2040 Vision Study: An Enlargement of Model Based Engineering

Presented by: Dr. Steven M. Arnold
Technical Lead: Multiscale Modeling
Material and Structures Division
NASA Glenn Research Center

Sponsored by Transformational Tools and Technologies (T^3) Project
Building on the success of the 2030 CFD Study

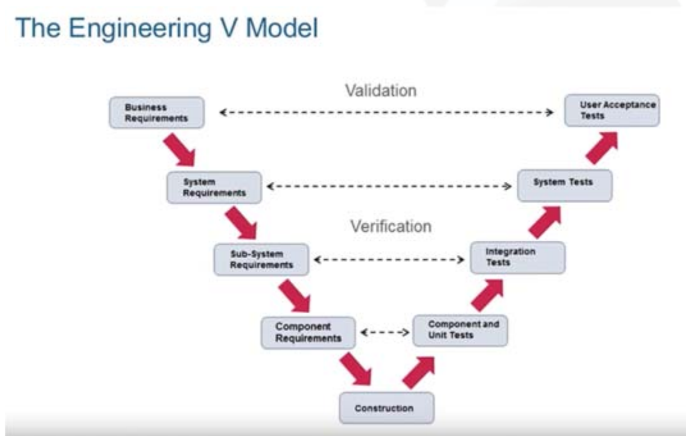
What is Model Based System Engineering?

- The core MBE tenet is that **models** are used (rather than documents) to drive all aspects of the product lifecycle and that data is ***created once and reused by all downstream data consumers.*** ... Engineers use models to convey product definition or otherwise define a product's form, fit and function. (www.3dcadworld)

- INCOSE defines MBSE as "Model-based systems engineering (MBSE) is the formalized **application of modeling** to support system requirements, design, analysis, verification and validation activities beginning in the conceptual design phase and continuing throughout development and later life cycle phases."

- WIKIPEDIA: Model-based systems engineering (MBSE) is a systems engineering methodology that focuses on creating and **exploiting domain models as the primary means** of information exchange between engineers, rather than on document-based information exchange. More recently, the focus has also started to cover aspects related to the model execution in computer simulation experiment, to further overcome the gap between the system model specification and the respective simulation software.

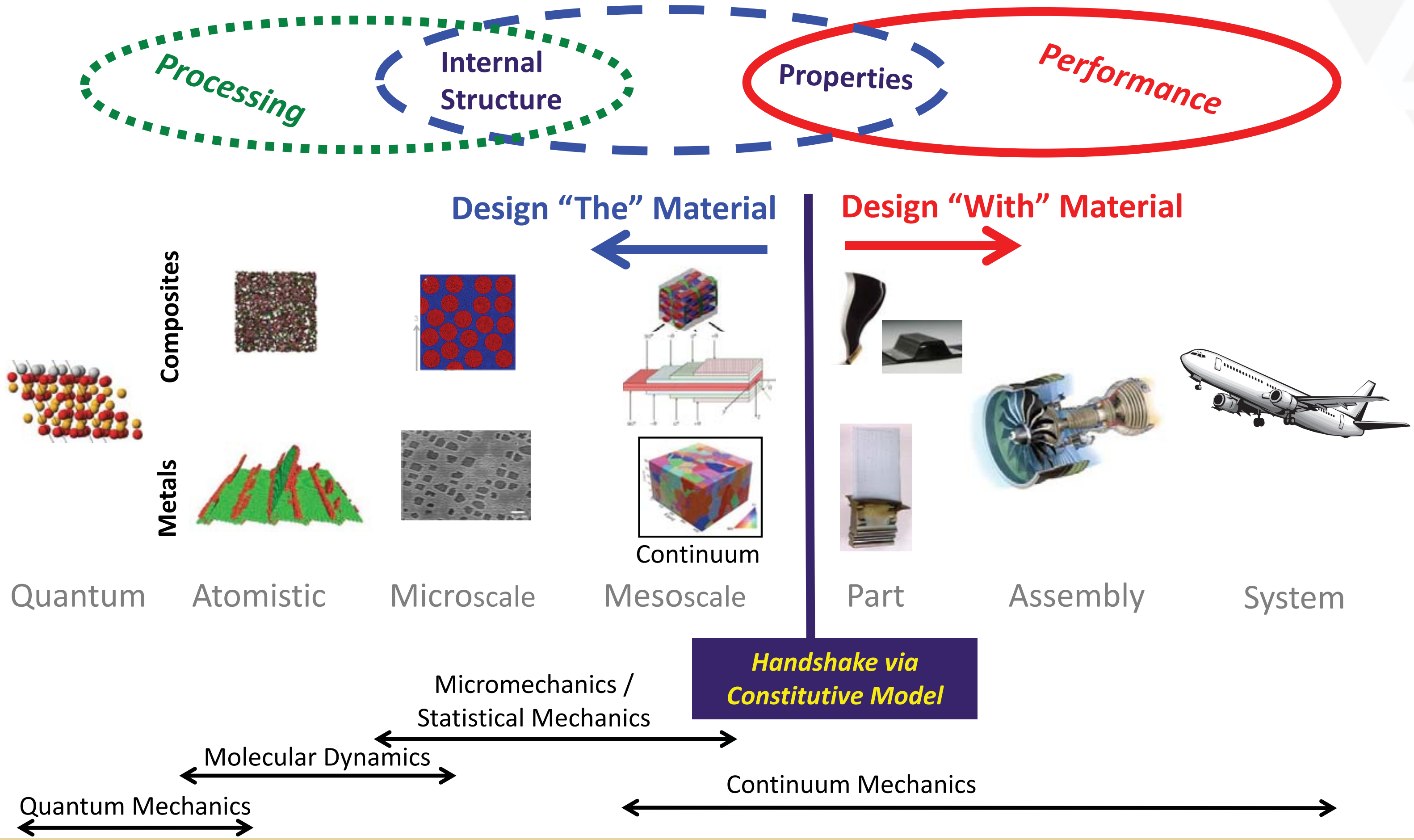
- DEFINITIONS OF MBSE, MBD, MBE AND MODEL BASED DEVELOPMENT (https://www.lifecycleinsights.com)
  - **Model Based Definition (MBD)** is a mechanical engineering initiative where a 3D model with Product Manufacturing Information (PMI) augments or replaces a 2D engineering drawing as design documentation. Model Based Enterprise (MBE) is a company wide initiative to augment 3D models with additional information to create new documentation deliverables beyond engineering.
  - **Model Based System Engineering (MBSE)** is a system engineering initiative to create a digital model of a system that is used by all engineering disciplines and other functional organizations within a company.
  - **Model Based Development** is a embedded software initiative where a two-sided model is used to verify control requirements and that the code runs on target electronic hardware.



Influence And Interaction Of Various Materials And System Engineering Software Products

CAD – computer aided design, CAE – computer aided engineering, MAT – material properties, PDM – product data management, SDM – simulation data management, MLM – material lifecycle management, PLM - product lifecycle management

Integrated Computational Materials Engineering (ICME) Is The Future



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

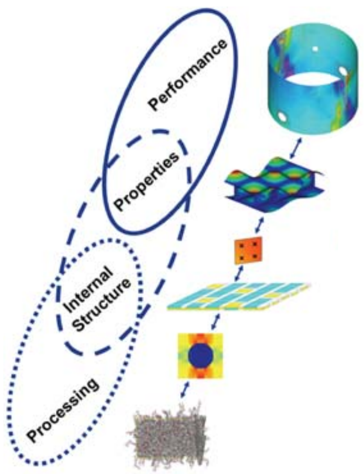
2040 Ecosystem Revolutionizes Design Paradigm

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***

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*

Study Identified 9 Key Element Domains

	Key Element	End State Characteristics With Most Connections to Gaps and Recommended Actions		
1	**Models and Methodologies** All models and methods, at all length scales, whether phenomenological, physics-based, data-driven, deterministic, or probabilistic. Also concerned with methods and protocols to characterize and validate models.	Robust	Interoperable	Adaptive
2	**Multiscale Measurement and Characterization Tools and Methods** Methods, practices, and measurement devices for observing, defining, and characterizing material and structural response and underlying causational mechanisms as associated with deformation, damage, and failure.	Robust	Accessible	Interoperable
3	**Optimization and Optimization Methodologies** Computational/numerical approaches and mathematical formalizations for optimizing or improving the performance of products, materials, structures, manufacturing processes, and design workflows for given applications.	Robust	Adaptive	Accessible
4	**Decision Making and Uncertainty Quantification and Management** The investigation, characterization, and management of uncertain or variable inputs to quantify prediction confidence, enhance the design process, enable optimal decision making for new material and component design, facilitate materials and component certification, and enable a response to regulatory requirements.	Traceable	Robust	Accessible
5	**Verification and Validation** Methods/practices associated with verification of algorithms and validation of models.	Accessible	User Friendly	Robust
6	**Data, Informatics, and Visualization** All aspects associated with the electronic capture, analysis, archival, maintenance, dissemination, and visualization of material and system data and metadata, whether experimental or simulation, at all length scales.	Traceable	Accessible	User Friendly
7	**Workflows and Collaboration Frameworks** Technologies associated with workflows and collaboration functions, both physical (e.g., human, organizational) and computational.	Accessible	User-Friendly	Traceable
8	**Education and Training** All aspects of curriculum development, education, and training opportunities for preparing the current, emerging, and future workforce in the capabilities and skills needed to realize and utilize the Vision 2040 end state.	Accessible	Robust	Interoperable
9	**Computational Infrastructure** All computer hardware, firmware, software, networks, platforms, and HPC architectures required to support the 2040 vision.	Adaptive	Accessible	Robust

