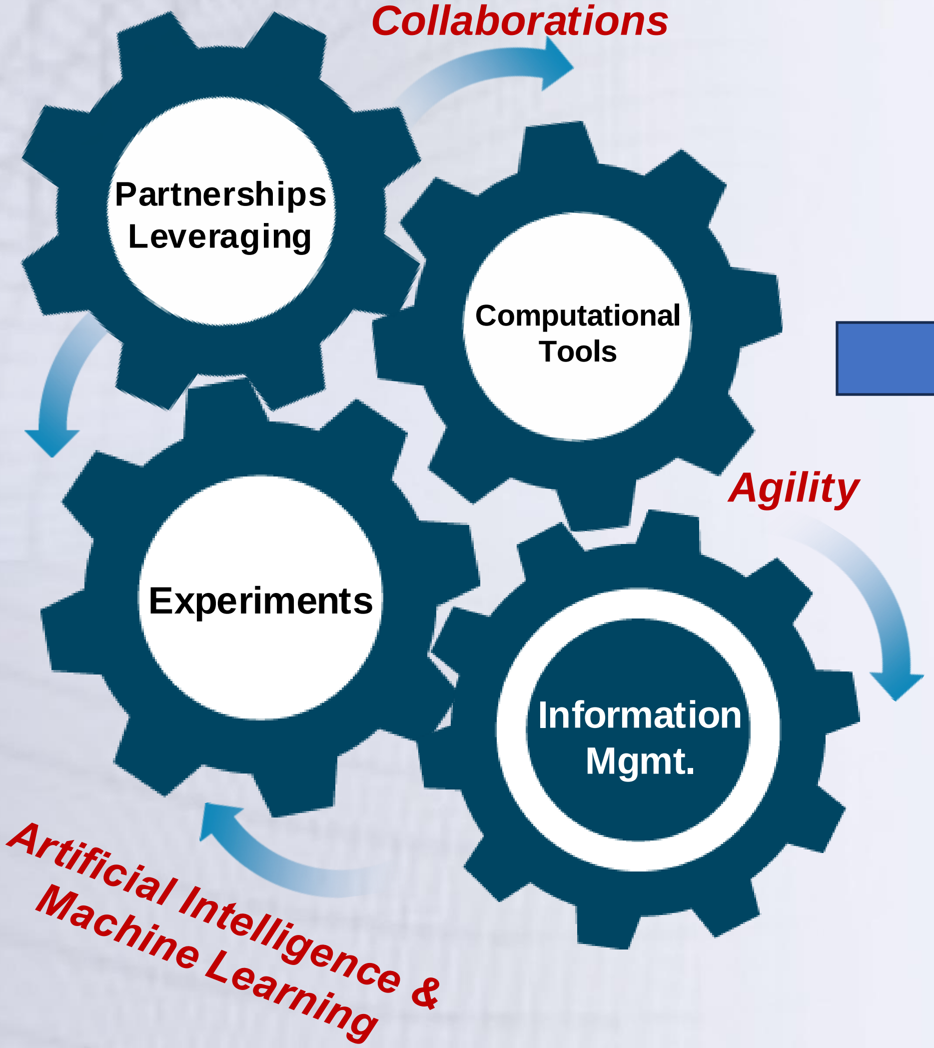
Contract #: 80NSSC18C0053 CFDRC Title: Integrated Fluid and Materials Modeling of Environmental Barrier Coatings

SBIR 2019 Phase I; Phase II (Completed)

Contract #: 80NSSC19C0263; N&R Engineering; Title: Probabilistic/Reliability Software Tool for Ceramic Matrix Composite/Environmental Barrier Coating Interface Modeling

M&S Operates to Maximize Outcomes

Each Focus Area Tightly Integrates Modeling (Physics-based and Data Driven), Experiments, Information Management Throughout Portfolio To Guide And Identify Sensitivities To Optimize Resources and Preserve Knowledge



Collaborations

Partnerships Leveraging

Computational Tools

Agility

Experiments

Information Mgmt.

Artificial Intelligence & Machine Learning

FY24 Accomplishments

- 5 Commercial & 23 Research Licenses
- 5 Patents
- 38 Journal papers & 74 Conference Presentations
- 21 invited Lectures with 4 being Keynotes
- 18 on-going SAAs with 3 pending
- 16 Awards
- 12 Interns, 1 Post Doc, 1 Pathway

FY21 – FY24 Leveraging and Partnerships

Over 100 partnerships (Industry, Academia, OGAs)

Leveraged over $7 Million non-T^3 funds ($2.4M in FY24) such as SBIRs, EPSCoRs, and STRGs

SBIR - Small Business Innovation Research
EPSCoR - Established Program to Stimulate Competitive Research
STRG - Space Technology Research Grants

Examples of TTT Successes Details

T^3 M&S Products: Models & Methodologies (KE1)

Physics Based:

- **SMA-GVIPS** - Advanced constitutive model for shape memory alloys applied to design and analyze spring tires for Mars Sample Return (SMD)
- **GVIPS** – Multimechanism Viscoelastoplastic constitutive model with stiffness and strength degradation (Abaqus UMAT with implicit integrator)
- ☞ **NASMAT** – NASA Multiscale Analysis Tool ; being applied to analyze
    - space-relevant 3D woven heatshields and thermoplastic composite joints
    - deformation and lifing of EBC/CMC specimens and Vanes
- **PRX-VCCT (**Progressive Release eXplicit Virtual Crack Closure Technique)
    - Recently implemented into **commercial Abaqus FEA code** enables efficient fracture analysis at the component level
- Phenomenological Durability Model Established for EBC Systems subjected to Steam Oxidation (NASA TM -2024-0000936)
- Numerous first principle & MD simulations for understanding mechanisms in Metals, SMAs, Batteries, and Cables

Data Driven Models:

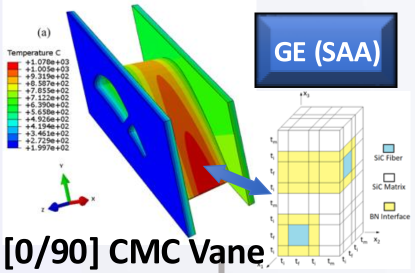
- ☞ **MicroNet** – Microscopy aware AI that enables automatic quantification of microstructure – critical for materials design
- Composite ply surrogate model used for performing accurate and efficient multiscale modeling of composites
- ML Fatigue Life Estimator

Multiscale Modeling Enables Engineered Materials

High-Performance Compute Enabled

- Tasks-based partitioned Parallelization
  - Enables Hierarchical Simultaneous Computation
- Integration with preCICE enables easy interoperability with 3rd party software
  - Macro/Micro problems operate independently

Industrialized Sized Problems



GE (SAA)

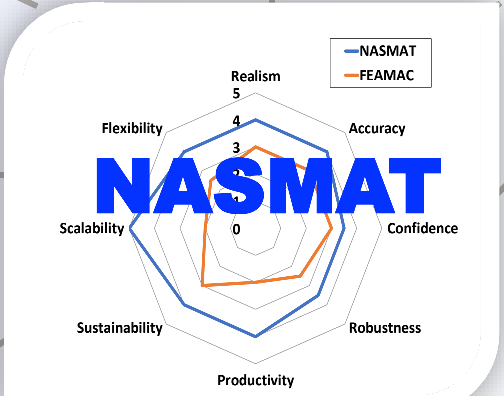
[0/90] CMC Vane

Machine Learning Informed Enhances Speed 100x

Collaboration
WMU (Gustafson)
NRAs (Kim, Stapleton)
SBIR II (Achuthan)

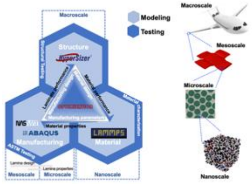
Educating Next Generation

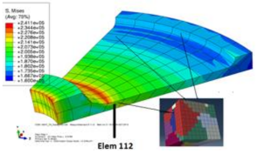
10+ Interns/Student Fellows
4 Faculty Fellows
2 Post-Docs
Numerous PhD committees
Multiple College Courses



Cross-cutting Capabilities Stimulates Collaboration

- UMass NRA team wins **2022 AIAA ICME Prize Competition**
- WMU – Study microstructure impact on AM
- PSU – Understanding Concrete Microstructure in Micrograviity
- SBIR II – Tailors microstructure of Turbine Disk for performance



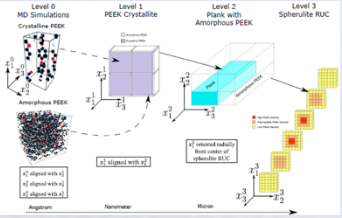


Signed SUA: U Tenn.-Knoxville; UMass Lowell; U Texas – Austin; Utah State; Boise State; Penn State; Army ERDC; Boise St. and U. South Carolina through ULI, AFRL; Michigan Tech; Western Michigan

Plug-Play Capable

Collaborations

- GE (SAA)
- STMD, ESM
- TDEA, ONR (Thermoplastics)

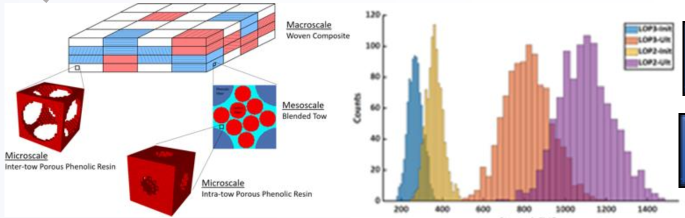


NASA Multiscale Analysis Tool

Thermoelastic Progressive Damage

- Metals
- Laminated CMCs
- 3D Woven
  - PMC, Phenolic, Hybrid tows
- Thermoplastics
- Porous Materials

UQ Integrated to Mitigate Risk



STMD (ESM)

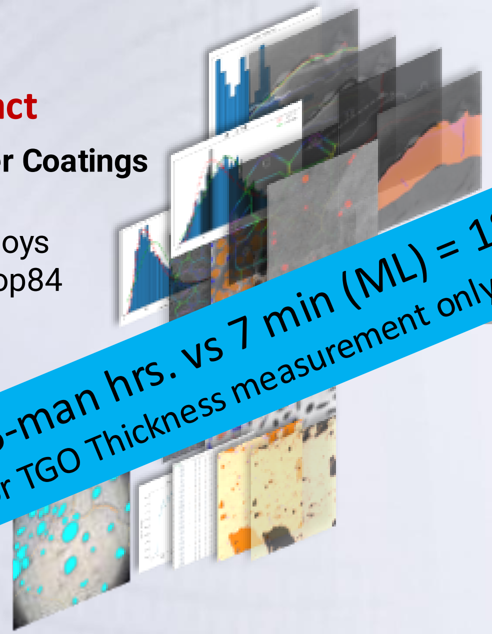
SBIR-II (N&R)

Sandia: Dakota

ML/AI Transforming The Way We Do Materials R&D

MicroNet Went "Live" in FY22

Automatic Quantification of Microstructural Feature Distributions



ARMD Impact

Environmental Barrier Coatings

HT Metals

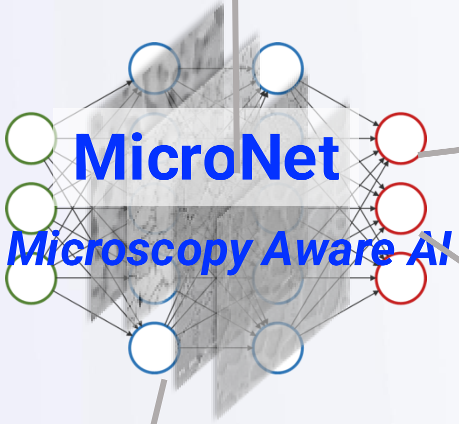
ODS; Ni-Superalloys

Inconel 718; GRCop84

Icing

Time Savings: 22.5-man hrs. vs 7 min (ML) = 180x

Man hour is for TGO Thickness measurement only



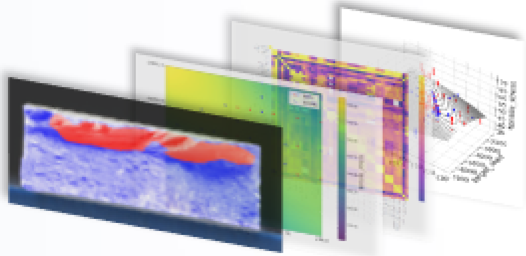
MicroNet

Microscopy Aware AI

Opensource Code

- 10,000 downloads in first 10 weeks
- https://github.com/nasa/pretrained-microscopy-models
- NTR 1613148106
- NTR 1638373122

