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Vision 2040: A Roadmap for Integrated, Multiscale Modeling and Simulation of Materials and Systems

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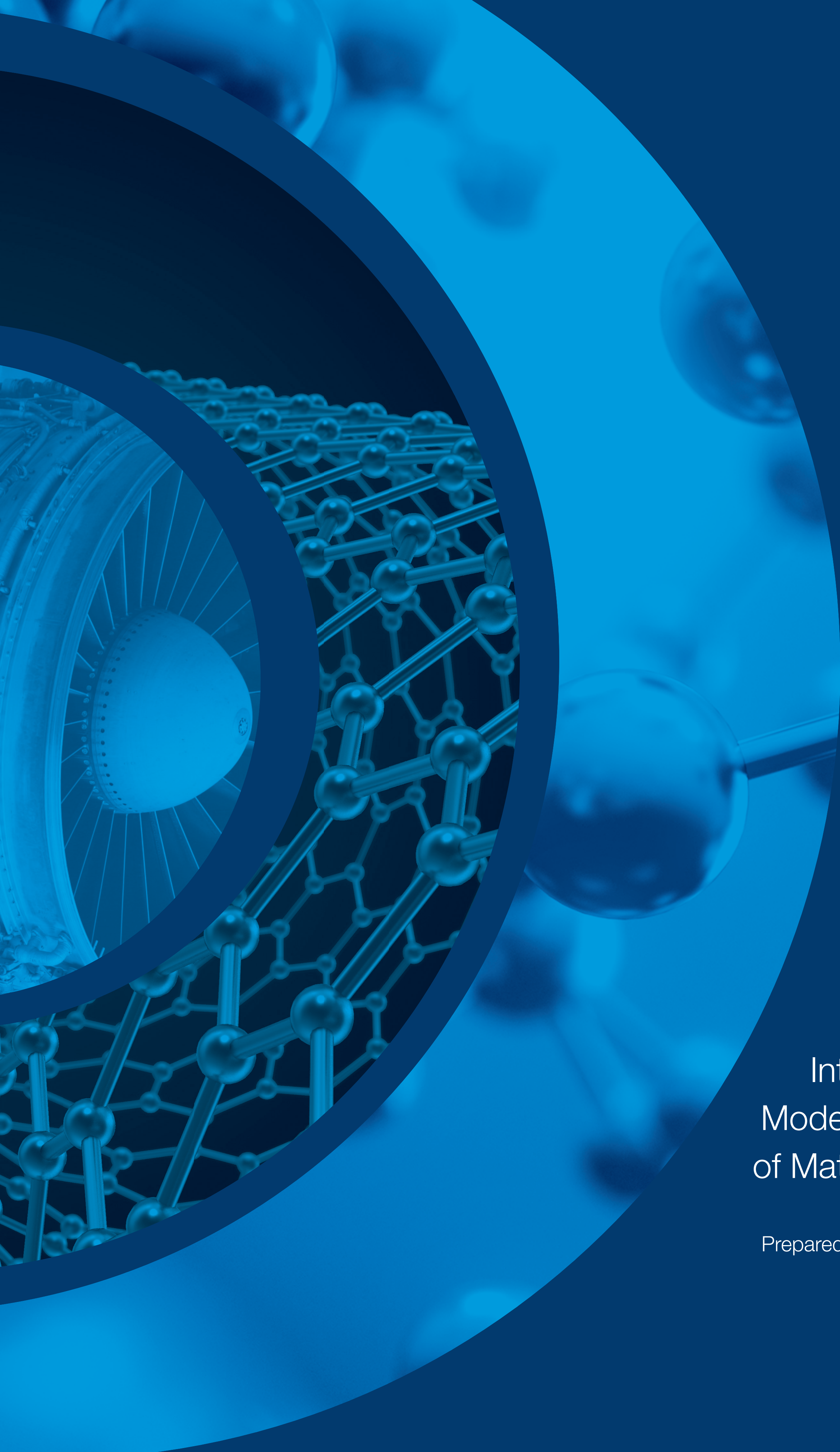

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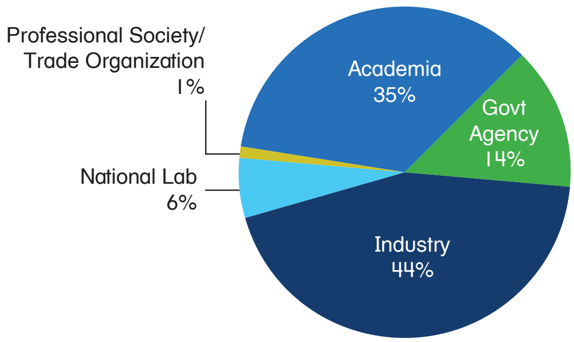
About This Study

Over the last few decades, advances in high-performance computing, new materials characterization methods, and, more recently, an emphasis on integrated computational materials engineering (ICME) and additive manufacturing have been a catalyst for multiscale modeling and simulation-based design of materials and systems* in the aerospace industry. While these advances have driven significant progress in the development of aerospace components and systems, that progress has been limited by persistent technology and infrastructure challenges that must be overcome to realize the full potential of integrated materials and systems design and simulation modeling throughout the supply chain.

In support of the NASA Aeronautics Research Mission Directorate (ARMD) Strategic Implementation Plan (SIP), the Transformational Tools and Technology (TTT) Project under the Transformative Aeronautics Concept Program (TACP) sponsored a study to define a potential 25-year future state required for integrated, multiscale modeling of materials and systems (e.g., load-bearing structures) to accelerate the pace and reduce the expense of innovation in future aerospace and aeronautical systems. Through a series of surveys, workshops, and validation exercises, this study called upon the combined expertise of over 450 contributors (250 as anonymous survey respondents) from throughout the materials science and engineering supply chain, nearly 200 of whom volunteered their time to provide input and insight to this study. Together, they identified not only the critical technical and cultural challenges/gaps facing the multiscale modeling community but also nine core technical work areas (Key Elements). These Key Elements must be matured to build within the aerospace sector the collaborative digital environment (i.e., tools, resources, practices, and people) necessary to efficiently, cost-effectively, and accurately design, manufacture, and certify future aerospace systems in the year 2040. This work was then reviewed by nine expert panels, one per Key Element, with an average of 10 non-team-member specialists. Through a series of working sessions spanning more than six months, the panelists vetted and enhanced the definition, state of the art, and all gaps and recommended actions within their respective Key Elements to ensure completeness and technical accuracy. In addition, they worked collectively to determine the criticality and priority of all the gaps and actions and then voted unanimously to endorse the findings of this study, demonstrating the true consensus nature of its content and recommendations.

FIGURE 1 VISION 2040 CONTRIBUTORS BY AFFILIATION (NEARLY 200 TOTAL WORKSHOP AND PANELIST CONTRIBUTORS)



*Systems is used here to broadly represent entities that need to meet specific requirements to achieve a given purpose. A specific example is that of a load-bearing system which is often referred to as a structure whereas a system that stores energy may be identified as a battery. This also includes entities that are multifunctional in nature that manage stress, temperature, electric, magnetic, and radiation fields simultaneously. In this report system will more often be utilized in the context of load-bearing or structural applications.

The 2040 vision study has been completed in two major phases. In the inaugural Phase 1, project partners Pratt & Whitney; BlueQuartz Software; ESI Group; Rolls-Royce; Boeing; University of California, Santa Barbara; and United Technologies Research Center worked with workshop and survey participants and the aforementioned supply-chain stakeholders to develop a community consensus vision for the state of integrated, multiscale modeling of materials and systems in the year 2040, as well as initial recommendations for the kinds of research and development (R&D) necessary to achieve it. In the subsequent Phase 2 portion of the study, a team comprising Pratt & Whitney, Nexight Group, BlueQuartz Software, ESI Group, and NASA technologists worked to build a community consensus strategy that aligned the vision with current capabilities and future technology development and implementation goals for aerospace and aeronautical systems. The resulting 2040 vision state, critical gaps, actions, and major recommendations contained in this report do not represent the vision of any one individual organization. Rather, this vision reflects a broad community consensus built from contributions of the nearly 450 volunteer experts from industry, government, and academia who contributed their expertise during two years of work to produce this report (see Appendix C for a more complete list of known contributors).

To achieve the collaborative environment (ecosystem) called for in this 2040 vision, new kinds of data, data-sharing, and data analytics tools, advances in modeling capabilities, greater interoperability, updated collaborative approaches, common standards, and a shift in culture and human factors are necessary to set the industry on a path to more cost-effective discovery, design, and manufacture of future aerospace systems.

Who Should Read This Report

While this 2040 vision for integrated, multiscale modeling of materials and systems is critical to enabling innovative future aerospace and aeronautical systems design, development, and application capabilities, this document is intended to provide far-reaching value for all U.S. agencies pursuing advanced engineering and manufacturing. Prioritizing future research and development initiatives based on the pathways and recommendations defined in this report will encourage more rapid and revolutionary advances in materials design, enabling a significant increase in the United States' global competitiveness.

In particular, the following stakeholders may benefit from this report:

- **Funding managers** at U.S. agencies pursuing advanced engineering and manufacturing programs or building infrastructure for the U.S. scientific enterprise may find inspiration or direction in this report. Such people may find value in particular in this report's recommendations and recommended actions, which define opportunities for R&D projects and programs that will advance multiscale modeling and simulation capabilities in mission-critical areas.
- **Corporate leaders** responsible for materials and process development, manufacturing and supply chains, and product certification should seek to understand how the integrated tools and practices contained within the proposed collaboration environment could lead to increased efficiency, reduced cost, and business growth, and build programs to support progress toward the vision. In addition to embracing the recommendations and actions, leading companies should strengthen their internal capabilities to address identified critical gaps, as well as adopt and promote the new tools, methods, and other technologies called for throughout the report. Together with their supply chain partners, these companies should also strive to prioritize and commercialize the capabilities that will emerge in the pursuit of the Vision 2040 end state.
- **Researchers** in industry, government, and academia who are building new characterization, modeling, optimization, and simulation tools and technologies; developing materials data resources; or otherwise working to advance the state of multiscale modeling of materials and systems will find value in each Key Element's current state of the art assessments and specific recommendations. Researchers may find particular value in the critical gaps and recommended actions, which highlight scientific areas where additional research effort is needed to advance the state of the art (see Table 5 and each Key Element section in the Findings section of this report).
- **Educators** training the current and next generation of scientists, designers, and engineers should review this report to identify ways that curricula and training courses should evolve to meet tomorrow's needs. Because workforce and cultural issues are at the heart of Vision 2040, the future workforce will require training not only in key skill sets but also new ways of grasping and embracing

the multidisciplinary and lifecycle nature of the envisioned end state. Therefore, educators will be particularly interested in the detailed Education and Training Key Element, which outlines a series of actions that can help transform current curricula, courses, and approaches.

How to Read the Report

Because of the breadth of detailed information included in this report, funding managers, corporate leaders, researchers, and educators may find it helpful to focus their attention on specific areas.

Vision 2040 Overview

Includes a detailed breakdown of the 2040 vision and its end state characteristics, as well as the strategy for encouraging shifts in the current paradigm to enable more rapid and revolutionary changes within the materials design community. Also outlines the most critical challenges that must be overcome to achieve the envisioned ecosystem, as well as a set of recommendations and priority actions that, undertaken, can move the broader materials science and engineering community along the pathway to 2040.

- **Best for: Funding Managers, Corporate Leaders, Researchers, Educators**

Detailed Vision 2040 Findings

Offers a detailed definition and analysis of each of the nine core work areas identified by the roadmap. Each section includes an assessment of the current state of the art, a view of the envisioned 2040 end state, and comprehensive lists of all identified gaps and panel-vetted recommended actions organized by cross-cutting streams that illustrate the similarities shared by each work area.

- **Best for: Researchers, Educators**

Ensuring Long-Term Study Relevancy

Since the Vision 2040 Roadmap forecasts more than 20 years into the future, it should be considered a living document, periodically re-evaluated and revised to remain current and relevant. To ensure the continued community consensus that is vital to achieving the end state, NASA, with input and support from the scientific community, should regularly revisit this roadmap as needed to provide updates not only within each Key Element work area but also with regard to

- Pacing of proposed development based on time, difficulty, and expense
- Efficacy of established metrics
- Emergence of disruptive technologies
- Changes in the legal, regulatory, and/or funding landscapes.

Vision 2040 Overview

Integrated, multiscale modeling of materials and systems is an emerging field that combines new and existing methods from a broad range of scientific disciplines to design and develop new materials, components, structures, processes, and systems concurrently. These methods rely on iterative, predictive approaches that integrate experiments and simulations to elucidate the behavior and response mechanisms of materials at various length- and time-scales. Multiscale modeling approaches rely on methods and tools that closely align with ICME and the Materials Genome Initiative (MGI), which aim to reduce the time and cost required to move materials from discovery to application [1].

2040 Vision

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.

The Vision for 2040

The future vision targets the use of computational materials tools and techniques that, combined with structural and systems engineering tools and associated "digital tapestry"**, will enable cost-effective, rapid, and revolutionary design of fit-for-purpose materials, components, and systems, be they structural or functional. Creating an adaptive collaboration environment that integrates the efficient and cost-effective use of multiscale modeling and simulation approaches is essential to the design and production of the hardware, tools, and other critical aeronautics technologies that will advance NASA's mission goals and the goals of other relevant agencies and industry stakeholders. Additionally, such an integrated multiscale materials and structures collaboration environment has the potential to have pervasive impacts on materials and systems (structural) engineering and manufacturing beyond the aerospace industry.

NASA and its partners envision other engineering communities (e.g., automotive, biomedical) also benefiting from this new framework. By leveraging the foundational elements and customizing them for their unique needs, other industries can also begin to address their own materials and structures challenges more efficiently and accurately. Formalizing infrastructure that enables linkage of materials models, component design, and structural analysis is critical for realizing the 2040 vision [2].

2040 Vision Statement

The project team worked together with key leaders, stakeholders, and subject matter experts to define a vision for the future of integrated multiscale modeling of materials and structures in the year 2040. The vision represents decades of combined work in

**Phrase used by Dennis Little, Vice President of Space Systems, Lockheed Martin in a July 2016 *Design Engineering* article entitled "The Digital Thread: A Digital Stitch in Time."

computational science and engineering, ICME, design, structural analysis, and component lifing.

To effectively guide future research and development activities, the team and its partners developed an expanded summary of the 2040 vision statement that articulates a set of ideal functions and features of the envisioned cyber-physical-social ecosystem for integrated multiscale materials and systems modeling and simulation:

- Interdisciplinary frameworks that demonstrate and incentivize collaborative research endeavors and support new and disparate engineering disciplines with transformative collections of skills in materials science, data analytics, computational methods, and integrated engineering design.
- Modular (interoperable) frameworks designed with open interface standards for variable-fidelity models at various length scales, streamlined data polling and aggregation, validation-ready modeling environments, and integrated design of models and experiments.
- Agile, flexible computational tool supply chains that rapidly adjust to focused project support needs and new computational software and hardware development.
- High-bandwidth networks, software platforms, and commodity computing for widespread, simultaneous access to computational resources and architectures.
- Educational programs and tracks that explicitly leverage industry-relevant technologies to facilitate learning, strengthen competencies, and impart multidisciplinary capabilities for next-generation engineers and materials scientists.

Equipped with these functions and features, the future cyber-physical-social ecosystem will have the following impacts on the supply chain:

- Modeling and simulation tools for materials, process, design, chemistry, structural analysis, physics-based performance, and manufacturing will seamlessly interact to predict the co-evolution of microstructure and properties throughout the entire supply chain from raw material to individual component/part to system level.
- Computationally-linked model-based definitions of materials, processes, components, and manufacturing will exist with associated measurements and uncertainties required to calibrate, verify, and validate predictions, as well as inform critical decision points.
- Concurrent optimization of multidisciplinary and ICME-based workflows will include systems-based approaches to problem formulation, coupling of multiple scales and physics, and use of non-deterministic factors throughout the research and development continuum, from conceptual materials design to intended in-use application to product disposal and reuse.
- Capture, analysis, dissemination, feedback, and maintenance of all necessary or relevant experimental and virtual data and metadata corresponding to all spatial and temporal scales will happen seamlessly throughout the complete lifecycle.
- Interactive digital information/knowledge management solutions and integrated security access controls for protecting proprietary information will be readily accessible to engineers who will have the appropriate skills to manage and exploit the infrastructure for advanced aerospace systems from cradle to cradle.

Characteristics of the 2040 End State

To achieve this ambitious vision, the desired ecosystem of 2040 must embody the set of characteristics shown in Table 1. These six characteristics describe the goals, features, and impacts of the envisioned end state. To ensure the relevancy of the content in this roadmap, each gap and recommended action ties to one or more of these characteristics, depending on which characteristic it is preventing or supporting. These end-state characteristics act as a guide to help steer collaborative research and development efforts toward the 2040 vision.

Vision 2040: A Transformative Step Forward

Achieving Vision 2040 will require a significant, sustained investment in research, development, demonstration, coordination, and workforce

TABLE 1 END STATE CHARACTERISTICS

END STATE CHARACTERISTIC	DEFINITION
Accessible	The ecosystem will be tailorable to roles and skill levels so that models, methods, best practices, tools, workflows, and information are widely accessible and available to appropriately skilled engineers and non-engineers including manufacturers, compliance officers, academic students, and supply-chain specialists.
Adaptive	The ecosystem will encompass models that will 1) incorporate physics, chemistry, and microstructural information at appropriate scales; 2) adapt to varying levels of empirical or physics-based fidelity; 3) support nimble zooming-in and zooming-out of scales to examine lower-level features or systems-wide attributes of interest; and 4) use highly informative lifecycle (meta)data with sufficient pedigree, provenance, and quality to enable re-use of materials and manufacturing models in future component and systems designs. The ecosystem will use adaptable software packages for leveraging modern high-performance computing (HPC) hardware of 2040, and will operate within a flexible and efficient computational paradigm that balances speed and accuracy trade-offs to resolve scales and models in the design and analysis of aerospace applications.
Interoperable	Platforms within the ecosystem will be interoperable, and will rely on standards, best practices, common formats, and "plug & play" functionalities to seamlessly link scale-specific models, test protocols, characterization methods, and all associated Key Elements both within and across physical and computational workflows.
Robust	The models in the ecosystem will be more physically, mechanistically, and phenomenologically based than those used in today's engineering design methods, and will rely on robust toolsets, instruments, data infrastructures, and network architectures that 1) provide accurate predictions (with quantified uncertainty) of behavior over a range of environmental conditions; 2) endure disruptions and/or readily respond to variable and uncertain inputs/parameters; 3) yield reliable analytical results and design solutions; and 4) improve overall understanding of underlying physics, mechanisms, and phenomena.
Traceable	The ecosystem will possess knowledge management systems that enable consistency, traceability, and reusability of nomenclature, data, and information throughout the lifecycle including inception, design, manufacture, certification, operation, end-of-life, and disposal.
User Friendly	The ecosystem will use platforms with advanced user interfaces to provide intuitive direction, role-specific guidance, and task assistance to 1) guide engineers through the concurrent selection of models, length scales, and time scales for location-specific materials behavior throughout the component; 2) visualize modeling outputs in multiple formats; 3) facilitate the integration of newly available models; and 4) ensure compliance throughout the product lifecycle.

development activities over the next two decades. While the resources needed are sizable, the transformative advances in the way materials and systems are designed, produced, and deployed will deliver even greater returns. Ultimately, the future ecosystem will **strengthen the capabilities and competitiveness of U.S. aerospace and manufacturing sectors in several ways:**

- **Increased reusability of materials data and computational design work.** One report by Granta Design Limited found during an international survey that 40% of materials test data was used once and then discarded [3]. The 2040 ecosystem will avoid such data loss and eliminate the need for duplication of effort. Doing so will radically increase the efficiency of the U.S. materials innovation endeavor by freeing and/or saving millions of dollars of resources to obtain actual value-added data and simulations instead of redundant work.

- **Federated information management architectures and schema** that connect disparate and geographically decentralized repositories, including public and private resources, through interoperable data formats, ontologies, standards, and protocols.
- **Improved return on investment on engineering tools and efforts.** Incorrect materials data and substandard models of materials and/or systems limit the effectiveness of significant investments made by U.S. government agencies and businesses into computational engineering tools. By establishing a collaborative ecosystem that provides traceable, pedigreed data; verified, validated models; and reliable linkage tools to translate across length and time scales, the 2040 ecosystem will enable designers throughout the entire supply chain to use the best resources available to produce improved designs.
- **Integrated "smart" testing** that leverage models and simulations, and multi-objective optimization approaches to help minimize costly, time-consuming delays from excessive physical testing.
- **Collaborative, multidisciplinary environments** that bridge conventionally siloed experts and design stages throughout the product lifecycle, including across discipline, organization, and sector (e.g., aerospace, automotive). Achieving this level of collaboration will require both technical and cultural advances called for in this report and can yield cross-industry adaptation that increases overall U.S. engineering and manufacturing competitiveness.
- **Substantially expanded design space and manufacturability** using novel multiscale optimization approaches, including more probabilistic, path-dependent approaches to modeling of material properties. Such approaches are particularly important to additive manufacturing, in which material properties are entirely path-dependent.
- **Faster time to market by enabling** new designs, developed more rapidly and accurately through modeling and simulation, to transition easily and seamlessly from concept to reality (manufacturing and certification).
- **A highly skilled U.S. workforce** equipped with the skills necessary to capture the full value of integrated, multiscale materials and structures modeling and experimental approaches will ensure the United States remains the destination of choice for global engineering and manufacturing firms adopting leading-edge approaches to materials and systems design and innovation.

The 2040 vision describes a new digital paradigm for designing, optimizing, and certifying materials, systems, and manufacturing processes in a concurrent manner. Understanding the envisioned design paradigm of 2040 and how it differs from the general design landscape of today, as described in Table 2 below, is the first step in pursuit of achieving the proposed vision.

TABLE 2 DESIGN PARADIGM, TODAY VS. 2040

TODAY	2040
DESIGN OF MATERIALS AND SYSTEMS IS DISCONNECTED. There are two distinct design viewpoints: designing systems/components with materials, and designing the materials themselves. The first approach uses material properties based on empirical factors or test data to design systems and components, while the latter focuses on designing a specific material (e.g., microstructure, process) to achieve the desired properties and response for a given application. Today, scientists and engineers design materials and systems separately, rather than treating materials properties as variables in a single, concurrent design process.	**DESIGN OF MATERIALS AND SYSTEMS IS INTEGRATED.** Designing with materials and the design of materials will be intimately connected, enabling the concurrent design and optimization of the material, system, and manufacturing process. This approach will allow for model-based materials and process definitions to be fully incorporated spatially into system and component design and structural analysis [2]. Manufacturability, physics behavior, and recycling/disposal will be considered factors from the beginning of the design phase.

TODAY	2040
STAGES OF THE PRODUCT DEVELOPMENT LIFECYCLE ARE SEGMENTED. The outputs of each stage are handed off as inputs to the next (often requiring manual reworking), with each stage typically representing a different silo of expertise that seldom communicates or collaborates with the others. Product development is therefore viewed as a linear process rather than an iterative, concurrent one.	**STAGES OF THE PRODUCT DEVELOPMENT LIFECYCLE ARE SEAMLESSLY JOINED.** Multidisciplinary project environments will enable greater collaboration and communication among experts and organizations at each stage, allowing for a faster, more efficient iterative product development process. A unified representation of data and knowledge with managed uncertainty will be shared throughout the supply chain to facilitate greater transparency and understanding.
TOOLS, ONTOLOGIES, AND METHODOLOGIES ARE DOMAIN-SPECIFIC. Engineers and technical communities frequently describe data, taxonomies, and schemata in ways that are specific to their organizations or areas of expertise. This often prevents connectivity and interoperability of tools and platforms and inhibits fruitful collaboration across disciplines and stages of the product development lifecycle.	**TOOLS, ONTOLOGIES, AND METHODOLOGIES ARE USABLE ACROSS THE COMMUNITY.** The use of standards, common language, and interoperable tools will ensure accessibility, reusability***, and ease of information flow among individuals, tools, projects, domains, and organizations.
MATERIALS PROPERTIES ARE BASED ON EMPIRICISM. Practitioners use experimental (often costly) tests to generate design curves that represent materials properties. Unlike model-based definitions that provide dynamic outputs, empirical design curves are static and unable to concurrently change with the design of components or processes. Materials data is often generated a decade or more in the past and not rapidly updated. As a result, long lead times separate research and design.	**MATERIALS PROPERTIES ARE VIRTUALLY DETERMINED.** Practitioners will use model-based definitions and no longer rely solely on empirical testing to determine the properties of a material. As a result, materials properties will be dynamic outputs that respond to changes in the design process†. Characterization will be less expensive and require significantly less time, as the need to validate models will drive the requirements for generating materials data. Validated models will define the "design space" for materials definitions and account for uncertainty in all application spaces.
PRODUCT CERTIFICATION RELIES HEAVILY ON PHYSICAL TESTING. Industry predominantly uses simulation to support a “building-block” approach to product certification that requires expensive physical testing at each step.	**PRODUCT CERTIFICATION RELIES HEAVILY ON SIMULATION.** Simulation will be performance-based at the system level and integral to certification, supported by physical testing only when necessary. Certification will also extend to software packages and the associated data for validating materials of application-specific components.

