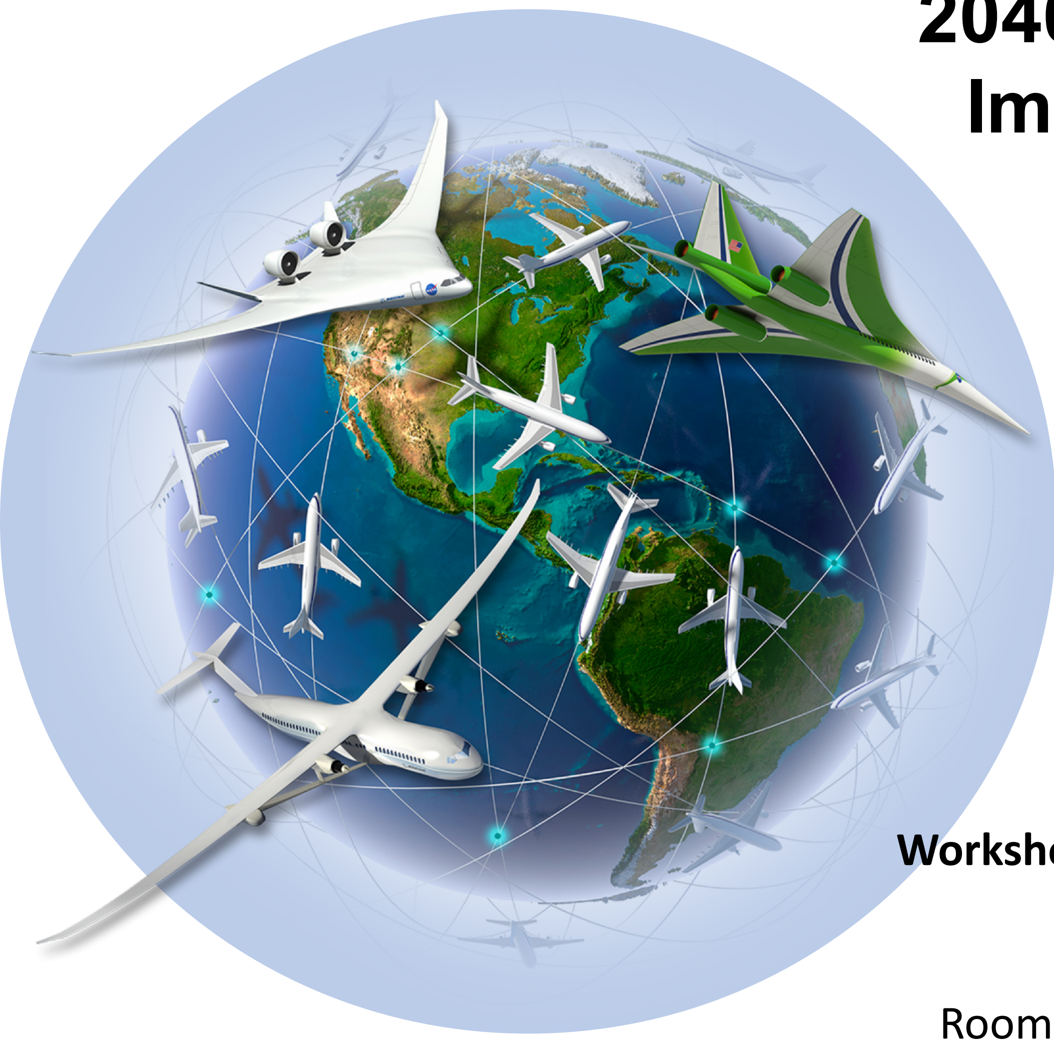


2040 Vision Study: NASA's Implementation Activities

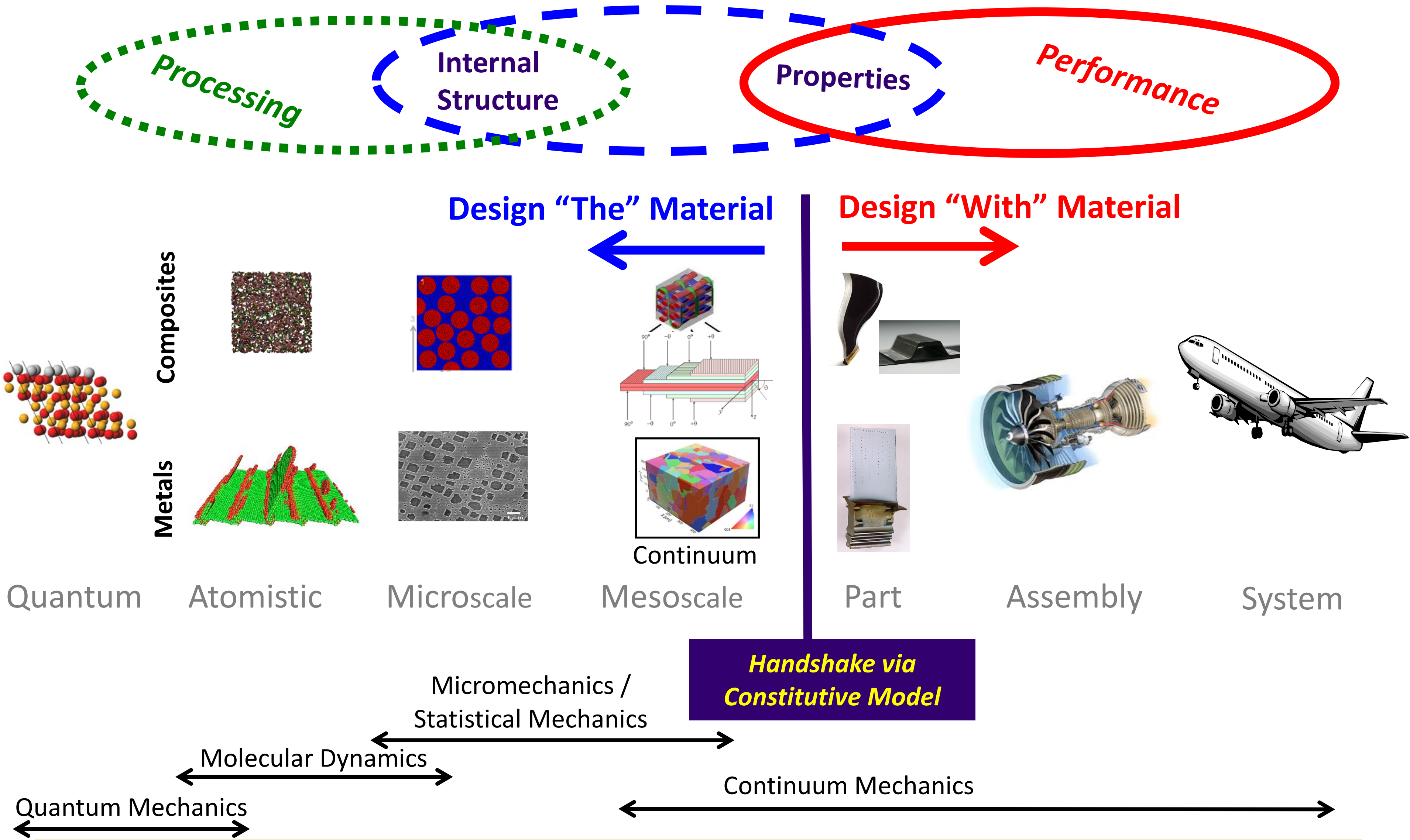
Steven M. Arnold
Material and Structures Division
NASA Glenn Research Center

Workshop on: "Data Analytics And What It Means To The Materials Community"
National Academy of Sciences building,
Room NAS120 at 2101 Constitution Avenue, NW.
July 16-17th 2019

Outline

1. Vision 2040 Background
2. Proposed: Integrated Multiscale Material/Structure Designer Ecosystem
3. Example Activities related to ML and Informatics

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**.

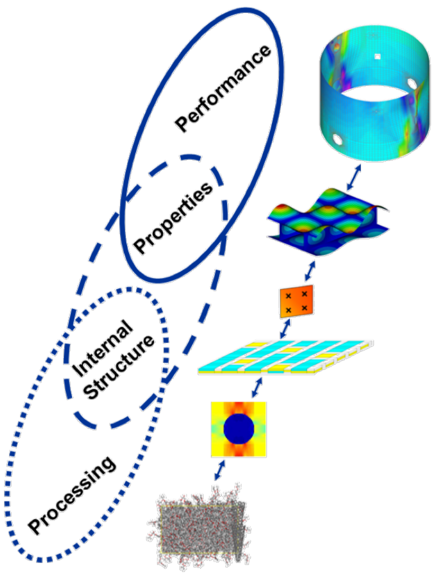
2040 Ecosystem Revolutionizes Design Paradigm

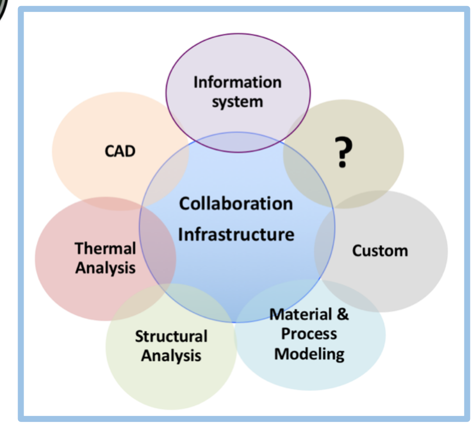
The cyber-physical-social ecosystem that marries "the design of materials" (material scientist viewpoint) with "the design with materials" (structural analyst viewpoint) approaches into one concurrent transformational digital paradigm.