Identified Critical Gaps & *Possible Subset of Actions Required To Close Each Gap*

Key Element	Critical Gap	Priority Action	Time Frame (2018 2020 2025 2030 2035 2040)	End State Characteristics
1	Underdevelopment of physics-based models that link length and time scales for relevant material systems	Multiscale V&V methods (5.6) Integration of uncertainty across scales (1.13) ICME-based fast process models (1.21) Multiscale models for rare-events/nucleation (1.22) Information framework for 3D/4D model dev. (2.11) Models for key uncertainty sources (1.23)		
2	Inability to conduct real time characterization and measurement of structure and response at appropriate length and time scales	Real-time measurement methods (2.14) Real-time visualization for experiment modeling (6.15) Lifecycle data: automated ingestion and storage (6.23) Protocols: link characterization, test data, models (2.10)		
3	Lack of reliable optimization methods that bridge across scale	New optimization formulation methods (3.13) Education modules: data analytics tools/methods (8.2) Optimization methods with uncertainty incorporated (3.11) Coupled multiphysics and optimization methods (3.5) Surrogate models for large scale optimization (4.15)		
4	Existing models and software codes are not designed to compute input sensitivities and propagate uncertainties to enable UQ	Benchmark characterization methods (2.3) Optimization methods with uncertainty incorporated (3.1) UQ: sensitivity analysis methods (4.19) Holistic test methods (2.16) Models for key uncertainty sources (1.23)		
5	Lack of guidelines and practitioner aids for multiscale/multiphysics (e.g., ICME) V&V	Best practices: data collection (5.7) Multiscale V&V standards and definitions (5.1) Student resources: industry V&V data (8.8) V&V training (5.2) Holistic test methods (2.16)		
6	No widely accepted community standards or schema for materials information storage and communication methods	Workflow data modeling: automation, recognition, tagging (7.1) Training: informatics framework interpretation & integration (6.21) Best practices: data federation (6.1) Best practices: defining multidisciplinary ontologies (6.3)		
7	Lack of open, community/industry standards defining inputs/outputs, needed functionality, data quality, model maturity levels, etc. for smooth operation in the envisioned ecosystem	Access-controlled example workflows (7.9) Best practices: multi-domain workflows (7.16) Data quality and model maturity standards (7.21) Access-controlled adaptive file formats (6.2)		
8	Education/training does not bridge the gap between "essential" or "fundamental" knowledge and industrially relevant skills	Education/Training: decision/UQ approaches (4.7) New computational certifications programs/tracks (8.14) Workforce transition training for students (8.5) V&V training (5.2) Student access to equipment/facilities (8.6)		
9	Lack of support, or adequate business models, for code development and maintenance, particularly for software used in engineering applications	Modernize existing codes (9.6) Best practices: multi-domain workflows (7.16) Web platform for code benchmarking (5.3) Open-source/alternative code writing tools (8.3) Early-stage collaborative code development (9.4) Initiative: support key modeling software tools (9.8)		

Ten Crosscutting Streams Identified To Help Organize Gaps And Recommended Actions Across Key Elements

These streams aim to show similarities among the challenges facing the various disciplines within the multiscale modeling and simulation community and the actions needed to overcome them:

1. Data Management
2. Data Analytics and Visualization
3. Information Sharing and Reusability
4. Multidisciplinary Collaboration
5. Institutional Paradigms
6. Benchmarking and Business Case
7. Scalability and Computational Efficiency
8. **Linkage and Integration**
9. Input / Output Confidence and Reliability
10. Behavior of Materials and Structures

Gaps Associated with Linkage and Integration Stream

Key Element	Gap	Accessible	Adaptive	Interoperable	Robust	Traceable	User-Friendly
KE1 Models and Methodologies	Models do not seamlessly link to actual certification analysis requirements (e.g., stiffness, strength, spectrum fatigue)			✓			✓
	V&V and UQ are typically addressed after the model development and calibration process rather than concurrently			✓	✓		
	Existing frameworks and models lack the adaptability to rapidly incorporate latest theories		✓	✓	✓		
	Limited interaction between "top-down" engineering requirements and "bottoms-up" performance modeling			✓	✓		
KE2 Multiscale Measurement and Characterization Tools and Methods	No standard protocols for linking quantitative data from standard characterization and test methods with models	✓		✓			✓
	Insufficient 3D/4D characterization methodologies for comparing simulation outputs to equivalent characterization results			✓	✓		
	No standard protocols or methods for defining models with respect to their corresponding physical specimens	✓		✓	✓		✓
KE3 Optimization and Optimization Methodologies	Limited modularity of high-fidelity models inhibits integration with other models in computational supply chains			✓			
	High-fidelity process models do not successfully incorporate the influences of manufacturing processes on material behavior/structural performance into optimization formulations			✓	✓	✓	
KE4 Decision Making and Uncertainty Quantification	Lack of systematic data fusion methods for combining and weighting multiple sources of information into single states of knowledge to inform decision making			✓			
	Need for established systems/protocols for quantifying and defining tolerable levels of uncertainties and errors at each step of the design process	✓		✓		✓	✓
	Lack of clear and consistent terminology for differentiating uncertainties from errors in models and algorithms	✓		✓		✓	✓
	Inability to quantify uncertainty when multiple model types and experimental datasets are employed to predict material properties and responses			✓	✓		
KE6 Data, Informatics and Visualization	Insufficient inclusion of spatially-defined materials data throughout material lifecycle, including evaluation and inspection data (i.e., spatial location on part geometry)			✓	✓		
KE7 Workflows and Collaboration Frameworks	Inability to automate the linking and execution of disparate models and computational methods with data from federated databases			✓			

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.

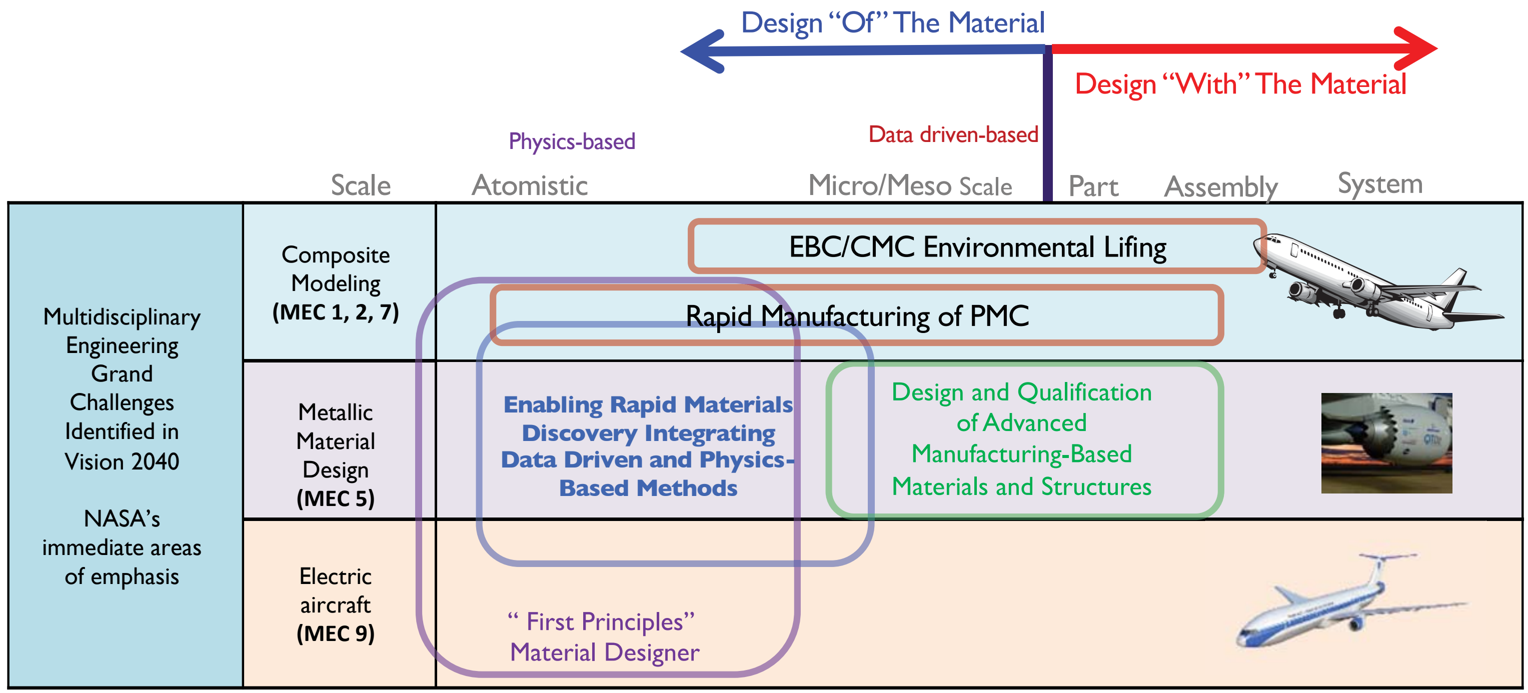
#11 NASA should engage with academia and industry stakeholders to **regularly update** this study and/or conduct follow-up studies • • •