The Vision Strategy

Scope

The 2040 vision targets a broad range of materials for aerospace and aeronautic systems and structures. These materials include but are not limited to

- Functional materials
- Energy conversion materials
- Advanced metallic materials
- Ceramic matrix composites (CMCs)
- Polymer matrix composites (PMCs)

For each of these materials, there are two predominant design viewpoints:

1. **Designing *with* materials (i.e., the structural analyst viewpoint):** The traditional approach of using experimentally measured material properties to design and produce systems/components based on application-specific requirements.
2. **Designing *the* materials (i.e., the materials scientist/engineer viewpoint):** Researching and discovering materials capabilities—in terms of process-structure-property relationships—and exploiting them as variables in the design of existing or emerging materials with tailored performance characteristics that fit spatially defined features and requirements for specific applications.

***Reusability is the degree to which both content (experimental or computational data) and systems can be readily exploited in an independent fashion, particularly where a new instance is implemented or used. This ensures that the content and system do not rely on instance-specific methods and services to function as expected.

†Enlargement of design/material space implicitly demands revolutionary enhancements in manufacturing approaches (e.g., additive manufacturing) to ensure producibility of these new materials with these properties.

Although these viewpoints are not mutually exclusive, the 2040 vision strategy aims to create a **cyber-physical-social ecosystem that marries these approaches into one concurrent, transformational digital paradigm**. The new paradigm, in alignment with the goals of ICME and the Materials Genome Initiative, provides the foundation for industry—and the broad materials science and engineering (MSE) community—to design and optimize materials, systems, and manufacturing processes in a concurrent manner. This vision is bold, but the benefits are substantial. Creating an ecosystem that supports this new concurrent digital paradigm throughout the entire supply chain demands a structured, multidisciplinary approach to transcend key technical and cultural barriers facing the multiscale materials and systems modeling community.

The future ecosystem will introduce a variety of transformative changes with respect to today's design paradigm. Some of those paradigm shifts include

- **Unified representations of data and knowledge** that are interpretable across applications and domains, and shared throughout the supply chain and product lifecycle
- **Federated information management architectures and schema** that connect disparate and geographically decentralized repositories, including public and private resources, through interoperable data formats, ontologies, standards, and protocols
- **Collaborative, multidisciplinary environments** that bridge conventionally siloed experts and design stages throughout the product lifecycle
- **Dynamic, "fit-for-purpose" materials and system design** with uncertainty quantification and management (UQ+M), manufacturing trade-offs analyses, and risk assessments conducted in real time
- **Substantially expanded design space and manufacturability** using novel multiscale optimization approaches
- Materials and systems designs that readily **connect across length and time scales**
- **Integrated "smart" test plans** that leverage model simulations and multi-objective optimization approaches to help minimize costly, time-consuming delays from excessive physical testing.

Perhaps the most influential impact permitted by the future ecosystem is the incorporation of model-based definitions into the design and structural analyses of systems and components [2]. Model-based definitions—which specifically apply to materials, processes, and components—are a major feature of the 2040 vision and the foremost representation of industry's transition into a "digital thread" infrastructure of the future. The incorporation of model-based definitions is already playing a major role in shaping the multiscale modeling landscape by

- Transitioning the broad community from 2D static engineering drawings to 3D dynamic, computationally-linked models
- Promoting a "digital thread" infrastructure that streamlines decision making through seamless inter- and intra-organizational communication and enhanced [meta]data accessibility and discovery
- Replacing static, empirically-based property specification minima and design curves with collections of property-specific models—across length and time scales—that provide dynamic, process-dependent, and spatially-defined outputs throughout the system/component design
- Supporting decision making throughout and beyond the system/component lifecycle to help ensure regulatory and organizational compliance—which can involve decades of data for certain aerospace applications.

Model-based definitions, which dynamically respond to component design changes, are digital specifications that link geometric features, microstructure, microstructural evolution mechanisms, and location-specific properties with manufacturing process paths. They integrate material models with rapidly evolving codes across design disciplines and are a powerful tool for adjusting sensitive variables and rapidly optimizing component designs. Maturing model-based material, process, and component definitions [4,5]—in combination with the Key Elements—will be crucial to maturing the 2040 vision as they will enable advanced system architectures and innovative designs for greater fuel efficiency, higher performance, and lower life cycle costs.

Though not explicitly mentioned, disruptive manufacturing technologies—such as additive manufacturing (AM)—are not excluded from the scope of this study. In fact, the ability to manufacture producible designs using advanced manufacturing technologies drives the need for the 2040 ecosystem and encourages the development of a new concurrent digital design paradigm. As the ecosystem matures, the consequences of disruptive technologies are likely to motivate a periodic reassessment of the specific role of advanced manufacturing methods in reshaping the 2040 vision.

The broad aerospace industry is firmly positioned to be the chief beneficiary of the 2040 ecosystem. While the space sector contends with extreme costs and risks associated with extreme environments, weight sensitivities, and the need to enhance product quality and safety, the aeronautical sector manages component lifecycles that span decades. Despite the focus on aerospace applications, the design paradigm of the 2040 ecosystem is actually applicable to nearly all materials systems and industries outside of aerospace. As the multiscale materials and systems modeling community implements the 2040 vision, other industries will inevitably adopt pieces of the multiscale modeling framework to accelerate design and analysis, collaborate across disciplines, increase the value of their work, and secure a competitive advantage.

Key Elements

The Vision 2040 strategy identifies nine interdependent Key Element (KE) work domains to organize not only the technical and cultural hurdles facing the multiscale modeling community but also the recommendations for pre-competitive research and development efforts to enable the 2040 vision. These core technical areas emerged from a broad examination of existing tools, techniques, and capabilities that are used across stakeholder groups for multiscale design and analysis of materials and systems. Together, these Key Elements represent a community-consensus foundation for fulfilling the 2040 vision for the entire supply chain. Table 3 provides a brief description of the domain of work that takes place within each of these Key Elements; more robust descriptions are provided in the next section of this report. The technologies associated with each Key Element are interrelated and will grow increasingly interconnected in the future, eventually coalescing to form the proposed 2040 end state. Figure 2 provides a visual representation of this integration from today, when these Key Elements are siloed, to 2040, when they will be seamlessly integrated into a single, interconnected ecosystem.

Advancing technology within these Key Elements will ensure that the researchers and engineers of the future will have the training and access to the technological infrastructure and tools necessary to

- Efficiently and accurately predict and simulate the performance (e.g., behavior and properties) of a design, including innovative designs that incorporate new materials and multifunctional aspects specifically designed to meet the performance requirements
- Establish, implement, and utilize specifically tailored experimental and virtual test programs to identify, manage, and mitigate risks
- Establish and/or improve the level of confidence in a design
- Manage the flows of information among all elements (e.g., models, tools, people) required to complete, manufacture, and certify an aerospace component/system.

While significant progress has been made over the past 20 years within industry to enhance and advance system/structural design and analysis technologies and the associated "digital thread" (e.g., Bell Helicopter's digital product journey[‡]), connection of this structural paradigm viewpoint with that of the design of materials paradigm, with all its potential impact, is still lacking and will require more work. Consequently, the authors of this report purposefully focused more attention on the issues surrounding multiscale modeling of materials and the infusion of the associated technologies (e.g., model-based definitions) into the systems design/analysis paradigm. As a result, the content of this report is more biased toward computational materials science and engineering than systems/structural design and analysis.

[‡]Jeff Cloud, Chief Engineer and Product Manager AW609 Tiltrotor, Bell Helicopter, Aviation Week Network presentation entitled "Creating the Ecosystem Behind Systems: Leveraging a Model-Based Enterprise", Sept 2016

TABLE 3 KEY ELEMENT DESCRIPTIONS

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

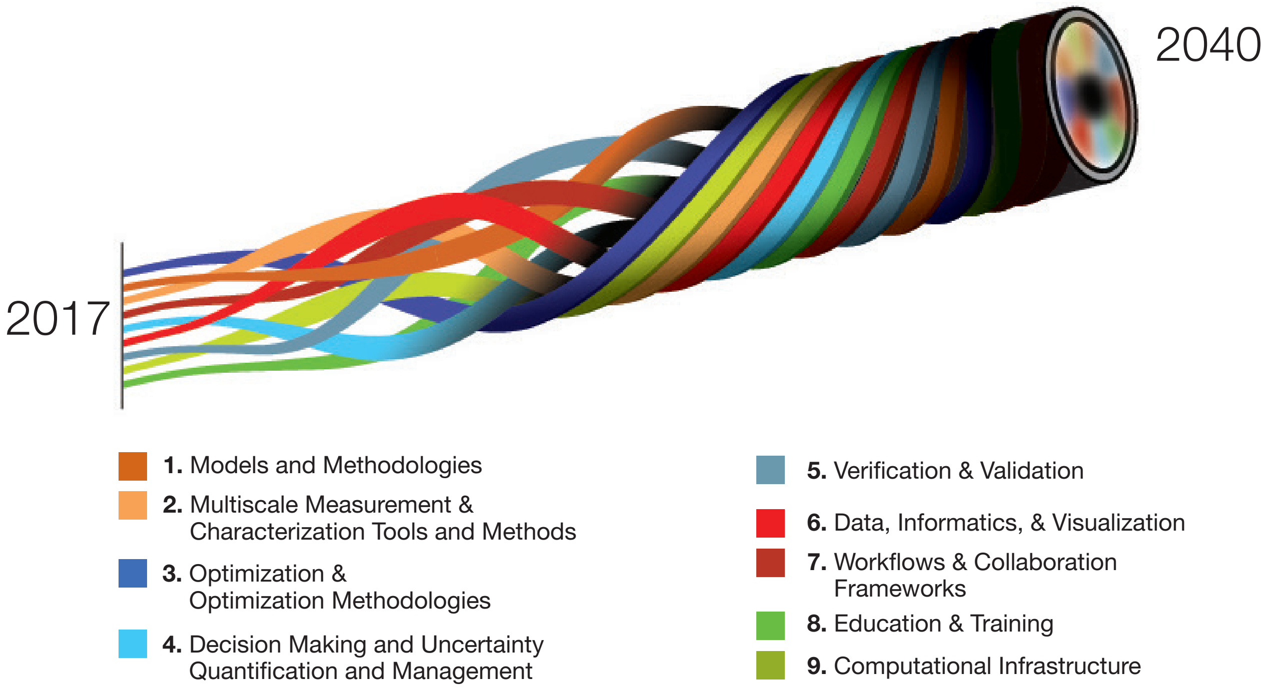


Figure 2 Each Key Element will need to overcome various gaps and challenges to become fully integrated with the others to achieve the vision for 2040. Collaboration and shared purpose across Key Elements will help make product design and development faster, more efficient, and more cost-effective in the envisioned interconnected environment of 2040.

Linkage with NASA Technology Roadmaps and Other Community-Wide Efforts

The collaborative goals of the vision are not just applicable to the U.S. aerospace sector but also the international communities focused on modeling and simulation of materials and systems. Various organizations have conducted similar, prior or parallel efforts [6] that identified overlapping challenges and paths forward that support the findings in this report. One such example is the UK SimBest Project [7], which set out to evaluate industry best practice and research state of the art for the high value-added manufacturing community to achieve greater efficiency savings and competitive advantages. The SimBest project surveyed efforts across eight technical areas—similar to this roadmap's nine Key Elements—in seven industrial sectors, including aerospace. While the project was not as broad in scope as the Vision 2040 Roadmap, the gap analysis between state-of-the-art capabilities and current industry best practices and future needs are in line with the findings of this report. The primary difference between these prior efforts and this one is that Vision 2040 calls for the holistic integration of materials, structural, and systems design and simulation needs within individual companies and, eventually, throughout supply chains. Prior studies looked primarily at similar technical challenges from either a materials or structures/systems perspective.

The Vision 2040 Roadmap is consistent with NASA's ARMD objectives, which recognizes six Strategic Thrusts that affect the aviation industry, the nation, and the world [8]:

1 **Safe, efficient growth in global operations**
Enable the continued development of a modernized air transportation system that will achieve greater capacity and operational efficiency while maintaining or improving current and future safety and other performance measures.

2 **Innovation in commercial supersonic aircraft**
Advance technologies to overcome the major environmental and efficiency barriers to market innovation in supersonic transport to both advance

‡Jeff Cloud, Chief Engineer and Product Manager AW609 Tiltrotor, Bell Helicopter, Aviation Week Network presentation entitled "Creating the Ecosystem Behind Systems: Leveraging a Model-Based Enterprise", Sept 2016

transcontinental and intercontinental transportation and maintain U.S. leadership in aviation systems.

3 **Ultra-efficient commercial vehicles**
Enable future generations of subsonic fixed wing and vertical lift commercial aircraft that lessen environmental impacts (e.g., noise, harmful emissions) while maintaining safety and improving operating economics.

4 **Transition to alternative propulsion and energy**
Enable the use of alternative fuels and foster a fundamental shift to innovative aircraft propulsion systems that have the potential to produce very low levels of carbon emissions relative to the energy used.

5 **Real-time, system-wide safety assurance**
Lead research into technology advances (sensors, networking, data mining, prognostics, etc.) to help demonstrate the feasibility of integrated, system-wide safety assurance (i.e., recognize safety risks as they develop in real time and implement strategies to prevent them from becoming issues).

6 **Assured autonomy for aviation transformation**
Advance new technologies in automation and autonomy for the safe integration of Unmanned Aircraft Systems (UAS) into the National Airspace System (NAS), verification and validation of innovative systems, advanced human-machine harmonization, and highly reliable trusted systems.

This report also aligns well with agency roadmaps published by NASA's Office of Chief Technologist in 2015. The NASA Technology Roadmaps [9] comprise a set of 15 distinct technology areas (TAs) that span a wide range of technologies and

TABLE 4 LINKAGES BETWEEN NASA TECHNOLOGY ROADMAPS AND THE VISION 2040 ROADMAP

Most relevant to the Vision 2040 Roadmap is the content of the roadmaps for TA 11: Modeling, Simulation, Information Technology and Processing and TA 12: Materials, Structures, Mechanical Systems and Manufacturing. Within TA 11 and 12, the technology areas that are most closely aligned with the content of the Vision 2040 Roadmap, include:

11.1.2	**GROUND COMPUTING** Includes exascale supercomputing and data storage, as well as quantum, cognitive, and other types of advanced computing for Big Data analysis and high-fidelity physics-based simulations for Earth and space science, as well as aerospace research and engineering.
11.3.5	**EXASCALE SIMULATION** Develops physics-based exascale environments that are needed to support the emerging requirements of multifaceted mathematics in complex systems, such as algorithms and analysis of methodologies for multi-scale and multi-physics simulation. These environments extend simulation performance and capability, the ability to seamlessly generate representative meshes, and the ability to numerically validate exascale data from various sources in near-real time.
11.3.6	**UNCERTAINTY QUANTIFICATION AND NONDETERMINISTIC SIMULATION METHODS** Identifies, classifies, models, and propagates all forms of uncertainty present in a system to enable understanding and management of their impact on system performance, robustness, reliability, and safety.
11.3.7	**MULTISCALE, MULTIPHYSICS, AND MULTIFIDELITY SIMULATION** Develops methods needed to represent physical processes at operative length and time scales and unify best-physics representations across multiple disciplines.
11.3.8	**VERIFICATION AND VALIDATION** Provides technologies needed to ensure that numerical solutions are correct and properly represent governing physical processes. Validation is heavily dependent on technologies for experimentation and measurement found throughout the other roadmaps.
11.4.2	**INTELLIGENT DATA UNDERSTANDING** Provides the ability to automatically mine and analyze datasets that are large, noisy, and of varying modalities, including discrete, continuous, text, and graphics, and extract or discover information that can be used for further analysis or decision making.
12.1.2	**COMPUTATIONALLY DESIGNED MATERIALS** Computational design of materials covers three major areas: prediction of life, design of materials with tailored or improved properties, and guided experimental validation. Improved properties and predictable performance will decrease developmental and operational costs while improving safety.
12.2.2	**DESIGN AND CERTIFICATION METHODS** Incorporation of model-based materials, manufacturing, and structural design methods with rational testing approaches to improve design and certification capabilities such as cost, schedule, and structural integrity.

capabilities needed to support the NASA mission during the next 20 years. In addition to a discussion of each technology, required capability, related state-of-the-art and performance goals, context is provided by the addition of representative NASA missions for which the technology is relevant. Most relevant to the Vision 2040 Roadmap is the content of the roadmaps for *TA 11: Modeling, Simulation, Information Technology and Processing* and *TA 12: Materials, Structures, Mechanical Systems and Manufacturing*. Specific links between those roadmaps and this one are noted in Table 4.

The Vision 2040 Roadmap is also consistent with materials-related elements of an internal NASA capabilities assessment developed during 2014 and 2015. The Materials Capability Leadership Team (MCLT), led by the NASA Technical Fellow for Materials and his deputies and consisting of members from each of the NASA centers, developed recommendations related to computational materials (CM). One of those recommendations was to recognize CM as an important materials sub-discipline by formulating an agency-funded, focused activity to develop CM tools for space exploration, given that CM methods will accelerate materials design and process development, reduce extent of material testing, and lead to physics-based life prediction (reliability) methods. Additionally, the team recommended that this sub-capability be well leveraged by current Department of Energy (DOE), Department of Defense (DoD), and National Institute of Standards and Technology (NIST) CM efforts.

These agency-wide planning efforts, together with numerous planning activities undertaken at NASA field centers during the past decade, come from the vision of the NASA research staff. In relation, this Vision 2040 Roadmap provides additional depth and perspective from the larger computational materials and structural community and offers a perspective on the future of the field that is consistent with these previous space-technology-oriented study recommendations and directions.

The Path Forward

Creating the interconnected ecosystem described in Vision 2040 is an ambitious goal. Focused, sustained, collaborative efforts by government, industry, and academia will be required to address the gaps and actions identified in this report (described in detail in each of the Key Element sections) to achieve this new level of interoperability for the aeronautics and space community, resulting in faster, more efficient, and more cost-effective innovation in materials and designs. Only by working collaboratively as a broad scientific and engineering community to address the gaps and recommended actions described in this report will the U.S. aerospace sector capture the full promise and benefits of interoperable integrated, multiscale modeling of materials and structures.

Critical Gaps and Recommended Actions

Gaps are the technical and cultural[§] challenges across industry, government, and academia that prevent the realization of the 2040 vision. These gaps—including underdeveloped technologies, poor data management practices, and workforce skill deficiencies—provide a baseline for identifying the technical and cultural actions needed to advance each Key Element toward the envisioned end state. As part of the study, a total of 118 gaps across all Key Elements were collected. Each expert panel prioritized its associated Key Element's gaps through a voting process, with the gap receiving the largest number of votes being identified as that Key Element's critical gap. The Vision 2040 Study identifies several of the most significant obstacles (or gaps) from the Key Elements that stand in the way of the future ecosystem (see Table 5).

Each of the study's Key Elements also generated a series of time-based recommended actions (a total of 180 across all Key Elements) for overcoming the key technical and cultural challenges/gaps to achieve the 2040 end state. These recommendations reflect the professional assessments of stakeholders from across the multiscale modeling and simulation community and encompass activities such as conducting basic research, improving existing technologies, and implementing community-wide standards. The study panelists identified, again through a voting process within each Key Element, a subset of high-priority recommended actions that will have the greatest impact on overcoming key challenges and realizing the future ecosystem.

[§]Note, history has indicated that cultural gaps/changes are by far the most difficult barriers to address regarding the successful creation and implementation of a new paradigm ("culture eats strategy every time").

Because the future is difficult to predict, there are many potential pathways to overcome the critical gaps identified in Table 5, as well as the others outlined in detail in each of the Key Element sections of this document. The color coding of each Key Element further illustrates how multiple actions from different Key Elements can be combined to close a given gap. These recommended actions should be strictly regarded as a possible strategy to address the closure of each Key Element's critical gap while approaching the 2040 end state. As the multiscale modeling and simulation landscape continues to shift due to emerging or disruptive technologies, certain gaps may necessitate additional or alternative action and approaches not listed in Table 5.

Each recommended action listed in Table 5 has been reduced to a short-form summary description for brevity; the full description of the recommendations for each action may be found by following the mapping number for the corresponding Key Element recommended action table in the Detailed Vision 2040 Findings section of the report. For example, details for the action labeled (5.3) may be found in the third row of the table for Key Element 5, Verification and Validation.

Multidisciplinary Engineering Challenges (MECs)

This report identifies a set of multidisciplinary engineering challenges (MECs). These MECs are problems that have never been holistically solved before and require advances in multiple Key Elements to fully solve. Focused R&D programs designed to address these MECs could deliver distinct, nearer-term value to the aerospace community by providing useful, real-world engineering solutions to important challenges while also tangibly advancing several Key Elements toward the longer-term Vision 2040. Brief descriptions of each proposed MEC are listed below; detailed descriptions of each can be found in Appendix A.

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 aerostructures and components
6. Automated readaptation 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

TABLE 5 CRITICAL GAPS AND PROPOSED RECOMMENDED ACTIONS

Accessible | Adaptive | Interoperable | Robust | Traceable | User Friendly

KEY ELEMENT	CRITICAL GAP	PRIORITY ACTIONS	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)	Adaptive, Robust
		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)	Robust
		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)	Adaptive, Interoperable, Robust
		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)	Robust, Traceable
		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)	Accessible, Traceable, User Friendly
		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)	Accessible, Interoperable, Traceable, User Friendly
		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)	Accessible, Interoperable, User Friendly
		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)	Accessible, Robust
		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)	Accessible, Adaptive, Traceable
		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)	

Major Study Recommendations

As previously noted, creating the interconnected ecosystem described in Vision 2040 will require sustained efforts by government, industry, and academia, working independently and collaboratively. The following overarching recommendations provide high-level suggestions for how to organize such efforts and position the United States to make meaningful progress toward the vision.

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

By establishing dedicated research programs associated with the Key Elements outlined herein, NASA and other federal agencies can accelerate closure of the critical gaps necessary to make the 2040 vision a reality. NASA should also establish public-private consortia and convene periodic community workshops associated with these Key Elements to address critical needs and assess progress between now and 2040. Other funding organizations should also seek to align their R&D programs to address the gaps and actions in this report in a manner that not only supports their own missions but also furthers the overall progress of the United States' capabilities and competitive advantages.

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.

The vision is far too ambitious and important to be addressed in a fragmented way; the data, knowledge, and tools developed under the effort will have broad value beyond NASA's mission and the aerospace sector. A coordinated federal strategy will be required to help mobilize the significant financial, human, and facility resources needed to achieve Vision 2040. NASA and other relevant agencies should persistently identify and fund development specifically in focus areas in which it has unique resources (e.g., expertise, experimental/characterization facilities, existing software codes and tools) or needs not addressed by another agency's activities. One possible mechanism is for NASA to establish a Model-Based Innovation Ecosystem (MBIE) working group to lead, guide, and establish the necessary collaborations with key research partners and industrial stakeholders within the broader engineering communities to champion the recommendations of this Vision 2040 Roadmap.

RECOMMENDATION #3:
NASA and other federal agencies 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.

NASA and other federal agencies (e.g., NIST) should establish interagency design standards and protocols to enable federated data infrastructure. These standards should explicitly address data ontologies and semantics necessary to permit communication across materials and system related disciplines and across associated length and time scales, as well as robust information management infrastructure to link experimental and simulation data at various length scales. NASA and NIST can encourage the adoption of this framework by developing best practices for data management and analytics, and disseminating conforming tools and processes throughout the relevant supply chains. Additionally, to extract the greatest value from investments in materials research, NASA should support the development of tools, for its and its partners' use, that capture and preserve materials data to enhance reproducibility, enable reusability, and allow in-depth analysis and visualization. Moreover, where possible, NASA and its partners should make databases and models widely available and encourage researchers to apply artificial intelligence and machine-learning tools to the datasets to pursue new insights.

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.