STMD Impact



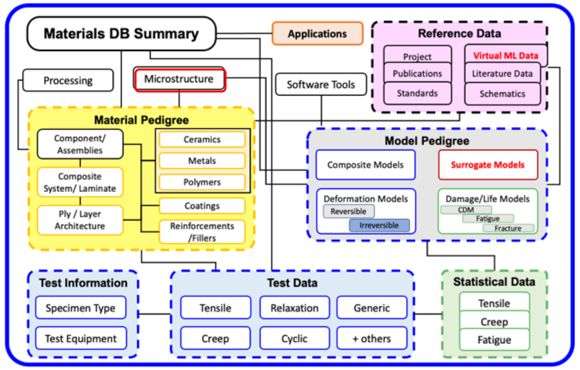
SLS Core Stage Welds

- Assisted NESC Investigation
- Quantified: defect features
- Found root cause of anomalous defects
- Recommended new process window

External Customers

BOEING	**NESC investigation of SLS welds**
GE	**HyTEC Combustor Liner Task: EBC**
ocas	**Belgian steel research organization**
ASM INTERNATIONAL	**AI/ML Microstructure Toolkit** • SAA with ASM International • Automatically featurize ANY microstructure • Used to establish PSPP relationships
	MDMI Simplify

Established ML Schema for ANSYS GRANTA MI



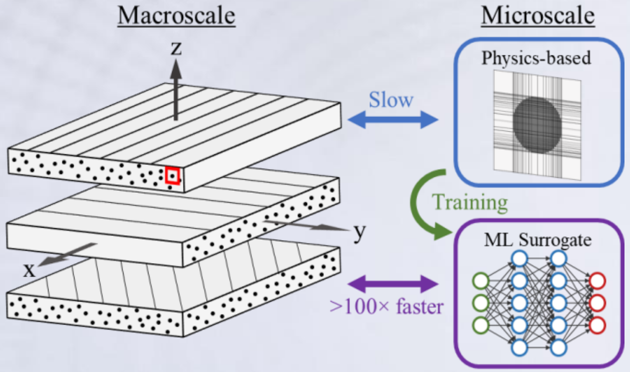
MicroNet's Output Enables Establishment of **Essential** Microstructure/Property Relationships

POC: Josh Stuckner (GRC)

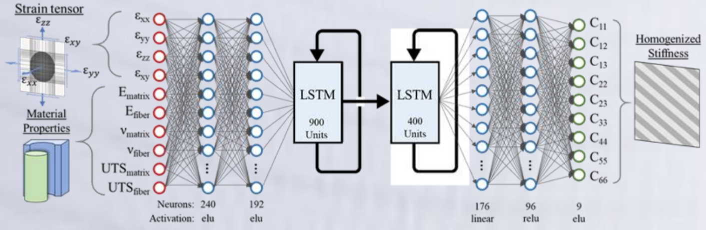
ML Surrogate Models Enables Ultra Efficient Simulations

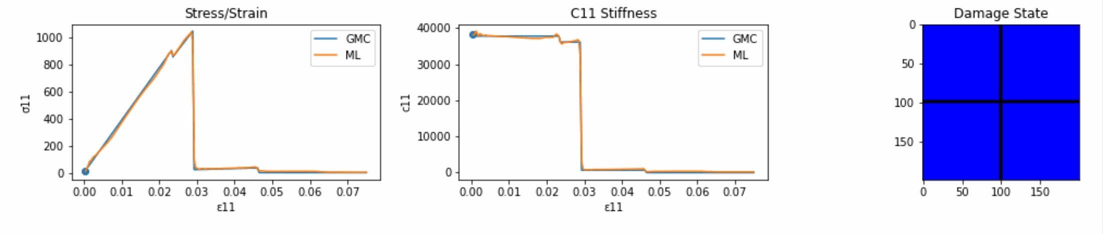
Multiscale model with embedded ML surrogate

- Calculates composite response **145 times faster** (with **98%** accuracy) compared to original physics-based model

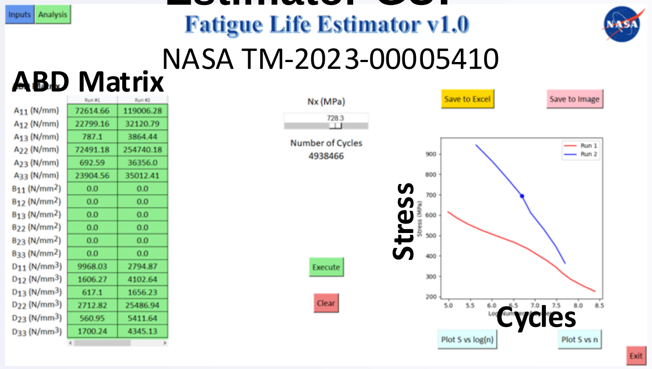


Schematic of LSTM surrogate model





ML Fatigue Life PMC Laminate Estimator GUI



Inputs Analysis

Fatigue Life Estimator v1.0

NASA TM-2023-00005410

ABD Matrix

	Run #1	Run #2
A_{11} (N/mm)	72614.66	119006.28
A_{12} (N/mm)	22799.16	32120.79
A_{13} (N/mm)	787.1	3864.44
A_{22} (N/mm)	72491.18	254740.18
A_{23} (N/mm)	692.59	36356.0
A_{33} (N/mm)	23904.56	35012.41
B_{11} (N/mm^2)	0.0	0.0
B_{12} (N/mm^2)	0.0	0.0
B_{13} (N/mm^2)	0.0	0.0
B_{22} (N/mm^2)	0.0	0.0
B_{23} (N/mm^2)	0.0	0.0
B_{33} (N/mm^2)	0.0	0.0
D_{11} (N/mm^3)	9968.03	2794.87
D_{12} (N/mm^3)	1606.27	4102.64
D_{13} (N/mm^3)	617.1	1656.23
D_{22} (N/mm^3)	2712.82	25486.94
D_{23} (N/mm^3)	560.95	5411.64
D_{33} (N/mm^3)	1700.24	4345.13

Nx (MPa)

728.3

Number of Cycles
4938466

Save to Excel Save to Image Execute Clear Plot S vs log(n) Plot S vs n Exit

Ultimate democratization toolset – micromechanics-based fatigue life analysis with **no training needed**

- 19 Input features (constituent prop, vol fraction, ply angles)
- Output ABD and S-N curve
- 15,000 hrs of training computations on single CPU
- ML ***very good*** estimate of the actual lives

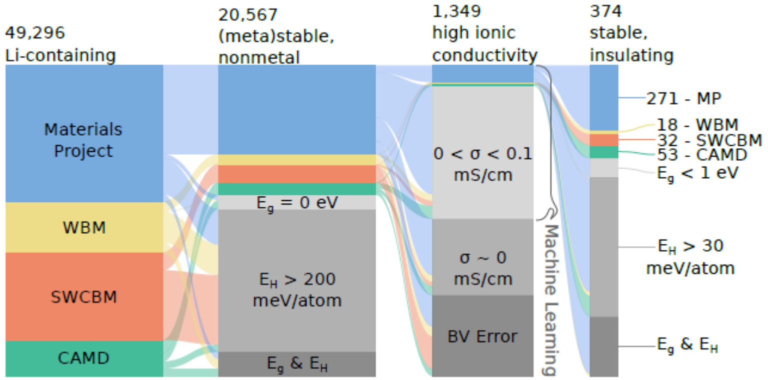
Probability prediction is within 2x = 0.92

Probability prediction is within 3x = 0.98

1,818x faster than PB Fatigue Life Estimation
3 secs vs 1.5 hrs on avg.

High throughput Screening of ~50K Battery Electrolyte Candidates

- *Data extracted from 4 Databases (blue, yellow, orange, green)*
- *Primary properties targeted*
  - ➢ *Thermodynamic stability*
  - ➢ *Electricity conductivity*
  - ➢ *Ionic conductivity*
- *Grey boxes indicate those rejected*



Identified 374 candidates, 35 suitable anode coating materials
~150,000 faster than high fidelity analysis
1 week vs. 3000 years (impossible)

T^3 M&S Products: New Materials (KE1,KE2,KE3)

Select examples of M&S innovation in FY24

Advanced (NiTiHfZr) lower cost Shape Memory Alloy (SMA) ingot under scaleup

- Scaleup has progressed with ~90lb heat produced via Plasma Arc Melted (PAM) under a cost-sharing agreement with external partners

Computationally identified new ultra-high temperature SMA (~500^{o}C)

- Stable actuation was achieved in binary RuNb alloys using a novel crystallographic transformation
- Established both computationally and experimentally. https://doi.org/10.1016/j.actamat.2024.120140

Actuators for **Quiet High Lift** (QHL) vortex generators produced and installed in VGs in conjunction with **FAA Continuous Lower Energy, Emissions and Noise (CLEEN) III Program**

☞ **GRX-810 Performance Improves 10x over previous advancement with Scale up**

Four co-exclusive commercial licensees:1) Carpenter, 2) Praxair / Linde, 3) Elementum3D, 4) PAC
23 Research licenses granted

☞ **Demonstrated superior high-temperature performance for a NASA-developed Disk Superalloy (compared to SOA)**

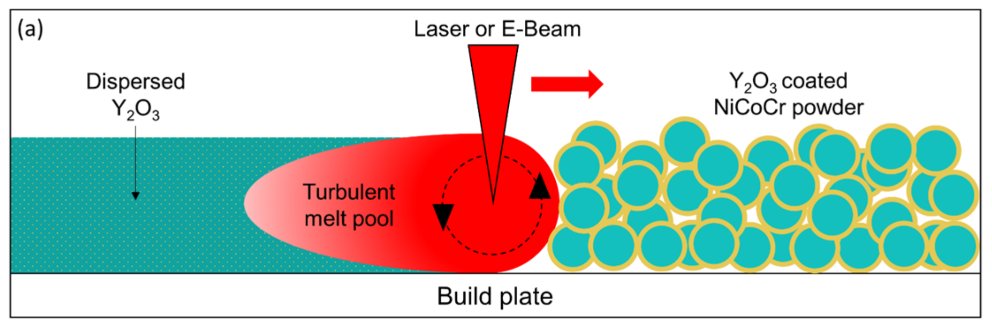
- TSNA-1 superalloy exhibited superior creep strength and fantastic crack growth rates over conventional superalloys