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**

Revolutionary Tools & Methods (RTM) Swim Lanes Tightly Aligned with 2040 MECs

Combine "design of the materials" (material scientist viewpoint) and "design with the materials" (structural analyst viewpoint) approaches into a *concurrent transformational* paradigm



Strategy aligned with Vision 2040 and supporting ARMD priorities

RTM - Materials and Structures Technologies Will Address These Vision 2040 Gaps

KE	Gaps
1	❖ Underdevelopment of physics-based models that link length and time scales for relevant material systems • Underdevelopment of models that simulate materials response against harsh environments or operating conditions (i.e., insufficient data to support these models) • Establish model building block approach for multiscale modeling methods and tools • Underdevelopment of atomistic models that simulate thermal behavior, chemical reactions, and electron transfer across time scales and phases with respect to specific operating conditions. • Lack of comprehensive material property database (e.g., physical, thermal, temperature, and strain-rate-dependent metallurgical properties) • Models that simulate systems behavior are commonly based on simplified linear approximations, and do not continuously adapt to unforeseen by-products which can lead to inaccurate results
2	❖ Inability to conduct real time characterization and measurement of structure and response at appropriate length and time scales • Lack of routine practices for accurately characterizing mixed mode failure behavior (e.g., delamination, crack growth) in advanced complex material systems
3	❖ Lack of reliable optimization methods that bridge across scale
4	• Lack of systematic data fusion methods for combining and weighting multiple sources of information into single states of knowledge to inform decision making
6	❖ No widely accepted community standards or schema for materials information storage and communication methods
7	• Inability to automate the linking and execution of disparate models and computational methods with data from federated databases
9	❖ Lack of support, or adequate business models, for code development and maintenance, particularly for software used in engineering applications

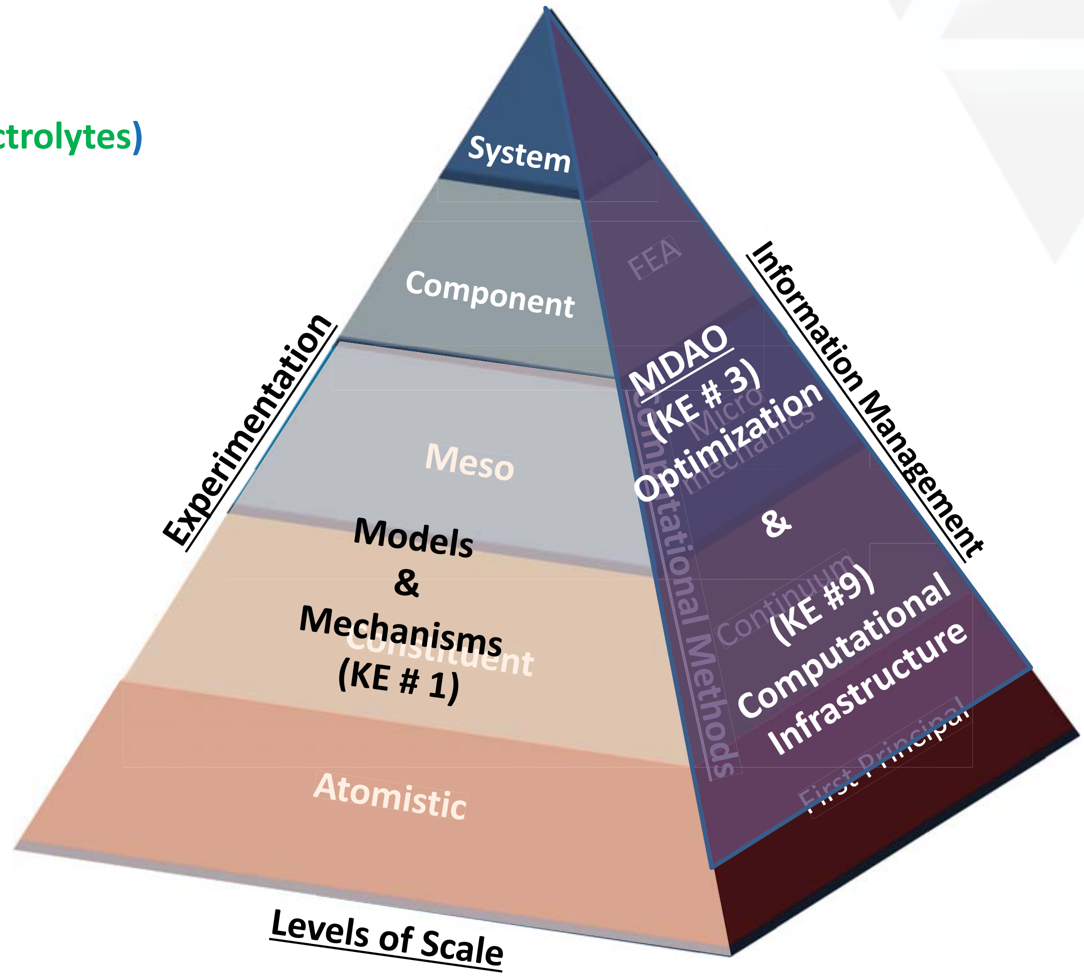
❖ Indicate Vision 2040 identified critical gaps within a Key Element Area

Building and Validating a Vision 2040 Ecosystem

RTM M&S Contribution Areas

Development/Research Areas

- Models & Mechanisms (KE1)
  - EBC/CMC Models **(TGO, Recession, CMAS)**
  - First Principle Models **(Coatings, SMA, Electrolytes)**
  - Micromechanics (**Power Cable Materials**)
  - ML surrogate models **(MAC/GMC)**
  - **Additive Manufacturing**
- Computational Framework (KE3 & KE9)
  - **NASMAT Multiscale Modeling**
    - Collaboration GE - SPFEA
    - Nanohub/MAC-GMC
    - Desire collaboration Sandia (SAW)
  - **Material Designer**
    - SMA Alloys
    - LPTS (Local Phase Transformation Strengthening) Alloys
    - Electrolytes
  - **Optimization**
    - Utilization of openMDAO framework

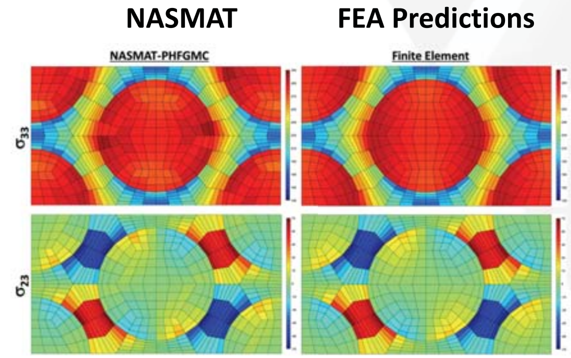


NASMAT: NASA's State-of-the-Art Multiscale Analysis Tool

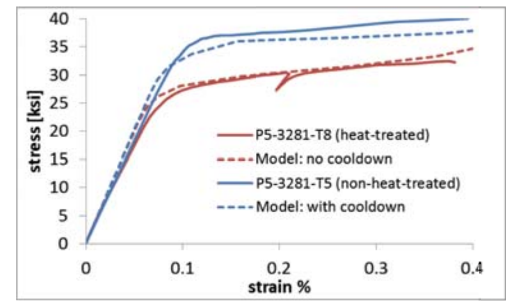
- **NASA's New State-of-the-Art Multiscale Analysis Tool – NASMAT** *is a new thread safe s*tate-of-the-art multiscale analysis software capable of executing industrial-scale multiscale structural analyses. It is based on the legacy multiscale analysis codes MAC/GMC and FEAMAC, first developed 20+ years ago, which do not effectively support parallel computing or modular functionality. Consequently, NASMAT has been designed for HPC platforms with enhanced upgradability, maintainability, interoperability, and distribution. **NASMAT** version 1.0 was recently released.