These benchmarked examples should include all data required for using the material within an application as well as for the digital thread or footprint for data and tool use (e.g., all time- and length-scale dependent data and documented tools and models describing the processing, structure, property, and performance relations for the application). Developing these benchmark examples will highlight any new or overlooked data, visualization, integration, and/or modeling needs, as well as provide needed validation datasets for emerging and/or disruptive technologies. Additionally, such an approach would allow research teams to avoid duplication of effort, build upon others' work, collaborate in more meaningful ways, and directly compare work done across teams, as well as create opportunities for advancing both data repository and data mining science by encouraging the compilation and comparison of multi-group data and efforts.

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.

NASA should apply its in-house expertise and world-class facilities to capture, analyze, maintain, and widely disseminate materials and systems information and knowledge throughout government, industry, and academia. An even larger, more diverse dataset could also be produced by NASA's coordinating with and leveraging the additional expertise and facilities of other government laboratories. By championing the dissemination of this data, through controlled and/or open access venues, NASA and its partners can facilitate independent model validation throughout the materials and design community. "Gold standard" datasets of material properties can also be highly valuable for advancing manufacturing process simulation capabilities. Plus, as the "gold standard" datasets grow, researchers can adapt and apply artificial intelligence (AI)/machine learning (ML) approaches to find new insights into materials and structural design based on the open data. Finally, significant portions of these datasets should be held in reserve as "blind" tests to enable accurate and authentic assessment of models and their uncertainties.

RECOMMENDATION #6: NASA and its partners 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.

Initially, NASA should work with partners to document existing, relevant case studies that demonstrate cost savings or other advantages, even if such case studies only incorporate a subset of the envisioned ecosystem (e.g., only multiscale material modeling without structural simulation). The primary purpose of the demonstration projects should be to document and publicize the benefits of using specific elements of the ecosystem for product design and development, rather than simply advancing the toolsets. Therefore, the projects should not involve restricted (e.g., International Traffic in Arms Regulations [ITAR]-controlled) information; the MECs may offer potential topics because they target high-interest challenges that require an innovative approach to previously unsolved problems. Additionally, these projects would be valuable for educators for identifying and showcasing tools and processes for conducting integrated materials and system design.

RECOMMENDATION #7:
NASA and other relevant federal agencies (i.e., National Science Foundation [NSF], DOE, DoD, and others) should increase fundamental research efforts to develop, characterize, and validate improved physics-based and data-driven materials models and implementation of model-based material and process definitions.

Specifically, these efforts should seek to

- Improve constitutive models (particularly those associated with nonlinear phenomenon), including first principles calculations and molecular dynamics/Monte Carlo atomistic modeling with density functional theory-based interatomic potentials.
- Improve measurement techniques at small size scales (e.g., *in situ* techniques for composite materials) to improve the ability to characterize and validate constitutive models, particularly under multiaxial loading scenarios.
- Use the improved measurement techniques to perform exploratory, characterization, and validation tests and provide uncertainty quantification (UQ) results for the improved constitutive models with levels of precision and accuracy not previously possible.

RECOMMENDATION #8
NASA and other federal agencies 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 and implementation of model-based material and process definitions.

Specifically,

- NASA should partner with all federal agencies engaged with the materials science engineering value stream to ensure expanded educational opportunities and sustained educational effectiveness within multiscale materials and structures modeling and simulation for engineering design and manufacturing (e.g., establish Collaboration Institutes of Education and Training [CIETs], encompassing different areas of multiscale modeling, to offer degree and/or certificate programs in computational materials and system engineering).
- NASA, in collaboration with the deans of leading colleges of engineering, should incentivize faculty to incorporate additional mathematics and statistics requirements into materials science and engineering undergraduate engineering curricula to better train graduates to apply multiscale modeling-based approaches to materials and systems design.
- NASA and other federal agencies should initiate a comprehensive campaign promoting engineering careers in computational materials science, simulation, and design, including fellowship and internship opportunities, as well as the development of the necessary educational and research infrastructure.

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.

NASA should strive to foster a multidisciplinary as well as transformative digital culture that integrates computational science and engineering, computer science and software engineering, and materials and manufacturing science. Simultaneously, universities should train the new workforce generation emphasizing this collaborative and digital culture. NASA should begin by establishing clear incentives for the community to share and contribute data and models to public and/or public/private databases. Federal agencies should also seek ways to encourage long-term thinking in the development and maintenance of testing and analysis infrastructure within government labs. Lastly, researchers should be afforded easier access to existing resources, support for learning to use those resources, and incentives for investing the time needed to do so.

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.

NASA should provide resources to ensure small businesses remain informed about the Vision 2040 effort and associated funding opportunities, including increased use of the Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs. NASA should also monitor innovative companies to help build connections between emerging capabilities of ICME-based businesses and critical gaps or actions called for in this report. NASA should support small businesses seeking to engage in the collaborative ecosystem by emphasizing the need for user-friendly platforms with easy data-sharing and collaboration capabilities. To help guide this effort, NASA should work with other federal agencies to identify and clarify specific or potential issues relating to export control requirements or related issues. Finally, federal agencies with high-performance computing resources should facilitate access to those resources by small businesses investigating problems of interest to the Vision 2040 effort.

RECOMMENDATION #11
NASA should engage with academia and industry stakeholders to regularly update this study and/or conduct follow-up studies to ensure the full realization of a cyber-physical-social ecosystem with a knowledge-based platform that is usable by human designers.

Vision 2040 calls for the integration of computational materials engineering and systems/structural design. Given the collective expertise of the stakeholders engaged in the study, this report addresses computational materials engineering extensively but requires additional work to further address the systems/structural design and analysis side of the envisioned ecosystem. By regularly revisiting the vision study and seeking input from the broad community, NASA can ensure the continued relevancy and value of this study. It is also important to acknowledge that the path forward must continually adapt based on the requirements for such a knowledge-based platform as identified by materials scientists, design practitioners, researchers, and computer scientists.

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Detailed Vision 2040 Findings

Key Elements

The Vision 2040 strategy identifies nine interdependent Key Element work domains to organize the technical and cultural hurdles facing the multiscale modeling and simulation community, as well as recommendations for pre-competitive research and development efforts to enable the 2040 vision. These core technical areas emerged from a broad examination of existing tools, techniques, and capabilities used across stakeholder groups for multiscale design and analysis of materials and systems. Together, these Key Elements represent a community-consensus foundation for fulfilling the 2040 vision for the entire supply chain.

1 Models and Methodologies
2 Multiscale Measurement and Characterization Tools and Methods
3 Optimization and Optimization Methodologies
4 Decision Making and Uncertainty Quantification and Management
5 Verification and Validation
6 Data, Informatics, and Visualization
7 Workflows and Collaboration Frameworks
8 Education and Training
9 Computational Infrastructure

Contributors to the 2040 vision established detailed descriptions of the Key Elements to define the boundaries of the efforts required to endorse the future ecosystem. The Key Elements' nine expert review panels comprised a range of stakeholder groups[*] and backgrounds[**] to capture the multifaceted nature of these broad technical areas—each providing a unique perspective on how the Key Elements will bring the broader community closer to the 2040 end state. Since the Key Elements are not mutually exclusive and may be classified in different ways, their functions will naturally overlap. Nevertheless, all nine Key Elements will coalesce to form the proposed 2040 end state.

FIGURE 3 THE SIX SECTIONS OF EACH KEY ELEMENT

1 Definition	2 Current State of the Art	3 2040 End State	4 Gaps	5 Recommended Actions	6 Relationships with Other Key Elements
List of roles and functions within the scope of the Key Element	Detailed summary of current technologies associated with the Key Element	Description of the capabilities required to achieve the envisioned design and simulation landscape of 2040	Technical and cultural challenges preventing the realization of the 2040 vision	Prioritized set of recommended actions with estimated funding levels and timelines to completion	The two-way relationships between the Key Element in question and the other eight Key Elements

Each of the nine Key Elements is divided into six sections, described in Figure 3.

To help the Key Elements coalesce into the 2040 end state, the roadmap defines 10 common themes, or crosscutting streams, to help organize the gaps and recommended actions. 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:** The Data Management stream deals with the capture, storage, description, and tracking of materials data and metadata, including data pedigree, provenance, ontologies, and collection modalities.

2 **Data Analytics and Visualization:** The Data Analytics and Visualization stream addresses the analysis and representation of data, including data mining and manipulation, artificial intelligence, machine learning, and uncertainty quantification.

3 **Information Sharing and Reusability:** The Information Sharing and Reusability stream focuses on the inter- and intra-organizational flow of information along the supply chain and throughout the product development lifecycle. It also encompasses information security (e.g., intellectual property [IP] protection, export controls) and availability (e.g., public databases, open source codes). The term "information" extends beyond data and metadata to include codes, methods, tools, assumptions, uncertainties, and any other shareable knowledge.

4 **Multidisciplinary Collaboration:** The Multidisciplinary Collaboration stream covers gaps and recommended actions that explicitly require the convening of experts, stakeholders, and domains (i.e., industry, government, and academia). Collaboration can take the form of consortia, workshops, or communication pathways and platforms among disparate groups that design, develop, or deploy aerospace materials and systems.

5 **Institutional Paradigms:** The Institutional Paradigms stream includes gaps and recommended actions that deal with traditional modes of working and operating in industry, academia, and government. This primarily includes challenges related to cultural and organizational inertia, and the potential strategies to overcome them. In general, institutions are slow-moving systems that resist change—from companies and universities to the people that work within them.

6 **Benchmarking and Business Case:** The Benchmarking and Business Case stream focuses on assessing and demonstrating current or emerging technologies and approaches. Assessments—such as validation, feasibility determination, or economic analysis—involve using standards to evaluate results, establishing benchmarks or example problems, and examining return on investment (ROI) via feasibility determination or economic analysis.

7 **Scalability and Computational Efficiency:** The Scalability and Computational Efficiency encompasses aspects of the ecosystem that address computational speed, complexity, and demand. This includes interfacing with HPC architectures, utilizing surrogate models, and developing more efficient or balanced computational methods.

8 **Linkage and Integration:** The Linkage and Integration stream covers gaps and recommended actions that deal with explicit linkages of models, methods, tools, instruments, databases, and spatiotemporal scales. Topics include compatibility, interoperability, and data fusion. Although similar to the Information Sharing and Reusability stream, Linkage and Integration focuses on non-human integration.

9 **Input/Output Confidence and Reliability:** The Input/Output Confidence and Reliability stream addresses the accuracy and robustness of inputs and outputs. This includes understanding, quantifying, or elucidating variables, constraints, uncertainties, and outputs from simulations, tools, and knowledge management systems.

10 **Behavior of Materials and Structures:** The Behavior of Materials and Structures stream

*academia, government, and industry

**modelers; experimentalists; specialized practitioners; researchers; design, materials, and structural engineers focuses on enhancing scientific understanding of the properties and physics associated with materials, structures, and processes. This includes materials characterization, response modeling, behavior mechanisms, and manufacturing environments.

Although the recommended actions are categorized into crosscutting streams, they are not limited to closing single gaps within the same stream.

Pursuing a recommended action represents a step toward realizing the 2040 end state and may address multiple gaps, across both streams and Key Elements. The gaps and actions presented in the tables in each of the Key Element sections that follow are each tied to the six characteristics of the 2040 end state (accessible, adaptive, interoperable, robust, traceable, and user-friendly) to highlight which attribute(s) of the envisioned 2040 ecosystem they are either preventing or enabling.

Key Element 1:

Models and Methodologies

Definition

This Key Element encompasses the following:

1 Deterministic and probabilistic mathematical models and numerical algorithms for elucidating, predicting, and/or representing the physics and range of expected behavior (chemical, electrical, thermomechanical, environmental, etc.) of materials at specific length and time scales, and across scales for various material and aerospace applications

2 Methods and protocols to identify, characterize, and validate model input/output parameters, both single and multiscale, relative to experimental data

3 Establishing physics-based and/or data-driven mathematical relationships that define process-structure-property-performance relationships of materials, thereby permitting the assessment of process-related materials reliability issues while effectively reducing trial and error approaches in materials design

Current State of the Art

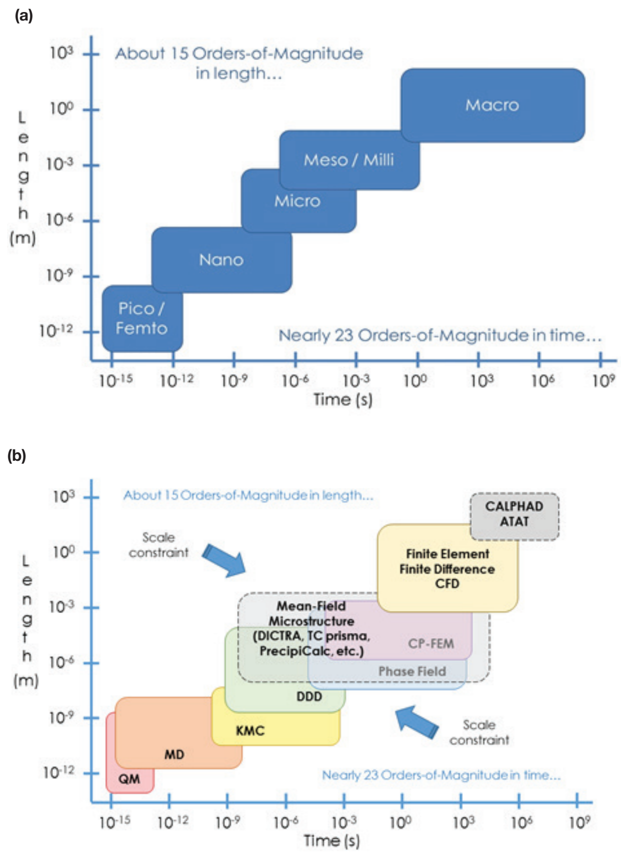
Role

Models permit studying the usage of materials and systems (e.g., structures) beyond those that are readily accessible through experiments. Models provide fully revealed results, yet approximate in-reality responses; experimentally measured responses represent full reality (environmental states, material conditions, etc.), yet provide only partially revealed results since only a subset of the full dimensional space is typically available. In today's design paradigm, this Key Element plays a central role in mathematically (i.e., using constitutive models) representing the behavior of materials in all system-level computer simulations—the majority of these being performed using the finite element method—regardless of organization.

When designing a given system, macro-level, continuum models are traditionally used to represent material behavior, whereas when designing "fit-for-purpose" materials or desiring to understand why a material behaves the way it does, lower length scale models—either continuum based (e.g., micromechanics), mesoscale or atomistic scale models—are used depending upon the material under investigation. Hierarchical materials structure information tied to models is not an explicit part of today's design and manufacturing paradigm. Thus, materials modeling is viewed fundamentally as an endeavor to develop constitutive relationships (e.g., a mathematical description describing the relationship between stress and strain, or applied fields and response fields) through a detailed understanding of the microstructural features that drive material responses, which then requires the observation and modeling of the material at each of the relevant scales of interest. A key purpose of integrated and multiscale materials and structures modeling—which is almost exclusively performed in research organizations—is

FIGURE 1.1 TODAY'S MULTISCALE MODELING PARADIGM (A) AND COMMON MODELING METHODS TO ADDRESS THESE REGIMES OF INTEREST (B)

QM = quantum mechanics (e.g., density functional theory, quantum chemistry); **MD** = molecular dynamics and accelerated molecular dynamics; **KMC** = kinetic Monte Carlo; **DDD** = discrete dislocation dynamics; **CP-FEM** = crystal plasticity finite element method (includes related spectral methods); **ATAT** = alloy theoretic tool kit; and **CALPHAD** = calculation of phase diagrams



to perform many times more instantiations of possible engineering designs than can be physically realized. Yet, within the current design paradigm, only isolated modeling and simulation methods are used to gain fundamental understanding, while empirical testing is used to evaluate material behavior and to deduce performance for both manufacturing and engineering design. There are few established standards taught across the spectrum.

Summary

Today's multiscale modeling paradigm develops single-scale methods and then seeks to pass parameters between scales, usually in a "bottom-up" (i.e., small scales to larger scales) fashion. Materials process engineers rely on finite element method (FEM)-based simulations tools that contain models for heat transfer, mechanics, and selected nonlinear materials behavior such as composites cure kinetics and properties, metal solidification, and finite-strain metal plasticity. Current development processes for such software incorporate lower scale physics based on semi-empirical understanding of materials and/or extrapolations based on large experimental datasets. These physics descriptions are typically parameterized across scales to run efficiently in the model or toolset. Selected parameters can be obtained using *ab initio* methods validated by experiments when available, while others are obtained from specialized experiments and materials characterization. The "computational supply chain" for the few models currently available has been synopsized for the multiscale modeling context in a recent TMS report [1]. The modeling and simulation supply chain supports well-developed simulation codes under various brand names for process modeling and macroscale structures analysis, including selected established and emerging tools for materials chemistry, alloy composition and kinetics.

Figure 1.1(a) depicts multiscale materials modeling from the materials physics, chemistry, mechanics, and materials engineering communities. This notional SoA view indicates single-scale simulation methods and implies data or information passing between scales, usually from the bottom up. The most advanced treatments consider methods for adaptively passing information between scales or for operating simulations at different scales by region of the domain that adapt in real time (e.g., the quasi-continuum method [2]). Additionally, Figure 1.1(b) depicts modeling method length scales as a function of the time scale that they access. The depictions are approximate and dependent upon the specific materials being studied and the specific simulation degrees of freedom.

Finite element, finite difference, and computational fluid dynamics methods are mainly macroscopic continuum methods, although they have many niche applications at other scales. The methods shown as gray box with dashed borders are methods for equilibrium conditions or mean-field methods that offer no spatially resolved information. They are intended to provide equilibrium information or average behavior. ATAT and CALPHAD methods are both examples of equilibrium methods. The reader is referred to the TMS multiscale modeling report for more extended descriptions of these methods [1].

The following sections discuss a more detailed review of models and methods applicable to the atomistic scale, mesoscale, and continuum scale.

ATOMISTIC SCALE

Electronic Structure, Density Functional Theory (DFT)

The most accurate and complete representations of the chemistry and molecular-level aspects of materials come from electronic structure methods where the atomic ions and electrons are explicitly included in the calculations [3]. Many of these methods, which have their origins in computational chemistry, are now routinely applied to materials. Electronic structure methods are required to evaluate material properties which depend on electronic behavior (e.g., band gaps, ionization potentials, optical spectra, electronic conductivity). In addition, these methods provide a high-accuracy description of ionic behavior, permitting the determination of crystal lattice properties such as lattice constants, phonon spectra, and elastic constants. These approaches, often called “first principles” or “*ab initio*” methods, represent approximate solutions to the quantum Schrödinger equation. They can be applied to arbitrary material compositions (i.e., they are “transferable”) without the need for further inputs or fitting parameters. However, this high degree of accuracy and generality creates a high computational expense resulting from including the electronic degrees of freedom in the problem; each electronic structure calculation computes the density of electrons throughout the material.

The most widely used *ab initio* method is Density Functional Theory (DFT), which expresses physical quantities, such as energy, as an approximate functional of the electron density function. This has proven to be a remarkably robust and computationally efficient approximation to the full quantum equations and has opened the door to treating significantly more complex systems than were able to be treated before. In addition to developments in the method, high performance software packages (e.g., VASP, *ab initio*, Quantum Expresso [4]) have matured significantly, making DFT a standard, widely used, and widely accessible tool for computational materials modeling. While early DFT studies were limited to a handful of atoms, current DFT computations can be performed on hundreds of atoms. Innovations in linear scaling methods [5] and other advanced approaches are expected to push that boundary into the thousands of atoms and higher in the near future. DFT methods need improved accuracy for certain classes of materials such as wide-band gap materials and highly correlated electron systems.

Another area which has begun to benefit from *ab initio* methods is computational thermodynamics [6]. The ability to compute accurate phase diagrams and other equilibrium properties (precipitates, diffusion, etc.) is critical for material design and processing. CALPHAD is a widely used phenomenological model that can generate phase diagram relatively quickly; however, CALPHAD requires large, carefully constructed, and experimentally derived input databases, and has a mixed record of predictive ability [7]. By definition, CALPHAD methods do not have established experimental databases. More recently, *ab initio*-based computations of free energies that use a combination of DFT, quasi-harmonic approximations, and cluster expansions have enabled first-principles, parameter-free evaluation of phase diagrams at 0 K (zero Kelvin) or ground state. This approach has been most successful when used for alloy development and design. The computational expense of such approaches has limited the complexity of possible alloys considered (e.g., the number of components). However, these limitations can be addressed through innovations in methods, computer power, software, and other areas. Further methodological work is needed for this approach to capture fully anharmonic effects and to treat mechanically unstable phases. A related approach with dramatically lower computational cost uses CALPHAD in conjunction with first principles methods [8]. Specifically, *ab initio* methods can be used to generate input parameters for CALPHAD, relaxing the necessity to obtain such parameters from experiments. This dual approach combines benefits of both methods: improved predictive ability with low computational expense.

Classical Molecular Dynamics and Monte Carlo

For applications that focus on the collective behavior of the atomic ions rather than the electrons, simulation methods that rely on classical mechanics using empirical interatomic potential energy function, rather than the solution of the Schrödinger equation, have proven very successful in describing the behavior of large systems of up to trillions of atoms in a crystal [9], and for a time period of up to 1 millisecond in protein folding simulations [10]. Trading the accuracy of the quantum mechanics for the simplicity of the classical mechanics at the level of atoms and molecules provides increased computational efficiency and enables massive parallelism of the calculations, solving problems in a variety of areas (e.g., thermodynamics of solids and liquids, transport properties, phase transitions, mechanical and thermomechanical properties at microscale, protein folding, self-assembly). Two major classes of classical atomistic methods are the molecular dynamics (MD) [11] and Monte Carlo (MC) methods [12].

Within MD, atomic-scale trajectories are evolved by solving the classical, dynamical equations of motion (i.e., Newton's Second Law) for the atomic "particle." In addition to accurately describing the kinetics of system evolution and non-equilibrium dynamics, an extensive theoretical formalism derived from statistical mechanics permits determination of a detailed set of properties from the particle trajectories, including thermodynamics, transport coefficients, mechanical response, thermal conductivity, and electrochemical processes.

The different types of MD approaches are distinguished by their definition of a particle and how the forces are computed. In classical MD, for instance, the particle is typically an individual atom and the corresponding interatomic forces and energies are obtained from an interatomic potential energy function which must be derived and/or fit to a database of properties either measured experimentally or computed with more fundamental methods such as DFT. Conceptually, the classical interatomic potential can be considered as being derived from an *ab initio* energy function where the electronic degrees of freedom have been integrated out. The result is a theory of atomic nuclei interacting via an energy function that captures both effective electronic (e.g., chemical bonding) as well as direct inter-atomic (i.e., nuclear) interactions. In reality, interatomic potential energy functions are rarely derived from first principles. Rather, they are more often postulated based on intuition and/or experience.

Instead of following atomic trajectories, MC methods randomly sample the configurational space of the system using the classical Boltzmann probability distribution of the system states with respect to the system energy. In the process of sampling, statistical quantities such as density of states and transition probabilities are used to directly determine the thermodynamics behavior of the system. MC methods are helpful in cases where the system dynamics are very slow, such as in solid solutions or dense entangled polymer networks where following atomic trajectories may take a prohibitively long time to explore a statistically meaningful part of the configurational space. Modern parallel computers allow simulation of multiple replicas of a system for much faster statistical sampling. Another benefit of MC methods is that they rely on only energy calculations, not interatomic forces, which helps simplify the computations.

Selection and derivation of appropriate interatomic potentials is a major challenge for MD/MC simulations. Potential energy functions must be parameterized for every chemical species being simulated and for all possible inter-chemical interactions for any system of interest. Such parameterizations, in general, do not exist for arbitrary chemical compositions, and are only available for a relatively small class of chemical elements. Simulations typically involve no more than two to three chemical species at a time, and there is a hierarchy of possible functional forms for interatomic potentials of varying accuracy, complexity, and computational expense. To date, parameterization of specific potentials has not been standardized, which has often resulted in a large number of different parameters sets for the same system and the same potential form. Furthermore, different parameterizations may be fit to different physical properties and therefore have differing levels of fidelity depending on the system and properties being simulated. A few "general purpose" potentials have been developed for organic systems (e.g., CHARM, OPLS), but these potentials often fail for applications beyond those originally envisioned. One important example is organic electrolytes for batteries where polarization effects from the ionic salts are not easily accommodated. Clearly, an application-specific, efficient, and systematic methodology is needed to generate appropriate potentials. MD/MC methods have proven most useful for parametric studies to investigate mechanisms in models of materials systems.