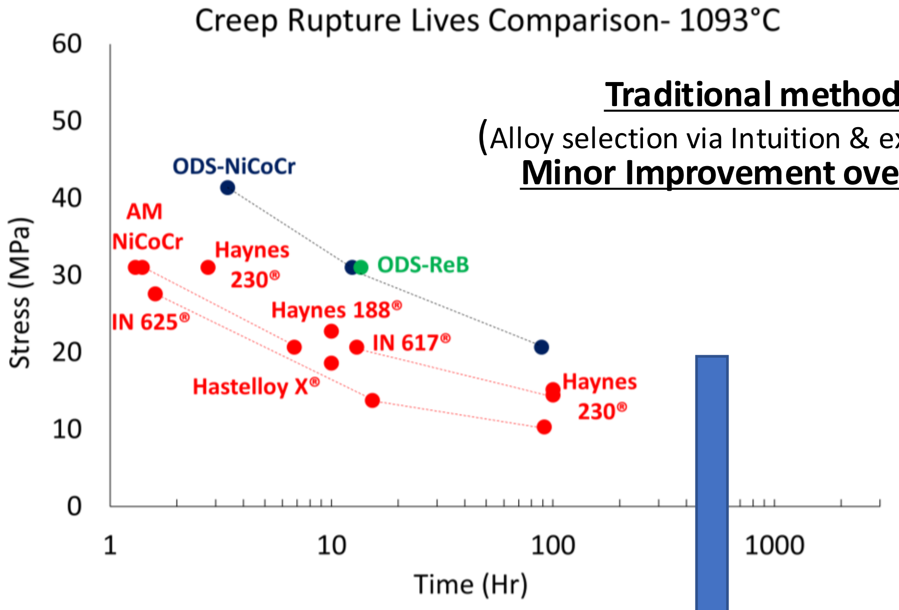
Machine learning enabled rapid discovery of candidate *non-flammable liquid electrolytes*

- 100s of safe liquid electrolyte candidates identified after screening ~1 billion molecules

ICME Improves Performance, Reduces Development Time/Cost

NASA Developed Advanced Dispersion Coating Technique



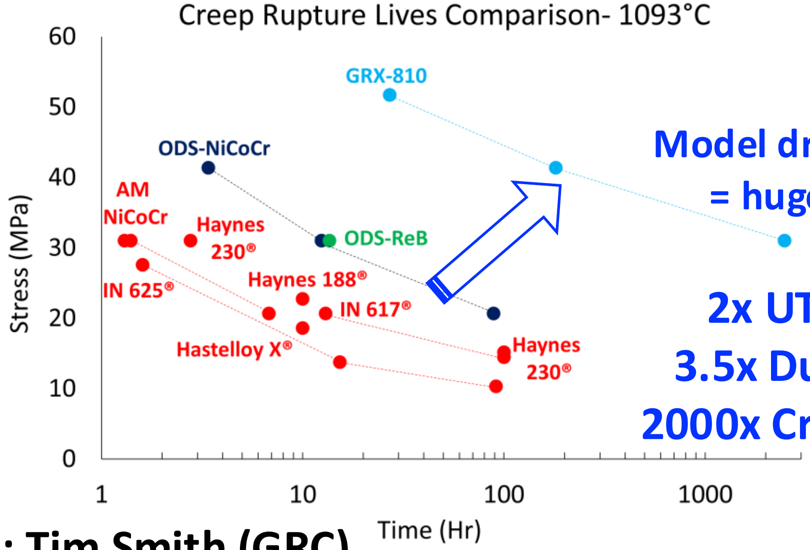


Traditional method

(Alloy selection via Intuition & experience)

Minor Improvement over SOA

Model Driven Design Resulted in Significant Performance Improvements



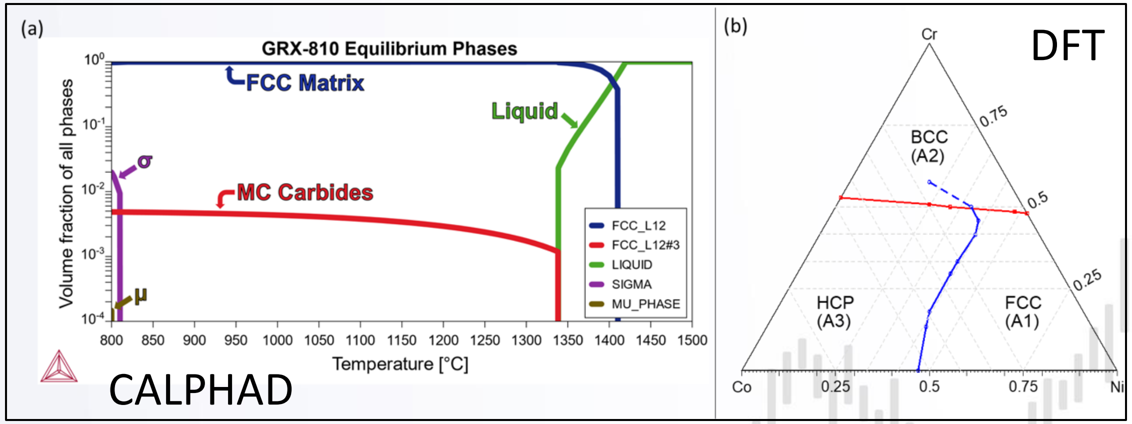
Model driven design = huge impact

2x UTS

3.5x Ductility

2000x Creep Rupture Life

Used Thermodynamic Modeling to Discover Optimal Alloy Chemistry



POC: Tim Smith (GRC)

Smith et al., A 3D printable alloy designed for extreme environments, Nature, Vol 617, 2023

Disk Superalloy Development

Forged TSNA-1 Disk alloy is providing significant improvements in HT creep & Dwell Fatigue

Challenge

Conventional disk alloys cannot operate in temperatures above 700°C – with creep being a rate limiting property.

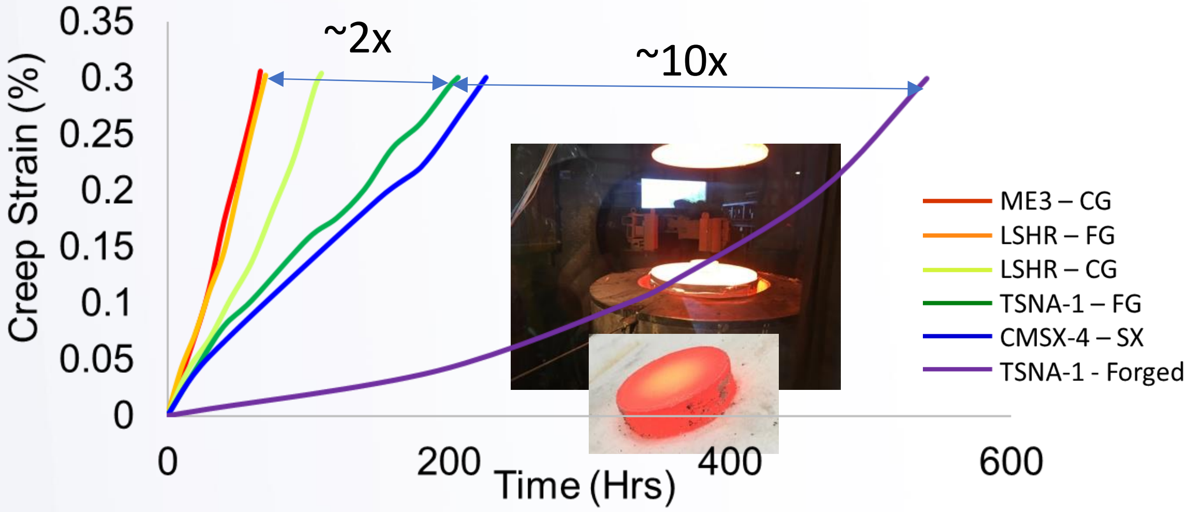
Actions

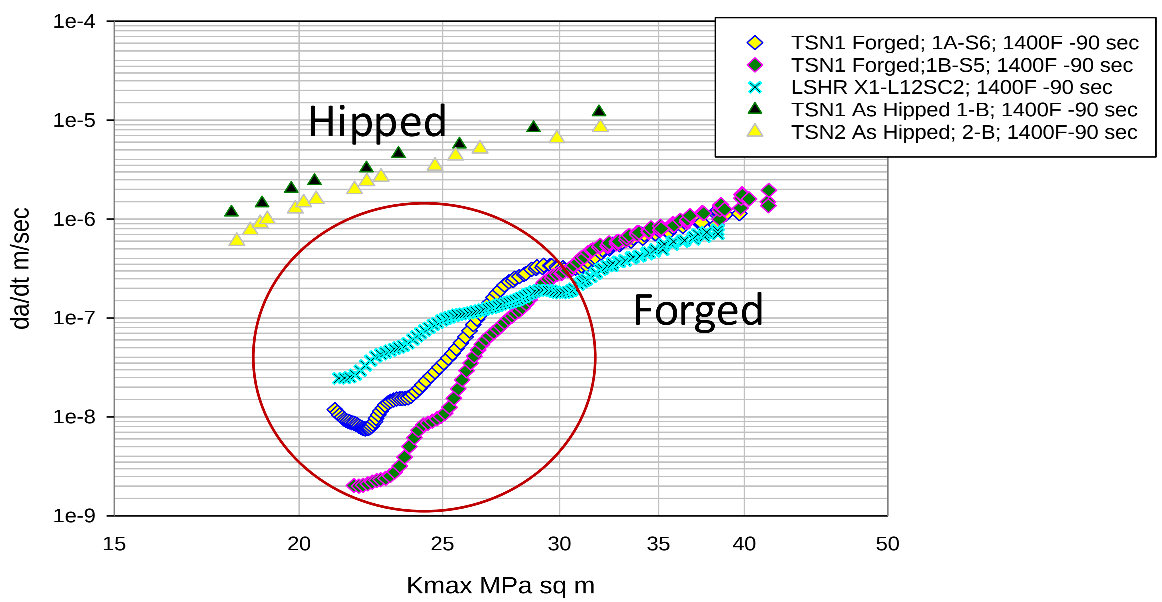
- Newly discovered atomic-scale strengthening mechanisms leveraged to produce high temperature capable disk alloys
- Optimal forging parameters were down selected and used for TSNA 1,2,and 3
- The forged disks were heat treated and machined to investigate improvements in properties.

Results and Benefits:

- Compression tests and forging trials prove that TSNA disk alloys can be processed into turbine disks
- Forged TSNA-1 provides almost ***a magnitude longer creep life*** to 0.3 strain at 760ºC compared to commercial disk alloys LSHR and ME3
- Forged crack growth and dwell fatigue results **reveal orders of magnitude better crack growth rates** compared to the As-HIPed TSNA alloys
- Forged TSNA-1 presents fantastic Creep and Dwell fatigue properties.
  - Dwell fatigue and Creep are considered properties that compete

760C/ 552MPa Creep Comparison





Kantzos, C., Smith, T., Telesman, J., Dempster, I., Gabb, T. (2024). Cyclic- and Dwell-Fatigue Crack Growth Behavior in a Phase Transformation Strengthened Disk Superalloy. In: Cormier, J., *et al.* Superalloys 2024. ISS 2024. The Minerals, Metals & Materials Series. Springer, Cham. https://doi.org/10.1007/978-3-031-63937-1_21

POC: Timothy Smith (GRC)

Atomistic Simulations Of The Effect Of Alloying Elements On Creep In TSNA: Nb vs Cr

CHALLENGE:

Creep (via twinning) is one of the most active deformation mechanisms in Ni-based superalloys above 700^{o}C. However, the *effects of solute additions are not well understood*.