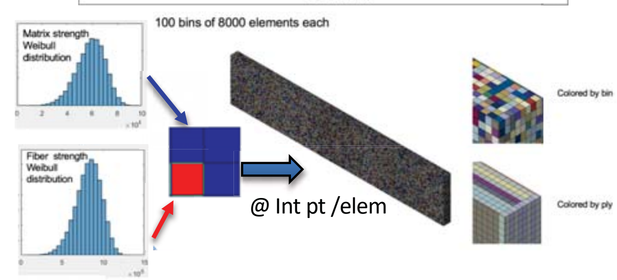
- The modularity of **NASMAT** was tested and verified by implementing two new micromechanics techniques, 1) the Parametric High-Fidelity Generalized Method of Cells (**PHFGMC**) – that allows for more general subcell geometries, 2) Carrera unified formulation (CUF)

- NASA's FEAMAC software was heavily **utilized and validated** by **GE** during an AFRL four year contract wherein they successfully ***predicted*** CMC smooth bar, open hole tension and single edge notch specimen behavior. Details were revealed during AFRLFA8650-11-C-5227 Final Review, Feb 2019.



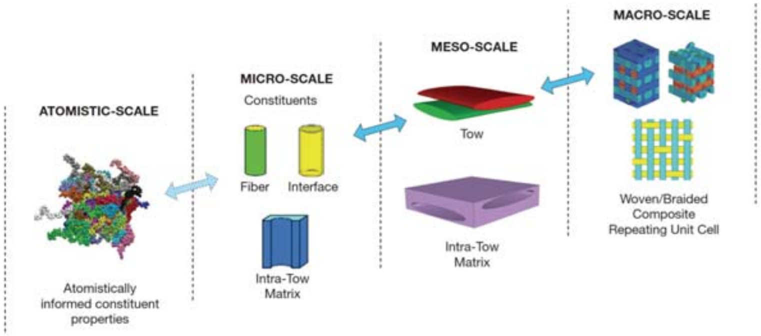
Smooth bar Predictions

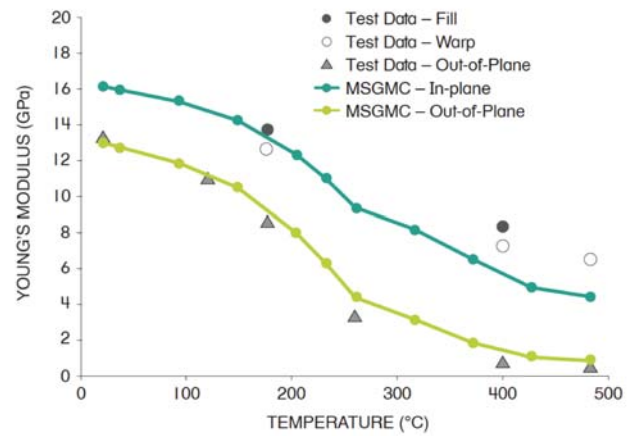




Single Edge-Notched Bend Simulations

Multiscale Modeling: Atomistic to Effective Properties





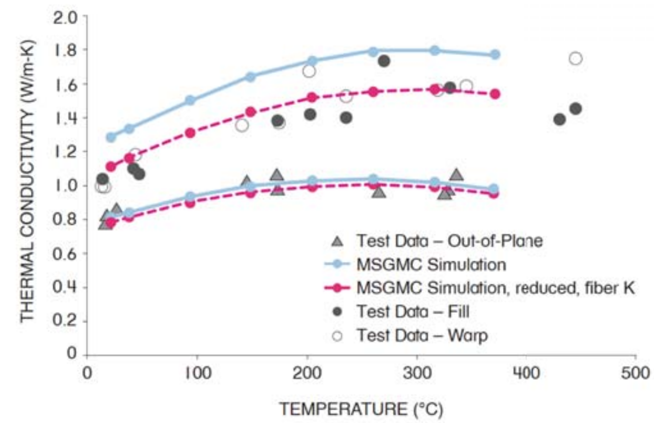
Significance for Vision 2040

MODELS & METHODOLOGIES
Methodologies based on Multiscale Generalized Method of Cells (MSGMC) will enable linkages with lower length-scale models.

CHARACTERIZATION
Quantitative structure definitions tied to models and test protocols will enable hierarchical characterization of complex failure mechanisms.

OPTIMIZATION
Improved predictive capabilities and analytical tools will help determine strength margins and optimum layup strategies for complex material architectures, such as composites.

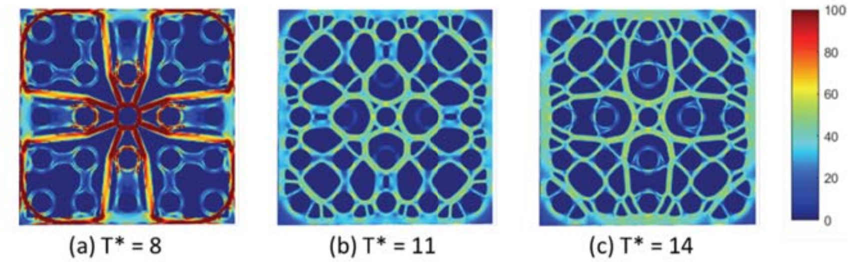
DATA, INFORMATICS, VISUALIZATION
Statistical descriptors and data structures will improve data quality and help automate the extraction of data from processing, characterization, and testing equipment.



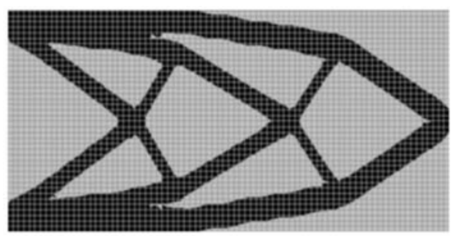
S.M. Arnold, et al., *Multiscale Modeling of Carbon/Phenolic Composite Thermal Protection Materials: Atomistic to Effective Properties*, NASA (Ohio: NASA, 2016).

openMDAO Is A Framework That Can Couple Materials + Structures For ICME

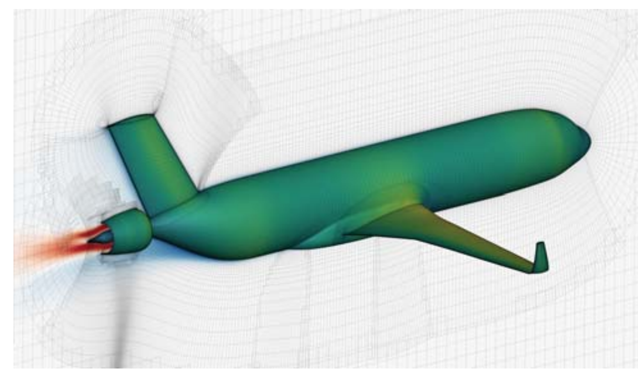
- Specializing in gradient based optimization with analytic derivatives
- Capable of integrating large scale PDE solvers (CFD, FEA)
- Has been used to solve coupled multi-physics topology optimization problems
- http://openmdao.org



Coupled structural-thermal topology optimization



2d topology optimization with discrete adjoint built entirely in OpenMDAO



Aeropropulsive design optimization of tailcone BLI thruster

Material Designer Currently Under Development

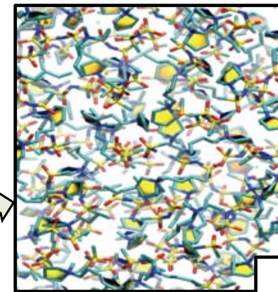
Steps in Design of Materials

1) Understanding SOA Materials
- a) High fidelity property predictions
- b) Physics based mechanisms discovered
- c) Property screening descriptor derived

2) Design of New Materials
- a) Database generation (exp. and/or comp.)
- b) High throughput screening
- c) Rapid property predictions (reduced order/ ML model)
- d) Optimization

3) Multiscale coupling to composites, structures, devices, chemical kinetics models, etc.