One recent development in this field is the construction of classical potentials (or force fields) by multi-dimensional interpolation between the energies in a massive DFT database (usually tens of thousands of atomic configurations). This is achieved by applying machine-learning (ML) approaches such as artificial neural networks [13]. The ML potentials are significantly slower than the traditional potentials, but they are orders of magnitude faster than straight DFT calculations. For simulations within the configurational domain of the training dataset, the accuracy of ML potentials can approach that of DFT calculations [14]. However, for new atomic configurations outside the training dataset, the accuracy of energy predictions is usually very poor. In the future, the accuracy of the extrapolation could be improved by combining the purely mathematical ML potentials with physics-based models of atomic bonding, such as bond-order potentials.

In addition to limitation on fidelity and chemical generality, and in spite of the significant progress in the computational efficiency achieved in the classical atomistic simulation, there is a need to be able to simulate experimentally relevant length and time scales. Impressive progress has been made recently in pushing both of these boundaries—accelerated MD methods, for example, have made longer time scales more accessible for selected systems [15]. However, considerable work remains to push these limits further and increase their applicability.

Ab Initio Molecular Dynamics; Reactive Force Fields

The surplus of possible potentials used in classical MD simulations can be circumvented to some extent by combining different *ab initio* methods (e.g., DFT with MD simulations, or *ab initio* molecular dynamics [AIMD]). In this approach, DFT supplies high accuracy interatomic forces that can be used for dynamical simulations without the need for an interatomic potential. The result is an accurate, highly transferable approach for materials of arbitrary chemical composition, though this incurs a high computational expense. In addition, current AIMD simulations are limited to hundreds of atoms, whereas classical MD has been used for systems of up to a billion atoms. Increases in computer power and innovations in software efficiency (e.g., scalability, parallelization) will continue to increase the number atoms that can be simulated with AIMD. However, classical, well-parameterized potentials will still be needed to consider increasingly complex and increasingly realistic systems of interest.

Classical MD simulations permit interatomic interactions (e.g., chemical bonds) that respond to their environment; however, they are limited in that bonds cannot be created or broken as occurs in chemically reacting systems. AIMD, on the contrary, allows for that reactive flexibility (though at high computational expense). Reactive force fields offer one approach to include bond breaking/formation events in classical simulations. Perhaps the most widely used reactive force field currently is ReaxFF (“reactive force field”), although others are under development [16].

Coarse Grained Molecular Dynamics; Dissipative Particle Dynamics

Another class of MD methods that attempt to access larger system sizes and longer time scales are “coarse grained” models [17]. In this class of methods, the notion of a particle is generalized to represent a collection of atoms. These methods can include united atom models where a generalized atom represents a specific chemical group (e.g., a –CH2, CH3, aromatic ring) for organic systems. Further abstractions, for example, include bead-spring models for polymers. With these models, the polymer is represented by a chain of single beads connected by relatively simple (e.g., harmonic) interactions. In addition to the advantage of computational efficiency, this class of models permits complicated systems to be decoupled and to have their individual attributes studied individually. For example, polymer material complexity comes from the combination of subtle chemical interactions and complex architectural effects due to polymer chain entanglement or network structure. The chemical and architectural effects can be decoupled by using a bead-spring approach to study different architecture in one set of simulations, while relying on an “all-atom” classical MD to consider more detailed chemical interactions.

An extreme case of coarse graining is Dissipative Particle Dynamics (DPD) [18]. In DPD, a particle can represent clusters ranging from several atoms up to hundreds of atoms. This class of methods extends particle dynamics into the mesoscale regime and provides a link between fully atomistic methods and quasi-continuum approaches for viscoelastic solids, fluids, and others. DPD is also highly advantageous for its faster dynamics due to the soft potential functions used. This permits the DPD beads to overlap and quickly move from one state to the other because they can partially pass through the other DPD beads in the systems.

MESOSCALE

Computational materials science at the mesoscale enables description of phenomena that cannot be accurately or efficiently simulated using either continuum or atomistic approaches. Unlike continuum descriptions where there is no material length scale, mesoscale descriptions typically include a length scale often related to dominant physical features within the material. Depending on the phenomena being considered, these length scales are typically on the order of a fraction of a micron to about a hundred microns.

An example of the differences between representations of a single class of phenomena is metal plasticity. Variants of plasticity theory include discrete dislocation dynamics (DDD), strain gradient plasticity, and crystal plasticity (CP-FEM). At length scales on the order of tens of microns or less, DDD can be used to simulate the generation, motion, accumulation, and annihilation of individual dislocations and systems of dislocations in an otherwise elastic medium. At somewhat larger length scales (tens to hundreds of microns) where homogenization of the effects of dislocations is required but where gradient effects dominate plastic mechanisms near discontinuities, strain gradient plasticity can be used to describe plastic deformation near a crack tip or in the presence of small precipitates. Finally, at even larger length scales that are relevant to deformation of individual grains (hundreds of microns to millimeters), crystal plasticity can be used to study plastic slip within a polycrystal that might contain tens, hundreds, or even thousands of grains.

Figure 1.2 below contains a summary of several commonly used mesoscale modeling methods that can be used to describe various physical phenomena. The current state of the art and breadth of application varies for each of these methods.

CONTINUUM-SCALE

Continuum models and methods constitute the foundation of computational analysis for representing material and system (in particular, structural) behavior, either linear or nonlinear. In essence, what delineates a structure from a material (i.e., the substance of which a body is composed) is the presence of a boundary. The structure's behavior is dependent upon the boundary as well as the material(s) that comprise it. In continuum mechanics, the material response to a given input is described by a constitutive model; the simplest example of this is Hooke's Law for linear elasticity ($\sigma = E\varepsilon$; that is, the stress tensor is linearly related to the strain tensor by the stiffness tensor).

System analysis, whether for simulation or optimization, relies heavily upon continuum-level constitutive models to represent material behavior throughout a given body. In the case of structural analysis, for instance, analytical solutions are only available for simple geometries, whereas numerical solutions (e.g., finite difference, finite element [FE]) are more widely used to handle arbitrary geometries and boundary conditions. Displacement-based FE analysis is currently the dominant numerical platform for solving continuum boundary value problems (BVPs). For instance, the structural analysis and design community typically uses FE-based simulation

FIGURE 1.2 COMMONLY USED MESOSCALE MODELING METHODS

METHOD	SOME CHARACTERISTICS	APPLICATIONS	REFERENCES
Discrete dislocation plasticity or dislocation dynamics	Dislocations are treated as line singularities in an elastic solid	Deformation, texture, fracture in metals	19-26
Nonlocal plasticity or gradient plasticity	Material length scale is incorporated directly into constitutive description	Deformation, texture, fracture in metals	27-36
Crystal plasticity	Continuum plasticity that considers plastic slip within individual grains of a crystalline material (length scale included in strain gradient crystal plasticity)	Deformation, texture, fracture in metals	37-46
Cellular automata	Transformation rules are applied to the sites of a lattice to determine the state of a site as a function of its prior state and the state of its neighbors	Solidification, recrystallization	47-52
Phase field methods	Based on thermodynamics and kinetics principles with material properties introduced by phenomenological parameters	Grain growth, recrystallization, phase transformation, deformation	53-57
Monte Carlo Potts model	Approximates a polycrystalline microstructure by assigning an integer "spin" to each lattice site with contiguous sites of the same spin composing a grain	Grain growth, recrystallization, phase transformation	58-63

codes for solving thermal, mechanical, and/or acoustic BVPs. The design engineers and analysts typically use linear, small-strain analysis (i.e., elastic models), while nonlinear analyses are used by experts and only when there are issues with selected designs that require higher fidelity. This is true for both quasi-static and dynamic analyses.

The current focus, with respect to the various commercial FE platforms (e.g., Abaqus, ANSYS, NASTRAN, LS-DYNA), is to include enhanced phenomenological-based deformation, damage, and lifing models, and incorporate multiphysics (e.g., combinations of structural, thermal, fluid/acoustic, electric, chemical/environmental) into these codes. There have been significant efforts to improve interoperability with other toolsets within the discipline (e.g., computer-aided design [CAD] and computer-aided engineering [CAE]) and across other disciplines (e.g., computational fluid dynamics [CFD] codes) and various workflow engines and platforms (e.g., Isight, MATLAB). 3D Experience (Dassault Systèmes Simulia) [64], Digital Enterprise (Siemens) [65], and Discovery Live (ANSYS) [66] are three examples of next generation commercial solution platforms, while COMSOL [67] is an example of a state-of-the-art multiphysics analysis platform.

Although it is beyond the current scope to conduct a complete review of the state of the art regarding the solution of structural or system level boundary value problems, it can be said that the solution portions dealing predominately with force and motion (i.e., stress and infinitesimal or finite strain) have reached a significant level of maturation. Two examples of ongoing development in this field that focus on improving the FE method are:

- Reduced-order modeling techniques (e.g., proper orthogonal decomposition [POD] [68]) to scale down the dimensionality of a large set of simulation equations, and
- The extended finite element method (XFEM) [69] to allow traditional FE platforms to model both internal and external boundaries—holes, inclusions, or cracks—without requiring the mesh to conform to these boundaries.

These efforts aim to significantly enhance solution robustness and speed.

Conversely, the constitutive model formulation (which connects forces and motion) remains an important and active area of research. Current commercial solutions predominately use constitutive models to represent a material at an integration point within the FE method. The ability to insert user-definable constitutive and failure models within most commercial codes (e.g., the UMAT routine within Abaqus) is proof of the variety of constitutive formulations.

At the core of continuum-based constitutive modeling is the concept of a homogeneous volume element of material over which the conjugate fields (e.g., stress and total strain) are assumed uniform. The material point does not explicitly account for any internal details (i.e., microstructure) within the material, such as inclusions, grains, or molecular arrangement. The effects of these details are accounted for implicitly through mathematical, thermodynamically consistent constructs that adhere to postulates of objectivity, physical admissibility, equipresence, and locality [70-72]. The most advanced nonlinear, continuum level, constitutive models to date are categorized as internal state variable (ISV) models, wherein both path-dependent, hereditary deformation (e.g., viscoelastoplasticity [73]) and damage (e.g., of the stiffness or strength degradation type) behavior are incorporated into the corresponding evolution equations [74-75]. The majority of these models, although often referred to as physics-based and motivated by underlying physical mechanisms, remain phenomenological in nature, as many of the associated model parameters require calibration or correlation with experimental response curves and are not explicitly associated with a given material mechanism, structure, or property. This is particularly true for anisotropic, effective (macro-level), constitutive, damage, and failure models wherein the macroscopic anisotropy is a byproduct of different phases or inclusions at a lower length scale. Regarding models for composite materials, for instance, the various directions must be characterized through extensive composite testing, as they do not, by definition, consider what is happening in each constituent (e.g., fiber/inclusion, matrix) at the appropriate physical scale.

Further, continuum constitutive models, whether isotropic or anisotropic, have proven to be well suited to predicting deformation response, although their ability to predict damage evolution and life remains problematic. This is understandable since failure mechanisms are influenced to a greater extent by underlying, lower-length scale features, which are by definition ignored. Fortunately, damage/life models can be enriched by linking with lower length scale features and modeling approaches while retaining the ability to interface with large-scale FE analyses of systems and applications. For example, in the case of composite materials or polycrystalline metals, researchers often desire to explicitly link the constitutive response of a material point (i.e., the continuum volume element) with internal, lower length scale features or details. To accomplish this, they require an additional theory beyond standard continuum mechanics (e.g., a micromechanics theory) where the effective behavior of the heterogeneous material is determined based on the behavior and interaction of the constituent phases (e.g., fiber and matrix in the case of composites, or grains in the context of polycrystalline metals), the respective volume fractions, and geometrical arrangements. Such approaches can be classified as multiscale, continuum-based methodologies that enable transitions of scales from the constituent-, to meso-, to macroscale through homogenization (i.e., up-scaling) and localization (i.e., down-scaling) procedures affiliated with a repeating unit cell (RUC) or representative volume element (RVE). In this way, a composite's effective behavior (be it linear or nonlinear) computed via micromechanics [76] can then be treated as a material point in higher-scale analyses.

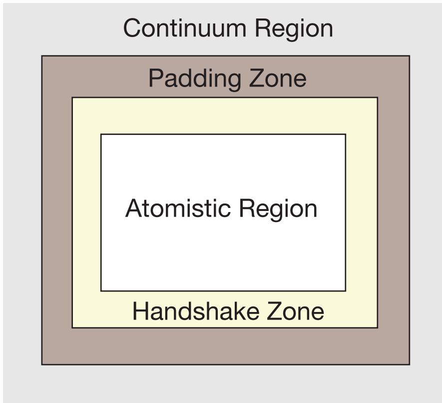
Currently, micromechanics-based material and structural analyses take place regularly within research organizations—see NASA Glenn's MAC/GMC (Micromechanics Analysis Code based on the Generalized Method of Cells) software [77]—and are present within commercial codes (e.g., Digimat [78], Autodesk HELIUS Composite [79] and Altair HyperWorks composite [80], and other software solutions [81]). However, such multiscale modeling techniques (see Case Study 1, Appendix B) are not routinely used by structural analysts/designers in industry because of lack of familiarity and accepted practice, increased complexity of analysis, and a design space limited to the linear thermoelastic regime. Although micromechanics grants access to both global and local fields (which enhances solution fidelity), the ultimate accuracy of such approaches is limited by the accuracy of the local (i.e., constituent) constitutive models (either deformation or damage), which are subjected by default to *in situ* multiaxial and non-proportional thermomechanical loading. It is imperative that such constitutive models be adequately verified and validated under complex loading conditions, yet this is not currently being done.

Finally, continuum models are now applied in various manufacturing processes that incorporate physics-based or semi-physics-based materials models. The aerospace sector, for instance, has used advanced forging simulations at the continuum level while incorporating physics-based materials models to design materials for manufacturing turbine components.

HYBRID APPROACHES

Hybrid models are defined herein as concurrent multiscale modeling techniques in which discretized continuum methods (e.g., finite element method [FEM]) are coupled with various types of atomistic methods (e.g., molecular static [MS] or molecular dynamic [MD]; see Case Study 2, Appendix B). Partitioned-domain methods is a specific type of hybrid approach wherein a body is divided into fully defined (both spatially and parametrically) independent coarse-scale regions (i.e., regions treated by continuum mechanics), and fine-scale regions (i.e., regions treated by atomistic methods such as MS or MD) [82, 83]. Such separation enables one to balance efficiency and fidelity in a more pragmatic manner. An essential feature of multiscale modeling approaches is the way communication is handled in the interface between the continuum and atomistic regions. Generically, the interface region (see Figure 1.3) is divided into two sub-regions: a "handshake" zone and a "padding zone." The size and nature of these zones depends on the specific type of multiscale modeling method. For non-equilibrium or dynamic methods, known complications in the interface zone may include spurious wave reflections caused by impedance mismatches between fine-scale and coarse-scale models or ghost forces that result from coupling local and non-local systems (e.g., FEM to MD, respectively). Furthermore, the thermal motion of atoms in the atomistic region of a coarse-scale grid can create entropy-like contributions which artificially affect the dynamics of coarse-scale models. In addition, different scales (particle versus continuum) may have different definitions of fundamental

FIGURE 1.3 SCHEMATIC OF GENERIC PARTITIONED-DOMAIN PROBLEM



quantities (e.g., stress, temperature), causing further complications. While static partitioned-domain methods and their associated errors are reasonably well established, dynamic models still require clarification [84].

According to Tadmor and Miller [71], there are four primary ways in which partitioned-domain methods differ:

1. **The governing formulation**, which can be subdivided into "energy-based" or "forced-based" approaches.
2. The coupling boundary conditions between the continuum and atomistic regions, which can be subdivided into "strong compatibility" and "weak compatibility", both being applied within the so-called padding region (see Figure 1.3).
3. The handshake region, wherein the transition can be abrupt with no handshake region or can exist and provide a gradual transition from the atomistic to continuum model.
4. Treatment of the continuum region itself, be they based on FEM, "meshless" methods (see [82,85]) or "coarse-grained molecular dynamic" (CGMD) [86], with the FEM being the most prominent approach in the literature.

Figure 1.4 summarizes a number of static methods for crystalline solids according to these four attributes [87].

Other multiscale "hybrid" approaches for coupling methods at various length—and perhaps more importantly, time scales—are actively in development [99-102]. These include

1. MS or MD methods and quantum calculations such as solid date density functional theory (DFT) (see extensive review by Bernstein et al. [103])
2. Full MD simulation with CGMD [104] and material point method coupled with molecular dynamics (MPM-MD) [105] in the area of amorphous polymers.
3. Coupled quantum mechanics (QM) and molecular mechanics (MM) models for developing a detailed quantum mechanical understanding of chemical reactions in complex molecules (see reviews by Sherwood et al [106], Friesner and Guallar [107], and Senn and Thiel [108] for biological systems).

Enhancing hybrid multiscale modeling techniques requires the development of an interoperable framework for coupling models and methods, that span both lengths and time scales, to efficiently and accurately analyze various materials (i.e., beyond pristine crystalline solids with "ordered" lattices that conform with the Cauchy-Born rule) contained within large scale structures or systems.

FIGURE 1.4 SUMMARY OF STATIC PARTITIONED-DOMAIN METHODS

METHOD	REF	GOVERNING FORMULATION	COUPLING BOUNDARY CONDITION	HANDSHAKE	CONTINUUM MODEL
Quasicontinuum (QC)	88	Energy-based	Strong	None	Cauchy-Born
Coupling of Length Scales (CLS)	89	Energy-based	Strong	None	Linear Elasticity
Bridging Domain (BD)	90	Energy-based	Weak	Linear mixing of energy	Cauchy-Born
Bridging Scale Model (BSM)	91	Energy-based	Weak/Strong Mix	None	Cauchy-Born
Composite Grid Atomistic Continuum Method (CACM)	92	Iterative Energy-based	Weak (avg. atomic positions)	None	Linear Elasticity
Cluster-energy Quasicontinuum (CQC-E)	93	Energy-based	Strong	None	Averaging of atomic clusters
Finite Element Atomistics Method (FEAt)	94	Force-based	Strong	None	Cauchy-Born
Coupled Atomistics and Dis-crete Dislocations (CADD)	95	Force-based	Strong	None	Nonlinear, nonlocal elasticity
Hybrid Simulation Method (HSM)	96	Force-based	Weak (avg. atomic positions)	Atomic Avg. for nodal B.C.	Nonlinear Elasticity
Concurrent Atomistic to Continuum (AtC	97, 98	Force-based	Strong	Linear mixing of stress and atomic force	Linear Elasticity

2040 End State

Simulations will fully link with models of materials structure and responses at multiple scales, allowing designers to conduct part- and system-level predictions informed by high-fidelity atomistic calculations. Such calculations will be enabled by highly parallelized code for multiphysics simulations that make effective use of exascale and beyond. As a result, developers will be able to tailor the microstructure and kinetics responses of materials at various scales to suit application-specific requirements. Furthermore, in 2040 models will allow exploration of materials and structures under loads and environments well beyond those accessible in laboratories, such as high Mach-number flight regimes, meteoric/atomic oxygen bombardment, or re-entry ionization conditions.

In 2040, model building will start with an informatics-based identification of gaps and limitations in prior model frameworks. Autonomous "bots" will then select among models and suggest structure, input parameters, and response protocols needed for parameterization while informing users about the predictive limits of the models.

Additionally, new classes of process simulation models will exist, perhaps based on large-scale data correlation and analysis, to provide revolutionary understanding and control of advanced manufacturing processes and products, including additively manufactured parts.

Gaps

The following gaps lie within five of the roadmap's 10 crosscutting streams, with the **Linkage and Integration** and **Behavior of Materials and Structures** streams containing the majority. Linking models to tools, databases, and other models presents a significant challenge, as does the ability to model complex physics at various scales. These gaps have a strong connection with the 2040 end state characteristic of **robustness**, and to a lesser extent, **interoperable** and **adaptive.** To create a robust ecosystem, the community's understanding of mechanisms and phenomena associated with materials and structures needs to take a considerable leap forward.

TABLE 1.1: MODELS AND METHODOLOGIES GAPS AND IMPACTED 2040 CHARACTERISTICS

AC Accessible **AD** Adaptive **IN** Interoperable **RB** Robust **TR** Traceable **UF** User Friendly Critical

GAPS	2040 CHARACTERISTICS					
	AC	AD	IN	RB	TR	UF
INFORMATION SHARING AND REUSABILITY						
Limited accessibility to common repositories for models and methods	AC					UF
Metadata tends to remain with simulation results of niche applications, and is seldom available for sharing across modeling platforms	AC					
Lack of comprehensive material property database (e.g., physical, thermal, temperature, and strain-rate-dependent metallurgical properties) • Limited availability of fundamental materials datasets at various scales precludes effective V&V and calibration	AC					
SCALABILITY AND COMPUTATIONAL EFFICIENCY						
Increasing microscale model complexity and computational expense inhibits characterization and validation of experiments at a higher length scales • Lack of experimental methods to verify models at small length and time scales		AD				
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		AD				
Reliance on large databases and empirical formulations limits predictive accuracy of computational thermodynamics methods (e.g., CALPHAD, constitutive models)		AD		RB		
LINKAGE AND INTEGRATION						
Models do not seamlessly link to actual certification analysis requirements (e.g., stiffness, strength, spectrum fatigue) • Models only manually support the certification process			IN			UF
V&V and UQ are typically addressed after the model development and calibration process rather than concurrently • Difficult to propagate uncertainty between spatiotemporal scales			IN	RB		
Existing frameworks and models lack the adaptability to rapidly incorporate latest theories		AD	IN	RB		
Limited interaction between "top-down" engineering requirements and "bottoms-up" performance modeling • Multiscale/hierarchical/concurrent approaches are poorly defined and do not integrate manufacturing-process-performance • Lack of useful automatic methods for linking models and passing information between scales			IN	RB		

GAPS	2040 CHARACTERISTICS					
	AC	AD	IN	RB	TR	UF
INPUT/OUT CONFIDENCE AND RELIABILITY						
Models and software packages lack robustness and user-friendliness • Commercial software packages often do not have robust materials databases integrated				●		●
BEHAVIOR OF MATERIALS AND STRUCTURES						
❖ Underdevelopment of physics-based models that link length and time scales for relevant material systems • Difficult to incorporate physics that connect lower length scales to higher length scales • Multi-component diffusion models are underdeveloped		●		●		
Lack of formal methods for defining model representative volume elements (RVEs) • No strong consensus on which RVEs are most representative of processes of interest • RVE methods do not sufficiently account for cracks/discontinuities and hierarchical microstructures				●		
Lack of fast process models for predicting materials properties				●		
Underdevelopment of models that simulate materials response against harsh environments (temperature, wear, radiation, etc.) or operating conditions (i.e., insufficient data to support these models)				●		
Inadequate models for simulating failure, nucleation, and non-equilibrium conditions (e.g., solid/liquid phase change)				●		
Underdevelopment of atomistic models that simulate thermal behavior, chemical reactions, and electron transfer across time scales and phases with respect to specific operating conditions • Fitting system-dependent interatomic potentials for atomistic simulations is too labor-intensive to permit efficient materials design and discovery • Lack of rigorous uncertainty quantification and predictive power in fundamental atomistic models				●		
Establish model building block approach for multiscale modeling methods and tools • Linkage with classical experimental building block approach • Include framework/guidelines for model parameter estimation at various length scales	●			●	●	

Recommended Actions

The following recommended actions lie within eight of the roadmap's 10 crosscutting streams, with the most actions (including high priority) under **Linkage and Integration** and **Behavior of Materials and Structures**. These are the same streams that contain the majority of the gaps for this Key Element. These recommended actions focus on developing new models and facilitating the linking of model inputs and outputs. The recommended actions have the strongest ties to the **robust, adaptive,** and **interoperable** characteristics of the 2040 end state.