TECHNICAL ACCOMPLISHMENT:

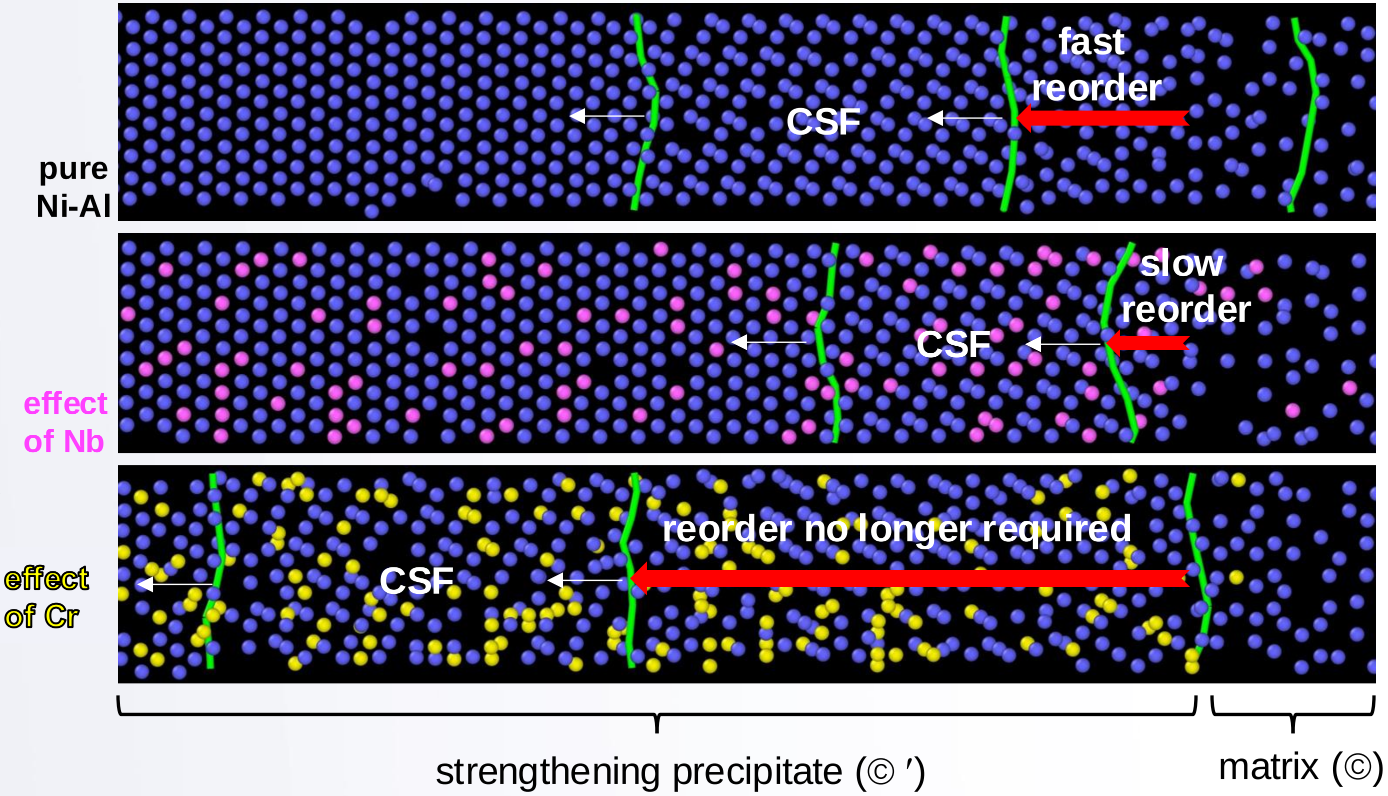
Atomistic simulations revealed the effects of Nb and Cr alloying additions on creep properties (see Figure). Creep deformation proceeds due to the passage of partial dislocation pairs which create *high energy* 2-layer complex stacking fault (*CSF*) that reorders into *low energy* super extrinsic stacking fault (SESF) via thermal diffusion. Slow diffusing Nb atoms significantly *reduce deformation*. Cr atoms reduce the energy of CSFs (reordering is no longer required for dislocation motion) and *accelerate deformation* creep. *Depending on concentration of Cr, the strengthening effect of Nb can be diminished*.

SIGNIFICANCE:

These results explain the experimentally observed effects of elemental composition of the alloy on creep resistance and *provide guidance for future development of Ni-based superalloys with improved creep properties*.

Effects of Nb and Cr additions on creep deformation

Dislocations (green); **Al** atoms (blue); **Nb** atoms (pink); **Cr** atoms (yellow);
Red arrows indicate deformation level



Dislocation pairs *form high energy CSF which reorders (top) into lower energy defect.* ***Nb*** *atoms suppress reordering, reducing deformation creep (middle).* ***Cr*** *atoms make strengthening precipitates weaker, accelerating deformation creep (bottom).*

POC: John Lawson (ARC)

T^3 M&S Products: Data Informatics (KE6)

JARIMIS *(Just a Rather Intelligent Materials Interrogation System)*

- Expert system that integrates various materials informatics tools (e.g., MicroNet, Surrogate ML models, Data management, etc.) to enable inverse design of materials and facilitate the application of machine learning (ML) and data science to rapidly discover and optimize new materials

NASA ICME Schema developed, published, and being adopted

- Enables digital transformation and capture of right information at right time, right format and right scale
- 5 TMs published to help community adopt our approach

AIMAOS - Automatic **I**nformation **M**anagement **A**cross **O**rganizations and **S**cales

- **First of its kind tool** to manage digital thread across length scale and organizations for the design of fit-for-purpose materials

Py MILab v2 enables automatic analysis and data management of test data

- Enhances **efficiency, consistency, and throughput** of thermomechanical test data analysis and minimizes data loss

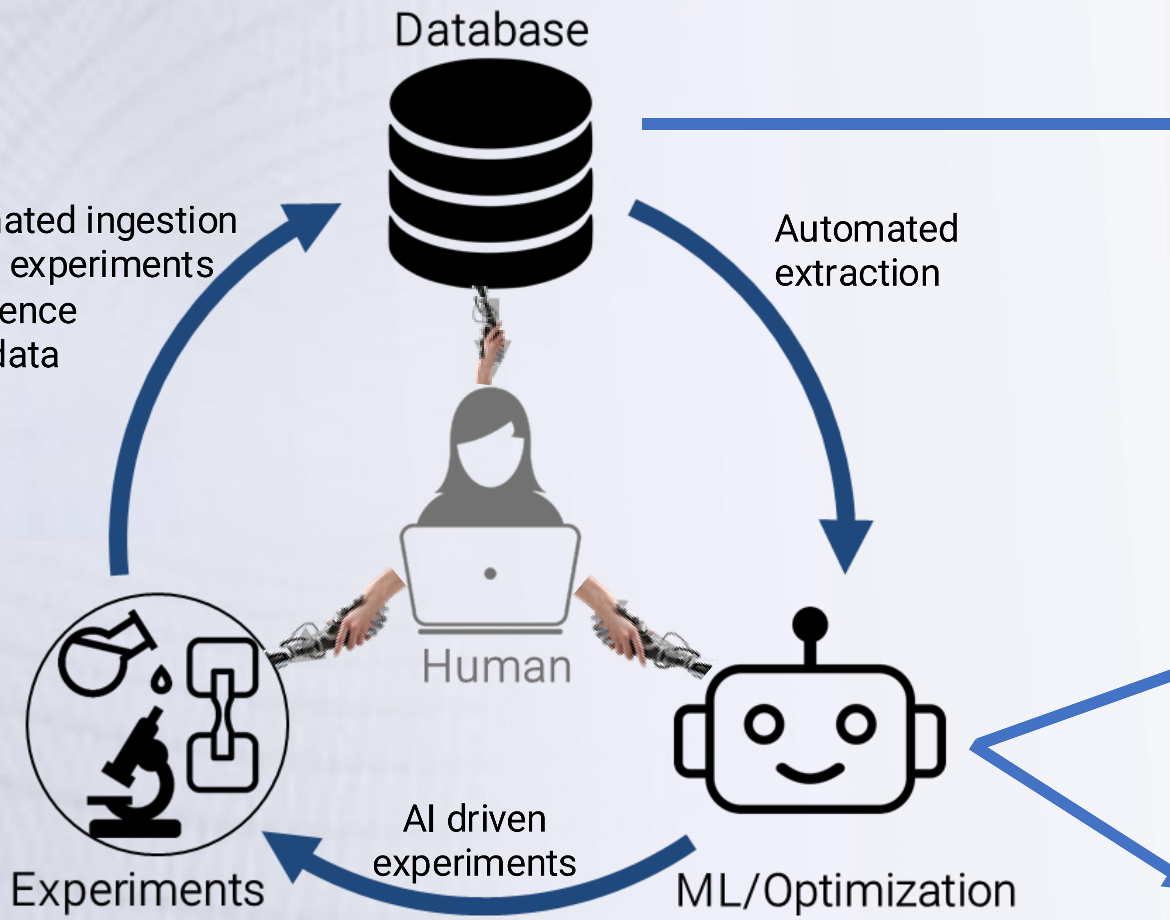
SMAnalytics - Software for the Automated Analysis, Summary, and Reporting of Shape Memory Alloy Tests https://software.nasa.gov/software/LEW-20278-1

SM^2ART – Shape Memory Material Analysis and Research Tool

- Database containing literature data on SMA, superelastic alloys, magnetic SMA, shape memory polymers and ceramics

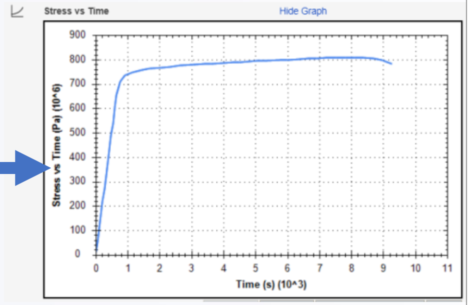
TRUST-AM Established Platform For All Physical And Computational Data And Methods To Support Computational Materials-Informed Qualification And Certification For Additive Manufacturing (RLCC)

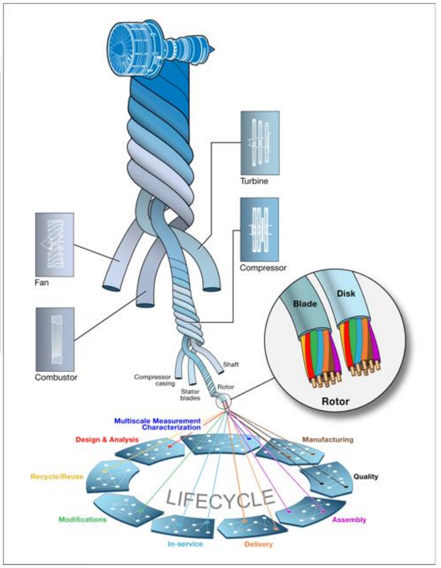
JARIMIS - Just a Rather Intelligent Materials Interrogation System



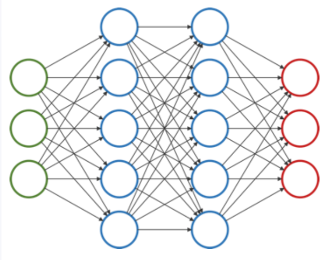
- Automated ingestion
- Virtual experiments
- Providence
- Meta data

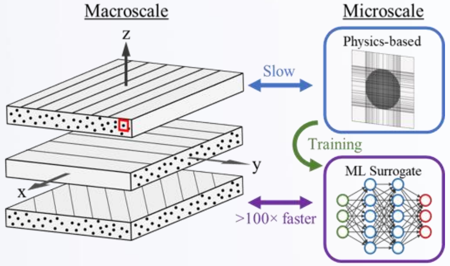
Information Management for Materials and Structures