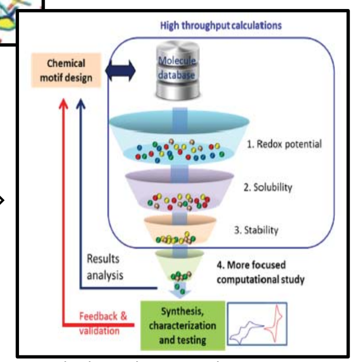
Design Rule Discovery



High Fidelity Simulations of SOA Materials

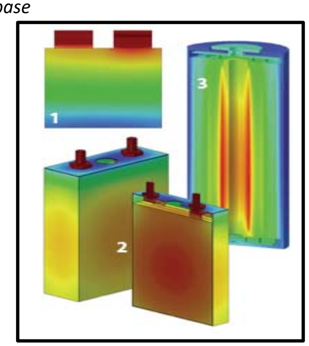
Target Materials
1) **Coatings**
2) **Alloys (SMA, LPTS)**
3) **Electrolytes**

Screening



High Throughput Database Screening for New Materials

Multiscale/Multiphysics Assembly



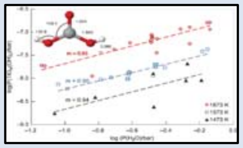
Multiphysics Coupling of Designed Materials

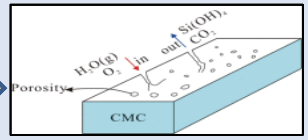
1) High fidelity models of SOA materials yield physics based mechanisms and screening descriptors
2) Descriptors and rapid property predictions enable detailed high throughput screening and validation
3) Designed materials coupled to larger structure, device, etc. with multiscale model

Material Designer Applications

Advanced coatings reduce emissions, noise and engine weight

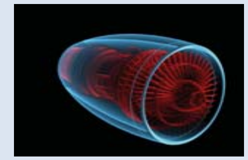
Coatings


High fidelity Thermochemistry

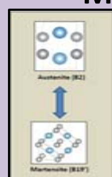


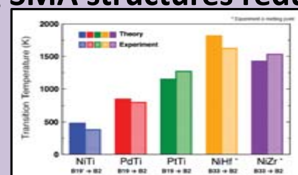
EBC Degradation Mechanisms

Advanced EBC Design

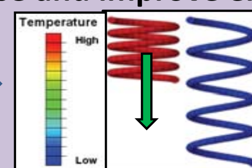

High Efficiency Engines

Morphing SMA structures reduce noise and improve energy efficient


Atomic Composition



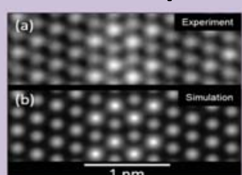
SMA Design Tool



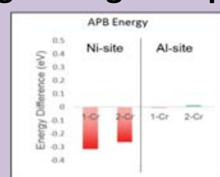
Tunable Actuation


Morphing Aircraft Structure

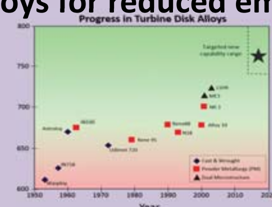
Computational design of high temperature alloys for reduced emissions and hybrid aircraft



Atomic Char & Sim



Comp Analysis of Defects

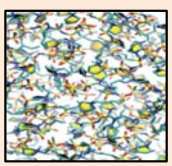


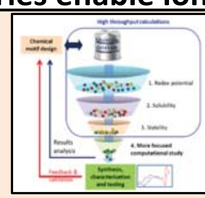
Superior HT Alloy Compositions

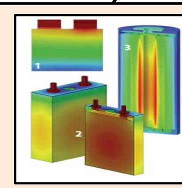
HT Small Core Turbines for Hybrid EAP

Ultra-high energy batteries enable long range, low noise, low emission electric aircraft

Batteries


Large Scale Simulations


High Throughput Screening


Novel Device Architectures

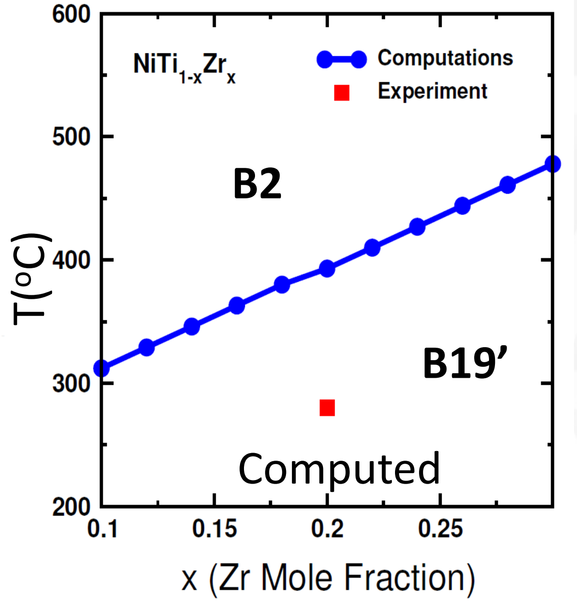

Long Range Electric Aircraft

First Principles Thermodynamics for SMA Ternaries

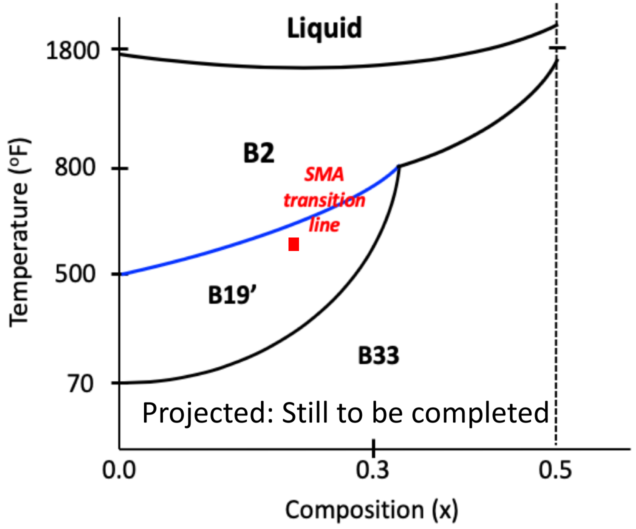
OBJECTIVE
- Apply high fidelity, first principles methods to predict thermodynamic properties of ternary shape memory alloys including phase behavior and phase transitions

APPROACH
- Computational method based on thermodynamic integration and *ab initio* molecular dynamics (AIMD) utilized to compute free energies of phases
- Ternaries are challenging because they are fundamentally *random* systems whereas previous work on binaries was *ordered*.
- Special quasi-random structures (SQS) were generated for each x as representative random structures to reduce computational cost

SIGNIFICANCE
- *First-of-its-kind* computations for ternaries performed to date



RESULTS
- Full thermodynamic analysis performed for $Ni_{0.5}\,Ti_{(0.5-x)}\,Hf_x$ and $Ni_{0.5}\,Ti_{(0.5-x)}\,Zr$ for x=[0, 0.5]
- *Phase diagram generated as a function of composition (x) and temperature (T)*
- A full analysis was performed including phase stability for the major phases (B2, B19', B19, B33) for each x and as a function of T
- Computational models use perfect, defect free single crystals. Therefore, they overpredict the experimental transition temperature. Similar behavior was seen with the binaries.
- *Correct trend of increasing T_M with x reproduced*



FUTURE WORK
- Complete description of phase diagram; other ternaries; mixed ternaries; predict mechanical properties, e.g. cycle life, work output, etc.; screening/design with ML

POC: John Lawson (ARC)

Discovery of a Novel Strengthening Mechanism for High Temperature Superalloys

OBJECTIVE

Evaluate the effect of recently observed atomic-scale stacking fault phase transformations have on creep strength in Ni-base Superalloys.

APPROACH

- Through state-of-the-art characterization and modeling techniques two different Ni-base superalloys with minor changes in refractory content were explored.
- Density functional theory (DFT) models provided groundbreaking insights into new atomic scale high temperature deformation mechanisms active for these alloys.
- Scanning transmission electron microscopy (STEM) confirmed the analysis performed using DFT.

SIGNIFICANCE

It was discovered that higher amounts of Tungsten facilitated a solid-state phase transformation along intrinsic stacking faults within the strengthening γ′ precipitates. Density functional theory models demonstrated that this phase transformation would inhibit further shearing of the precipitate improving the overall creep properties of the alloy. This is one of the first studies to explore the effect stacking fault segregation has on the creep properties for this class of alloys and this finding may have strong implications in how future high temperature alloys are characterized and designed.

New TTT alloy represents a **3x** improvement in creep life for this environment over SOA LSHR alloy, also performs as good as single crystal (CMSX4) alloy!!!