TABLE 1.2 MODELS AND METHODOLOGIES RECOMMENDED ACTIONS AND METRICS

FUNDING: $ <0.5M/year $$ 0.5-2M/year $$$ 2-5M/year $$$$ >5M/year

AC Accessible **AD** Adaptive **IN** Interoperable **RB** Robust **TR** Traceable **UF** User Friendly ✱ High Priority

ACTION	2040 CHARACTERISTICS						TIMEFRAME FOR COMPLETION			FUNDING
	AC	AD	IN	RB	TR	UF	NEAR 2017-2022	MID 2022-2035	LONG 2035+	
DATA ANALYTICS AND VISUALIZATION										
(1.1) Develop calibration tools that incorporate V&V and UQ methods to automatically fit model parameters			IN	RB	TR		■	■		$
(1.2) Deploy machine learning (ML) approaches to enable development of models that predict materials behavior		AD		RB	TR			■	■	$$$$
INFORMATION SHARING AND REUSABILITY										
(1.3) Create manufacturing process-structure-property databases to inform models that simulate extreme conditions	AC			RB	TR		■	■		$$$$
(1.4) Define model (and data) usage and IP issues to facilitate interoperability and sharing	AC		IN				■	■		$$
INSTITUTIONAL PARADIGMS										
(1.5) Increase transparency of assumptions used in models					TR		■			$
BENCHMARKING AND BUSINESS CASE										
(1.6) Ensure models can calculate cost vs. performance to allow economic tradeoff studies		AD	IN	RB			■			$
(1.7) Collect case studies of successes and failures to illustrate value of modeling to industry (especially subject matter experts	AC						■	■		$$
SCALABILITY AND COMPUTATIONAL EFFICIENCY										
✱ (1.8) Enhance micromechanics-based modeling approaches to take advantage of HPC architectures and enable analysis of large-scale problems		AD		RB			■	■		$$$
✱ (1.9) Foster user capability to selectively trade accuracy (fidelity) for speed in order to optimize computational efficiency • Combine composition approaches with surrogate models to automatically refine the surrogate (e.g., DOE ExMatEx Project)		AD				UF		■	■	$$$$

ACTION	2040 CHARACTERISTICS						TIMEFRAME FOR COMPLETION			FUNDING
	AC	AD	IN	RB	TR	UF	NEAR 2017-2022	MID 2022-2035	LONG 2035+	
SCALABILITY AND COMPUTATIONAL EFFICIENCY, CONTINUED										
(1.10) Develop novel computational methods (e.g., wavelet-based calculations) and other multi-time scaling techniques to enable lower length-scale or fast time scale physics in modeling activities		●		●			▨	▨		$$
(1.11) Develop a robust environment for interoperable open source and commercial codes	●		●	●				▨		$$
LINKAGE AND INTEGRATION										
✱ (1.12) Tie models to experimental measurements for V&V benchmarking activities and development of fundamental 3D/4D datasets • Link results to certification analysis			●				▨	▨		$$$$
(1.13) Develop consistent methodologies for integrating uncertainty from various sources into methods and/or models across scales			●				▨	▨		$$$$
(1.14) Identify input-output requirements to enable “hand-shaking” between scale-specific models			●				▨			$$
(1.15) Launch a digital platform (e.g., automated expert system) that guides the selection and linkage of models (within and across length scales) to form multiscale workflows for specific problems • Automated expert systems with tutorials, supported by digital libraries or marketplaces of multiscale models • Create functional model units by combining necessary models	●		●	●	●	●		▨	▨	$$$$
(1.16) Enable small spatiotemporal models with robust connections between microscale properties and higher length scale performance characteristics			●	●			▨			$$
(1.17) Link process model results to structure design			●		●		▨			$$$
(1.18) Develop accelerated dynamic modeling methods across length scales from atomistic to macro scale to enable modeling of experimental time scales at appropriate length scales		●	●	●			▨	▨		$$
INPUT/OUTPUT CONFIDENCE AND RELIABILITY										
(1.19) Create best practices for defining model fidelity and boundary conditions • Define process windows in models (i.e., controllable variables associated with specific performance criteria)	●			●		●	▨	▨		$$$$
(1.20) Develop industry-wide methods for systematic design and use of material mechanisms	●			●				▨	▨	$

ACTION	2040 CHARACTERISTICS						TIMEFRAME FOR COMPLETION			FUNDING
	AC	AD	IN	RB	TR	UF	NEAR 2017-2022	MID 2022-2035	LONG 2035+	
BEHAVIOR OF MATERIALS AND STRUCTURES										
✱ (1.21) Create fast process models that: • Simulate materials behavior at vastly different length scales within the same system • Permit highly accurate prediction of materials microstructure and properties • Integrate computational materials engineering/design approach				●			■	■	■	$$$
✱ (1.22) Develop/enhance predictive models at different length scales that simulate rare events and nucleation				●			■	■	■	$$$$
✱ (1.23) Develop physics-based models that address key sources of uncertainty in physical understanding				●				■	■	$$$$
✱ (1.24) Develop methods to automatically generate interatomic potentials to enable molecular dynamic simulations of arbitrary reactive and non-reactive systems	●		●	●			■	■		$$
(1.25) Establish a statistics-based approach for defining hierarchical RVEs of models based on response testing protocols and characterization methods • Incorporate into educational curricula to teach best practices for quantifying stochastic variations across scales of hierarchical materials structures • Enable support for future/unforeseen paradigms/ methodologies • Develop process-specific RVE approaches, or enable matching of processes and RVEs				●			■			$$
(1.26) Develop models for discontinuous phenomena (e.g., damage and fracture models)				●				■		$$$
(1.27) Develop and validate high fidelity models for homogeneous and heterogeneous systems (e.g., constitutive damage, fracture, fatigue, and creep models)				●			■	■		$$$$
(1.28) Enhance image-based modeling/tools for heterogeneous regions and data capture to feed computational tools				●		●	■	■		$$$$
(1.29) Develop automated methods for generation of chemical kinetic models from reactive MD simulations and/ or computational chemistry to simulate corrosion, catalysis, chemical processing, etc.			●	●			■	■		$$
(1.30) Develop computational thermodynamics methods based on *ab initio* methods for the complete phase diagrams of materials of arbitrary composition including solid-solid transformations, melting, precipitates, etc.			●	●			■	■		$$
(1.31) Develop non-equilibrium simulation methods to accommodate large property gradients (temperature, voltage, time evolution, etc.)		●		●			■	■		$$

Relationships with Other Key Elements

The Models and Methodologies Key Element will coordinate across core technical areas to mature modern computational and statistical physics methods, and robust analytical tools for the selection and linkage of multiscale variable-fidelity models within a system-based reciprocity framework.**

TABLE 1.3 EXAMPLE INTERRELATIONSHIPS OF KE1 (MODELS AND METHODOLOGIES) AND OTHER KEY ELEMENTS

OTHER KEY ELEMENTS	INTERRELATIONSHIP	THIS KEY ELEMENT
KE2 Multiscale Measurement and Characterization Tools and Methods	Create forward models of 3D/4D characterization tools to maximize information reliability and model parameter estimation	KE1 Models and Methodologies
	Experimentally replicate simulations, identify mechanisms and scale transitions, and provide data for model parameter characterization and validation	
KE3 Optimization and Optimization Methodologies	Enhance optimization algorithms for expanded design space via coupled multiscale/-physics models	
	Couple design problems for cross-scale modeling tool integration and increased solution and sensitivity analysis reliability	
KE4 Decision Making and Uncertainty Quantification and Management	Forward modeling of 3D/4D characterization tools to bound measurement uncertainty and error	
	Illuminate errors, bound error propagation, and enable model-based material and probabilistic component definitions	
KE5 Verification and Validation	Create industry-wide standards, protocols, and model formats to enable V&V tool and method applications	
	Validate models via concurrent companion modeling	
KE6 Data, Informatics, and Visualization	Provide model-based material hierarchies that define data structures	
	Define materials structures; enable capture, analysis, and dissemination of all relevant data; and integrate data-driven models via informatics framework	
KE7 Workflows and Collaboration Frameworks	Generate cost-benefit models for collaborative activities	
	Use collaboration frameworks for joint development and validation of models, and automate linking and execution of disparate models	
KE8 Education and Training	Produce multiscale modeling educational platforms, and translation of academic models with interoperability and user-friendly interfaces	
	Develop and deploy educational modules for multiscale/multiphysics computational methods, industry-relevant ICME models, and methods for government regulator acceptance of ICME approaches	
KE9 Computational Infrastructure	Catalyze scalable computations via reduced order/simplified models	
	Form frameworks for managing/accessing modeling results and governing simulation speed-accuracy tradeoffs	

**Reciprocity relationships describe measured properties and mechanisms in terms of mutually dependent connection among models, simulation codes, characterization protocols, and manufacturing methods.

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Key Element 2:

Multiscale Measurement and Characterization Tools and Methods

Definition

This Key Element encompasses the following:

1 Methods, practices, and devices for measuring, observing, defining, and characterizing

- Physical and chemical makeup and properties of a material within a given volume as well as its response to stimulus such as processing and thermal, mechanical, electromagnetic, and environmental loading
- Operative response (e.g., deformation and damage) mechanisms in response to simple and complex loading conditions (e.g., uniaxial, multiaxial, uniform, or gradient loading conditions)

2 Exploratory, characterization, and validation measurements associated with the identification and assessment of concepts and models at specific and/or transitioning length and time scales for the explicit purpose of establishing and improving models and the engineering simulation framework

3 Establishment of the underlying mechanisms inherent in or foundational to development of process-structure-property-performance relationships of materials and structures

Current State of the Art

Role

Multiscale measurement and characterization tools and methods refer to the approach, planning, and execution of experimental activities, both physical and computational, to establish robust multiscale modeling tools and methods. Physical, experimental investigations are foundational to physics-based material mechanism identification, model development, characterization, validation, and establishment of model uncertainty within the systems paradigm. While physical experiments fully represent and partially reveal reality, models fully reveal yet only approximate reality. Consequently, judicious use of both is required to maximize benefits while minimizing costs.

A systems-based approach to multiscale materials and structural modeling is required to ensure rapid, complete, and well-understood mechanistic modeling tools and methods. Experimental plans are either driven by the development of new mechanistic models or based on uncertainty exhibited in existing models, which drive the need for special, focused characterization of a material and representative models. These plans guide experimentation, either physical or computational, that is “for purpose,” specifically for exploratory testing, focused characterization for specific purpose, and validation of mechanisms and models.

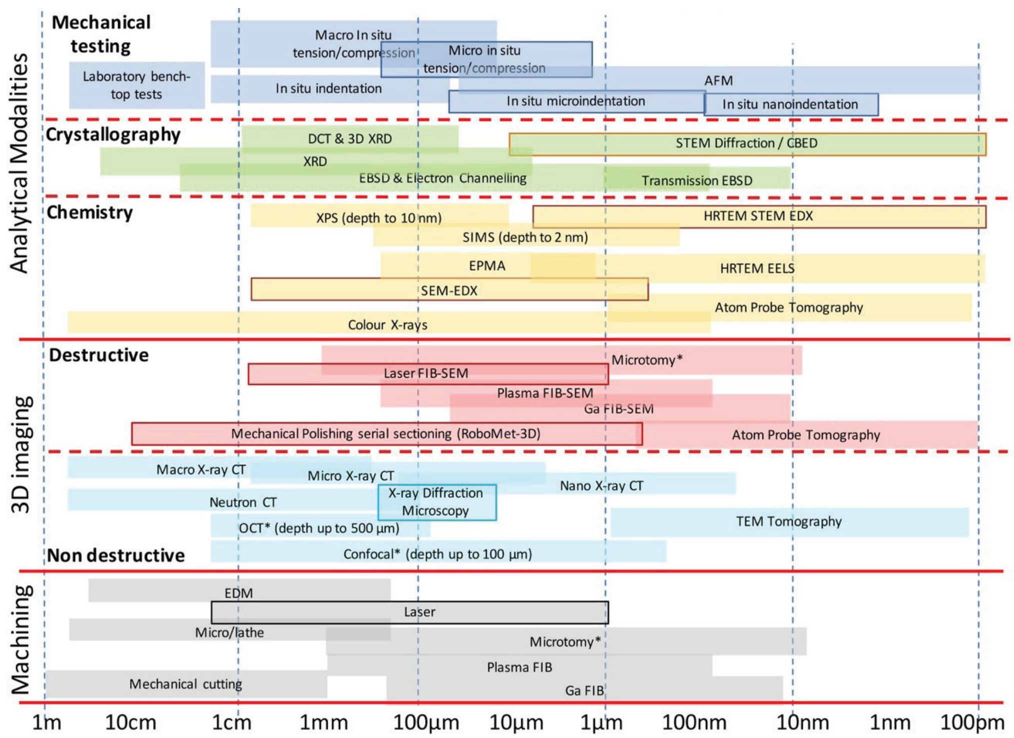
Summary

Characterization Instruments and Techniques

Professor Philip Withers, at the University of Manchester, United Kingdom, devised a convenient depiction of the current state for multiscale instrumentation that has been adapted, as shown in Figure 2.1. Figure 2.1 [1] depicts current capabilities for obtaining materials structure and mechanical testing characterization data across scales. The left axis of the figure shows three major types of information that may be needed (i.e., analytical information, three dimensional material structure information, and machining methods for preparing test and evaluation samples.) The bottom axis of the figure shows the associated length scales.

and likewise obtain materials structure information in 3 or 4 dimensions. Methods will become routine, rapid, quantitative, and cost-effective over the next twenty-five years and include new methods for filling the mesoscale gap. Further, methods such as dynamic transmission electron microscopy and synchrotron-based X-ray methods will expand access to time-resolved materials data and chemical reactions at nanoscales and beyond. Although these new tools and methods will become standard over

FIGURE 2.1: SYNOPSIS OF MATERIALS AND STRUCTURES CHARACTERIZATION INSTRUMENTATION FRAMEWORK OF TODAY, TAKEN AFTER P. WITHERS ET AL. [1].



Accordingly, each method is plotted to show the length-scale range over which data may be obtained. The figure is not a complete depiction of methods; however, it does depict the SoA for readily obtainable and selected developmental methods.

There has been a remarkable expansion in available, reliable tools for both destructive and non-destructive evaluation of hierarchical material structures and properties extending to the atomic level. Today, one can quantitatively characterize chemical information at the atomic scale for many materials

time, methods and tools will experience continuous innovation.

Selected techniques that are expected to provide particularly important information for models are identified by a framed box within some of the characterization domains. Neither dynamic material behavior under thermochemical or other imposed field environments, nor the modeling frameworks needed for their use, are depicted. Those frameworks are under-developed today, but may be radically expanded over the next 25 years. Further, the community does not have, as of yet, a holistic and structured data methodology, simulation suite, or materials analytics and machine-learning framework that is integral to these experimental methods.

Over the last decade, nano-to-microscale testing methodologies for mechanical behavior emerged, as did an understanding of phenomena at those scales [2-5]. These methods permit a probe of certain mechanistic behaviors of materials at small scales and a parametrization of models for coarse-scale predictions [6,7]. The methods led to direct measurements of scale-free dislocation responses for metal plasticity and a deeper understanding of these scientific challenges [8-13].

Also noteworthy is the emerging suite of tools for non-destructive characterization that includes high-energy X-ray diffraction microscopy (HEDM) and related techniques [14-16]. Today, highly specialized SoA methods permit one to non-destructively probe the internal 3-dimensional spatial evolution, and even the 4-dimensional time evolution, of grain structure of crystalline solids across scales, using near-field HEDM (nf-HEDM), diffraction contrast tomography (DCT) and dark-field X-ray microscopy [17-19]. Today's emerging technologies can provide 3-dimensional grain structures at voxel resolutions of about 1-3 micrometers (μm) and grain-averaged stress tensors for loaded materials at scales of ~40 μm or greater using the far-field HEDM method (ff-HEDM) [20]. The methods were demonstrated as concurrent measurements, which included the use of computed tomography contrast to detect opening up and propagation of cracks during loading. While beam-line energy, detectors, and data reconstruction and interpretation algorithms are currently limited to materials having average grain sizes in the range for 30-100 μm, cross-section samples that are within ~1 millimeter (mm), microscale voxel dimensions, and time scales of minutes to hours, they are expected to improve over the next twenty years. These methods will be expanded to broader spatiotemporal domains, potentially ranging from tens of nanometer (nm) voxel sizes up through multiple millimeter sample dimensions. Once the methods are coupled to real-time material and experiment simulation and machine learning, they will provide unprecedented capabilities for model construction, evaluation, and validation. These advanced X-ray methods, together with advancements in multiscale response testing, will open entirely new capabilities that follow form and flow into direct representations of microstructure within a computational model. They will also enable the use of statistically representative microstructural models to assess the distribution of properties associated with the variation of microstructure.

Emerging sensor data streams provide indicators for materials characterization and possible model development. Though their analyses are not yet tied to models for materials and processes, recent progress suggests that these data streams will be particularly valuable for additive manufacturing (3D-printing) processes [21]. Manufacturing settings typically have broad suites of non-destructive evaluation (NDE) methods available for flaw or heterogeneity detection. These are being developed via models that incorporate 3D material structure for non-destructive materials characterization—going well beyond conventional NDE methodologies.

However, dramatic advancements in instrument capability and techniques bring associated escalations of instrument cost and, thereby, reduced access to these capabilities across the materials and structures community. The current trend is for advanced characterization methods to exist within highly specialized centers of excellence and for these centers to be managed in a similar way to current facilities (e.g., synchrotron–based X-ray or neutron scattering facilities). By 2040, much of the needed characterization for models will likely have to take place at "beam-lines" while working with specialized experts, perhaps operating within consortia of specialized practitioners. A recent example of this is the NSF Materials Instrumentation Platforms (MIPs) program, where centers of excellence provide access to specialized equipment with professional support staff (e.g., providing access to equipment that can model crystal growth of compounds for functional materials applications).

Challenges to advanced materials instrumentation occur with software and "big data." Some experiments produce so much data that 6-12 months are required solely to process and analyze the data, which is at odds with the high-throughput design process. In addition, the wide variety of materials taxonomy and metadata structure across the suite of instruments creates a bottleneck when attempting to analyze their data. This barrier can be resolved using instrumentation consortia and advanced software that can easily translate data formats and build data provenance in an automated fashion. For 3D and 4D data, "in-line" data analysis and reconstruction would also permit more efficient use of instruments and easier analyses of the large datasets that are generated in these instruments. There are still basic research issues that limit the merging of data collected on a given material with different instruments, despite the fact that parallel/correlated "data channels" would substantially enhance the understanding of a wide spectrum of materials phenomena. Finally, given that datasets will continue to increase in size and resolution as computer architectures continue to advance, mechanisms for sharing data and workflows for processing the data will need to be developed (see Case Study 3, Appendix B). Lessons learned from the biology and astronomy communities should be leveraged.

Experimental Methods and Plans

Currently, the first step in devising an experimental plan is to identify or propose physical mechanisms that control the behavior within a material—usually a selected mechanism that may or may not account for the multiscale aspects of a material behavior. In this respect, experiments are designed to isolate given mechanisms at a prescribed scale, or to assess quantities—such as deformation fields or damage statistics—that encompass aggregated mechanisms at the scale of measurement. To confirm the mechanism within a material, a simulation of a material behavior based on the modeled mechanism(s) is performed and evaluated. For this procedure, it is critical to understand both experimental and model assumptions, including the material structure definition and how the measured fields are represented in the models (i.e., how the models predict the measured fields).

Next, materials are tested for controlled materials structure and external testing boundary conditions under an assumption of the initial conditions of the materials state, which is fed back to the models (illustrating the "reciprocity" between these aspects). An assessment of the experimental results relative to the model predictions provides insight into the validity of the proposed model. This approach can also assess the structure and application domain of the proposed mechanism, with the model providing guidance for specific structure and test conditions to study.

The overwhelming majority of today's materials tests are performed using one-dimensional (or uniaxial) normal or torsional loads comprising simple one- or two-load segments (e.g., tensile, creep, relaxation, cyclic). Test samples are easy to machine and require minimal quantities of materials, and test rigs are readily available. The loads and strains are generally uniform in the gage section—or at least assumed to be so—and are therefore easy to calculate. These tests facilitate basic materials characterization and estimation of model parameters for design and analysis purposes. Unfortunately, the majority of components operate in more complex (multiaxial) stress and strain states. Moreover, realistic applications of parts and components involve frequent temperature changes/gradients and other environmental effects (e.g., oxidation, erosion). All of these conditions act simultaneously on the part, greatly affecting material behavior and expected life. Consequently, it is highly problematic to shift from material models based on uniaxial data to predicting component responses under true service conditions. Current models are typically insufficient for predicting life and deformation—especially outside of the elastic regime—when evaluated under multiaxial or non-proportional loading, and other complex combinatorial states (e.g., temperature, environment). Materials with initial and/or evolving textures or anisotropic properties (e.g., composite materials) cause additional complications such as specimen preparation, instrumentation requirements, the required amount of uniaxial testing, and the complexities of the models themselves.

As a result, the current testing paradigm is expanding to include a diverse range of conditions to aid in the exploration, characterization, verification, and validation of material behavior models. Examples may include sequential loading sequences (i.e., multiple loading segments) and combined test types (e.g., creep-fatigue, load history effects, thermal cycling), while measuring strains in various directions (via full-field) and monitoring damage development. Rather than conducting hundreds of common (e.g., tensile) tests, it may be more suitable to conduct a few well-conceived tests to characterize and vigorously exercise the model (assumptions, functional forms, etc.).

There is a significant need to conduct multiaxial validation tests (e.g., axial-torsion, in-plane biaxial tests) at both the coupon and sub-element levels. Simple tests, such as bend tests, have limited value as they only measure single point displacement and may inadvertently introduce multiaxial stress states. Actual values within the sample are assumed to be uniform and based on simple beam theory calculations. However, multiaxial tests require special load frames and are therefore much costlier than their standard uniaxial counterparts. Internal pressurization can invoke other unique stress states, but is rarely used (particularly at high temperatures) due to safety concerns regarding high-pressure fluids.

Moreover, sample machining for multiaxial tests is an order of magnitude more expensive than uniaxial tests, and requires much greater quantities of materials. For example, in-plane biaxial samples, which are often cruciform in shape, require complicated designs to minimize premature failures in areas of high stress concentration. For simple metallic systems, samples can cost up to $10,000 each. Non-metallic materials, which are often fabricated into near net shapes, can be even costlier even though such tests rarely involve heating and atmospheric controls. Stress and strain rates are extremely difficult to determine, and must otherwise be derived using finite element analysis (FEA) and/or measured (in the case of strain) using full field photogrammetry. Because of this, multiaxial tests are considered pseudo-structural tests, requiring concomitant resources for both testing and data analysis, yet they are a crucial next step in bridging the gap between uniaxial coupon and full-scale component data and modeling.

A similar importance can also be given to benchmark testing and sub-component tests (e.g., structural members, plates, shells, discs) whose data output is extremely valuable for model verification. Because these tests are highly specialized and expensive, access to such data is rare. The 2040 effort should emphasize concerted efforts in testing complicated or combinatorial modes, developing new associated test methods, and widely distributing the results to directly benefit the multiscale materials and structures modeling community. Actual mixed-mode component test data, which is often scarce and proprietary, would yield enormous benefit to the community for its ability to confirm the accuracy of material behavior models and methodologies.

Experimental plans and test methods are covered in the Verification and Validation (V&V) Key Element, wherein decision making and uncertainty quantification (UQ) management further support the development of experimental plans. If a response mechanism is confirmed, it may be sufficient for a qualitative end purpose and providing direction for material and/or process optimization or control. For quantitative application of a mechanistic model, specific material properties or parameters are needed to support calibration of the proposed model, as most models are simplifications of the entire physics-based process. Achieving higher accuracies and lower uncertainties requires increased experimentation. The proposed model and methodology, which includes the appropriate V&V approach and UQ tools, drives the quantity and specific type of physical experimentation. Greater knowledge about input sensitivities is crucial for designing efficient experimental plans, enhancing model UQ, and reducing unnecessary testing.