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





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
Data Analytics and Visualization *Stream*

Key Element	Gap	Accessible	Adaptive	Interoperable	Robust	Traceable	User-Friendly
KE4 Decision Making and Uncertainty Quantification	Existing models and software codes are not designed to compute input sensitivities and propagate uncertainties to enable UQ						
	Lack of standards/best practices for decision making and for quantifying and presenting uncertainties in data across multiple length and time scales						
KE6 Data, Informatics and Visualization	Lack of community-accepted practices or standards for mining and quantifying complex materials information and datasets between experiments and models						
	Many materials information frameworks are not sufficiently developed for compatibility with state-of-the-art data analysis and management technology						
	Human involvement in thresholding and segmentation limits the suitability of 2D/3D/4D images for analysis						
	Limited ability to capture and represent time dependent data (4D)						
	Limited ability to represent translucency among multiple layers of data						
	Deep Learning and Machine Learning (ML) techniques are not implemented across MS&E disciplines, and across length scales						
	Workforce not sufficiently trained in data science, machine learning, programming, and analysis • Not yet accepted as vital aspect of materials and structures engineering disciplines						
KE8 Education and Training	University curricula—especially for non-computer science disciplines—are not sufficiently imparting undergraduates with the skills needed to transition to industry • Data analysis; Code development; Version control; Quality assurance • Familiarity with commercial modeling and simulation software packages						
[KE9] Computational Infrastructure	Lack of methods capable of using artificial intelligence/machine learning to improve scalability						

Major Recommendations: Vision 2040

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

RECOMMENDATION #2:
NASA and other relevant federal agencies should form ***an interagency coordinating body*** to not only affect alignment of federal investments but also coordinate those federal investments with industry investments to ensure government, industry, and academia work in concert to achieve the 2040 vision.

RECOMMENDATION #3: NASA should engage with government, industry, and academic stakeholders to develop an agreed-upon interoperability framework for the envisioned ecosystem, with emphasis on data-exchange mechanisms

Software Forum/Panel Session @ SciTech 19; San Diego, CA , Jan 2019

RECOMMENDATION #4: NASA should partner with other government agencies and professional societies to ***identify and pursue benchmark materials, systems, and applications*** to focus early efforts on addressing critical gaps and actions identified in this report.

Intension is to solicit help from AIAA to help coordinate

RECOMMENDATION #5: NASA and other government agencies (e.g., NIST) should lead a coordinated effort to 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.

Major Recommendations: Vision 2040

RECOMMENDATION #6:
NASA should lead **demonstration projects** that document and publicize the broad benefits (e.g., cost savings) of model-based concurrent design, development, and deployment of materials and systems

RECOMMENDATION #7: NASA and other relevant federal agencies (i.e., NSF, DOE, DoD, and others) should increase fundamental research efforts to ***develop, characterize, and validate improved physics-based and data-driven materials models***.

RECOMMENDATION #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 and develop a highly skilled future materials science and system engineering workforce

*Collaboration Institutes of Education and Training (CIETs)

RECOMMENDATION #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.

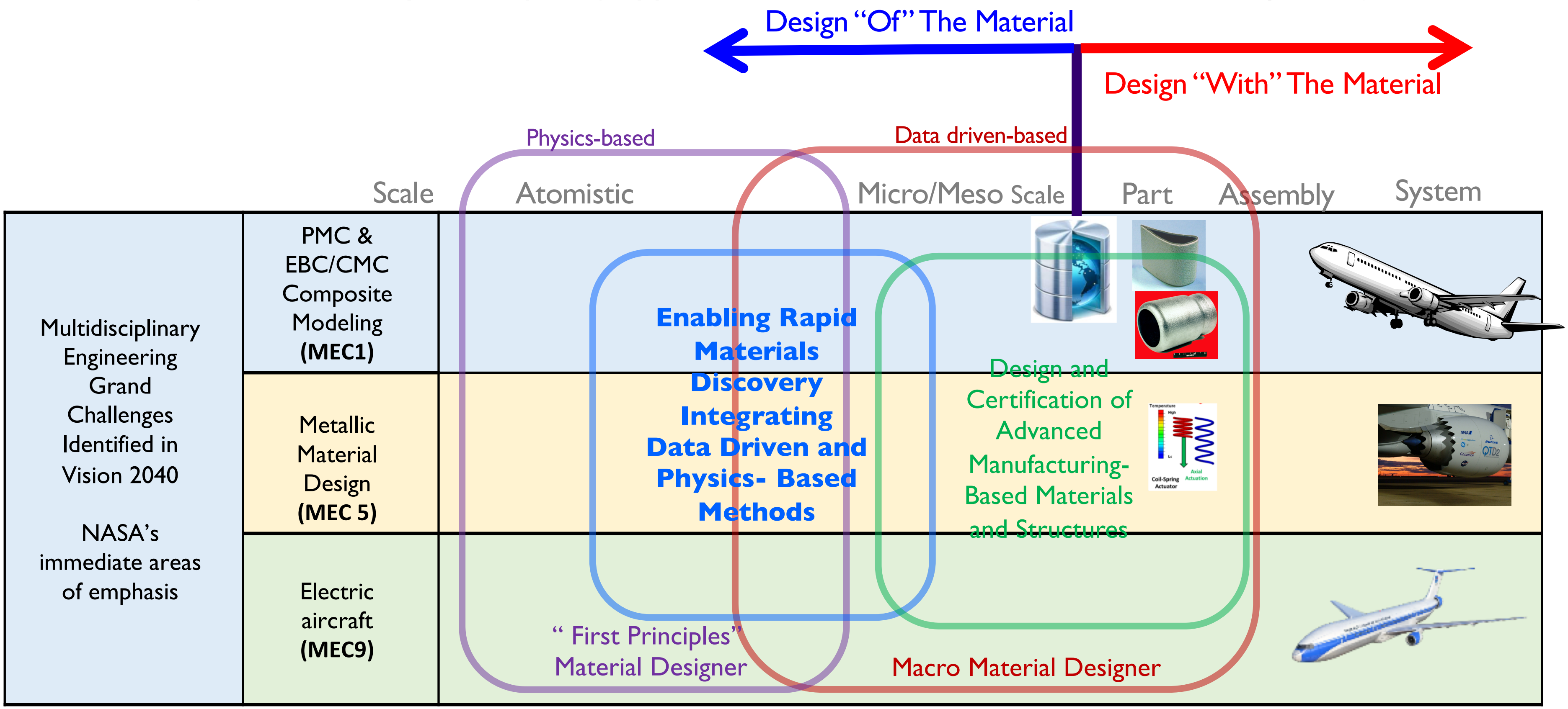
RECOMMENDATION #10 NASA and other federal agencies should support the growth of small businesses working in ICME to strengthen U.S. manufacturing competitiveness and establish U.S. leadership in this emerging field.