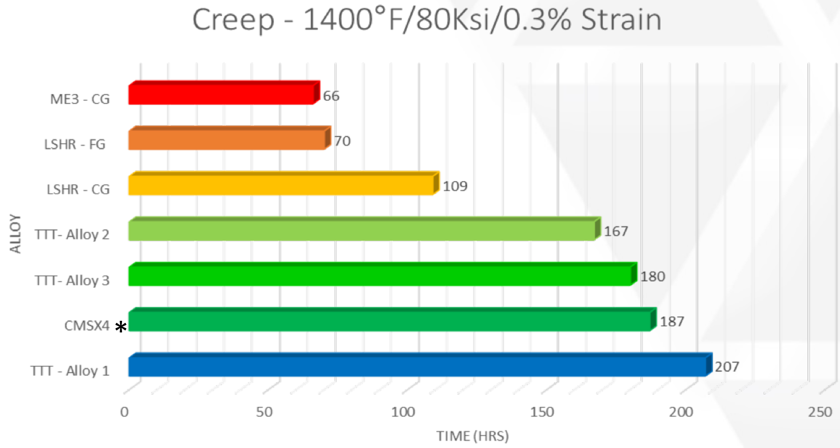


Figure 1: Creep performance of current state-of-the-art disk superalloys ME3 and LSHR compared to the TTT developed superalloys at 1400°F and 80 Ksi. Alloy 1 represents a 3x improvement in creep life for this environment

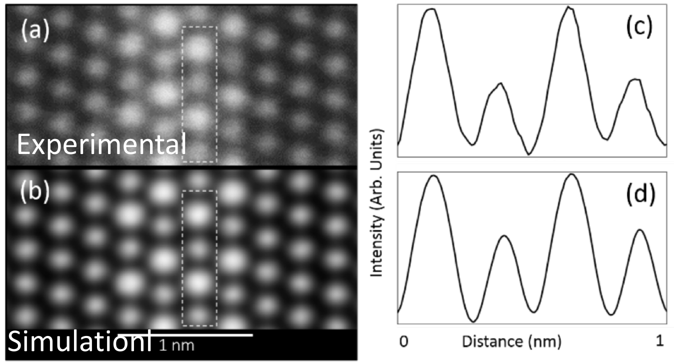


Figure 2: (a) Experimental and (b) simulated HAADF image of a intrinsic fault in LSHR. (c) Experimental and (d) simulated averaged intensity of the atomic columns moving down the fault as highlighted the boxes in (a) and (b).

POC: Tim Smith, Brian Good, Tim Gabb, Laura Evans, Steve Arnold (GRC)

Building and Validating a Vision 2040 Ecosystem
RTM M&S Contribution Areas

Development/Research Areas

Data, ML, Visualization (KE2)

Data Management

- Granta MI (ICME schema)
  - CMC
  - EBC
  - CMAS

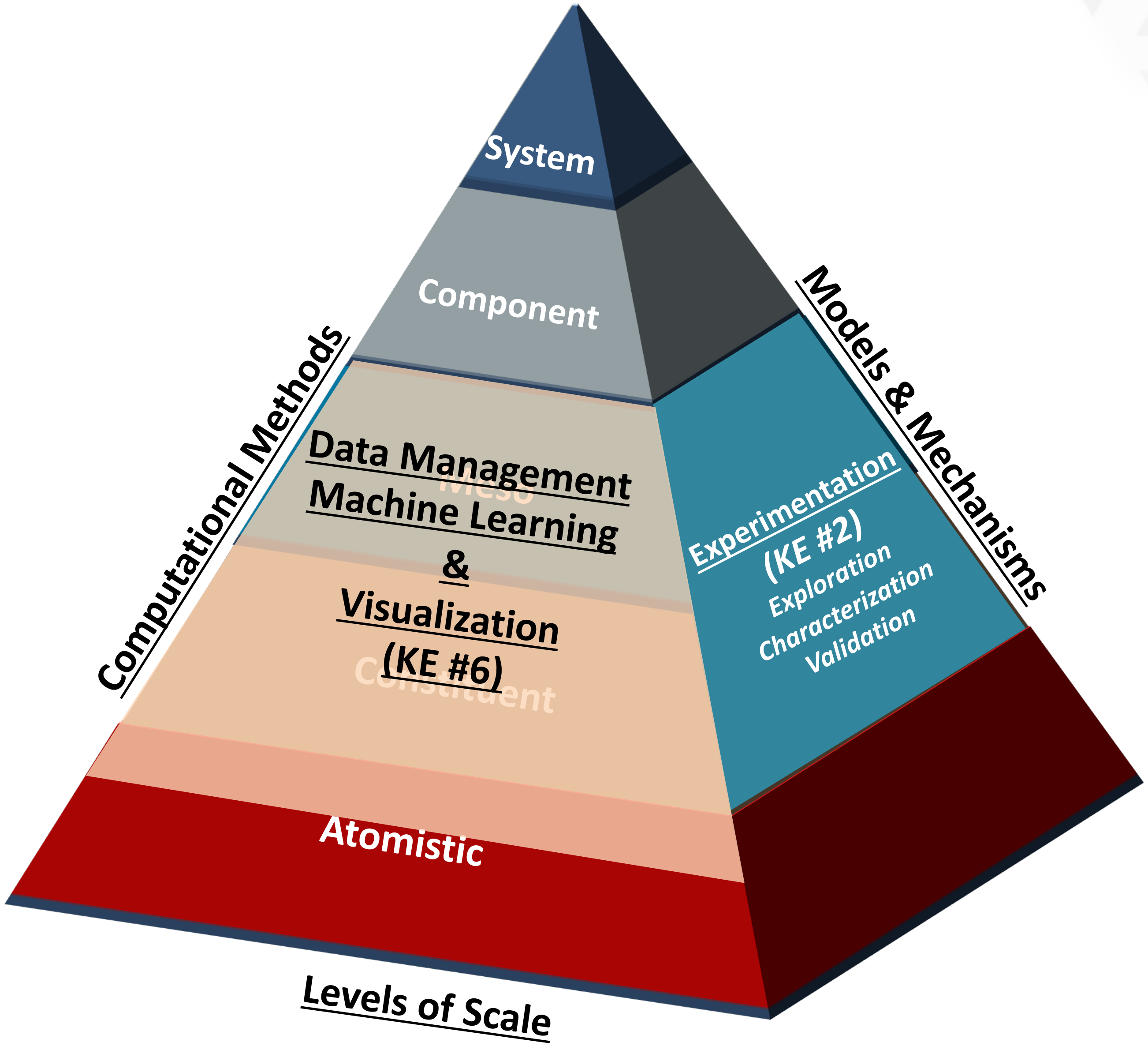
Machine Learning

Optimal Experimental Design

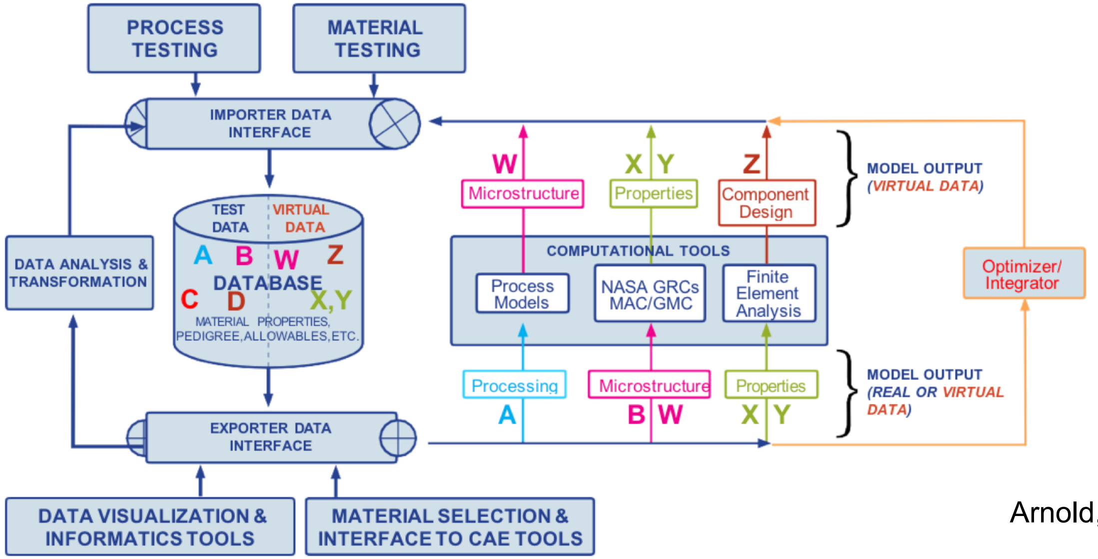
- Deep Learning NN (Neural Network)
  - MAC/GMC - Laminate (Tensile & Fatigue)
  - Atomistic (Anharmonic Energy)
  - Polymers for Rapid Manufacturing
  - Physically-Informed NN EAM Potentials
- Estimation Theory
  - Stochastic Optimization

Visualization

- Multiscale



Information Management Enabling Multiscale Modeling Within ICME Paradigm



ICME infrastructure for housing both modeling and testing information

Arnold, et al.; *"Combining Material and Model Pedigree is Foundational to Making ICME a Reality"*, IMMI, 4:4, 2015.

Significance for Vision 2040

DATA, INFORMATICS, & VISUALIZATION
Coupling data management libraries and visualization software suites will drive the ecosystem for generating fundamental 3D/4D datasets, thereby enabling the validation of crucial physics-based models.