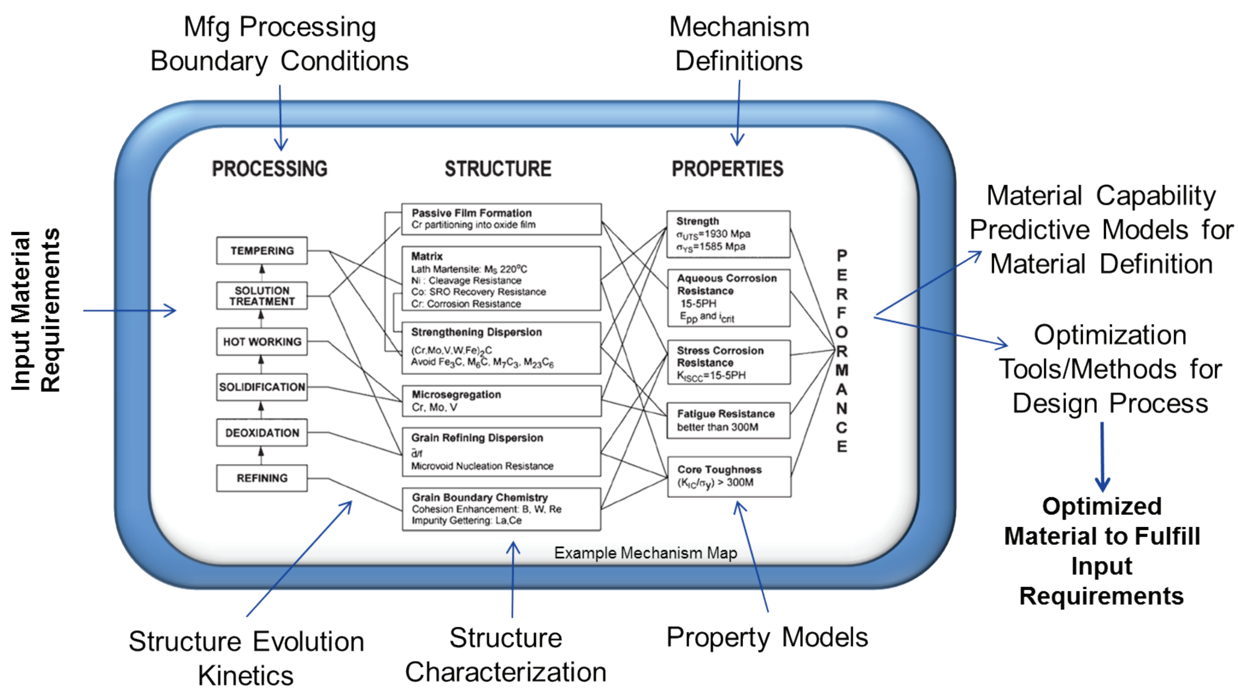
Systematic application of experimental methods guides the development of multiscale models as well as the physical test methods needed to quantify and validate underlying physics-based mechanisms. New mechanisms can be activated under specific material structure and environmental conditions. Exposing materials to the unique environments and conditions (e.g., times, temperatures, loads) of other design spaces can lead to the discovery of previously unreported behavioral mechanisms. As use environments become more extreme, the materials evolution becomes more extreme, and so must the experimental plans evolve to assess these new conditions. These discoveries are guided by characterizing materials at new application spaces and comparing behavior to that predicted from proposed mechanism models. As model predictions deviate from measured experimental results, the proposed model is either incorrect or does not completely describe the actual behavior for the material at differing operating conditions. This experimental method and approach drove the discovery that micro-twinning in nickel-based superalloys was the rate-limiting mechanism at application temperatures above those previously characterized and modeled [22]. Focused metallographic experimentation was required in this example to identify the mechanism, which established a model that can now be used to predict creep behavior when this mechanism is operative.

Similarly, experimental methods linked proposed models and careful material characterization in a fuel cell case study (see Case Study 2, Appendix B). The desired macroscopic behavior of the polymer membrane fuel cell drove the experimental plan to characterize and validate proposed models that described the mechanisms at atomistic, molecular, microstructure, and macrostructure levels.

application and optimization. This formalization of alloy design provides a systematic approach to define required experimental methods for both model application and physical testing activities.

By linking modeling and physical experimentation, it is possible to rapidly screen material, process, and structure space by design of critical experiments.

FIGURE 2.2 EXAMPLE OF AN OLSON DIAGRAM

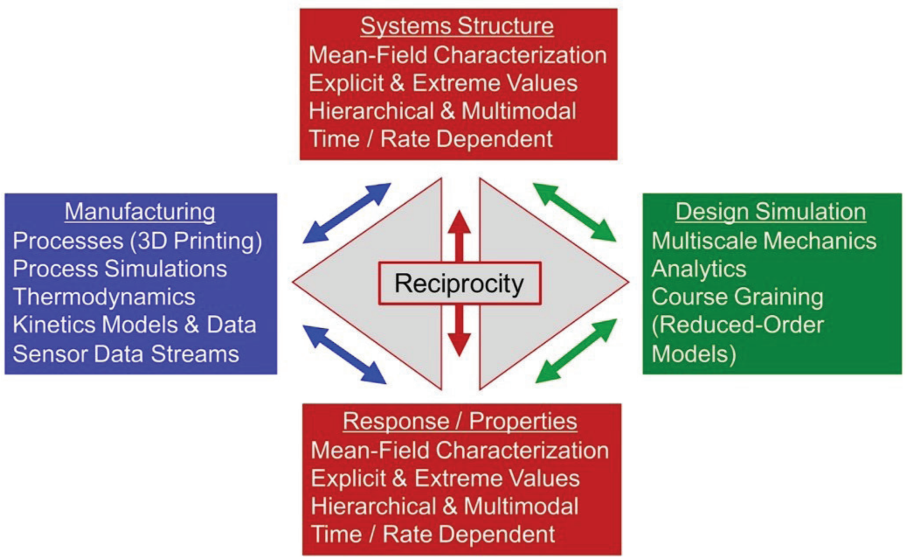


A systematic approach for the design of new materials based on the previous Defense Advanced Research Products Agency (DARPA)-sponsored Accelerated Insertion of Materials (AIM) program is a formalization of the Processing-Structure-Property-Performance relationship [23]. Figure 2.2 shows one example approach in a formalized map, which may be called an "Olson Diagram." In this example, a steel material can be designed using the definition of mechanisms that relates structure to properties, and then using models that relate processing to structure. The models guide the experimental method development to screen applicable alloying elements and material structure. These models are multiscale and link to structural models for component

Critical experiments provide insight into whether desired mechanisms are active in a material that is being designed. Additionally, advanced characterization tools and methods are supporting efficient and cost-effective experimental methods to achieve the development or optimization of a material. High-throughput testing methods are being effectively linked to computational modeling methods, such as multi-component diffusion couples [24-26], gradient chemistry samples, and gradient structure samples (e.g., gradient solution heat treatment bars or Jominy End Quench Test bars [27]). The ability to rapidly develop large quantities of data that can be used to validate models and operative mechanisms further refines experimental methods.

Experimental methods, though strictly thought of as addressing the design and development of new materials or models, can also be applied to quality control and component and process validation. The aerospace community has begun using physics-based models to predict the critical-to-performance structure and properties on a component location-specific basis. This linked model and physical testing approach for component qualification and certification can provide a cost-efficient experimental method that enables further understanding of the production component, the manufacturing process, and the applied model. The experimental plan for component qualification can provide data to update the physics-based model through Bayesian updating methods [28,29]. This experimental method and analysis approach has been refined for application within an ICME framework under a U.S. Air Force-sponsored Foundational Engineering Problems (FEP) project for bulk residual stress modeling, prediction, physical development, and validation in nickel-based disk components [30].

FIGURE 2.3: SYSTEMS RECIPROCITY RELATIONSHIP PARADIGM



Characterization for Hierarchical Systems Reciprocity

Within today's industry settings, both materials structure and response characterization are somewhat detached from multiscale modeling environments. Materials testing data for models is often produced following ASTM standard. experimental test protocols developed outside of symbiotic models of the physics being evaluated and countless company-proprietary or industry-preferred methods for empirically evaluating materials' macroscopic aspects [23]. These data form the basis for statistical and other analyses to arrive at "design allowables," or handbook materials property "curves" (i.e., models) for design. This is a static process that neither readily adapts to advances in simulation or information technologies, nor dynamically captures the hierarchical microstructure aspects of materials.

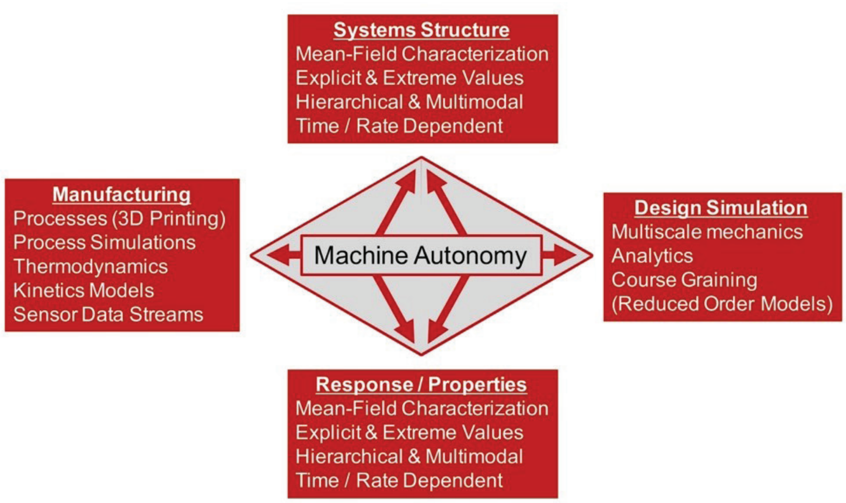
The static nature of current day processes presents an obstacle for "location-specific" materials definitions and for wide-spread design and implementation of multifunctional or hybrid materials and structures for aeronautics systems. To capture the hierarchical nature of materials processes, today's design paradigm either treats phenomena at single scales, or attempts to configure processed samples in ways that represent changes to the material at particular scales. For composites, one often tests configurations at multiple single scales in relative isolation from behaviors at higher or lower scales, ultimately relying upon full-scale component and system testing for qualification in the absence of models. Within today's multiscale framework for materials, the hierarchical aspects of materials and their structures are largely inferred rather than explicitly tied to models and characterization with established hand-offs across the scales. There is no established engineering basis for other methodologies.

Having objective, structured and hierarchical methods based on reciprocity between models, structure characterization, and response, it is natural to extend the reciprocity relationships into the broader engineering framework over the next 10-20 years. A similar paradigm forms the basis for systems biology [31,32]. Figure 2.3 captures these extended relationships by showing that fully integrated information from manufacturing, materials structure, and measured materials responses, and between structure definition, measured responses, and engineering design, can both follow the notion of structure-property reciprocity. Today's SoA functions by passing some information along the lower pathway of Figure 2.3, flowing from manufacturing to measured responses and up through to design. Over time, organizing the information flow and coupling hierarchical definitions for the materials and the engineered structure will lead to broader information flow throughout the system. In this sense, the multiscale engineering system (See Case Study 1, Appendix B), from design to manufacturing, becomes tractable within a systems reciprocity framework that focuses and manages the models, simulations codes, characterization protocols, and manufacturing methods.

The proposed systems paradigm has an analogy to current-day navigation systems (e.g., Google Maps). Those systems organize spatial information in a hierarchical way that permits the user to observe greater fidelity by focusing over differing scales of geography. That framework permits the management of image data contained in the "street views," or the locations of businesses and other database information tied to hierarchical geography. The 2040 vision systems reciprocity paradigm will be analogous in that spatiotemporal materials structure information, from local chemistry to macroscopic engineering, will tie to the engineering design. However, the multiscale materials and structures modeling challenge is larger in terms of scope and complexity of the information being managed; examples include CAD drawings, hierarchical materials structure information—defined by models and chemistry information—as well as models tensorial and response field data and testing results. The complexity and size suggests that hierarchies of systems will need to be built and advanced as unit entities for design. Over time, these will merge to complete the system. In so doing, multiple modeling approaches to the same data and experiments will be compared and stochastically combined, using stochastic model fusion methods as is done in SoA weather forecasting.

Over the coming decade, expanding the systems reciprocity relationships methods will have important impacts on the multiscale framework. Currently, the missing component is the vital role of hierarchical systems structure for building the relationships. Within the new paradigm, materials hierarchical structure gives way to "systems structure" to include the structure contained in the digital data associated with manufacturing and engineering design, as is done in additive manufacturing. In this sense, the new materials spatiotemporal-structure-centric reciprocity paradigm builds on the analogous schema to current-day geospatial data and analysis methods at much higher levels of information complexity.

FIGURE 2.4 MULTISCALE MATERIALS AND STRUCTURES PARADIGM



Over many years, increasing levels of machine based data management, model building, and design optimization will lead to convergence of cyber and physical systems within a common framework. Figure 2.4 suggests that artificial intelligence and autonomous systems will emerge as the focal point for the framework wherein the materials, manufacturing parameters, and optimal design are almost entirely managed by autonomous decision making, leaving the engineering design process open to focus on engineering constraints for the system rather than on the details of selected hardware part or component manufacture. Indeed, such systems are currently being explored for biological systems and selected materials challenges [33,34].

2040 End State

In 2040, characterization tools and methods will integrate seamlessly with modeling and simulation tools to deploy and exploit experimental work more efficiently and, at times, autonomously. Researchers and designers will use a formalized, standard approach for experimental methods that link with models, simulation, and physical characterization methods. For example, quantitative representative volume element (RVE) frameworks will benefit from expanded reciprocity relationships that include the response models, experimental tests, and characterization methods. Modeling and data frameworks will fully integrate with response testing and hierarchical structure characterization, so that models may be used to bound the characterization descriptor sets and protocols. Materials analytics and machine-learning frameworks will become integral to characterization methods, in part by establishing forward models of characterization methods and use-modes within a characterization protocol.

Experimental tools will incorporate advanced methods to sense and autonomously acquire data within characterization instruments. For example, modeling tools will interact with experimental testing rigs to enable real-time, iterative modifications of experiments, model parameter characterization, and simulation outputs. Automated data collection will include a structure or framework for correlating data from different methods (e.g., chemical, crystallographic, deformation data) as well as across length and time scales.

Designers will benefit from the significantly enhanced realism of virtual design, including being able to accurately forecast a structure's lifetime, enabled by the ability to instantiate many stochastically equivalent realizations of a material's internal spatiotemporal hierarchy in models, and to use them in simulations for reliable forecasting. Such simulations will be accurate even at extreme-value conditions that are difficult to measure experimentally.

Gaps

The following gaps lie within six of the roadmap's 10 crosscutting streams, with the **Input/Output Confidence and Reliability** stream containing the most gaps. Accounting for and establishing confidence in measurements and characterization data is a fundamental challenge for this Key Element. These gaps have the strongest ties to the **robust** and **accessible** characteristics of the 2040 end state. To realize a robust model-based ecosystem by 2040, inputs to and outputs from characterization tools must be well-understood.

TABLE 2.1 MULTISCALE MEASUREMENT AND CHARACTERIZATION TOOLS AND METHODS GAPS AND IMPACTED 2040 CHARACTERISTICS

AC Accessible **AD** Adaptive **IN** Interoperable **RB** Robust **TR** Traceable **UF** User Friendly ❖ Critical

GAPS	2040 CHARACTERISTICS					
	AC	AD	IN	RB	TR	UF
INFORMATION SHARING AND REUSABILITY						
Sharing and integration of materials lifecycle data is costly and generally not incentivized across the materials and structures research community	AC		IN		TR	
INSTITUTIONAL PARADIGMS						
Graduate students and industry practitioners have limited access to and use of existing sophisticated characterization/testing frameworks: • Equipment costs and set-up times are prohibitive • Advancements in instrumentation/capabilities exceeds the number of specialized experts in both the equipment and methodologies	AC					
SCALABILITY AND COMPUTATIONAL EFFICIENCY						
Materials instrumentation/software generates substantial volumes of data, requiring excessive data processing time • E.g., one week of synchrotron data requires 6-12 months of data processing	AC	AD				
LINKAGE AND INTEGRATION						
Insufficient 3D/4D characterization methodologies for comparing simulation outputs to equivalent characterization results			IN	RB		
No standard protocols for linking quantitative data from standard characterization and test methods with models	AC		IN			UF
No standard protocols or methods for defining models with respect to their corresponding physical specimens • By integrating the procedures and including both destructive and non-destructive characterization of the initial and tested specimens, the means exist to define the material behavior within validated models	AC		IN	RB		UF
INPUT/OUTPUT CONFIDENCE AND RELIABILITY						
❖ Inability to conduct real time characterization and measurement of structure and response at appropriate length and time scales • Limited ability to do real-time detection, tracking, and measurement of failure initiation/evolution at earliest stages to generate dynamic validation data for physics-based models				RB		
Lack of statistical characterization approaches for monitoring variability (i.e., as sources of uncertainty)				RB		
Variability between characterization instruments precludes the accurate and reliable measurement of residual stress states and some thermophysical and thermochemical fundamental quantities of systems across scales		AD	IN	RB		

GAPS	2040 CHARACTERISTICS					
	AC	AD	IN	RB	TR	UF
INPUT/OUTPUT CONFIDENCE AND RELIABILITY, CONTINUED						
Lack of standard procedures for using the broad spectrum of available filters and parameters available across characterization instruments	✓					✓
Certain datasets used in mechanics models cannot be measured or may not be available via small-scale/fundamental computations (e.g., molecular dynamics) • No acceptable or tested approaches for making inferred measurements		✓		✓		
BEHAVIOR OF MATERIALS AND STRUCTURES						
Lack of routine practices for accurately characterizing mixed mode failure behavior (e.g., delamination, crack growth) in advanced complex materials systems	✓			✓		✓
Underdevelopment of nano-to-microscale testing methodologies: Challenging to test dynamic material behavior at short time scales or lifetime-limiting mechanisms at large time scales • Underdeveloped methods for investigating fracture and crack propagation due to incomplete understanding and control of both initial material conditions and test boundary conditions				✓		

Recommended Actions

The following recommended actions lie within six of the roadmap's 10 crosscutting streams, with the most actions (including high priority) under **Linkage and Integration** and **Behavior of Materials and Structures**. Strategies to advance this Key Element toward the 2040 end state focus on developing and improving test and characterization methods and ensuring the outputs from these methods integrate with the modeling framework. The recommended actions have the strongest ties to the **robust**, **interoperable,** and **accessible** characteristics of the 2040 end state.

TABLE 2.2: MULTISCALE MEASUREMENT AND CHARACTERIZATION TOOLS AND RECOMMENDED ACTIONS AND METRICS

FUNDING: $ <0.5M/year $$ 0.5-2M/year $$$ 2-5M/year $$$$ >5M/year

AC Accessible **AD** Adaptive **IN** Interoperable **RB** Robust **TR** Traceable **UF** User Friendly * High Priority

ACTION	2040 CHARACTERISTICS						TIMEFRAME FOR COMPLETION			FUNDING
	AC	AD	IN	RB	TR	UF	NEAR 2017-2022	MID 2022-2035	LONG 2035+	
DATA ANALYTICS AND VISUALIZATION										
* (2.1) 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		✓					✓	✓	✓	$$$$
(2.2) Explore statistical methods that use process-structure data to represent extreme-value responses of materials in predictive models				✓			✓			$$
BENCHMARKING AND BUSINESS CASE										
* (2.3) Benchmark capabilities and relative accuracies of current/emerging characterization methods—in terms of the mechanisms controlling materials behavior—to provide means of validating predictions of proposed mechanistic models • Publish results to enable assessment of new characterization	✓			✓			✓	✓		$$$
(2.4) Assess and demonstrate commonalties of multiscale modeling frameworks, methods, and protocols across materials classes • Common frameworks address competitive nature of structural materials within application domains				✓				✓	✓	$$$
SCALABILITY AND COMPUTATIONAL EFFICIENCY										
(2.5) Improve software capabilities for conducting systematic assessments of models and experiments relative to quantified uncertainty		✓		✓			✓	✓		$$$
LINKAGE AND INTEGRATION										
* (2.6) Foster characterization, modeling methods, and approaches for reliably establishing correlations between coupon specimens and hierarchical materials structures • Cultivate standards for quantitatively defining hierarchical materials structure within the context of models			✓	✓			✓	✓	✓	$$$$

ACTION	2040 CHARACTERISTICS						TIMEFRAME FOR COMPLETION			FUNDING
	AC	AD	IN	RB	TR	UF	NEAR 2017-2022	MID 2022-2035	LONG 2035+	
LINKAGE AND INTEGRATION, CONTINUED										
✱ (2.7) Identify key 3D/4D characterization tools and create forward models for all instrumentation apparatuses • Demonstrate/quantify enhancements in speed and quality of information		●	●	●			●	●	●	$$$$
✱ (2.8) Establish common procedures for merging multimodal data gathered from multiple instruments	●		●		●	●	●	●		$$
✱ (2.9) Integrate in-service environmental effects and chemical reactions into modeling capabilities			●	●			●	●	●	$$$
(2.10) Establish protocols for linking quantitative characterization and response test data with models	●		●		●	●		●		$$
(2.11) Define a framework that permits direct integration of 3D/4D materials information into current and emerging physics-based models			●	●				●		$$$
(2.12) Expand forward modeling approach to NDE methodologies by coupling direct measurement of structure with models of hierarchical structure and NDE interrogation signals/modes			●	●				●		$$$
(2.13) Incorporate response models into the structure-response reciprocity relationships of quantitative model frameworks			●	●				●		$$
INPUT/OUTPUT CONFIDENCE AND RELIABILITY										
✱ (2.14) Enable real-time sensing telemetrics and measurement methods to obtain and analyze spatiotemporal response fields of interest (as opposed to post-failure microscopy, sectioning, characterization and imaging)				●			●	●		$$$
(2.15) Formalize model-based methods to determine the quantitative data required to validate constitutive models and mechanisms (e.g., polycrystalline deformation)				●				●		$$$
BEHAVIOR OF MATERIALS AND STRUCTURES										
✱ (2.16) Establish test methods by material class and length scale for exploration, characterization, and model validation: • Investigate fundamental mechanisms and dynamic materials behavior • Characterize material response under extreme environmental conditions • Identify material-specific properties and quantify model input parameter sensitivities	●			●		●		●	●	$$$
✱ (2.17) Establish test facilities to advance accelerated lifetime tests for simulating highly complex loading scenarios (e.g., thermal, mechanical, electrical, chemical)				●				●		$$$$

ACTION	2040 CHARACTERISTICS						TIMEFRAME FOR COMPLETION			FUNDING
	AC	AD	IN	RB	TR	UF	NEAR 2017-2022	MID 2022-2035	LONG 2035+	
BEHAVIOR OF MATERIALS AND STRUCTURES, CONTINUED										
(2.18) Adopt standardized simulation methods to hierarchically define and bound models • Couple methods with measurement protocols • Determine best practices and protocols for controlling initial and test boundary conditions	●			●		●	●			$$$
(2.19) Formalize a series of RVE/SERVE methods and define their applicability within the various hierarchical domains: • Explore approaches for scale separation conditions that invalidate RVE-based approaches • Identify mean-field conditions • Extend into overlapping scales			●	●			●			$$$
(2.20) Examine solutions for treating damage accumulation and life-limiting attributes of structures				●				●		$$
(2.21) Develop advanced experimental methods for characterizing reaction kinetics that influence the manufacturing process (e.g., kinetics controlling chemical vapor deposition [CVI] process)				●			●	●		$$$
(2.22) Improve high-energy X-ray methods and respective models and validation methodologies • Use pedigree measurements to develop sufficient, affordable lab-scale measurement techniques	●			●			●	●	●	$$$$

Relationships with Other Key Elements

This technical area will work in concert with the other Key Elements to develop analytical methods, machine learning frameworks, autonomous systems technologies, and formalized approaches to intimately connect models, hierarchical systems structures, and test protocols in support of model development and validation.

TABLE 2.3 EXAMPLE INTERRELATIONSHIPS OF KE2 (MULTISCALE MEASUREMENT AND CHARACTERIZATION TOOLS AND METHODS) AND OTHER KEY ELEMENTS

OTHER KEY ELEMENTS	INTERRELATIONSHIP	THIS KEY ELEMENT
KE1 Models and Methodologies	Experimentally replicate simulations, identify mechanisms and scale transitions, and provide data for model parameter characterization and validation	KE2 Multiscale Measurement and Characterization Tools and Methods
	Create forward models of 3D/4D characterization tools to maximize information reliability and model parameter estimation	
KE3 Optimization and Optimization Methodologies	Collect key data to support simplified modeling optimization methods at the engineering design level	
	Provide virtual multiscale optimization of engineering designs and methods for model parameter estimation at various length scales	
KE4 Decision Making and Uncertainty Quantification and Management	Deliver data for model input sensitivity assessments, efficient experimental designs, and enhanced model UQ	
	Introduce probabilistic methods for structural characterization and component analysis	
KE5 Verification and Validation	Enable integrated parameter sensitives and error propagation studies for enhanced model validation	
	Assess physical and computational method linkages, and optimize experimental plans to support V&V	
KE6 Data, Informatics, and Visualization	Provide experimental/characterization systems-based material hierarchies that define data structures	
	Provide informatics framework to house characterization and response data to facilitate integration and application of machine learning tools	
KE7 Workflows and Collaboration Frameworks	Provide systems-based materials structure paradigms that define local workflow connections	
	Accelerate materials characterization via automated generation and execution of coupled physical/computational workflows	
KE8 Education and Training	Develop in-line data analysis and reconstruction methods for efficient use of measurement/characterization instruments	
	Translate systems-based characterization for models approach for classroom curricula and laboratory courses	
KE9 Computational Infrastructure	Support linked experimental data generation and computational analysis	
	Support linked experimental data generation and computational analysis	

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Key Element 3:

Optimization and Optimization Methodologies

Definition

This Key Element encompasses the following:

1 Computational/numerical approaches and mathematical formalizations for finding the minimum or maximum performance (solution) of products, materials, structures, manufacturing processes, and design workflows for given applications. This includes the development and use of reduced order methods and surrogate models suitable for optimization.