MicroNet and Surrogate Modeling

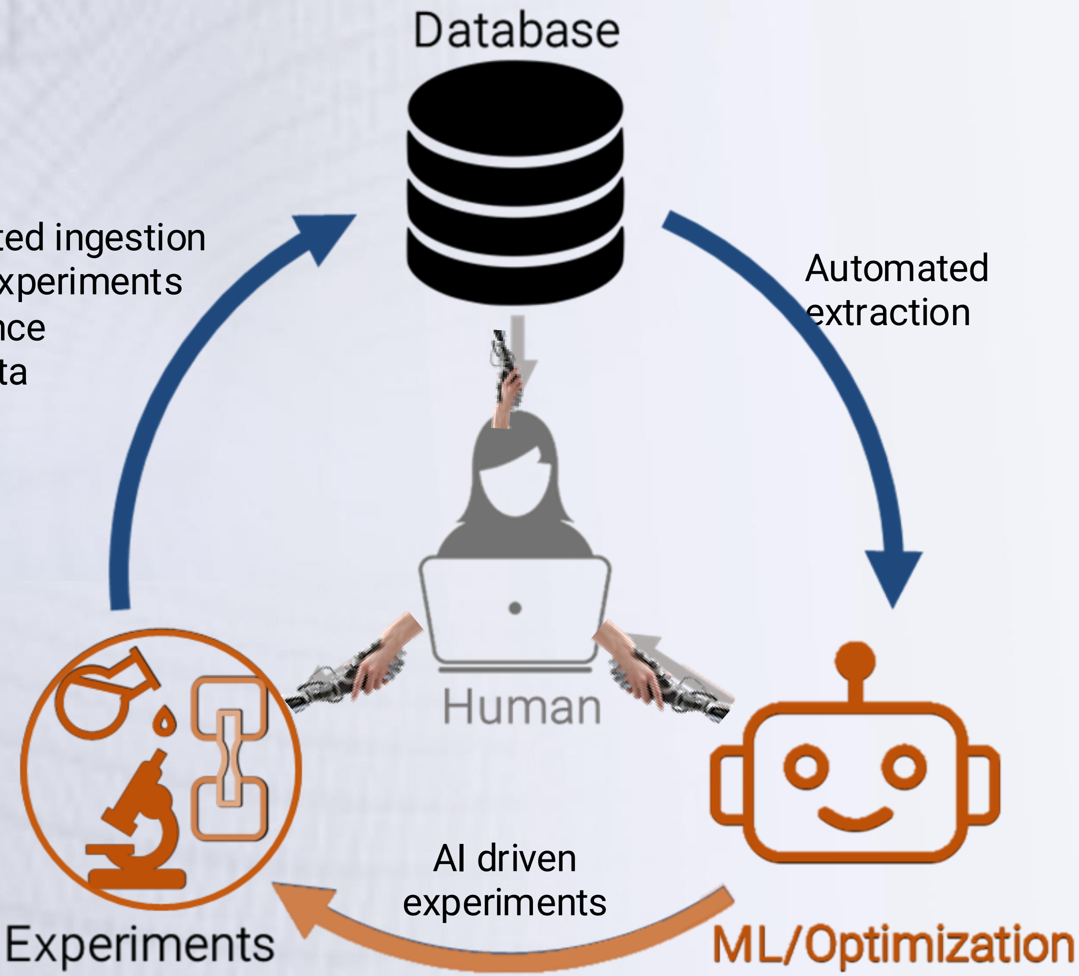




- ML algorithms
- Property prediction
- PSP Relationships
- Optimization
- Simulations

Test Case: Autonomous Laboratory using JARIMIS

- Automated ingestion
- Virtual experiments
- Providence
- Meta data



Database

Automated extraction

Human

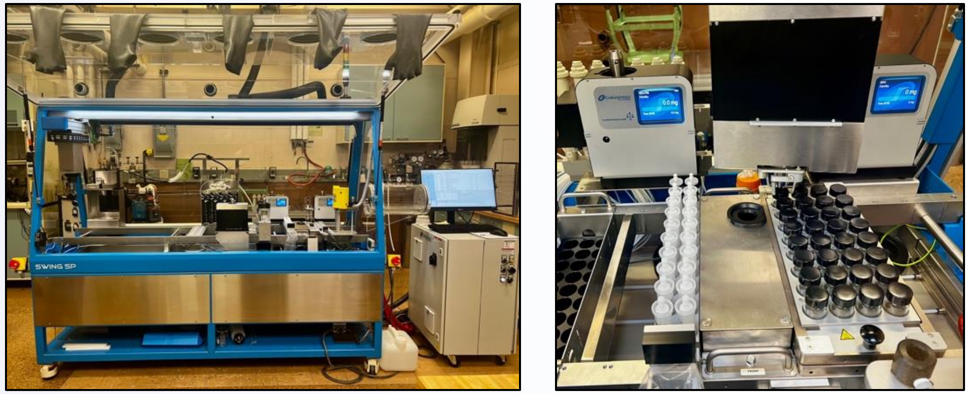
ML/Optimization

AI driven experiments

Experiments

Established Automated Materials Laboratory for Electric Insulation Materials Optimization

- Self-driving laboratory that iteratively designs, executes, and learns from materials science experiments in a fully autonomous loop.
- Provides capability to demonstrate rapid materials development integrated with AI and ML
- Reduces time to discovery of materials with targeted properties for challenging applications



32 samples prepared at the same time in AML

Turnaround speed is 10-20X over current state

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:

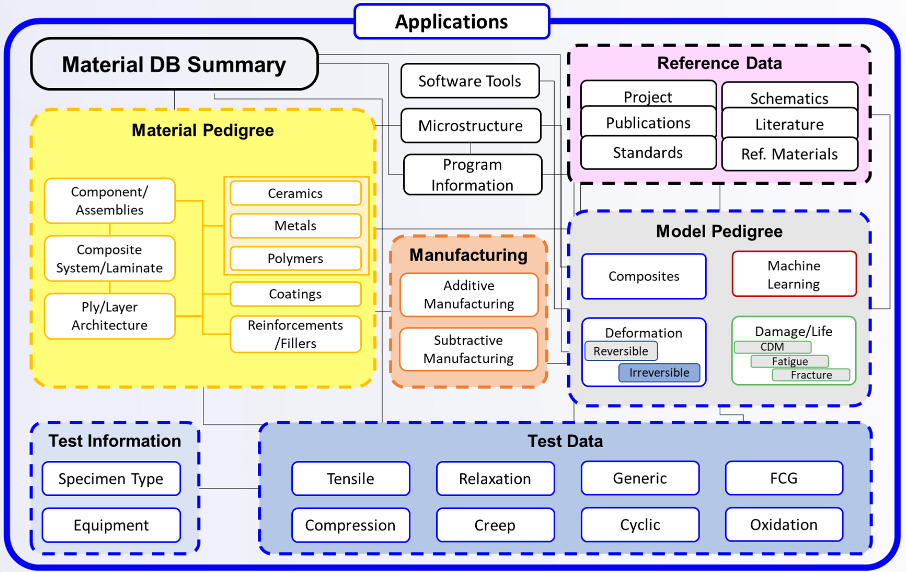
- Required establishment of Material Pedigree, Manufacturing, Microstructure, Model Pedigree, and Software Tools Tables within Granta MI
- Digital Thread / Digital Twin
- **Six key accomplishments**

Additive Manufacturing

ICMAMS 2023, Aug 9, 2023

Application Table

NASA TM-2022-00184033


Applications

Material DB Summary

Software Tools

Microstructure

Program Information

Reference Data: Project, Publications, Standards, Schematics, Literature, Ref. Materials

Material Pedigree: Component/ Assemblies, Composite System/Laminate, Ply/Layer Architecture, Ceramics, Metals, Polymers, Coatings, Reinforcements /Fillers

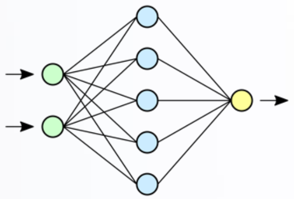
Manufacturing: Additive Manufacturing, Subtractive Manufacturing

Model Pedigree: Composites, Machine Learning, Deformation (Reversible, Irreversible), Damage/Life (CDM, Fatigue, Fracture)

Test Information: Specimen Type, Equipment

Test Data: Tensile, Relaxation, Generic, FCG, Compression, Creep, Cyclic, Oxidation

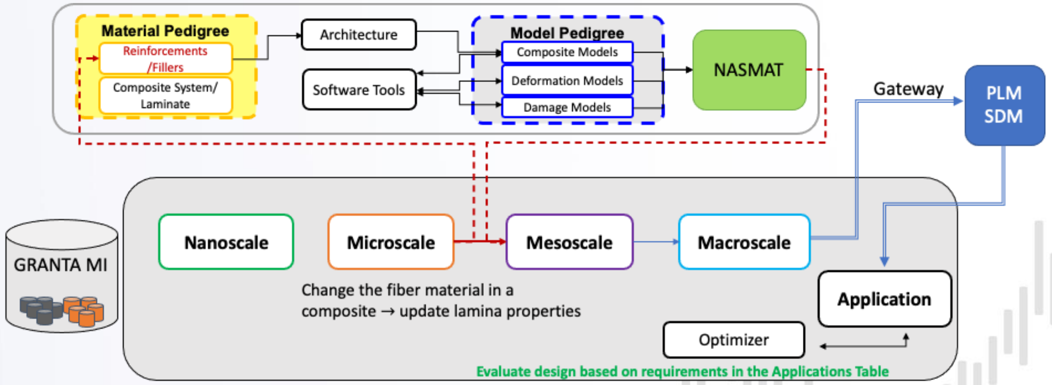
NASA GRC ICME Schema: Executive Summary
NASA TM-2023-0018337



Machine Learning Table

NASA TM-2022-0017137

AIMAOS: Automated Information Management Across Organizations and Scales (TMS ICME, May 21, 2023; **NASA TM-2024-0010796**)


Material Pedigree: Reinforcements /Fillers, Composite System/ Laminate

Architecture

Software Tools

Model Pedigree: Composite Models, Deformation Models, Damage Models

NASMAT

Gateway

PLM SDM

GRANTA MI

Nanoscale

Microscale

Mesoscale

Macroscale

Change the fiber material in a composite → update lamina properties

Application

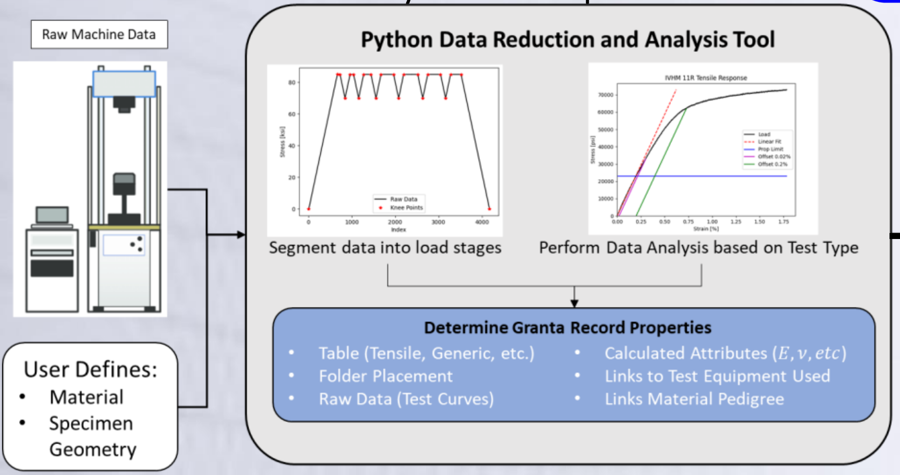
Optimizer

Evaluate design based on requirements in the Applications Table

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

Py-MILab (NASA TM-2024-0012389)

Data Analytics and Importer


Raw Machine Data

User Defines:
- Material
- Specimen Geometry

Python Data Reduction and Analysis Tool

Segment data into load stages

Perform Data Analysis based on Test Type

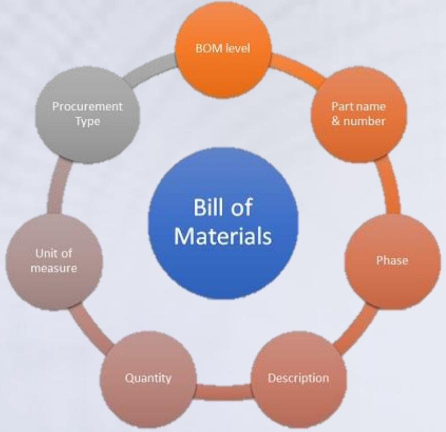
Determine Granta Record Properties
- Table (Tensile, Generic, etc.)
- Folder Placement
- Raw Data (Test Curves)
- Calculated Attributes (E, ν, etc)
- Links to Test Equipment Used
- Links Material Pedigree