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

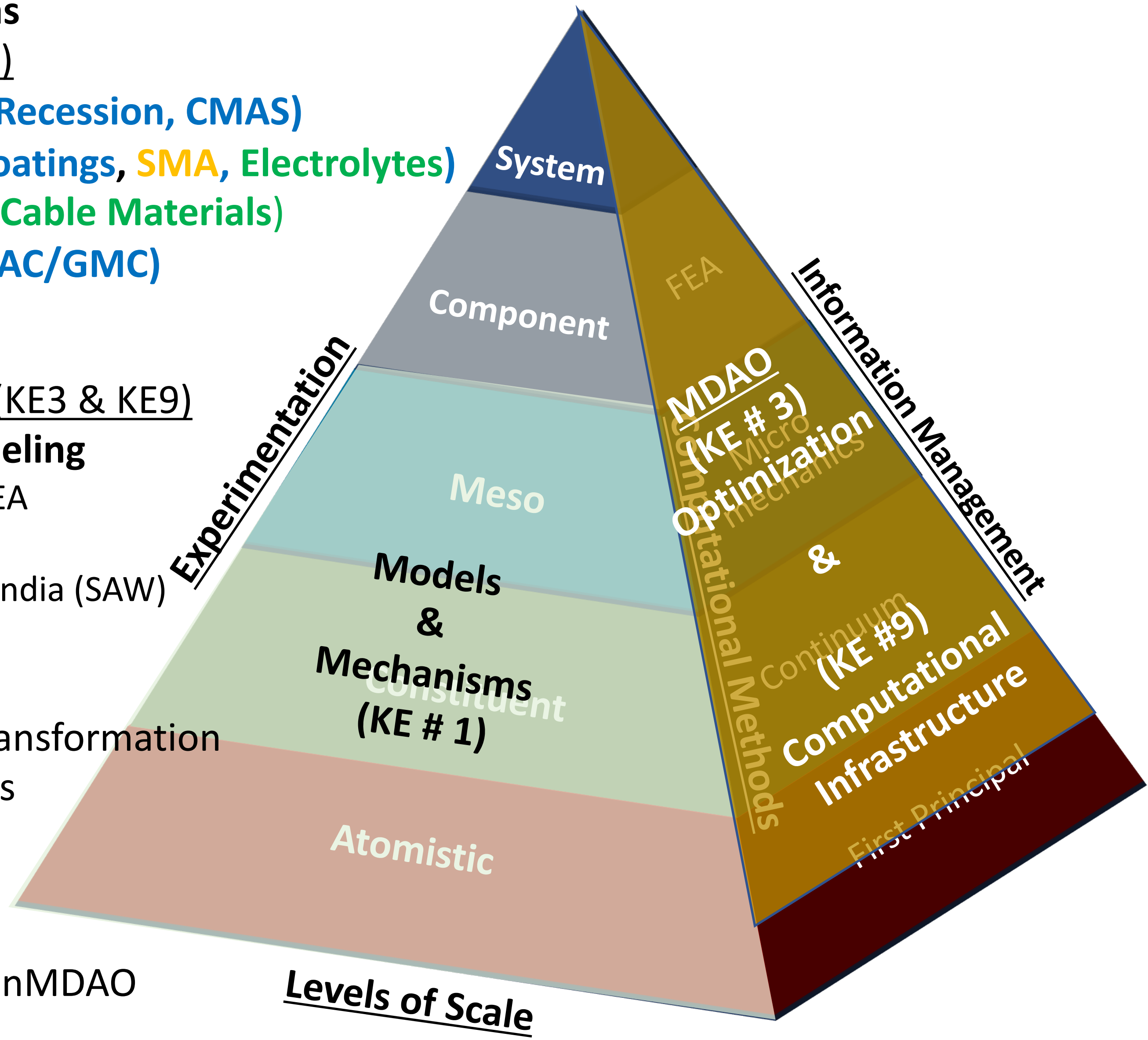
❖ Indicate Vision 2040 identified critical gaps within a Key Element Area

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

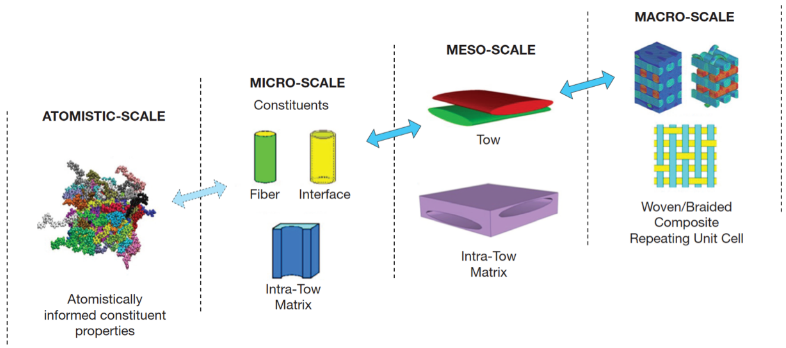
Development/Research Areas

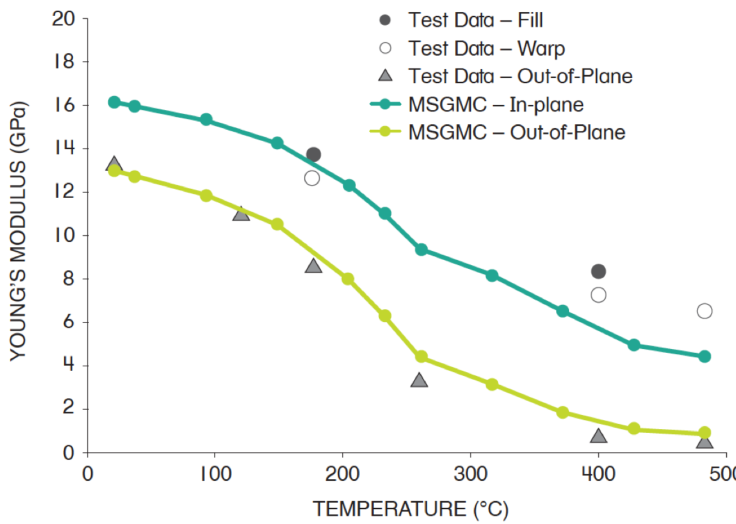
- Models & Mechanisms (KE1)
  - EBC/CMC Models **(TGO, Recession, CMAS)**
  - First Principle Models **(Coatings, SMA, Electrolytes)**
  - Micromechanics (**Power Cable Materials**)
  - ML surrogate models **(MAC/GMC)**
  - **Additive Manufacturing**

- 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**
    - Connection with openMDAO framework



Multiscale Modeling: Atomistic to Effective Properties





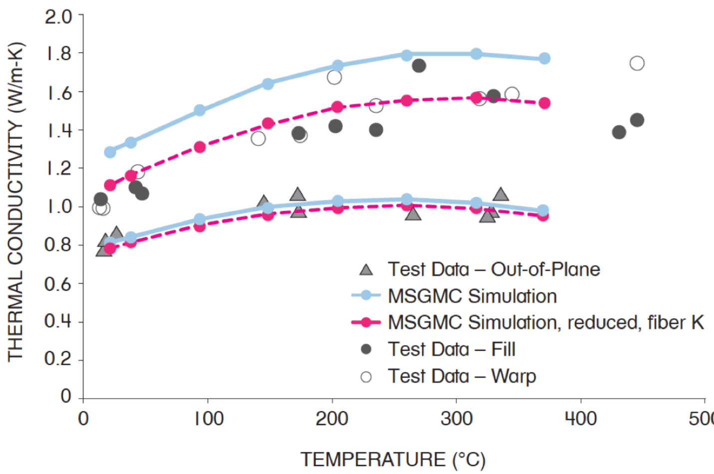
Significance for Vision 2040

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.



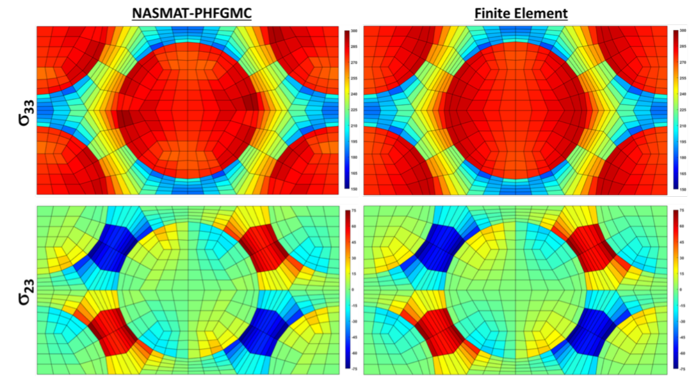
S.M. Arnold, et al., *Multiscale Modeling of Carbon/Phenolic Composite Thermal Protection Materials: Atomistic to Effective Properties*, NASA (Ohio: NASA, 2016).

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

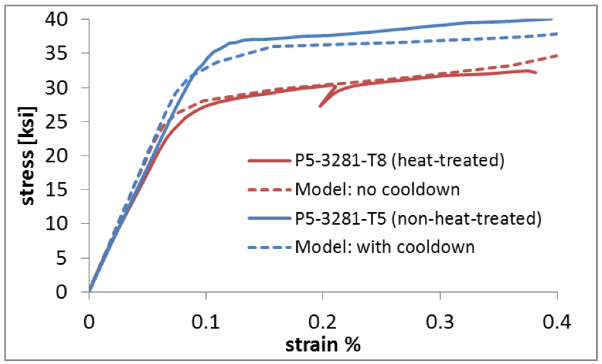
- **NASMAT: NASA’s New State-of-the-Art Multiscale Analysis Tool – NASMAT** *is a new thread safe* state-of-the-art multiscale analysis software capable of executing <u>industrial-scale</u> multiscale structural analyses. It is based on the legacy multiscale analysis codes MAC/GMC and FEAMAC, first developed 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 a new micromechanics technique– the Parametric High-Fidelity Generalized Method of Cells (**PHFGMC**) – that allows for more general subcell geometries.