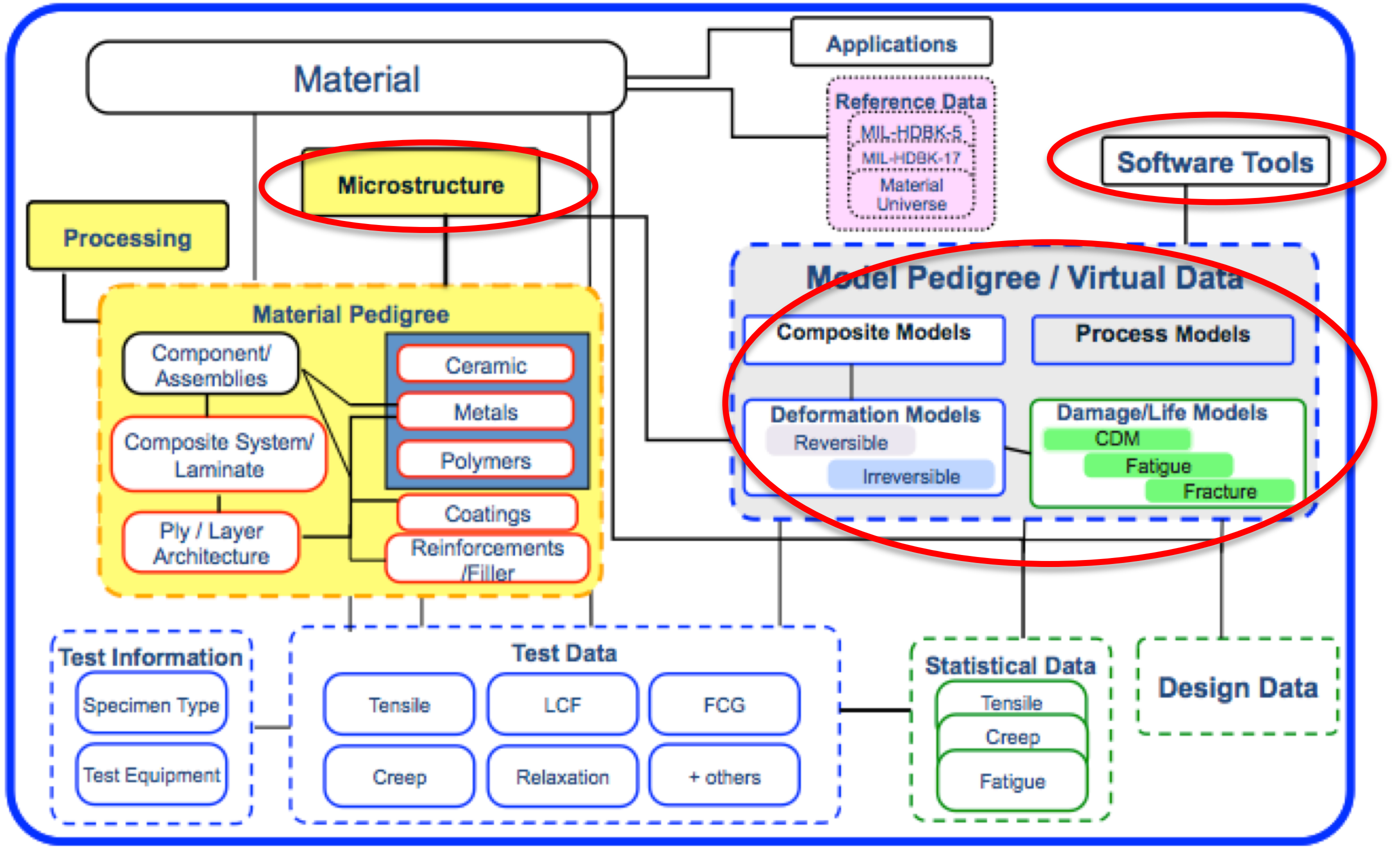
CHARACTERIZATION
Robust model-structure-response definitions will provide the foundation for reliable methods of managing error and uncertainty

WORKFLOW & COLLABORATION FRAMEWORKS
Database and optimization software suites will enhance workflow functionalities and facilitate cross-organizational sharing of data, tools, and models.

COMPUTATIONAL INFRASTRUCTURE
Machine learning and analytical tools will help design software suites take advantage of novel HPC paradigm and various hardware configurations.

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

To accomplish this introduced Model Tables in addition to Microstructure and Software Tools Table

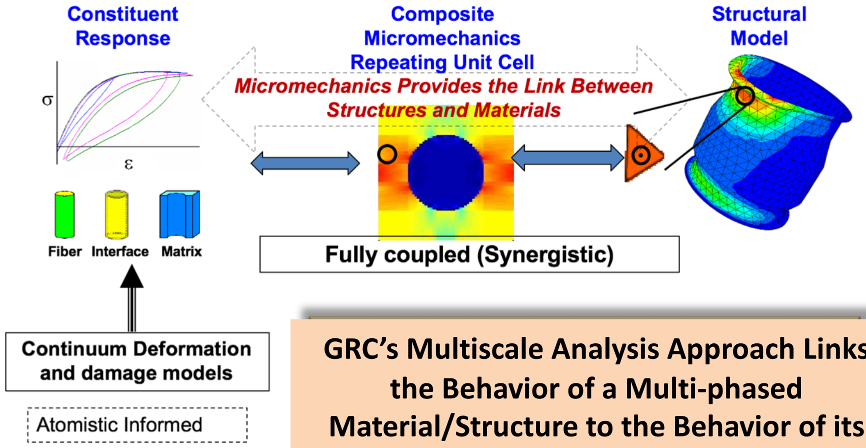


Arnold, S.M., Holland, F. and Bednarcyk, B.A.; (2014). Robust Informatics Infrastructure Required For ICME: Combining Virtual and Experimental Data, 55th AIAA/ASME/ASCE/AHS/SC Structures, Structural Dynamics, and Materials Conference, National Harbor, Maryland, 13 - 17 January 2014, AIAA-2014-0460

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

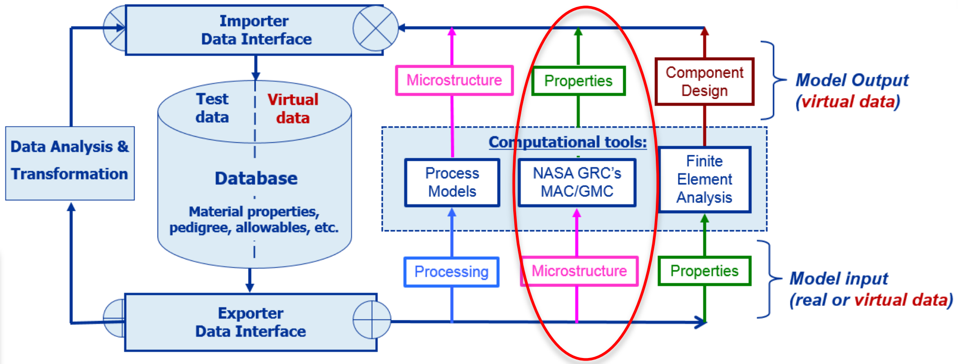
Arnold, S.M., Holland, F.A., Bednarcyk, B.A., and Pineda, E.J.;(2015) "Combining Material and Model Pedigree is Foundational to Making ICME a Reality", Integrating Materials and Manufacturing Innovation, IMMI, 4:4 DOI 10.1186/s40192-015-0031-2.

Granta MI Software Coupled with GRC's MAC/GMC to Enable ICME of Composites



GRC's Multiscale Analysis Approach Links the Behavior of a Multi-phased Material/Structure to the Behavior of its Constituents

Coupling between testing and simulation data is key to realizing ICME

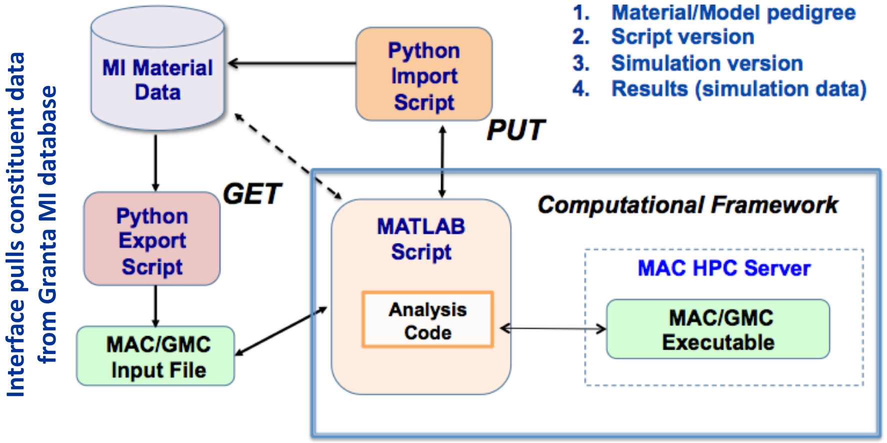


- Linkage to Granta MI software done in collaboration with Granta Design Ltd.