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

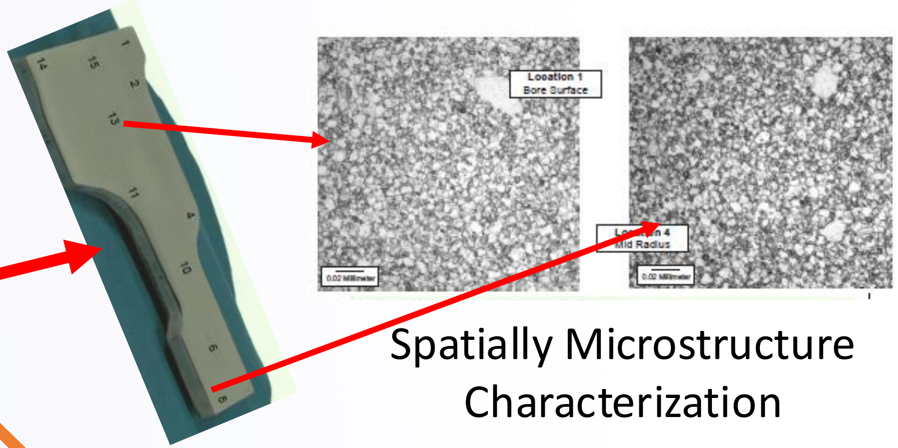
- Application Table links part requirements, microstructure information, material properties, geometry, employed models, relevant analysis, and performance

NASA/TM-20220018403

Application

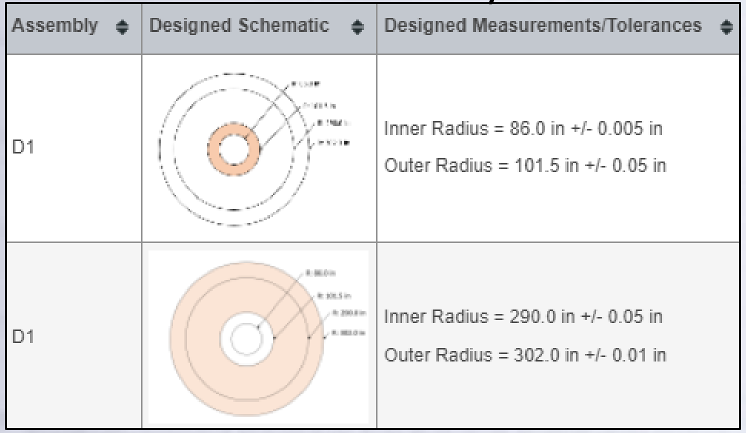


Summary of material properties



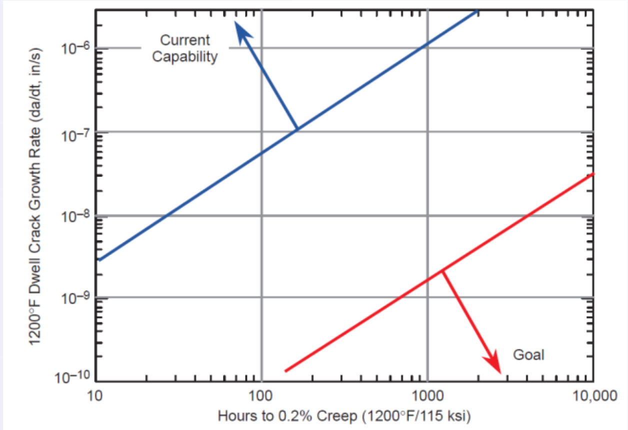
Spatially Microstructure Characterization

Part Geometry

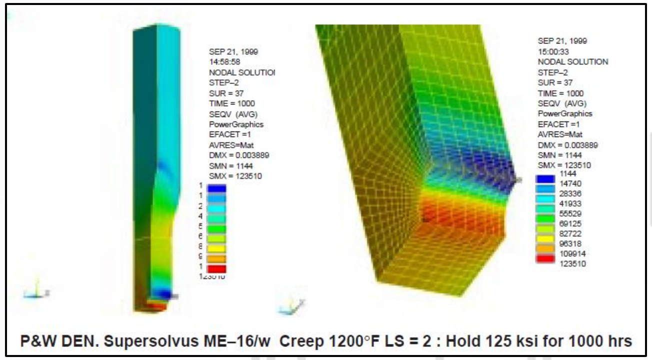


Assembly	Designed Schematic	Designed Measurements/Tolerances
D1		Inner Radius = 86.0 in +/- 0.005 in Outer Radius = 101.5 in +/- 0.05 in
D1		Inner Radius = 290.0 in +/- 0.05 in Outer Radius = 302.0 in +/- 0.01 in

Performance Requirements



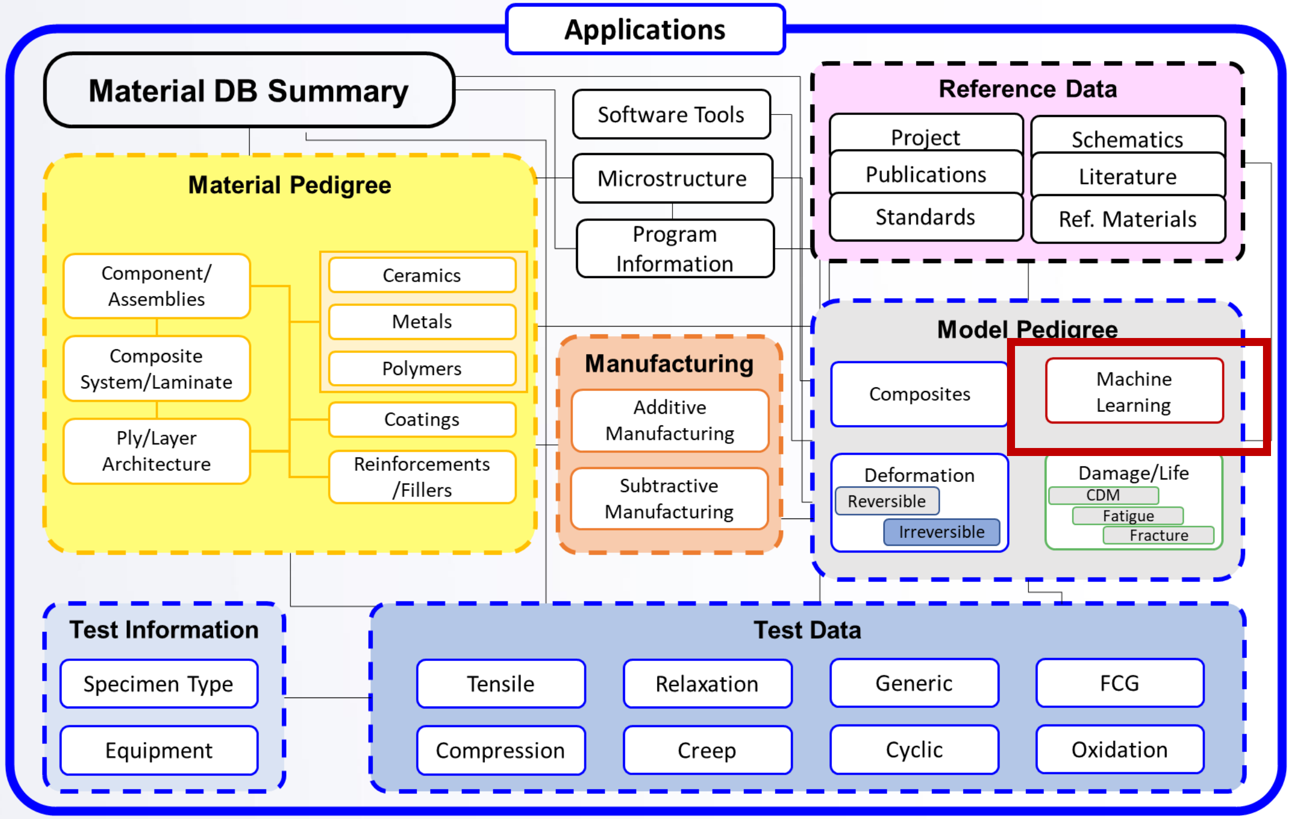
Summary of Relevant Analyses with Links to PLM/SDM



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

Effective Data Management for Machine Learning Data and Models

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



Applications

Material DB Summary

Software Tools
Microstructure
Program Information

Reference Data
Project
Publications
Standards
Schematics
Literature
Ref. Materials

Material Pedigree
Component/ Assemblies
Composite System/Laminate
Ply/Layer Architecture
Ceramics
Metals
Polymers
Coatings
Reinforcements /Fillers

Manufacturing
Additive Manufacturing
Subtractive Manufacturing

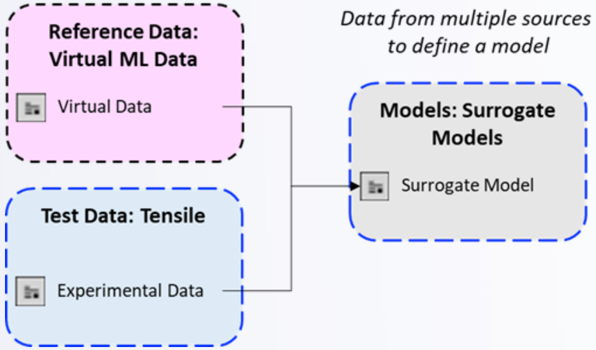
Model Pedigree
Composites
Machine Learning
Deformation
Reversible
Irreversible
Damage/Life
CDM
Fatigue
Fracture

Test Information
Specimen Type
Equipment

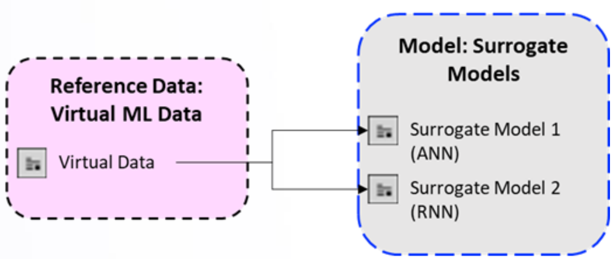
Test Data
Tensile
Relaxation
Generic
FCG
Compression
Creep
Cyclic
Oxidation