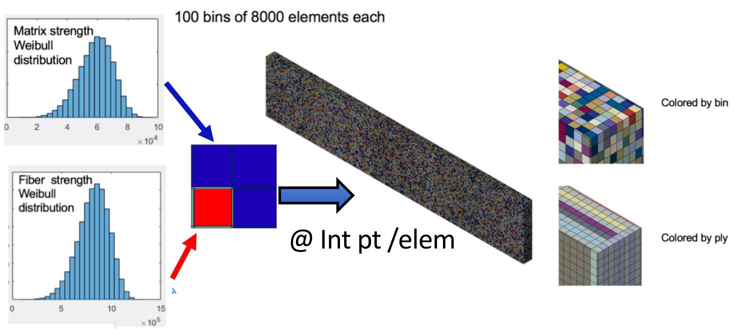
- NASA’s FEAMAC software was heavily **<u>utilized and validated</u>** by **GE** during an AFRL four year contract wherein they successfully ***predicted*** CMC smooth bar, open hole tension and single edge notch specimen behavior. Details were revealed during AFRLFA8650-11-C-5227 Final Review, Feb 2019.

NASMAT **FEA Predictions**



Smooth bar Predictions





Single Edge-Notched Bend Simulations

Material Designer

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

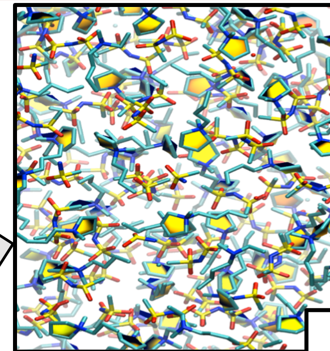
Steps in Design of Materials

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

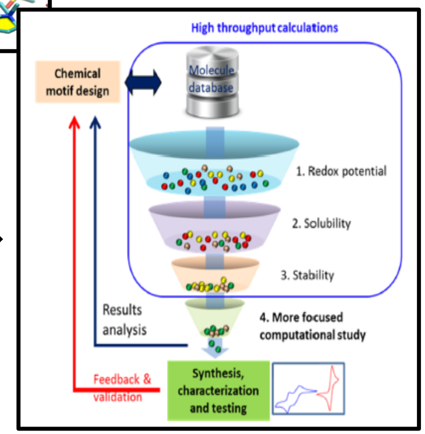
3) Multiscale coupling to composites, structures, devices, chemical kinetics models, etc.

Design Rule Discovery



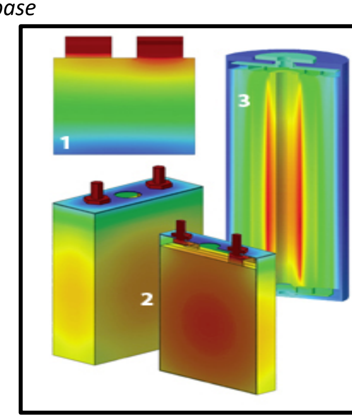
High Fidelity Simulations of SOA Materials

Screening



High Throughput Database Screening for New Materials

Multiscale/Multiphysics Assembly



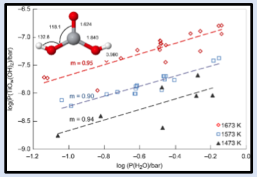
Multiphysics Coupling of Designed Materials

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

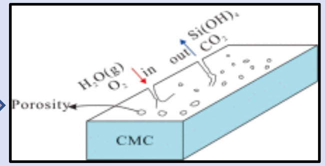
Material Designer Applications

Advanced coatings reduce emissions, noise and engine weight

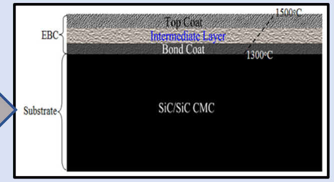
Coatings



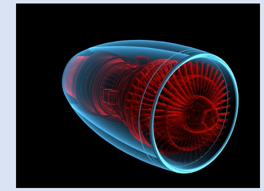
High fidelity Thermochemistry



EBC Degradation Mechanisms

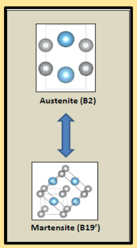


Advanced EBC Design

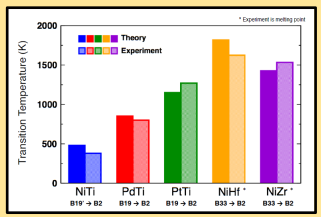

High Efficiency Engines

Morphing SMA structures reduce noise and improve energy efficient

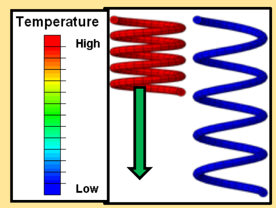
Metallic Alloys



Atomic Composition



SMA Design Tool

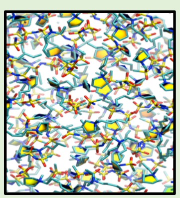


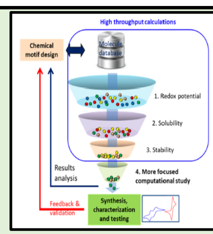
Tunable Actuation


Morphing Aircraft Structure

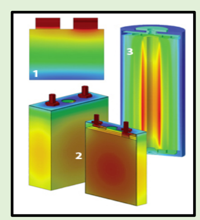
Ultra-high energy batteries enable long range, low noise, low emission electric aircraft

Batteries


Large Scale Simulations



High Throughput Screening



Novel Device Architectures


Long Range Electric Aircraft

Simple Parameterizations Hint at Reduced Order Models for SMA Predictions

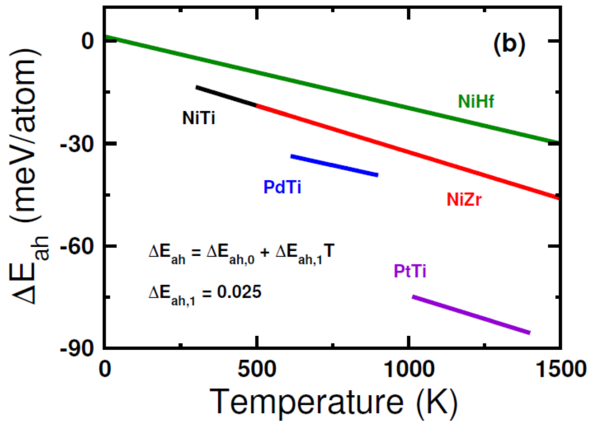
OBJECTIVE
First principles thermodynamics *prediction* of SMA transition temperature for arbitrary ternary high temperature SMA (HTSMA)

APPROACH
Ab initio molecular dynamics simulations used to compute thermodynamic phases of HTSMA. Transition temperatures and other thermodynamic information (specific heats, thermal expansion, etc) obtained as spin-offs

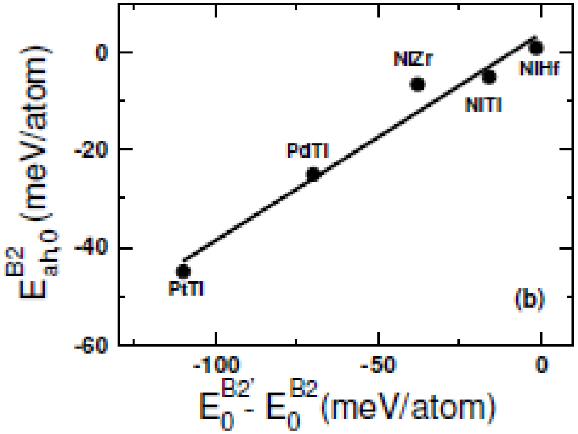
SIGNIFICANCE
- Traditional HTSMA development has been empirical
- Phenomenological models, e.g. CALPHAD, require large, expensive databases to fit models and can give wrong answers.
- First principles methods give high fidelity, parameter-free, predictions with no databases and no fitting.
- Computational tool can be extended beyond thermodynamics to include other properties (actuation work output, cycle life, etc).
- HTSMA design rules obtained from fundamental insights
- Reduced order models derived for rapid properties predictions.

RESULTS
- Anharmonic energies E_{ah} are crucial for SMA predictions but currently require months of supercomputer simulations
- Recently developed *linear parameterizations* of E_{ah} (top figure) hint at possible reduced order models that may enable rapid predictions and avoid costly, lengthy supercomputer simulations.
- Model has two parameters ($E_{ah,0}$ and $E_{ah,1}$). The first is material dependent and also *linear* (bottom plot) while the second is universal (0.025)

FUTURE WORK
- Couple simple parametrizations to machine learning algorithms
- Extend computational tool to include SMA cycle life, work output, etc.



Simple linear parameterizations of difficult to compute anharmonic energies hints at possible reduced order models which may enable rapid SMA predictions.



Constant term in linear model can be fit to crystal energy differences. Remarkably this relationship is linear as well for NiTi, NiZr, NiHf, PdTi and PtTi.

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.

ACCOMPLISHMENTS

- Creep tests on two microstructurally similar superalloys were performed.
- Post-test microstructural and deformation analysis was performed using high resolution scanning and transmission electron microscopy.
- A journal article entitled, "Effect of Stacking Fault Segregation and Local Phase Transformations on Creep Strength in Ni-base Superalloys" was recently published in Acta Materialia.
- Future work will explore new superalloy chemistries that may leverage the new strengthening mechanism recently discovered.