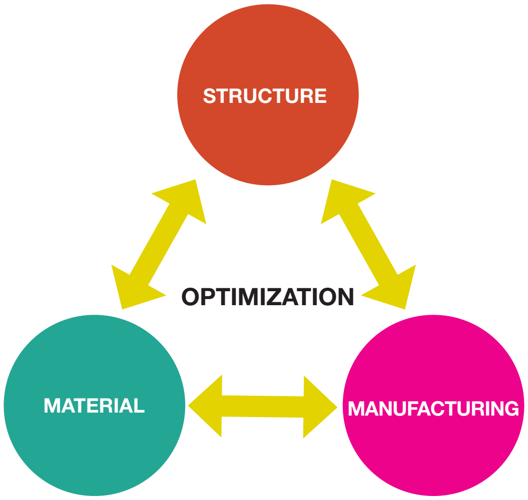
Current State of the Art

Role

The role of optimization is to integrate the wide range of research advances identified in this document and maximally exploit them in engineering designs. The complexity of multiscale and multiphysics structural-material systems means that design based on human intuition alone is likely to be highly challenging. Consequently, optimization is critically needed to aid the creativity and intuition of the design processes. The Optimization and Optimization Methodologies Key Element focuses on two primary research questions: (1) how to formulate an optimization problem that results in meaningful design, and (2) how to solve the optimization problem such that the optimum solution(s) is(are) found. Here, the plural form of solutions is intentionally used to recognize that engineering design problems are likely to have multiple solutions, thereby permitting a range of design options and their implications. Optimization is essentially a design tool that provides insight into the design space and assists the creativity and intuition of a design engineer.

In the context of engineering design, the three primary components to consider are structural design, material design/selection, and manufacturing/processing. A structure is at the top scale, requiring multiple functionalities and commonly subject to multiphysics and multidisciplinary environments with the associated performance objective and constraint functions. These multiphysics functionalities can be provided by the top-scale structural design and/or lower-scale material design. In this sense, material design (i.e., "designing *the* materials" paradigm) is subject to the functional requirements defined at the structural scale. In other words, optimum material properties are dictated by the functional requirements of the structure that one or more materials constitute. The material design is thus optimized for a particular target property (or set of properties) determined by the needs at the structural scale. This paradigm is a significant departure from the traditional material design/selection philosophy wherein a specific material is selected for a given property or set of properties (e.g., conductivity or stiffness), is maximized or minimized so as to best fit applications in general rather than optimize or tailor the material for the specific applications. The other significant contributor to engineering design, which was not typically considered during an early design phase, is manufacturing and material processing.

FIGURE 3.1 ROLE OF OPTIMIZATION



While advanced manufacturing technology enables more complex multiscale features to be built, the resulting material properties can vary, depending on the geometrical features as well as manufacturing techniques and processing parameters. This means manufacturing techniques and processing parameters and the variability associated with them need to be considered during design to ensure the safety and reliability of the resulting structures. It is therefore clear that design of modern structural-material systems is a highly coupled multiphysics multiscale problem, often involving complex and emergent behaviors well beyond human intuition. Consequently, determining how to formulate an optimization problem to reflect these complex design needs and to define a design space that will allow an optimization method to find a useful design solution are key research questions. It is noted that an optimization problem may involve a wide variety of considerations including full product life cycle, supply chain management, overall profit, and functional performance. Some of the research questions, particularly in management and processes, have long been considered under the heading of Operations Research, expanding the scope to applied mathematics, management, finance, and artificial intelligence. For the purpose of this document and in balance of the key elements identified in the NASA 2040 vision, the discussion will be focused on design optimization. However, this does not mean that the research advances in Operations Research and their potential integration with design optimization should be excluded.

Given the formulation of the optimization problem, the other main research question is how to solve an optimization problem (i.e., optimization methodology). These two research questions are separated here for the simplicity of the discussion but, in practice, are intimately linked and usually considered together as a design space is defined by the problem formulation and the characteristics of the design space indicates a suitable optimization methodology. The optimization problem arising here is likely to be a large-scale, nonlinear, non-convex, and computationally expensive simulation that connects multiple scales and physics. Therefore, given these computational challenges and the difficulties of accurately representing the true engineering design problem, substantial research needs exist associated with optimization methods.

More specifically, optimization research encompasses the following:

- Optimization formulation and methods for coupling multiple scales to simultaneously design an integrated material-structural system, thereby enabling materials to be tailored to the specific functional and performance requirements defined at the structural scale.
- Optimization formulation and methods to integrate manufacturing and processing such that manufacturing/processing parameters are considered directly as design variables and constraints, using the process-structure-property model.
- Optimization methods that will create multiple and unintuitive new designs (independent of the initial designs) to aid the engineers revolutionizing the future designs (e.g., topology optimization).
- Scalable computational frameworks for multiscale and multiphysics optimization (e.g., Dassault Systèmes 3DExperience Platform).
- Fundamental mathematics for optimization and numerical methods.
- Optimization problem formulation and mathematical/computational methods to account for uncertainties in the physical systems as well as in the numerical models propagated across scales, including reliability-based robust optimization.

- Simulation and modeling suitable for sensitivity analysis and optimization, including physics-based, data-driven, and surrogate models.
- Recognizing that many engineering problems are ill-posed, algorithms to assist the engineers to define a meaningful design problem and/or dynamically evolving the problem definition as optimization "learns" about the design space.

Summary

There has been a substantial body of research in multiscale and multiphysics modeling where, given a specific design, the behavior of interests is analyzed. In contrast, optimization aims to determine a design given the specific behavior of interests. To this extent, optimization can be considered the inverse of modeling but there has been surprisingly little research in this area. However, engineering and design optimization has been an active research area for the last five decades or so and the following will discuss them.

STRUCTURAL OPTIMIZATION

Structural optimization can be interpreted in two ways: (1) it optimizes a structural configuration* or (2) it considers structural mechanics as the driving physics and assumes that the primary functionality is load-carrying. Design optimization finds its root in structural optimization to mean both (e.g., truss cross-sectional sizing optimization) for the minimum weight subject to a stress constraint.

One of the first structural optimization works was published in 1904 and established optimum truss lay-outs for a few structural configurations [1]. As the computational power grew with the introduction of the finite element method, modern structural optimization initiated in the 1960s with truss optimization [2]. The complexities grew to shape optimization where the boundary shapes are optimized then to topology optimization. Structural optimization includes truss, shape, and other optimization where the driving physics and functionality are mechanical load-carrying and the design space is parameterized such that the configuration does not fundamentally change. Consequently, the final solution is dependent on the initial design, and the potential gain is relatively limited. Parameterization here can be cross-sectional areas of a truss [3,4], thickness of each plate element in a continuum model hence the optimum thickness variation of a 2D structure [5], shape of the boundaries [6], and geometric sizing variables [7]. Structural optimization, aside from topology optimization, is considered a mature approach.

TOPOLOGY OPTIMIZATION

Topology optimization, although quite general, can be considered a subset of structural optimization, although much research has applied it to many different physics other than structural mechanics. Many research questions in topology optimization remain unresolved, with a high level of low TRL activities still current. There are several commercial software packages that use topology optimization in structural mechanics (e.g., OptiStruct, ANSYS, NASTRAN, Abaqus, and Genesis), but their application in engineering practice is somewhat immature. The rise of additive manufacturing (AM) is fueling interest in topology optimization as an ideal design method. A distinguishing characteristic of topology optimization is the ability to change topology, sizing, and shape of a part or component. Hence, it is considered the most general form of design optimization for achieving a final solution *independent* of the initial solution. This means the potential gain can be substantial and the resulting design can be unintuitive and revolutionizing.

The most popular problem formulation for topology optimization is the minimization of strain energy subject to the maximum volume constraint [8-10]. One reason for this is that this is a relatively well-behaved problem and the Michell Structures [1] (still used extensively for validation purposes) can be used to benchmark and validate the methods being developed. Topology optimization has been developed to investigate optimum designs under a wide range of physics characterized by the objective and constraint functions. They include piezoelectric [11], photonic [12-13], acousto-elastic [14], electrothermal [15], fluid-structure [16,17], aero-elastic [18], natural frequency(ies) [19]), stress, [20,21], compliant mechanism [22], nonlinearity [23]. Topology optimization has also been extended to simultaneously optimize additional design variables such as location of Dirichlet boundary conditions [24] and graded material distribution [25]. Buckling is a constraint that is still considered challenging despite its prevalence as a failure mechanism in many engineering applications [26]. The availability

*That is, with geometrical variables such as cross-sectional geometry dimensions of truss members or shape and layout of a structural configuration.

of these various functions in engineering practice via commercial software has lagged and thus the uptake of various topology optimization in industry has been slow.

There are two classes of topology optimization methods. One is based on density where each finite element's density is considered a design variable and the density can be penalized to yield a near black-and-white solution by material interpolation schemes, commonly used being SIMP [27] or RAMP [28]. This density-based method arose from the homogenization-based method in 1988 and is the more mature of the two classes of the methods, hence it is found in all commercial software. An advantage of the density-based methods arises from this maturity in that it is reasonably well-understood and has been demonstrated to work well in a wide range of challenging single and multi-physics problems. Numerical instabilities such as the checkerboard formation is well-understood and is commonly circumvented by applying sensitivity or density filtering. A disadvantage of the density-based methods, however, is that solutions often have a staircase (jagged) representation of structural boundaries, which may require smoothing to properly capture behavior for boundary-dominated physics (e.g. stress and/or fluid flow along a boundary) and for integration with CAD packages. Existing commercial efforts have shown varying degrees of success to integrate a suite of software into a framework to enable a seamless design workflow. For example, Dassault Systèmes—which owns CAD, simulation, and optimization IP—offers a bi-directional link between the optimized topology and the parametric geometry. While research needs to continue to develop a robust software solution, it is important to note the multi-faceted dimensions to integrate traditionally disparate science/engineering software with issues such as licensing, business models, end-users, and supply chains.

The other class of topology optimization is boundary-based topology optimization [29]. Today, the most popular approach is level set-based topology optimization [30-32] in which there are several variations. The level set method primarily employs the level set implicit function to represent the boundaries and uses the level set equation based on advection to smoothly move the boundaries. Since the structural boundary is directly moved, a clear boundary definition is available (i.e., no gray elements without penalization), and smooth boundaries mean no staircase representation. Thus, there is no need for post-processing, and the level set method can offer a natural representation of the design solution within the solid modeling/CAD and manufacturing environment—although rigorous investigations have yet to be conducted. It has also been shown that filtering is not needed since no checkerboards are formed. The finite elements can now be cut by a boundary and research is on-going to develop a suitable general purpose computational mechanics method for the analyses of the Eulerian structural discretization. This can be done adaptively or on a fixed mesh, as is typically done with density-based methods. As the boundary methods were introduced after the density-based methods and are considered less mature and somewhat more difficult, they have yet to be widely adopted within commercial software packages. However, efforts within the open MDAO community [33] are beginning to make the level set topology optimization available beyond the academic research community. Yet, additional fundamental research still remains to make the methods more reliable and robust.

It is worth commenting on the mesh dependency of topology optimization. Several papers claim mesh independence through numerical treatments such as filtering in the density-based methods. As the boundary-based methods allow partial elements to be removed, they too show reduced sensitivity to mesh. While efforts are seen in topology optimization to reduce the mesh dependency, it remains mesh dependent, as expected, since finite element methods employ discretization and the sensitivities are fundamentally dependent on the mesh. For further details on the status of topology optimization research, readers should review references [34-36] as well as [37] for details of the various methods under consideration.

In recent years, there has been some interest in topology optimization accounting for specific constraints associated with additive manufacturing [38]. Two constraints have been studied extensively in the literature. The first is the overhang constraint where the layer-by-layer construction means a poorly supported structural feature with a low acute angle cannot be reliably manufactured. Additive manufacturing currently builds a supporting structure which can be eliminated after manufacturing. Many of the topology optimization approaches aim to impose a geometry constraint that limits the overhang angle, eliminating the need for supporting structures and thereby reducing the need for post-processing, material usage, and build time [39-46]. The other constraint is the length scale control where additive manufacturing cannot build small structural features. Again, this is considered as an additional geometry constraint in topology optimization [47-52].

While active research efforts have seen some successes in many structural optimization problems demonstrating the revolutionizing potential and capabilities, their applications in engineering industry have been surprisingly limited, indicating that further research is needed to translate the academic research into practice. In addition, many outstanding challenges still require low-TRL research, including topology optimization considering coupled multiphysics, nonlinearities, buckling, transient, and manufacturing constraints.

MATERIAL OPTIMIZATION

There have been optimization studies dedicated to exploring the material design space for a range of materials, including graded materials with gradient-based properties [25], systems with two or more discrete materials [53], and architected or periodic or lattice-structured materials [12,54]. Architected materials were especially relevant in the context of metamaterials (i.e., materials with properties not commonly found in nature). Despite existing research activities focused on demonstrating low-TRL feasibility, few have successfully transitioned to engineering design practice.

Optimization methods for fiber-reinforced composite materials, which are predominantly used in structural mechanics applications, are widely available in a range of commercial software packages. These optimization methods encompass two-dimensional fiber composites (i.e., optimizing straight fiber angles, stacking sequence, thickness, and number of plies [13, 55-59]) and two-dimensional two-steered fiber composites with continuously varying fiber orientation angles [60-62]. Few research studies address the design and optimization of three-dimensional composites.

Research in lower length scale optimization of materials is scarce (i.e., material microstructure, grain level, and lower [63-64]), including attempts to link their design to the continuum-level scale.

MULTIDISCIPLINARY DESIGN OPTIMIZATION/ MULTIPHYSICS OPTIMIZATION

Coupled Multidisciplinary Design Optimization (MDO) has been developed under systems engineering. Actives areas of research have focused on the mathematics and science of coupling complex and often conflicting multidisciplinary needs in engineering systems design as well as the associated computational environment. Such MDO approaches are now common practice in industry outside the materials domain (see [65] for a comprehensive summary of MDO methods). Most MDO studies do not consider that materials as an integral element of optimization. However, it is anticipated that some generic methodologies and coupling frameworks would be applicable to structural-material system optimization. MDO is accessible via a range of tools:

1. Isight & Simulia Execution Engine [66]: Used to combine multiple cross-disciplinary models and application together into simulation process flows, automate their execution across distributed computational resources, explore the resulting design space, and identify the optimal design parameters subject to required constraints.

2. General purpose optimization methods available in other commercial software like MATLAB [67], R [68], and SAS [69] are not used except in rare cases in industry. Specific tie-ins to FEM software such as Abaqus [70] require specific codes to be written for materials of interest using physics at the level of interest.

3. Some optimization tools exist in design-specific software like Siemens NX PLM (e.g., for geometry optimization [71]), but these are still emerging and often not used; even when they are used, they can only handle simplified models. More complicated situations, especially taking into account material behaviors, cannot be optimized in the current state.

4. Software for visualizing the large magnitude of data produced by optimization studies does exist but is almost unknown and not used (Tecplot Chorus [72] and its competitors).

5 Optimization frameworks such as OpenMDAO which builds the foundation for MDO on an advanced HPC environment. This library of solvers and optimizers, written in Python, allows implementation and solution of various problems quickly in an environment that manages the user's models.

6 Tools for optimizing complex geometries (mesh-morphing). There are on-going initiatives to develop these tools (e.g., Air Force Research Labs initiatives like the PACE consortium).

In the context of material and structural design, the term *multiphysics* is more commonly used than *multidisciplinary*. Coupled multiphysics topology optimization has been demonstrated in a wide range of single-scale designs, including piezoelectric [11], photonic [12-13], acousto-elastic [14], electrothermal [15], fluid-structure [16-17], and aero-elastic [18] materials.

High-fidelity multiphysics and multiscale methods with integrated optimization features for searching high-dimensional-parameter spaces have received surprisingly little attention, despite successful research results at low TRLs. In general, high fidelity methods offer opportunities to explore a greater dimensional design space which is proportional to the expected performance gain and a level of reliable and creative design solutions. This is, of course, at the expense of computational resources (i.e., efficiency). Consequently, this is a critical area of fundamental research which, if successful, will enable designers to take advantage of sophisticated modeling techniques.

RELIABILITY AND ROBUST OPTIMIZATION

Optimization for uncertainties can be classified into two general categories: reliability optimization and robust optimization. Reliability-based optimization presents uncertainties as constraints with quantified probabilities (e.g., failure), while robust design optimization aims to find a solution insensitive to uncertainties. Both are commonly employed in practice for conducting low-fidelity, low-dimensional design optimization [73].

In the context of large-scale topology optimization, reliability-based topology optimization (RBTO) was first introduced by Kharmanda and Olhoff [74] to treat probabilistic constraints. The objective function remained deterministic. The RBTO research primarily considers the loading magnitude and direction of uncertainties as well as the material properties in the context of structural mechanics [74-80]. In contrast, less effort has been seen in the area of robust topology optimization.

A popular approach to robust topology optimization is to approximate the random field of uncertainties as a set of discrete cases. Because the applied loading is often considered to be the uncertain parameter, this approach is sometimes referred to as the multi-load formulation. This transforms a stochastic problem into a deterministic one with multiple conditions, which the existing topology optimization methods are equipped to solve [81-83]. An alternative to the multi-load approach is to minimize the worst case, which turns the optimization into a min-max problem [84-89]. While generating a safe design, this approach can lead to an overly conservative solution.

Research has shown that fast and efficient methods are possible for some classes of problems in topology optimization. Moreover, the results indicate that the topological solution can fundamentally change due to the presence of uncertainties [83]. However, this has not been applied beyond the academic demonstrative studies. Further research to consider generalized uncertainties and formulating a fast and reliable method have not continued and they are generally not accessible in engineering practice.

SURROGATE MODELING AND REDUCED ORDER MODELING

Surrogate modeling, metamodeling, and Reduced Order Modeling (ROM) [90] refer to methods typically used for reducing computational cost of highly expensive analyses or simulations. This is particularly relevant in the design optimization context where an analysis is required at every iteration as the design is modified and optimized. In cases where a single analysis can take hours or even days, repetitive applications of such evaluations make optimization prohibitive. Surrogate modeling or ROM offers an efficient way to estimate the response so that an optimum solution can be found.

There are a variety of surrogate modeling methodologies [91], with Kriging [92] and Radial Basis Function (RBF) [93] more commonly seen in structural optimization. Example applications have been seen in crashworthiness modeling involving highly nonlinear dynamic finite element analyses [94], optimization of helicopter rotor blades [95], rocket propulsion components [96], or shape optimization of an aircraft engine nacelle [97]. The fundamental principle of surrogate modeling is to estimate the response from the known responses. This means the success of using a surrogate model in the context of optimization is critically dependent on the availabilities of responses; this approach suffers from the curse of dimensionality with its computational cost rapidly increasing with large datasets and high dimensional spaces. Discontinuities can present challenges to a surrogate model. Adding to this, the surrogate model can contain numerical oscillations, meaning that the response estimates may be reasonable but the gradients may not be. Many surrogate-based modeling optimization approaches employ a gradient-free optimizer such as a genetic algorithm and particle swarm optimization. These two factors limit the utilization of surrogate modeling to lower-order (i.e., a low number of design variables) optimization problems.

Surrogate modeling techniques like RBF poorly handle discontinuities and are computationally expensive with respect to larger datasets. Until sensor technologies became more prevalent in manufacturing operations, data were collected in smaller experiments. Today, machine learning algorithms can help to create surrogates of tens of billions of rows of data, and hundreds of features (including field data).

If surrogate modeling is to be utilized in large-scale optimization, substantial low TRL research is needed to efficiently build and adapt a high-order surrogate model together with reliable sensitivity estimations.

OPTIMIZATION PROBLEM FORMULATION

While it is clear that there are huge gaps in knowledge that require TRL 1 fundamental research to enable the NASA 2040 vision, the literature survey so far has also revealed that substantial research at low TRL has not translated to engineering practice. One reason is that engineer design problems are ill-posed and the solution is a function of the optimization problem definition. Although the majority of optimization research assumes that an engineer knows how a problem should be formulated, this is far from the reality. Without the knowledge of specialists, there is little information available on how to iterate and reformulate the optimization problem when the first attempt does not yield a meaningful solution [98]. This challenge will only be compounded in complex multiscale problems with emergent behavior and coupled nonlinear multiphysics.

Emerging research has demonstrated an algorithm that revises and updates an optimization problem as optimization progresses [99-100]. While only a handful of papers with demonstrations on simple low-order problems currently exist, the results are promising. Further research in this area is critical to ensure that low TRL research in optimization translates and is employed effectively in practice.

MULTISCALE OPTIMIZATION

While there has been a considerable amount of research in developing numerical multiscale models (i.e., predicting behavior or performance of a design —both material and structural—or configuration), there has been little research in inverse of multiscale models or optimization (i.e., determining the design configuration for the optimum behavior or performance). In particular, it is apparent that a structural shape and configuration is dependent not only upon the applied loading, but also on material properties (i.e., material performance), thus making the material performance an integral part of structural or functional design. Consequently, the design or tailoring of the material properties depends on the optimum target properties which can only be deduced from the specific performance requirements of the structure. This means it is critically required to intimately couple the "design with" and "design the" paradigms (see Case Study 4, Appendix B). The lack of studies in crossing the structural scale to the material scale has been widely recognized but, without this link, the optimum material properties cannot be communicated to the materials design so the meaningful tailoring of material microstructure, for example, cannot be achieved. There have been a few recent research studies in multiscale optimization linking the structural scale to architected material using topology optimization [101-105]. Results show that topology optimization is a promising approach in incorporating high-fidelity methods and enabling the exploration of the largest design space. They also show that the real benefits of multiscale design arise in coupled multiphysics problems with conflicting needs.

Such research, although still in its infancy, suggest that these challenges need to be addressed at the fundamental (low) TRL level. To date, unfortunately, there has been no research to attempt to link the structural scale design to the scale below the architected material or to consider manufacturing constraints or material variabilities. There have been few attempts to consider coupled multiphysics in multiscale optimization. Therefore, low TRL research is a critical need for developing multiscale optimization.

2040 End State

By 2040, optimization will seamlessly tie materials science to design, processing, and manufacturing. Engineers will regularly use optimization methodologies to design material-structures systems that integrate computational multiscale modeling and multiphysics simulations to optimize fit-for-purpose materials and their associated components/structures/vehicles. Uncertainty in material properties, manufacturing processes, and operating environments will be readily accounted for in design optimization. Expanded metrics will include sustainability (both environmental and economic) and end-of-life requirements for recycling and cradle-to-cradle use of materials and structures. At universities and national laboratories around the world, an engaged research community will focus on developing optimization methods, using an active forum to exchange open-source models, best practices, and benchmark problems.

Gaps

The following gaps lie within five of the roadmap's 10 crosscutting streams, with the **Input/Output Confidence and Reliability** stream containing the most critical gap. While scalability is a noteworthy barrier that precludes optimization tools and methods from handling an increasing number of design parameters and vast amounts of generated data, the most significant challenge facing this Key Element is the inability to substantiate confidence and reliability in optimized design solutions. These gaps have the strongest ties to the **adaptive** and **robust** characteristics of the 2040 end state. The adaptiveness of the envisioned ecosystem will depend on the ability of optimization tools and methods to efficiently handle design problems of varying levels of complexity.