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

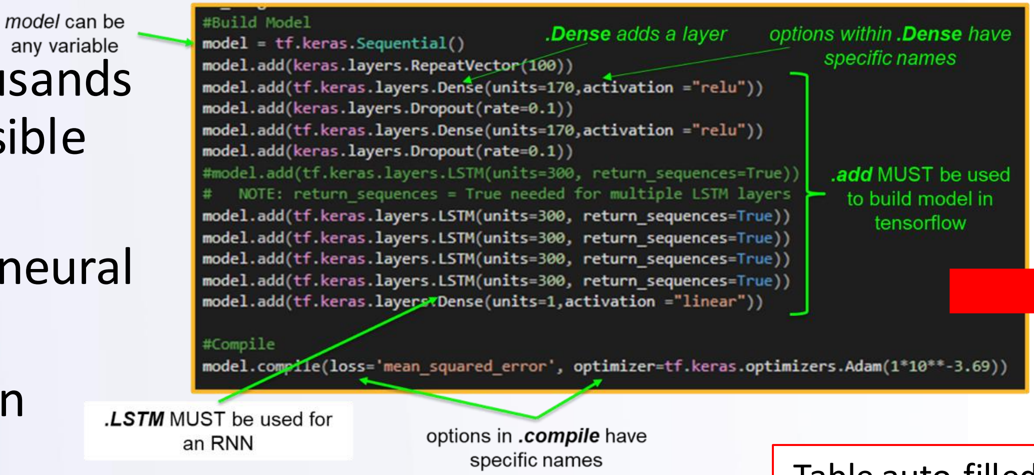


Data from multiple sources to define a model



Multiple models trained from one set of data

- 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



```
#Build Model
model = tf.keras.Sequential()
model.add(keras.layers.RepeatVector(100))
model.add(tf.keras.layers.Dense(units=170,activation ="relu"))
model.add(keras.layers.Dropout(rate=0.1))
model.add(tf.keras.layers.Dense(units=170,activation ="relu"))
model.add(keras.layers.Dropout(rate=0.1))
#model.add(tf.keras.layers.LSTM(units=300, return_sequences=True))
#   NOTE: return_sequences = True needed for multiple LSTM layers
model.add(tf.keras.layers.LSTM(units=300, return_sequences=True))
model.add(tf.keras.layers.LSTM(units=300, return_sequences=True))
model.add(tf.keras.layers.LSTM(units=300, return_sequences=True))
model.add(tf.keras.layers.LSTM(units=300, return_sequences=True))
model.add(tf.keras.layers.Dense(units=1,activation ="linear"))

#Compile
model.compile(loss='mean_squared_error', optimizer=tf.keras.optimizers.Adam(1*10**-3.69))
```

model can be any variable

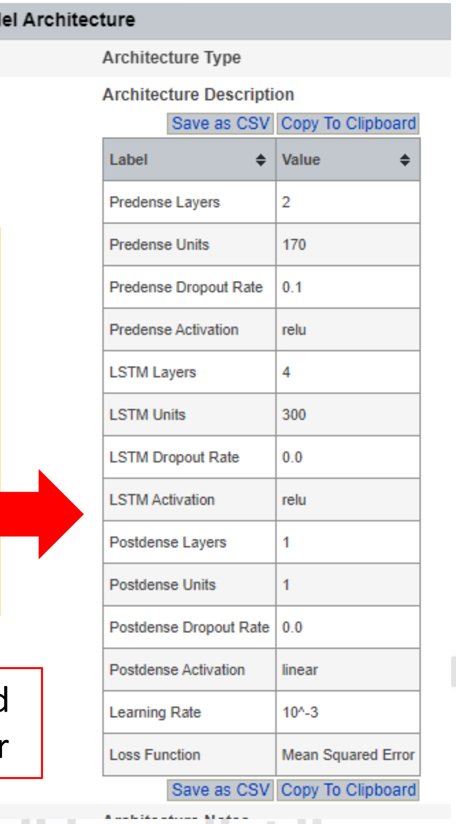
.Dense *adds a layer*

options within ***.Dense*** *have specific names*

.add MUST be used to build model in tensorflow

.LSTM MUST be used for an RNN

options in ***.compile*** have specific names



Model Architecture

Architecture Type

Architecture Description

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

Table auto-filled out in importer

NASA TM-2022-0017137

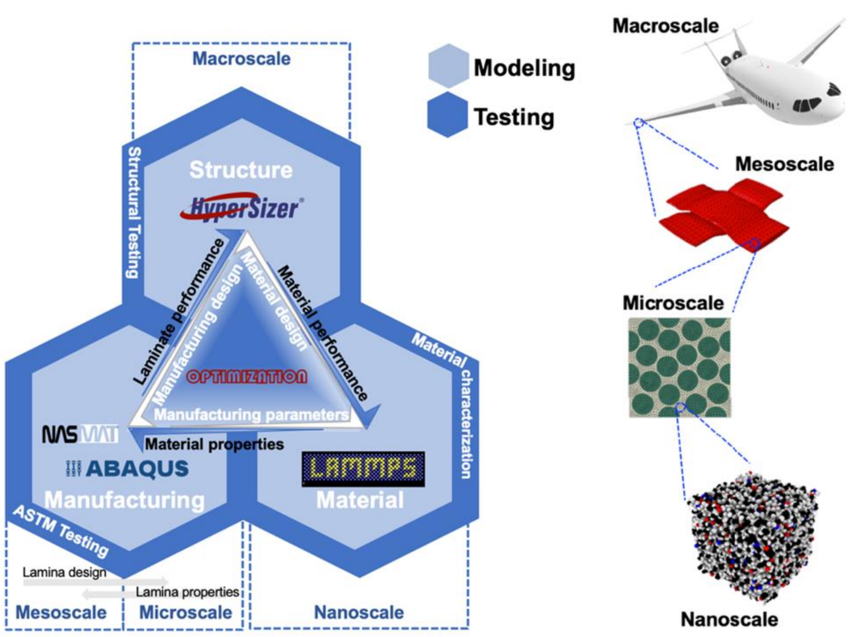
ICME Optimization of Advanced Composite Components of the Aurora D8 Aircraft: Digital Twin/Digital Thread

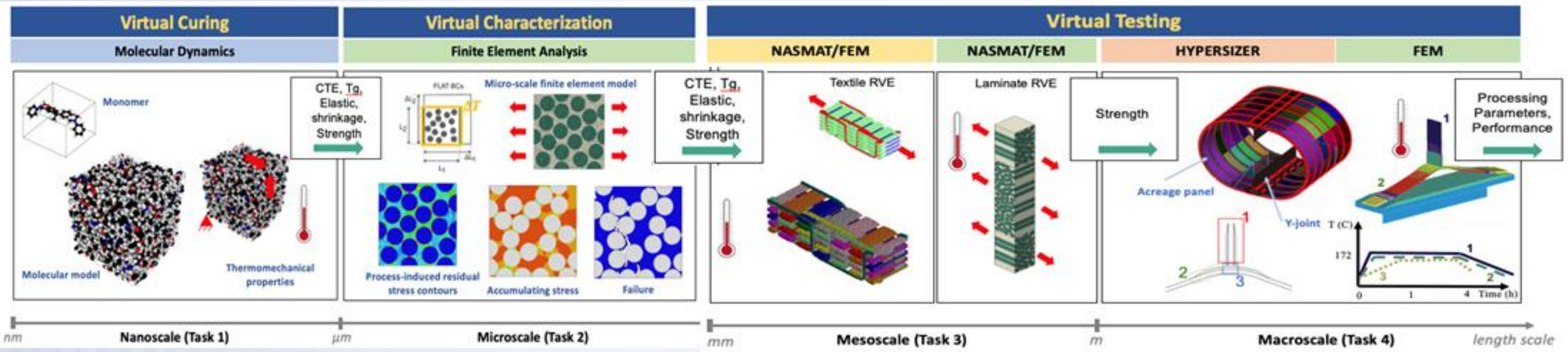
Multi Org. NRA Collaboration: Univ Mass Lowell, Univ Michigan Tech, NASA, Aurora, Collier

AIAA 2022 ICME Prize Winner

- Objective is to develop an **integrated approach** to design and optimize the composite Y-joints and composite acreage panels used in the Aurora D8 aircraft
- Approach - link material models, structural models, and experiments at multiple length scales
- Benchmark problem will serve to demonstrate the benefits of the ICME (compared to traditional approach)
  - **Digital Twins** at each scale
  - Input/output from each scale will constitute the **digital thread** of this ICME framework
- Use case within AIAA Digital Twin Implementation paper (Multiscale – ICME Schema)

Recommendation #6

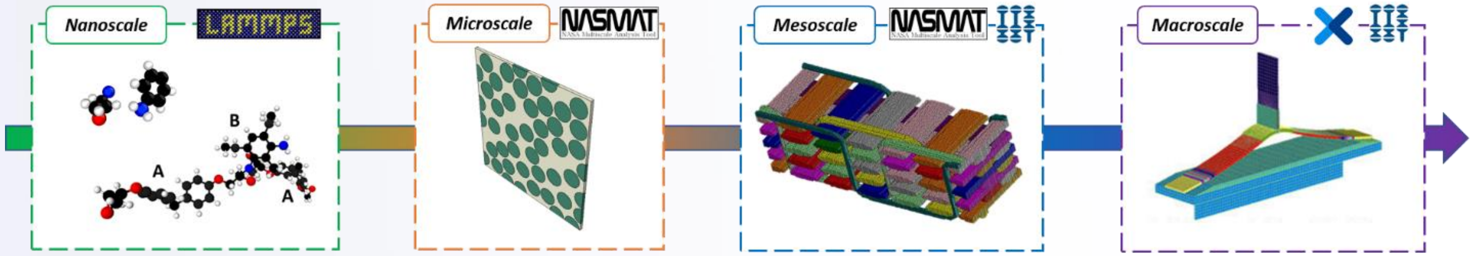




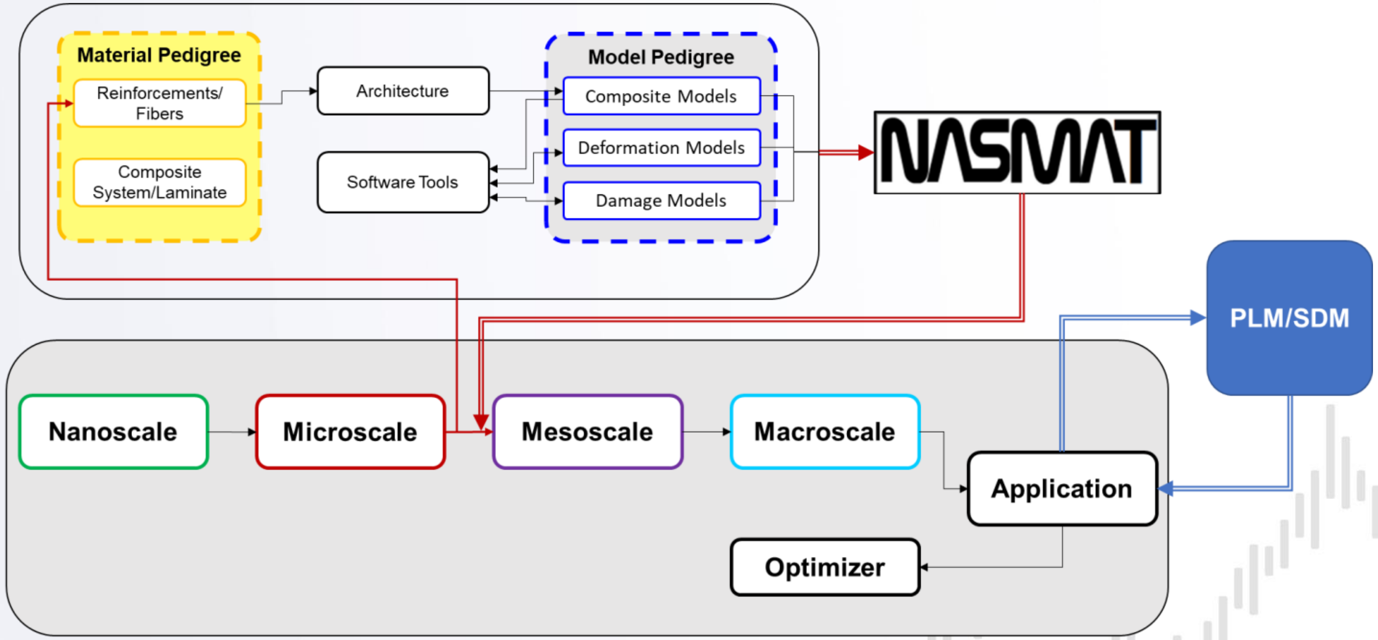
AIMAOS Assists Digital Thread Management in ICME

AIMAOS – **A**utomatic **I**nformation **M**anagement **A**cross **O**rganizations and **S**cales

- Python GUI automatically propagates material information across scales through interaction with simulation tools (e.g., LAMMPS, NASMAT, FEA, HyperX)
  - Users define constituents, lamina, and laminates
  - Automatically generate input/output decks at each scales
    - Become part of the digital thread



- As changes are made at lower length scales, the relevant material properties, models, and tools are used to generate the correct input file and run the new analysis to ensure the digital thread is maintained
  - Changes are stored in the GUI at each length scale to provide traceability