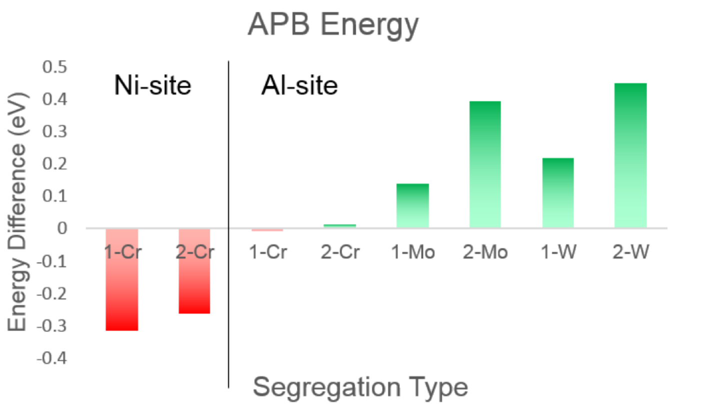


Figure 1: The change in APB energy when Cr, Mo, and W segregate to the Al-site or Cr along a Ni-site. The number associated with each bar represents the number of solute atoms (Cr, Mo, or W) included in the calculation

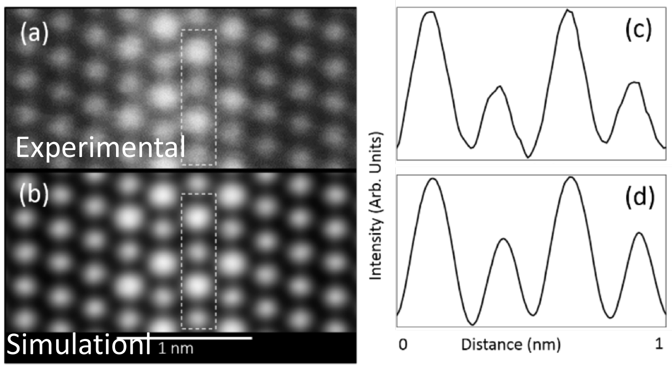


Figure 2: (a) Experimental and (b) simulated HAADF image of a intrinsic fault in LSHR. (c) Experimental and (d) simulated averaged intensity of the atomic columns moving down the fault as highlighted the boxes in (a) and (b).

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

Experimentation (KE2)

Exploration

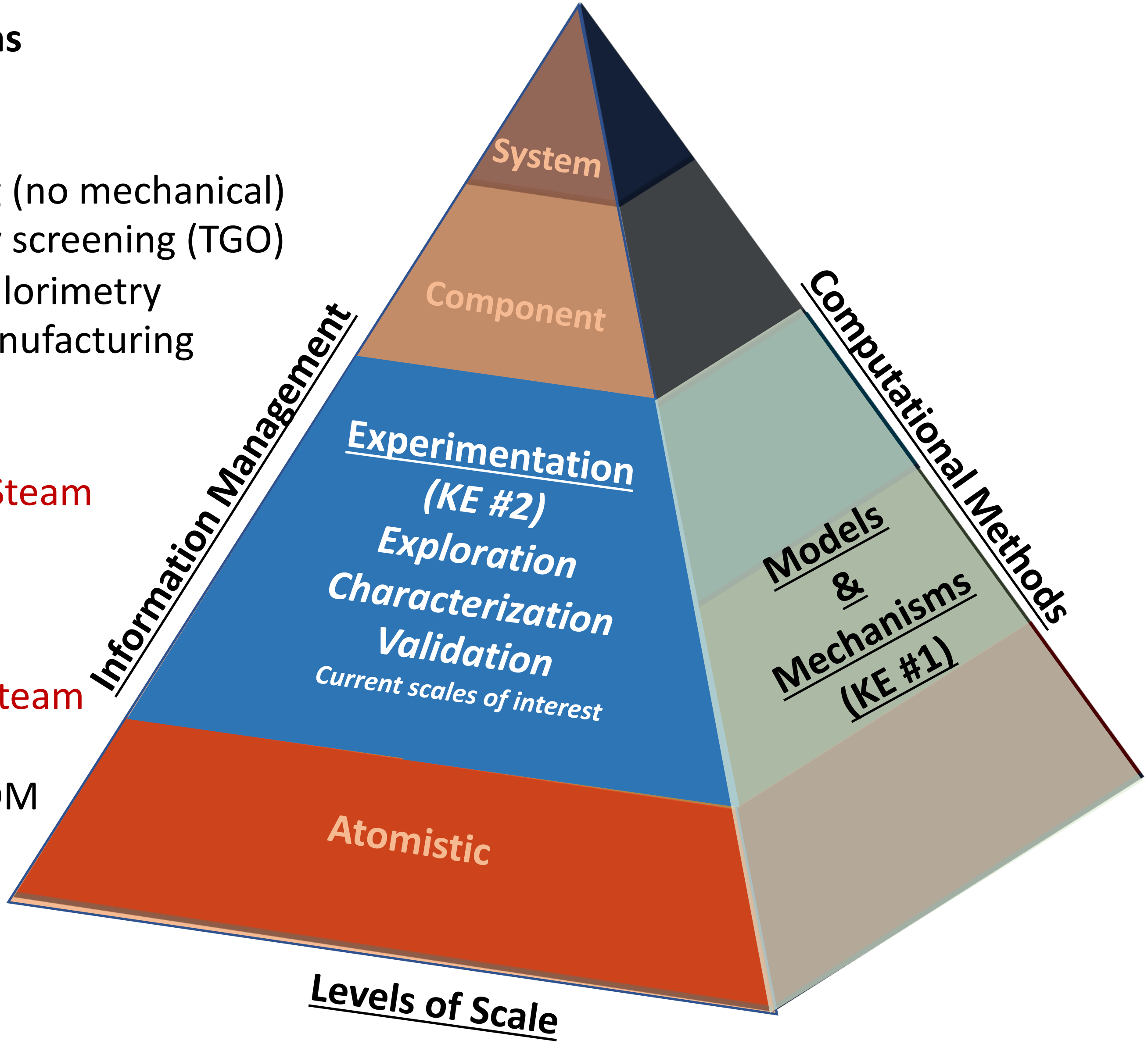
- EBC/CMC steam cycling (no mechanical)
  - Coating chemistry screening (TGO)
- High Temp Reaction Calorimetry
- Open SLM additive manufacturing

Characterization

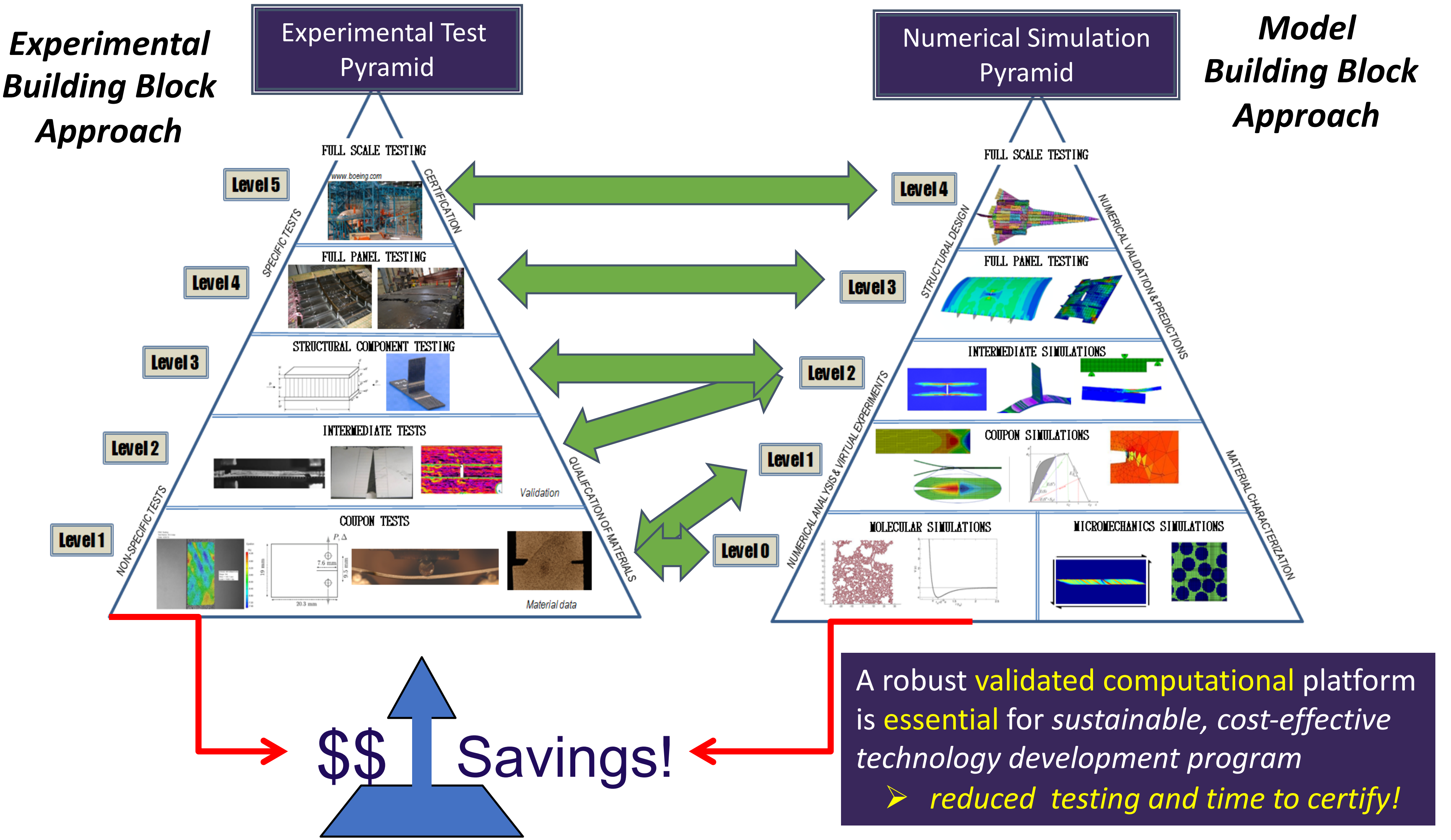
- EBC/CMC Testing 2700 in Steam
  - Creep
  - Fatigue
  - SPLCF
- Mini EBC/CMC Testing in Steam
  - Creep/Fatigue
- Argonne/APS – DXR & HEDM
- Plasma FIB In-situ testing