Linkage Established through Workflow and Python Scripts

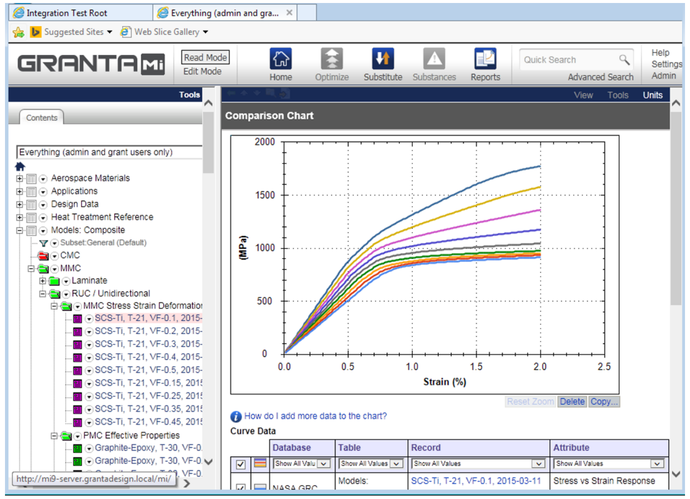
Workflow enables full traceability

1. Material/Model pedigree
2. Script version
3. Simulation version
4. Results (simulation data)



Workflow captures GRC's MAC/GMC simulation data, with full model pedigree, within Granta MI

Simulation results, including nonlinear curves, are captured and stored in Granta MI database, along with all relevant metadata

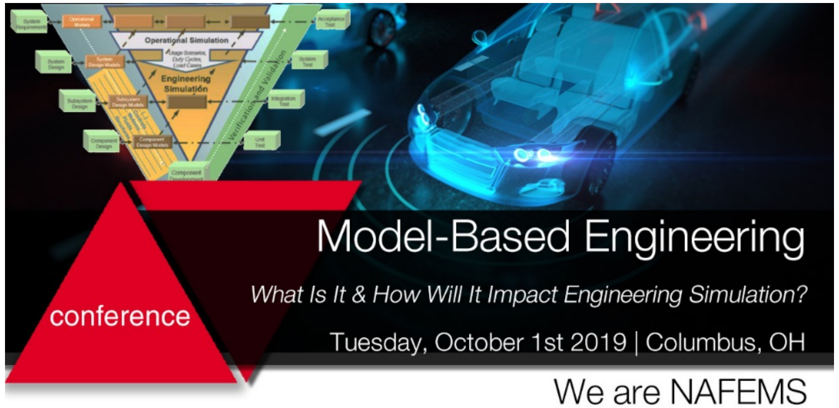


Future 2040 Funding Opportunities

- NASA Research Announcement (NRA) **due to be released Fall 2019** – see https://nspires.nasaprs.com/external/solicitations/solicitations.do
- SBIR/STTR - see https://sbir.nasa.gov/prg_sched_anncmnte
- Anticipating a new $8 Mil funding wedge to begin in FY21 (Oct 2020) targeted toward revolutionary materials development

NASA CR 2018-219771

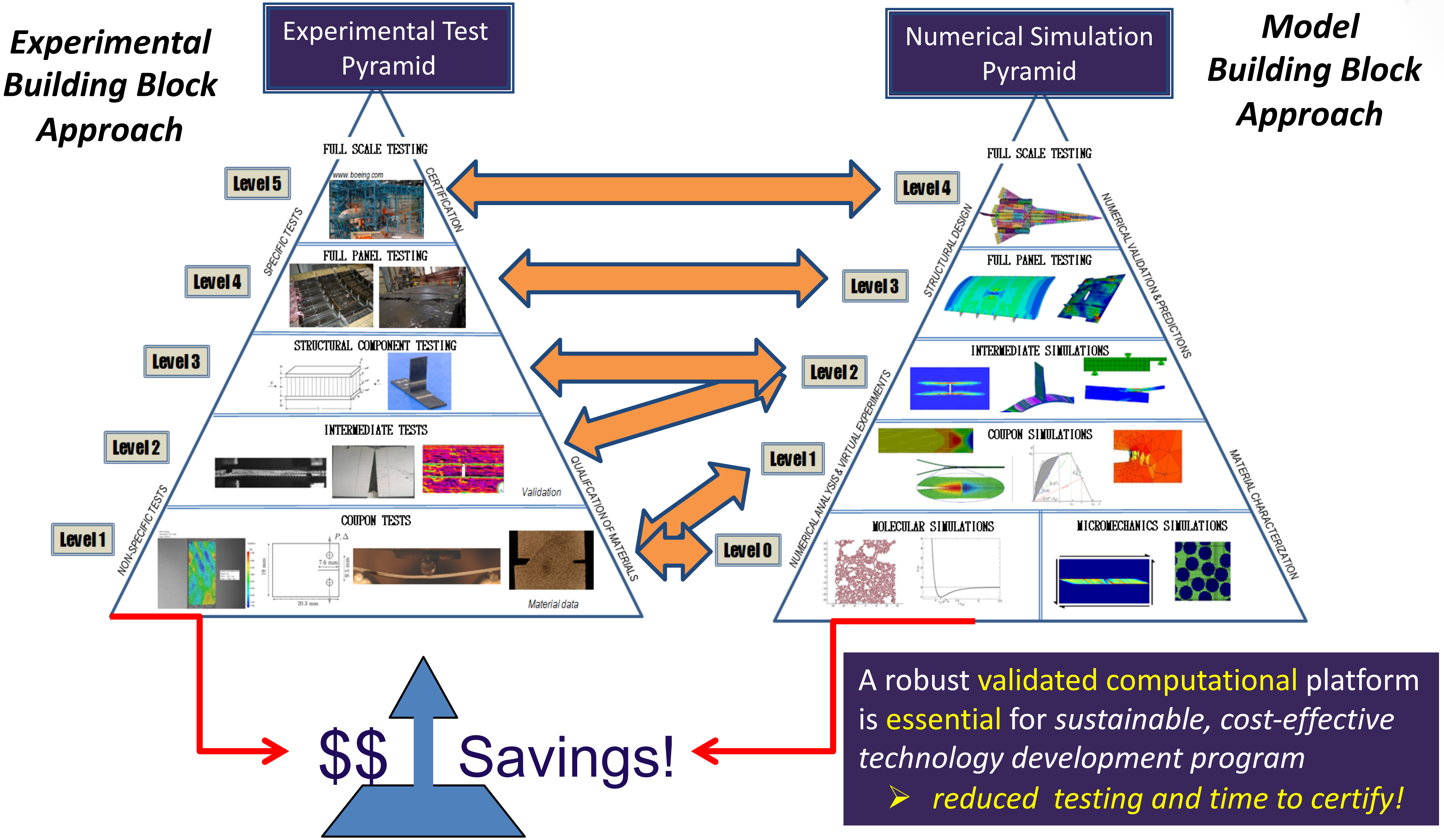
https://ntrs.nasa.gov/archive/nasa/casi.ntrs.nasa.gov/20180002010.pdf



Thank You!

Contact: Steven.M.Arnold@nasa.gov

Virtual Testing Can Enable Significant Cost Savings in Certification Process



A robust validated computational platform is essential for *sustainable, cost-effective technology development program*

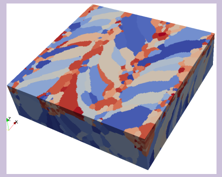
- *reduced testing and time to certify!*

Rapid Manufacturing and Qualification Supporting Commercial and Urban Aviation

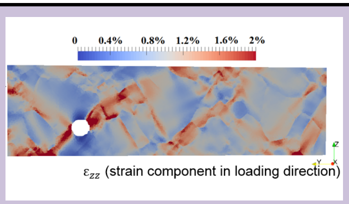
Computational Materials Enables Next Generation Qualification of AM

Additively Manufactured Metals

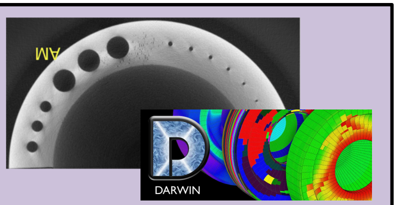
Configurable Architecture Additive Testbed



Process-Microstructure



Microstructure-Performance



Engineering Capabilities for Material Qualification

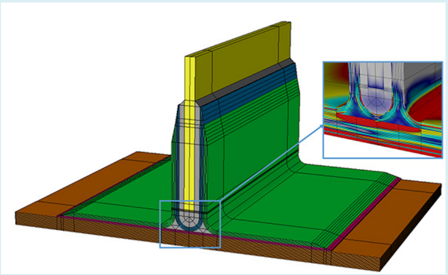
Unitized Structures are Enabling to Rapid Manufacturing of Commercial and UAM Vehicles

Unitized PMC Composites

Computational NDE-Informed Inspection Capability

Laser Ablation Techniques for Surface Preparation

Simulation Software for Bond-Performance and Defect Assessment



Rapid Manufacturing of Unitized Commercial and UAM Vehicle Components

Vision for UAM