Material Pedigree

Reinforcements/ Fibers

Composite System/Laminate

Architecture

Software Tools

Model Pedigree

Composite Models

Deformation Models

Damage Models

NASMAT

PLM/SDM

Nanoscale

Microscale

Mesoscale

Macroscale

Application

Optimizer

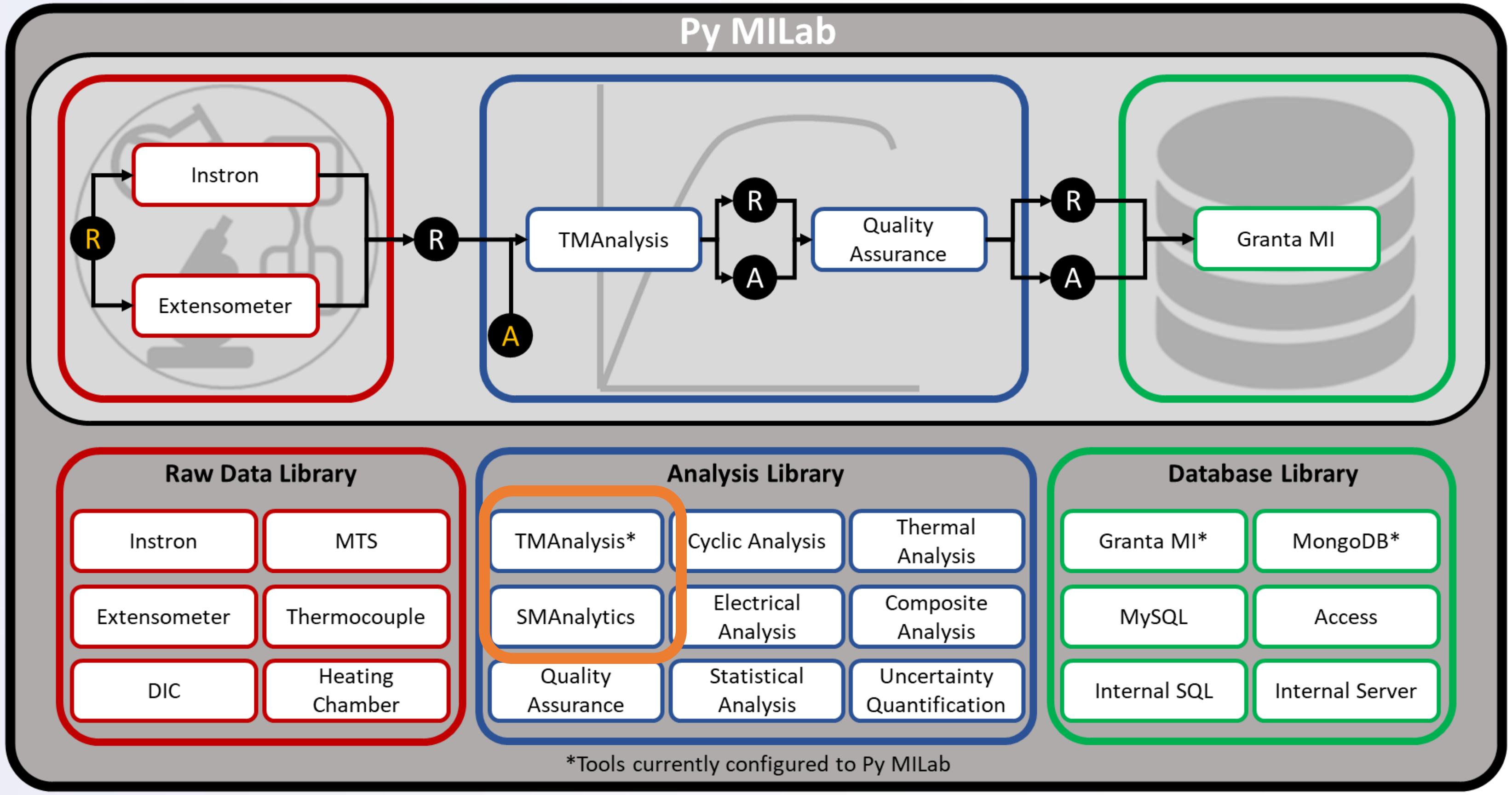
GRANTA MI

NASA TM-2024-0010796

POC: Brandon Hearley (GRC)

Py MILab: Automating Test Data Management Throughout the Data Life Cycle

- 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
- Modules are interfaced via neutral file formats (e.g. JSON)
  - Plug-and-play capability
  - Chain analyses together



Py MILab

R
Instron
Extensometer
R
A
TMAnalysis
R
A
Quality Assurance
R
A
Granta MI

Raw Data Library

Instron	MTS
Extensometer	Thermocouple
DIC	Heating Chamber

Analysis Library

TMAnalysis*	Cyclic Analysis	Thermal Analysis
SMAnalytics	Electrical Analysis	Composite Analysis
Quality Assurance	Statistical Analysis	Uncertainty Quantification

Database Library

Granta MI*	MongoDB*
MySQL	Access
Internal SQL	Internal Server

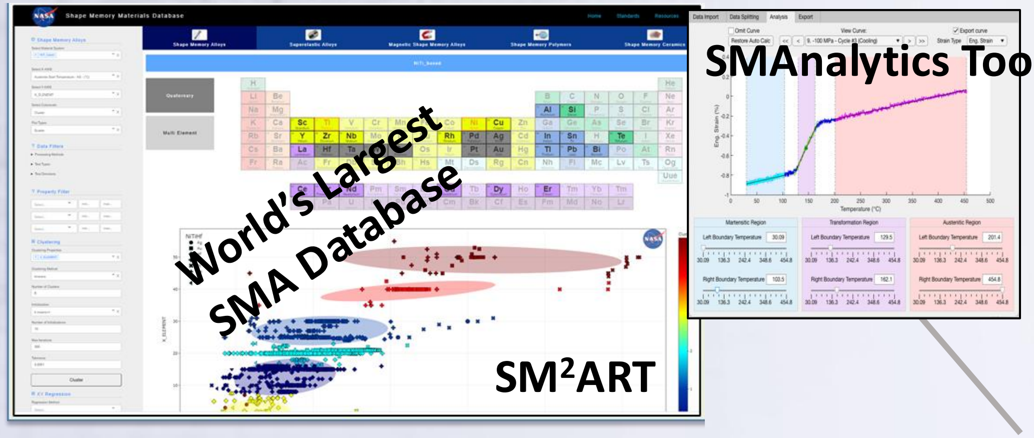
*Tools currently configured to Py MILab

R Template Raw Data Neutral File
R Populate Raw Data Neutral File
A Template Analysis Neutral File
A Populate Analysis Neutral File

POC: Brandon Hearley (GRC) **NASA TM-2024-0012389**

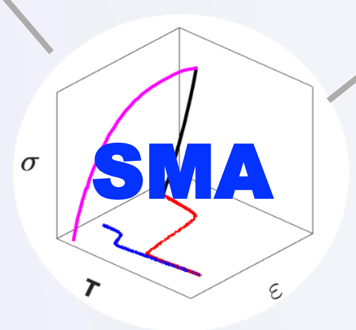
World’s Largest SMA Database Enables Development of Two New SMAs In One Year

eco Demonstrator PROGRAM



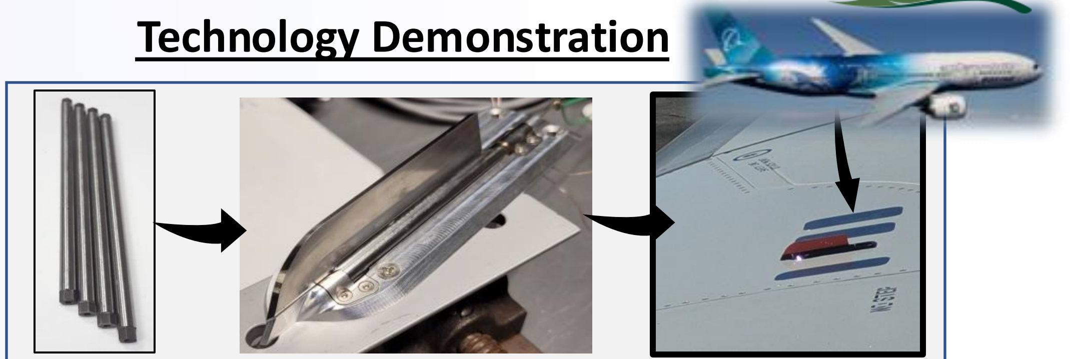
Shape Memory Materials Database & Analysis Tool was launched online via a web portal
https://shapememory.grc.nasa.gov/

1) Completed the database functionality for ALL materials category
   - Significance: Enable faster, efficient, accurate design of SMAs (in line with Vision 2040)
2) Tool publicly launched via a web application
   - Significance: Promote database growth & data mining via direct scientific community contributions



POC: Othmane Benafan

Technology Demonstration



SMA tubes (completed)
Wind tunnel test (completed)
Flight integration (completed)

BOEING Deharde APPROVED APPROVED

- Actuation: Altitude activated + Aircraft triggered
- New alloys: TWO alloys designed (Torque tubes)
- Conditions: Standard day+ hot day + partial cold day

- NiTiPdPt alloy stowed at -22°C, or on-demand
- Altitude:: Fully stowed at 32,000’

SMART-VG "2nd Generation" prototype systems (4 VG's in total) were successfully installed and operated for 24 flights on the ecoDemonstrator 777-200ER flight test campaign. Data & CFD analyses confirm drag performance.

T^3 M&S Contributing Expertise to Community (KE8)

Select examples of M&S sharing expertise

TTT staff supports Professional Society committee positions: member, chair, vice chair, secretary, steering committee, conf organization committee, etc.

International Leadership for Shape Memory Alloys

Top Prize Poster at 2024 International Shape Memory & Superelastic

Japan Metal Bulletin

30周年記念講演を開催

形状記憶合金協、祝賀会も

Invited talks at science center in Japan

NASA Team led International 6th CASMART Student Design Competition

Expert Consults for High Voltage Electric Materials

- Development of HV Standards Committee
- Aerospace Information Report (AIR) on safe and reliable electrical wiring systems
- Other NASA projects, companies, and OGAs
  - Astrobotics (SBIR), Raytheon, Dupont, General Cable (Prysmian Group), FAA, AEPS

Authoring Mil Handbook and Position and Implementation papers:

Ceramic Matrix Composite Handbook

AIAA Digital Twin: Ref Model, Realization… ;

AIAA Digital Thread: Definition, Value and Ref Model

COMPOSITE MATERIALS HANDBOOK

5

Ceramic Matrix Composites

DIGITAL TWIN: REFERENCE MODEL, REALIZATIONS & RECOMMENDATIONS

DIGITAL THREAD: DEFINITION, VALUE, AND REFERENCE MODEL

Concluding Remarks

- Integrated Computational Engineering has and will continue to impact the way we do business – accelerate innovation/discovery
- The Vision 2040 ecosystem will transform current design paradigm
  - Most likely there will be multiple ecosystems developed
  - Expert panels believe technical goals are achievable
  - However, organizational cultural issues will be the real stumbling block
    - “culture eats strategy” every time
- NASA T^3 M&S portfolio is aligned with 2040 Vision and has made significant progress toward closing several of the identified technical gaps
- ML/AI will play a pivotal role in the coming ecosystem
  - **Surrogate models** enable **ultra efficient** utilization of physics-based models
- Additive Manufacturing is an essential enabling technology to literally make the 2040 Vision a reality
  - In near future, hope to update 2040 Vision to include AM discipline
- Solution will most likely ***not*** be a single toolset/environment or “database” (i.e. multiple ecosystems) therefore essential to identify/specify requirements for communication.
  - Toolsets developed at NASA GRC interact with a database to enable ***judicious*** automatic capture, analysis, maintenance, and dissemination of data to realize ‘fit-for-purpose’ materials

Thank You !

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