Validation Testing

- QARE2
- CE-5 Rig Testing



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!*

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

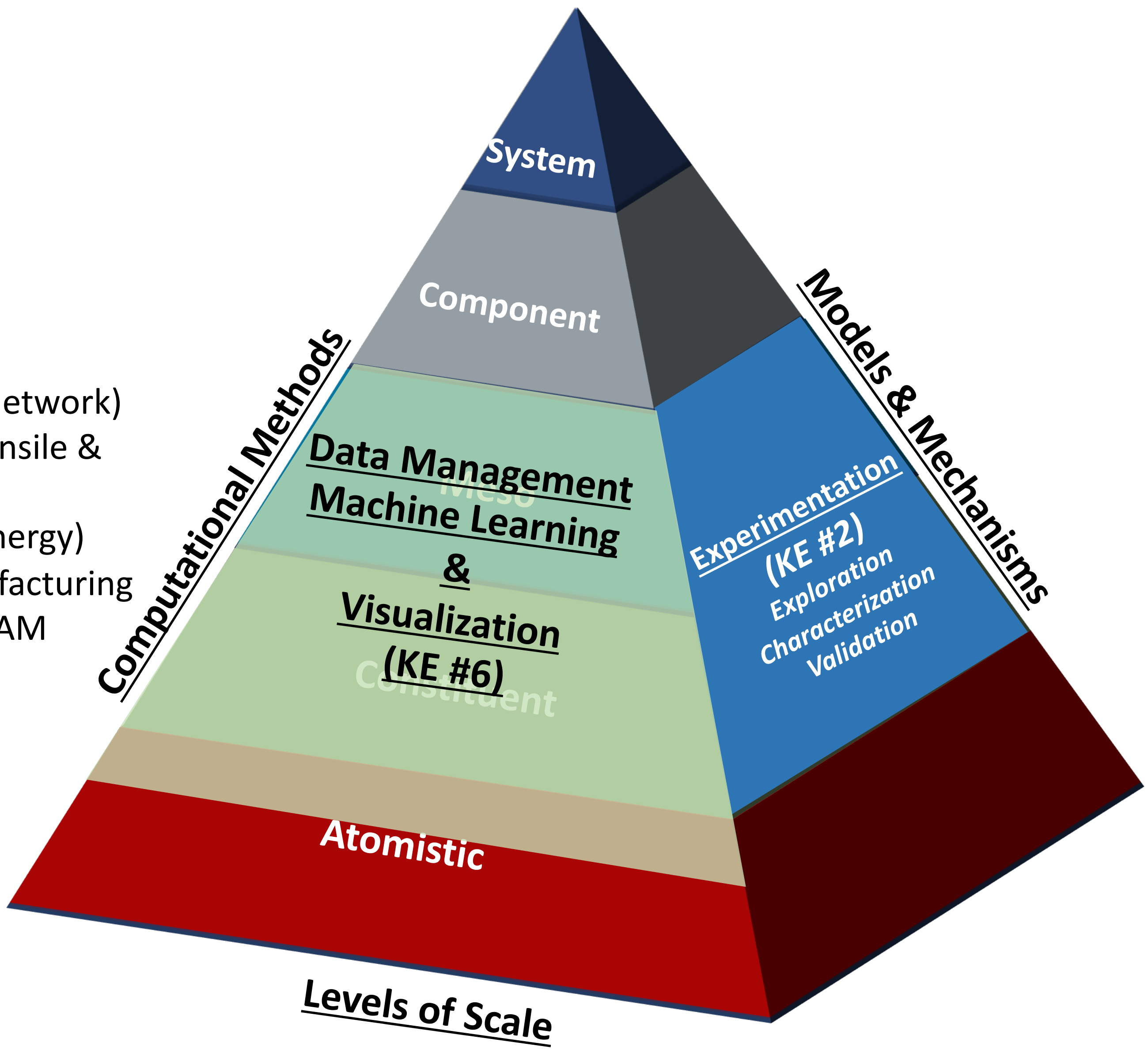
Machine Learning

Optimal Experimental Design

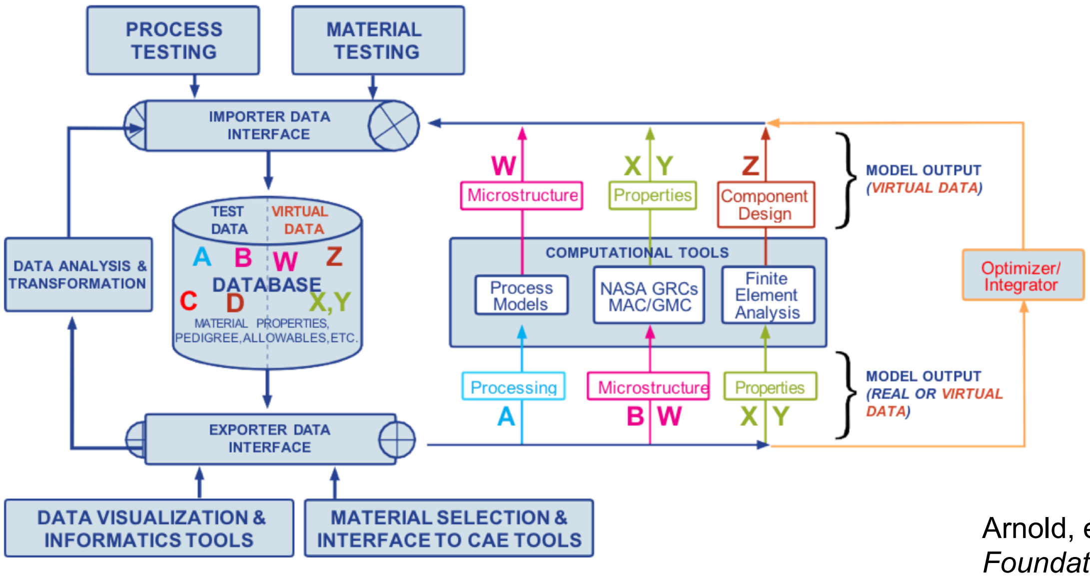
- Deep Learning NN (Neural Network)
  - MAC/GMC - Laminate (Tensile & Fatigue)
  - Atomistic (Anharmonic Energy)
  - Polymers for Rapid Manufacturing
  - Physically-Informed NN EAM Potentials
- Estimation Theory
  - Stochastic Optimization

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 .

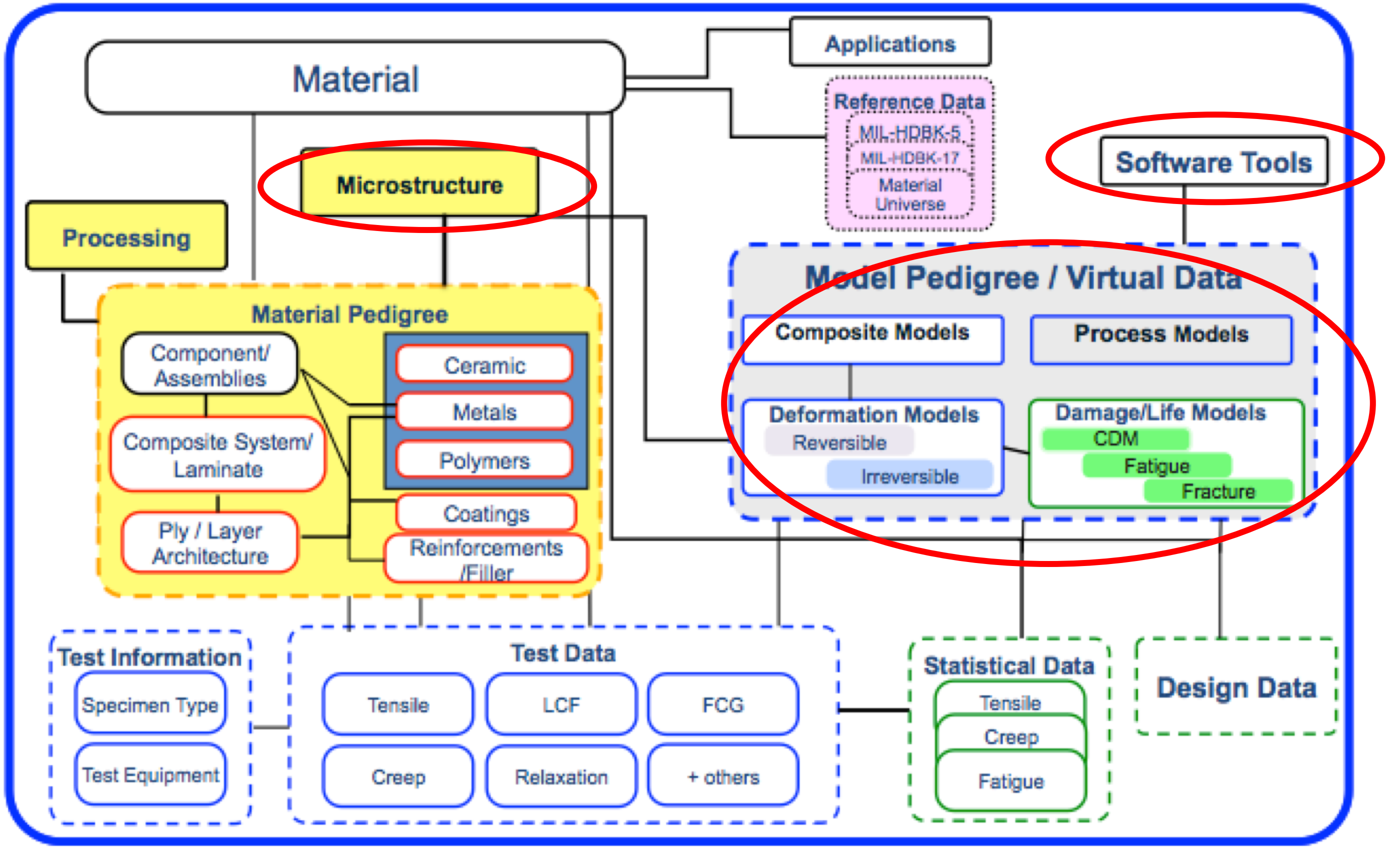
CHARACTERIZATION
Robust model-structure-response definitions will provide the foundation for reliable methods of managing error and uncertainty

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

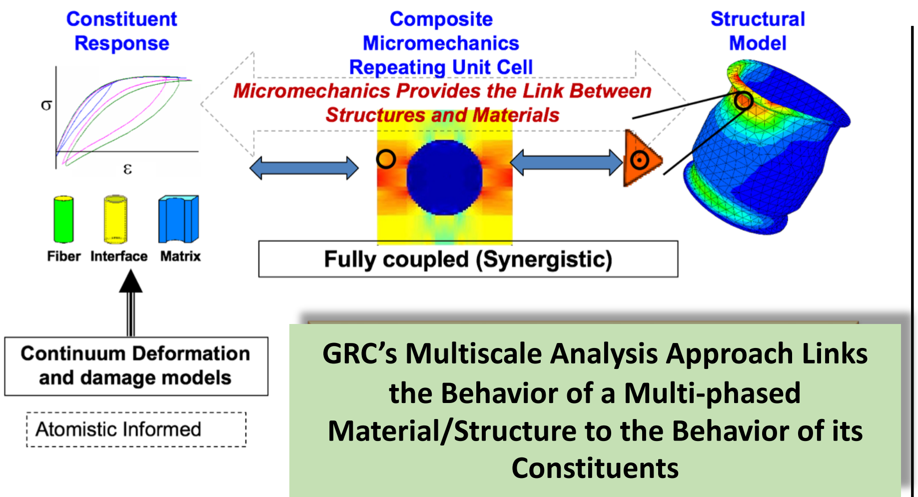


Arnold, S.M., Holland, F. and Bednarcyk, B.A.; (2014). Robust Informatics Infrastructure Required For ICME: Combining Virtual and Experimental Data, 55th AIAA/ASME/ASCE/AHS/SC Structures, Structural Dynamics, and Materials Conference, National Harbor, Maryland, 13 - 17 January 2014, AIAA-2014-0460

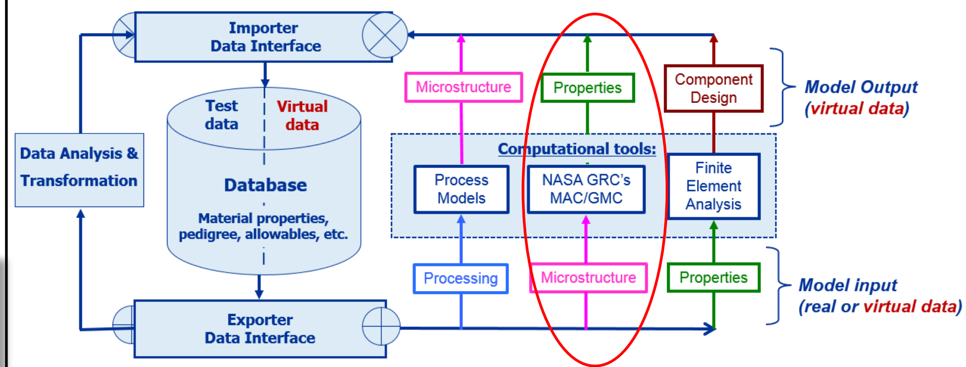
Arnold, S. M., et. al (2015). ; "Microstructural Influence on Deformation and Fatigue Life of Composites Using the Generalized Method of Cells", 56th AIAA/ASME/ASCE/AHS/SC Structure AIAA SciTech 2015, ICME Special Session, Kissimmee, FL, 2015; AIAA 2015-0202

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



Coupling between testing and simulation data is key to realizing ICME

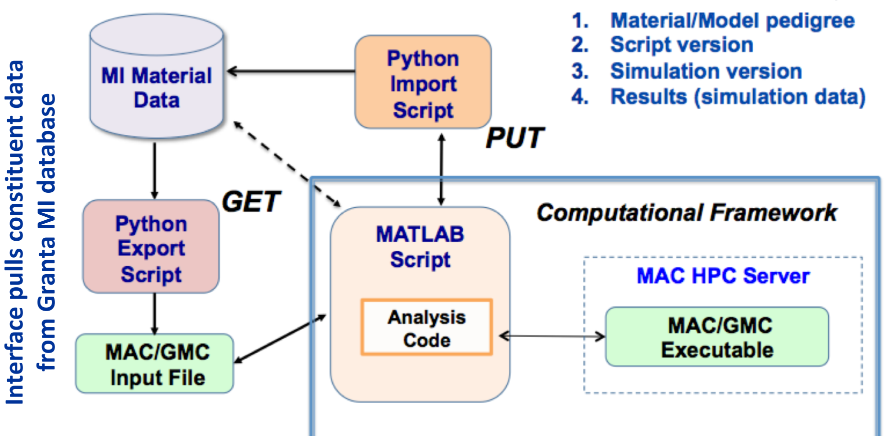


- Linkage to Granta MI software done in collaboration with Granta Design Ltd.

Linkage Established through Workflow and Python Scripts

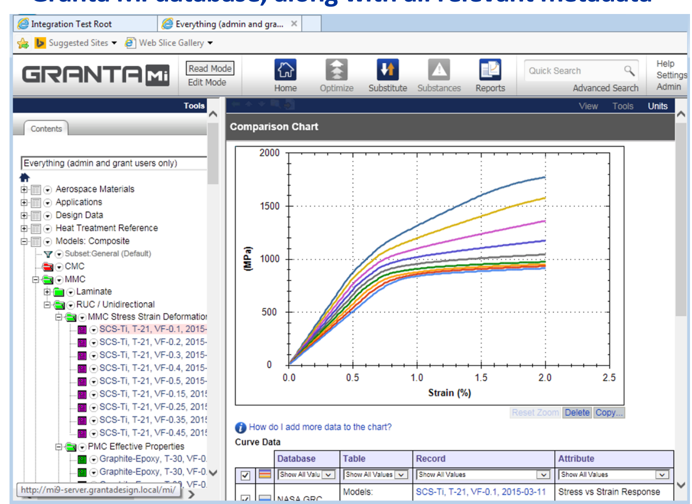
Workflow enables full traceability

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

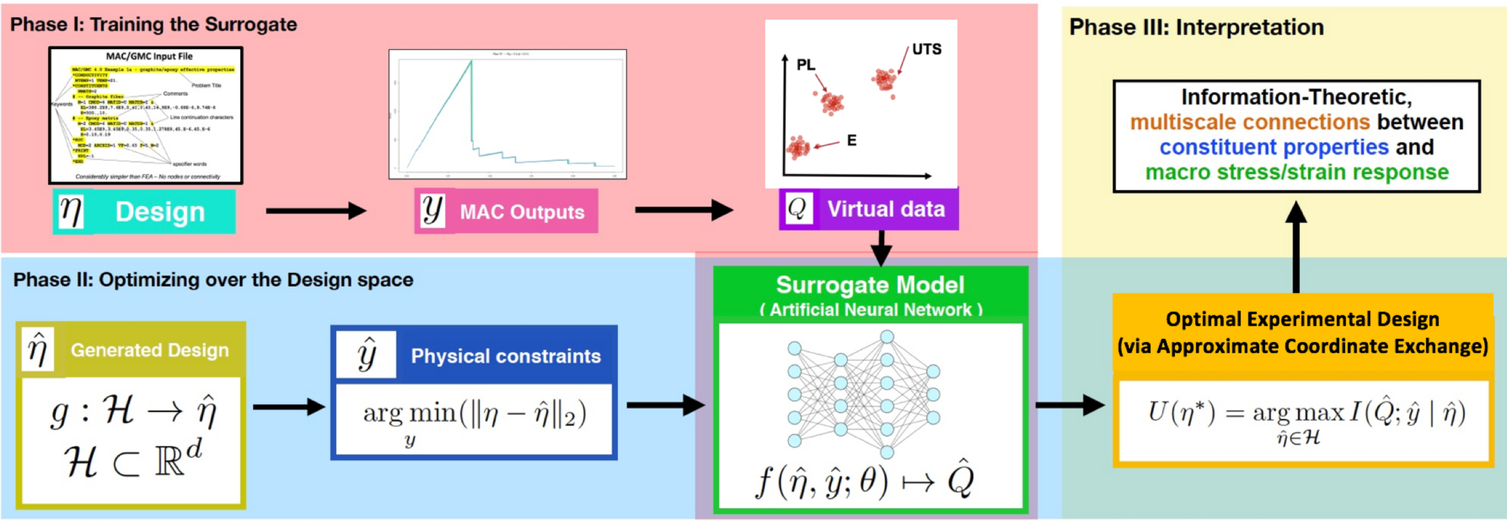
Simulation results, including nonlinear curves, are captured and stored in Granta MI database, along with all relevant metadata



Composite Material Discovery Using ML

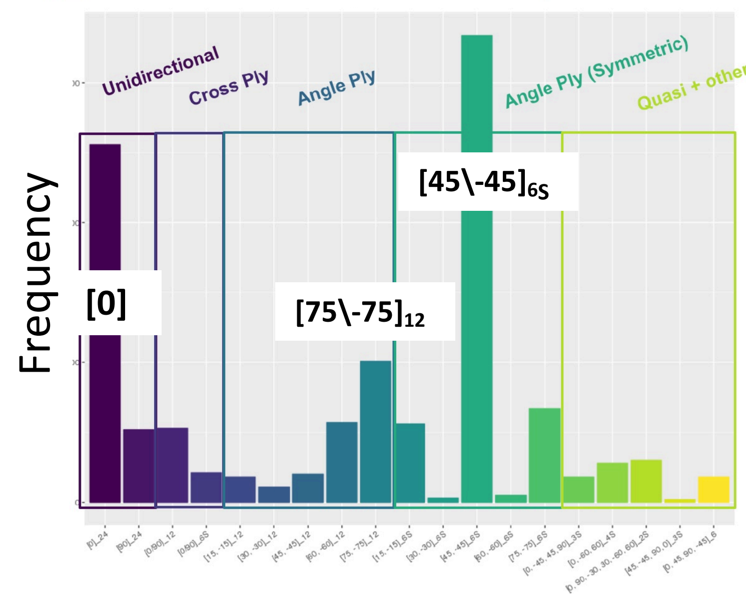
PROBLEM

Develop a general workflow for creating interpretable, high-fidelity surrogate models trained on virtual composite data coupled with optimal experimental design framework to obtain insight into lower length scale information.



ACCOMPLISHMENTS

- Established a framework that incorporates artificial neural network (ANN) model and optimal experimental design algorithm to enable extraction of information relative to multiscale material behavior (constituent, macroscale) given 5 point-wise properties E, PLS and UTS (for both stress and strain).
- Surrogate (ANN) model represents PB micromechanics model (MAC/GMC) within 2% accuracy. Enables millions of calculations in seconds. Ran 19 laminates, 10,000 cases for training.
- Initial results appear promising. Provided "most informative" laminates to test.



POC. Matthew Piekenbrock and Steve Arnold

Future 2040 Funding Opportunities

- NASA Research Announcement (NRA) **due to be released Aug/Sept 2019** – see https://nspires.nasaprs.com/external/solicitations/solicitations.do

- SBIR/STTR - see https://sbir.nasa.gov/prg_sched_anncmnte

- Anticipating a new $10Mil 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

Thanks for Your Attention

Questions

Contact: Steven.M.Arnold@nasa.gov

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Actions Associated with Data Analytics and Visualization Stream

Key Element	Recommended Action							Near Term	Mid Term	Long Term	Funding
[KE1] Models and Methodologies	Develop calibration tools that incorporate V&V and UQ methods to automatically fit model parameters			X	X	X		X	X		$
	Deploy machine learning (ML) approaches to enable development of models that predict materials behavior		X		X	X			X	X	$$$$
[KE2] Multiscale Measurement and Characterization Tools and Methods	Develop and integrate analytical tools (e.g., **machine learning** and autonomous systems technology) or software packages to support large-scale characterization datasets; Examine industry practices across bioinformatics community		X					X	X	X	$$$$
	Formalize methods to recognize and use unexpected data (e.g., anomalies) relative to proposed mechanistic models					X		X	X	X	$$
	Explore statistical methods that use process-structure data to represent extreme-value responses of materials in predictive models				X			X			$$
[KE4] Decision Making and Uncertainty Quantification	Establish decision-making strategies and/or toolsets for highly complex environments that draw upon principles from diverse fields/specialties including risk analysis, decision support, and reasoning under uncertainty				X	X	X	X	X		$$$
	Devise novel UQ methods that uses low-fidelity physics based surrogate models to balance computational efficiency with convergence accuracy		X					X	X	X	$$
	Devise novel methods for interpreting large uncertainties that are intrinsically generated by computationally inexpensive surrogate-based models		X		X			X	X		$$$
	Investigate creative approaches (e.g., **machine learning**) for interpreting, visualizing, and summarizing quantified uncertainties and decision making processes		X			X	X	X	X		$$$

Actions Associated with Data Analytics and Visualization Stream

Key Element	Recommended Action							Near Term	Mid Term	Long Term	Funding
[KE6] Data, Informatics, and Visualization	Develop and standardize fast-acting **machine learning** (e.g., natural language processing), data mining, and data analysis approaches and incorporate them into model development for cohesive materials data analysis: Apply techniques to "learn" data schemata; Use **ML** to quantify level of confidence in statistical model-based prediction results; Direct collaboration with experts in computer science and **machine learning** to drive symbiotic development		X	X	X			X	X	X	$$
	Develop methods to quantify the quality of data					X	X	X	X		$$
	Develop adaptive 2D/3D/4D microstructural segmentation techniques to reduce human error and boost quantitative visualization of materials and structures		X		X		X	X	X		$$
	Enhance the accuracy and speed of visualization of unstructured, high dimensional data (e.g., through translucency) to show relationships between multiple layers of data	X			X		X	X	X		$$
	Design immersive 3D displays for increased data interaction • Significant potential in additive manufacturing design	X					X		X		$$
	Create user-friendly, easy to learn interfaces using the latest in natural user interface technology (voice, gestural, etc.)						X		X		$$
	Develop real-time visualization (e.g., "auto-pilot") for condition-based real-time monitoring of experiments						X	X	X		$$
[KE7] Workflows and Collaboration Frameworks	Incorporate informatics and **machine-learning** tools into collaboration networks to facilitate engineering design and optimization of collaborative tools and networks	X	X	X			X	X			$

Actions Associated with Data Analytics and Visualization Stream

Key Element	Recommended Action							Near Term	Mid Term	Long Term	Funding
[KE8] Education and Training	Develop advanced instrumentation methods/practices for universities to teach rapid generation and analysis of engineering data (multimodal, combinatorial, spatial, etc.) and improve algorithms to analyze and reconstruct data for student instrumentation use	X			X	X		X	X	X	$
	Develop focused education and training modules—including web-based approaches—in data management/analytics tools and methods, and deploy throughout MSE programs (and other engineering programs) in United States; Focus on an industry-supported emerging simulation platform	X			X	X		X	X		$
[KE9] Computational Infrastructure	Develop approaches to use technology such as **machine learning**, AI, and cognitive computing to improve and implement algorithms on new hardware		X			X		X	X		$$$