TABLE 3.1 OPTIMIZATION AND OPTIMIZATION METHODOLOGIES GAPS AND IMPACTED 2040 CHARACTERISTICS

AC Accessible **AD** Adaptive **IN** Interoperable **RB** Robust **TR** Traceable **UF** User Friendly ❖ Critical

GAPS	2040 CHARACTERISTICS AC	AD	IN	RB	TR	UF
DATA MANAGEMENT						
Limited ability to manage vast datasets generated by real-time optimization searches and make subsequent decisions about the results • Lacking advanced visualization and post-processing techniques needed for agile decision making					✓	✓
INSTITUTIONAL PARADIGMS						
Limited understanding of how to formulate optimization problems and sensitivity analyses in concurrent design of materials and structures	✓					✓
SCALABILITY AND COMPUTATIONAL EFFICIENCY						
Inadequate scalability of methods for optimization under uncertainty for high-fidelity, high-dimensional problems • Optimization methods do not sufficiently address uncertainty propagation across multiple scales		✓		✓		
Insufficient computational/numerical methods and fundamental mathematics to reliably solve problems with a reasonable level of computational resources. • Optimization is too computationally intensive for numerical models that are incompatible with intrusive optimization methods (e.g., gradient-based optimization)		✓				
LINKAGE AND INTEGRATION						
Limited modularity of high-fidelity models inhibits integration with other models in computational supply chains • No existing multiscale design optimization framework that accounts for manufacturability constraints at each scale			✓			
High-fidelity process models do not successfully incorporate the influences of manufacturing processes on material behavior/structural performance into optimization formulations			✓	✓		
INPUT/OUTPUT CONFIDENCE AND RELIABILITY						
Lack of robust optimization methods/routines for multiscale modeling of emergent material behavior (e.g., time-dependent effects, microstructural evolution, discontinuities)		✓		✓		
❖ Lack of reliable optimization methods that bridge across scales (e.g., topology optimization for multiple length scales, physics, and functionalities) • Incorrect and unverified outputs from complex simulation can corrupt optimization runs		✓	✓	✓		

Recommended Actions

The following recommended actions lie within seven of the roadmap's 10 crosscutting streams, with the most actions (including high priority) under **Scalability and Computational Efficiency**. Many of these recommended actions are centered on speeding up optimization approaches and establishing best practices so that optimization routines are consistent across the community. The recommended actions have the strongest tie to the **robust, accessible,** and **adaptive** characteristics of the 2040 end state.

TABLE 3.2 OPTIMIZATION AND OPTIMIZATION METHODOLOGIES RECOMMENDED ACTIONS AND METRICS

FUNDING: $ <0.5M/year $$ 0.5-2M/year $$$ 2-5M/year $$$$ >5M/year

AC Accessible   **AD** Adaptive   **IN** Interoperable   **RB** Robust   **TR** Traceable   **UF** User Friendly   ✱ High Priority

ACTION	2040 CHARACTERISTICS						TIMEFRAME FOR COMPLETION			FUNDING
	AC	AD	IN	RB	TR	UF	NEAR 2017-2022	MID 2022-2035	LONG 2035+	
MULTIDISCIPLINARY COLLABORATION										
✱ (3.1) Develop or adopt a standard set of open-source materials and structural analysis models to encourage collaboration within and between industry and academia	AC					UF	▨	▨		$$
(3.2) Develop training programs in optimization methods for industrial materials and structures design	AC			RB			▨	▨	▨	$
BENCHMARKING AND BUSINESS CASE										
(3.3) Determine industry-accepted guidelines for determining optimization methodologies by problem classes (e.g., optimization-by-shopping, gradient-based optimization methods, sensitivity analyses, robust design optimization)	AC					UF	▨	▨		$
✱ (3.4) Create benchmark optimization problems to provide industry with a means to evaluate optimization algorithms with multiple performance requirements	AC						▨	▨		$$
SCALABILITY AND COMPUTATIONAL EFFICIENCY										
✱ (3.5) Combine high-fidelity multiphysics methods with optimization approaches to search high-dimensional parameter spaces		AD	IN	RB			▨	▨	▨	$$$
✱ (3.6) Develop models that are designed from the ground up for efficient derivative computation, to enable multiphysics optimization		AD		RB				▨	▨	$$
✱ (3.7) Improve the scalability of surrogate-based optimization methods to solve computationally intensive and high-dimensional design problems at an accelerated pace		AD		RB			▨	▨		$$

ACTION	2040 CHARACTERISTICS AC	AD	IN	RB	TR	UF	TIMEFRAME FOR COMPLETION NEAR 2017-2022	MID 2022-2035	LONG 2035+	FUNDING
SCALABILITY AND COMPUTATIONAL EFFICIENCY, CONTINUED										
✱ (3.8) Enable human-in-the-loop optimization approaches	✓	✓					✓	✓		$$
(3.9) Incorporate automatic verification of model assumptions as an optimization constraint		✓						✓	✓	$$
(3.10) Establish best practices for the development and use of emulators/surrogates to speed up optimization and improve model accuracy over design space of interest	✓	✓		✓			✓	✓	✓	$$
LINKAGE AND INTEGRATION										
✱ (3.11) Establish/improve practices for incorporating uncertainty into optimization methods			✓	✓			✓	✓		$$
(3.12) Determine best practices for incorporating processed-property interactions into process models			✓	✓				✓	✓	$$
INPUT/OUTPUT CONFIDENCE AND RELIABILITY										
✱ (3.13) Create and/or articulate a set of new/improved optimization methods and problem formulation approaches for coupled multiscale material-structural systems including specific classes of materials or commons types of modeling problems	✓			✓		✓	✓	✓		$$
(3.14) Develop set of approaches for validating optimum solutions: • How/why the optimizer arrived at the solution • Determine whether the solution meets the user requirements • Sensitivity analysis of constraints/variables	✓			✓	✓	✓	✓	✓		$$
(3.15) Improve and promote best practices for optimizing manufacturing time and cost	✓	✓		✓		✓	✓	✓		$$
BEHAVIOR OF MATERIALS AND STRUCTURES										
(3.16) Formulate appropriate models and analysis methods for sensitivity analysis suitable for optimization				✓	✓	✓	✓	✓		$$
(3.17) Improve optimum layup strategies for advanced materials (e.g., composite architectures)				✓			✓	✓		$$

Relationships with Other Key Elements

Critical to adopting ICME, this area will draw upon the other Key Elements to enable algorithms and computational frameworks that expand the materials/systems design space, support decision making with uncertainty, budgets, permit interoperability with advanced HPC environments, and increase the ubiquity of optimization formulations methods across disciplines and organizations.

TABLE 3.3 INTERRELATIONSHIP OF KE3 (OPTIMIZATION AND OPTIMIZATION METHODOLOGIES) AND OTHER KEY ELEMENTS

Note: Interrelationships among KEs vary. Equal weight should not be inferred.

OTHER KEY ELEMENTS	INTERRELATIONSHIP	THIS KEY ELEMENT
KE1 Models and Methodologies	Couple design problems for cross-scale modeling tool integration and increased solution and sensitivity analysis reliability	KE3 Optimization and Optimization Methodologies
	Enhance optimization algorithms for expanded design space via coupled multi-scale/-physics models	
KE2 Multiscale Measurement and Characterization Tools and Methods	Provide virtual multiscale optimization of engineering designs and methods for model parameter estimation at various length scales	
	Collect key data to support simplified modeling optimization methods at the engineering design level	
KE4 Decision Making and Uncertainty Quantification and Management	Support optimization algorithms with integrated UQ information for enhanced decision making	
	Provide manufacturing constraints with integrated uncertainties for readily manufacturable solutions	
KE5 Verification and Validation	Foster model-based optimization routines for V&V activity planning and selection	
	Calibrate and validate estimated uncertainty in optimization routines	
KE6 Data, Informatics, and Visualization	Deliver optimization algorithms that retain and expand knowledge of previously solved problems	
	Build common data infrastructure, standardized data formats, and multidimensional visualizations for improved optimization routines	
KE7 Workflows and Collaboration Frameworks	Link design problems for efficient workflow construction	
	Develop interdisciplinary collaboration tools for holistic multiscale systems-level optimization	
KE8 Education and Training	Establish industry criteria and benchmark problems to explicitly describe optimal designs	
	Create clear education and training modules incorporating best practices in optimization at university and industry level	
KE9 Computational Infrastructure	Automate code optimization for optimal performance with computational infrastructure	
	Standardize computational environments to enhance multiscale/multiphysics optimization and stimulate collaboration	

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Key Element 4:

Decision Making and Uncertainty Quantification and Management

Definition

This Key Element encompasses the investigation, characterization, and management of uncertainty (both aleatoric and epistemic) to quantify prediction confidence, enhance the design process, enable optimal decision making for new materials and component designs, facilitate materials and component certification, enable responses to regulatory requirements, and support maintenance planning and system retirement. This includes

1 Tools, methods, and protocols to
- Enable the accurate evaluation and management of material, component, and/or system-based design options in the presence of various sources of uncertainty in both simulations and experiments
- Reach a sufficient level of design accuracy without foregoing computational efficiency within a reasonable cost and uncertainty budget
- Replicate the stochastic nature/behavior of materials and structures
- Incorporate uncertainty variables or inputs into risk-averse decision strategies

2 Methods for quantifying, tracking, and managing the magnitude and propagation of uncertainty throughout the time and length scales associated with models and decisions that must be made regarding both materials and structures for a given application

3 Methods for cataloging uncertainties and their sources such as parameter values, model form in representing physics, and experimental protocols and methods used to produce validation datasets

4 Objective methods and approaches for informing critical decision points throughout the design process in the presence of uncertainty

Current State of the Art

Role

Technological advances in novel characterization methods and high-performance computing have allowed engineers to model increasingly complex multiphysics simulations of materials and structures at various length and time scales. Because of this growing reliance on high-fidelity computational modeling approaches for the design of materials and structures, formalized approaches that establish confidence in the results of modeling predictions are needed. These methods are crucial for mitigating risk and driving highly consequential decision making.

Experimentation, characterization, computational modeling, and other aspects of engineering design use inputs and constraints under a state of uncertainty to bound activities and drive decision making. As part of the future engineering design framework, uncertainty quantification and management can reduce design variations, avoid costly downstream design modifications, and ultimately ensure that a chosen design approach results in a consistent, reliable end product.

Summary

UNCERTAINTY QUANTIFICATION IN DESIGN

While much of aerospace design still relies on traditional deterministic methods that fail to account for uncertainty in high-fidelity modeling, design practices are changing in response to pressure from customers, management leaders, and quality management organizations within industry. These new design practices, for both experiments and computational simulations, take advantage of modern computing tools and frameworks to more effectively account for uncertainty during design.

Traditional design methods are largely deterministic; inputs and design features are treated as fixed values akin to blueprint-nominal geometry in hardware, Gaussian distributions are often used to express variable model parameters, and fixed assumptions are coupled with simple yes/no criteria to determine if the design meets the specific requirements. If requirements are met, the design proceeds to testing and eventual production. Cost and time constraints drive a persistent need to minimize the degree of pre-production testing. Yet, in traditional deterministic design, testing is considered the last chance to evaluate—and subsequently mitigate—any variation or uncertainty in the nominal design prior to the production stage. Unfortunately, if unnoticed, the impacts of significant variations or uncertainties can ultimately result in costly fixes or corrections—especially if a technology has reached a production-level stage. Moreover, concurrent development of new or improved materials is largely out of sync with the rate of next-generation product designs and prototypes; the uncertainties associated in each of these endeavors are largely uncoupled and unquantified.

Even in cases when a designer attempts to account for uncertainty using conservative assumptions (e.g., two or three standard deviations), undesirable scenarios are still not explicitly modeled, captured, or explored, especially for high-fidelity simulations of complex features or in-service conditions. Undetected uncertainties can lead to a range of undesirable outcomes, from slightly exceeding tolerable design limits to major out-of-specification errors. This inability to fully reveal or quantify uncertainty has motivated the aerospace industry to pursue more modern design approaches and paradigms.

By and large, designers assume that fixed inputs are nominal or conservative, although there is often no real data to support such labels. In fact, a designer's assumption may actually be over- or under-projected. In the case of a conservative assumption, a design may over-perform with respect to meeting design qualifications, leaving the designer with a missed opportunity to use less costly materials or manufacturing methods without sacrificing required performance. Similarly, designs that demonstrate an improvement in other key metrics like weight, manufacturability, or repairability may be mistakenly classified as not meeting performance requirements.

By embracing and building upon recent advances in uncertainty quantification (UQ), designers can be in a better position to modify materials designs and respond to new product needs without experiencing delays or interruptions to the development process. While deeply dependent on modification to the status quo of design practices, the appropriate use of UQ can help avoid such design problems. For design in the presence of uncertainty, the designer—usually working with a team of experts representing multiple disciplines within a common or relatively similar design field—establishes a model (typically as a statistical distribution) of the uncertainties, variations, and measurement errors for each major design parameter. The design team examines how interdependent processing steps affect and often compound uncertainties. For example, in part geometry, uncertainty may be modeled as blueprint tolerance limits. For environmental parameters, it may be defined using historical data from aircraft operators or, in the absence of any data, expert experience and judgment. Design teams may also estimate "model uncertainty" depending on the outputs of interest, such as fatigue life or maximum temperature. This type of uncertainty is often accounted for by testing alternative versions of the same design model or by comparing model output to data collected in the physical world for calibrating physics-based computer models.

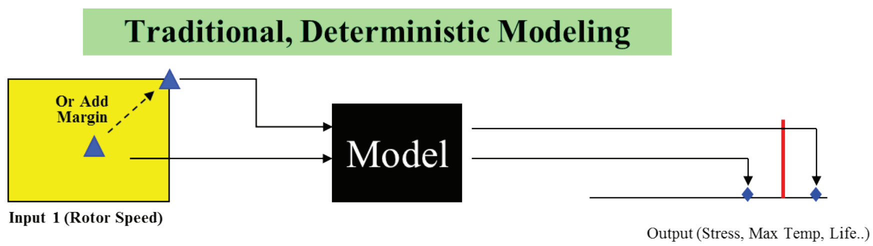
After defining "suitability representative models," designers use analysis methods like Monte Carlo simulations and/or design of experiments methodologies to evaluate all possible combinations of design parameter values to determine which ones satisfy design requirements. The primary objective is to estimate the percentage of parts for a given design that will or will not meet design requirements and by how much.

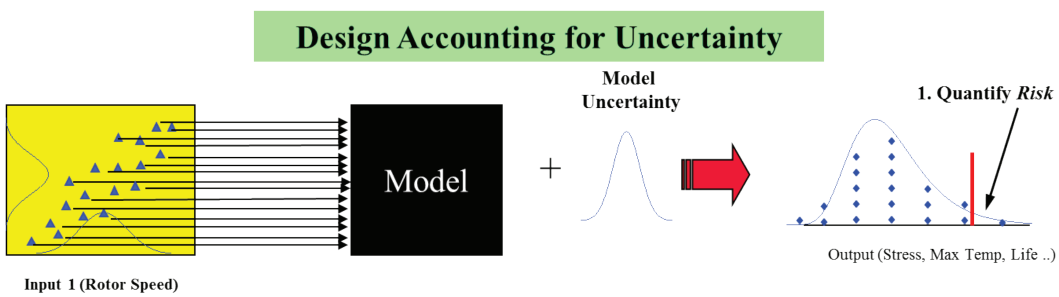
Figure 4.1 depicts a comparison of traditional and next-generation design methods. The latter design approach accounts for uncertainty in experiments, model forms, and model parameters used in the forward estimation of outputs based on a set of given inputs. Accounting for uncertainty requires intensive use of computational resources—often for the process of iterative design—and frequently uses parallel computing to execute computer codes on high-performance systems for optimum efficiency.

There are additional advantages to designing with uncertainty. After considering all possible combinations of inputs into models or metamodels, designers can use this data to compare options and identify an "optimal" design (based on the discretion of the designer). The data can also be

The major OEMs in the aerospace sector, as well as many of their suppliers, already use design tools that account for uncertainty (e.g., design of experiments, Monte Carlo simulations, sensitivity analyses). However, these tools are most often used in one-off projects or small pockets of design activities; the practice is not yet become a standard design practice, with no well-established guidelines or requirements. Although there is some effort to standardize the practice of accounting for uncertainty in design, no requirements currently exist in the aerospace sector (references [2] and [3] detail OEM efforts to address uncertainty quantification in design).

FIGURE 4.1 SIMPLIFIED COMPARISON OF TRADITIONAL DETERMINISTIC DESIGN MODELING APPROACHES WITH THOSE THAT ACCOUNT FOR UNCERTAINTY





used to conduct local or global sensitivity analyses to understand variabilities present in design model inputs or in the materials processes and manufacturing methods. Designers may also use the data to run a sensitivity analysis to rank uncertain inputs in the design model to elucidate their unique impacts on final design performance. These sensitivity analyses can help designers evaluate the feasibility of single-point optimal designs versus robust designs less sensitive to variations of design inputs [1]. Since failure may occur at the joint or interface between two parts, is it necessary to comprehend the uncertainty around a part as well as the bonded system.

DECISION MAKING WHILE ACCOUNTING FOR UNCERTAINTY

To date, some progress has been made to establish decision-making methods and practices that account for uncertainty in design, with several major companies having engaged in design of aerospace components (e.g., aircraft gas turbine design), including General Electric, Pratt & Whitney, and Rolls-Royce. Remarkably, systems-level design approaches that consider uncertainty are less developed than the field of uncertainty quantification. Numerous means to quantify uncertainty are under active development, including Gaussian pseudo-likelihood representations, Bayesian updating/learning approaches, Markov chains for uncertainty propagation, fuzzy set and interval probability representations, information uncertainty in coarse-graining, and others [4-8]. When the Air Force Research Lab (AFRL) teamed up with the aforementioned aerospace companies in an initiative known as the PACE (Probabilistic Analysis Consortium for Engines) consortium, they universally agreed on a key opportunity: "lack of methods and procedures for developing design criteria and requirements that are intended to apply to models with built in uncertainty quantification." The work being pursued under the PACE consortium on this topic is breaking new ground and will ultimately play an influential role in transforming the way that designers create and manage both part-level and system-level design criteria to account for uncertainty in design.

Designing in the presence of uncertainty requires engineering systems-based approaches to quantify, budget, and manage uncertainty throughout the process (i.e., preliminary design exploration, materials design and development, product manufacture, prototyping, and detail design) to help facilitate early-stage assessments of downstream risk and cost. The concept of ICME is based on facilitating decision support for materials design and development (see Case Study 4, Appendix B) regardless of whether designers use highly predictive computational methods and tools (e.g., DFT, molecular statics/dynamics), highly calibrated methods and tools (e.g., finite element method, computational fluid dynamics), or discrete modeling of defects in materials. Several other challenges in ICME-based design approaches require further attention [9].

References [1] and [10-11] cover current SoA in decision support for materials design and development for next generation-competitive products. QuesTek Innovations LLC developed and advanced an approach for the concurrent design of materials for specific application requirements [12] based on Olson's pioneering top-down materials design foundations [13]. The approach embraces a classical preliminary design process followed by detailed design—employing first principles modeling and thermodynamic databases—to suggest feasible candidate materials solutions that offer potential to meet ranged sets of performance requirements. With limited experimental prototyping and subsequent analysis, the approach typically uses several design iteration loops to converge on satisfactory solutions, then facilitates design trade-offs by considering multiple performance objectives and constraints (e.g., strength, environmental degradation). Engineering finite element analyses of components provide bounds on operating conditions of stress, for example, while considering realistic 3D models of microstructure to assess inherent material variability and its effect on responses of interest.

Multiscale modeling is not equivalent to materials design but rather serves the latter by providing quantitative decision support as necessary [9-10]. Hierarchical rather than concurrent multiscale modeling methods are typically pursued and generally preferred due to the considerations for specific scales and mechanisms when providing quality decision support. When linking various models via concurrent multiscale modeling schemes (i.e., two-way, bottom-up, and top-down), the uncertainty expressed at different length and time scales is generally high. The materials modeling community has not adequately addressed the quantification and propagation of uncertainty through model chains. Model-based design approaches for reducing uncertainty, which range from high-fidelity models to surrogate, or reduced order models (ROMs), emphasize the key physical principles that play the biggest role in driving decision support for the materials design and development process [14]. Experiments often play a key role in process-microstructure and microstructure-property relationships, and it is essential to quantify uncertainty in both experimental protocols and surrogate model interpretation of experimental results, with data science methods increasingly playing a role in this regard [15].

Materials design and development approaches for expressing uncertainty in both models and experiments are rapidly evolving and providing a way to track the propagation of uncertainty from material process route through material structure and properties. Materials properties are mapped onto ranged sets of multiple performance requirements, subject to design constraints, to search for feasible design solutions. Typically, feasible solutions represent a Pareto frontier from which each user or designer can select a solution based on variability, uncertainty, and preference. The monograph by McDowell et al. [1] clearly defines materials design as an extension of engineering systems design methods that makes use of compromise decision support problems for multiple design objectives. Approaches can range from tracking uncertainty propagation in materials design and development (as demonstrated in the DARPA AIM program [16]), to compiling uncertainty propagation distributions for projected performance based on uncertainty in design variables [17-18], to extensions of Taguchi-based robust design (i.e., lack of sensitivity of responses or design targets to process variables [1,11,19]). Recent examples of the Inductive Design Exploration Method (IDEM) approach [1,19] have considered the design of ultra-high-performance concrete [20] and other applications [21].

2040 End State

By 2040, there will be robust, probabilistic risk assessment and uncertainty quantification for material and process design across all length and time scales. Computationally guided systems will manage materials, manufacturing parameters, and optimal design using automated decision making that provide quantified levels of uncertainty. This will allow the design process to focus on engineering constraints for the system rather than the details of selected part or component manufacture. The autonomous systems will quickly deliver answers to prevent designers from waiting for prolonged periods of time to rapidly achieve the desired results. Quantified and trusted understanding of uncertainty will reduce the required amount of qualification and certification testing, accelerate time to delivery, and reduce costs. Higher confidence levels in materials-, component-, and system-level assessments will facilitate optimum maintenance schedules, reduce risks of failure, and avoid unnecessary costs.

Gaps

The following gaps are spread throughout all 10 of the roadmap's crosscutting streams, with the most critical gap falling within the **Data Analytics and Visualization** stream. One common theme throughout this Key Element is a lack of methods and protocols for understanding, quantifying, and documenting uncertainties throughout the design process. The identified gaps have the strongest ties to the **accessible, robust,** and **traceable** characteristics of the 2040 end state. Access to common UQ methods and protocols is a requirement to establishing the ecosystem of the future.

TABLE 4.1 DECISION MAKING AND UNCERTAINTY QUANTIFICATION AND MANAGEMENT GAPS AND IMPACTED 2040 CHARACTERISTICS

AC Accessible **AD** Adaptive **IN** Interoperable **RB** Robust **TR** Traceable **UF** User Friendly ❖ Critical

GAPS	2040 CHARACTERISTICS					
	AC	AD	IN	RB	TR	UF
DATA MANAGEMENT						
Lack of standards or common formats for presenting and documenting the inputs and outputs of decision-making processes (i.e., assumptions, data inputs, models employed, uncertainties, critical decision points)	AC				TR	UF
DATA ANALYTICS AND VISUALIZATION						
❖ Existing models and software codes are not designed to compute input sensitivities and propagate uncertainties to enable UQ				RB	TR	
Lack of standards/best practices for decision making and for quantifying and presenting uncertainties in data across multiple time and length scales	AC		IN		TR	UF
INFORMATION SHARING AND REUSABILITY						
Limited availability of material and process datasets with documented uncertainty to use as parametric inputs for informing both deterministic and non-deterministic models	AC				TR	
Industry is reluctant to reveal UQ and/or calibration data/methods for fear of liability	AC				TR	
MULTIDISCIPLINARY COLLABORATION						
Decision making and UQ methods are largely inaccessible and/or poorly communicated to others across engineering fields	AC		IN		TR	UF
INSTITUTIONAL PARADIGMS						
Lack of engineers and scientists trained in data-analysis, decision making, and UQ management practices, including modeling approaches to stochastic modeling and statistically based methodologies	AC					
BENCHMARKING AND BUSINESS CASE						
Lack of available benchmarking studies on existing decision-making tools	AC			RB		
Lack of methods/tools that examine the business cases for making decisions throughout the design process				RB	TR	
SCALABILITY AND COMPUTATIONAL EFFICIENCY						
Calculations accounting for uncertainty are computationally expensive		AD		RB		

GAPS	2040 CHARACTERISTICS					
	AC	AD	IN	RB	TR	UF
LINKAGE AND INTEGRATION						
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			✓	✓		
INPUT/OUTPUT CONFIDENCE AND RELIABILITY						
Lack of established protocols or best practices for selecting UQ methods based on design requirements	✓					✓
Insufficient databases of known uncertainties (e.g., at individual scales) that support propagation of uncertainty through multiple scales			✓	✓		
Insufficient tools for assessing the reliability of probabilistic modeling outputs				✓		
BEHAVIOR OF MATERIALS AND STRUCTURES						
The ability of UQ analytical methods to quantify confidence in the prediction of material and component behavior across length scales and at all levels of complexity is limited by: • Computational inefficiencies • Mathematical inconsistencies of multiscale modeling algorithms • Gaps in physical understanding of materials, data, and measurement capabilities				✓		
Limited understanding of uncertainty related to manufacturing environment variability				✓	✓	
Sources of uncertainty related to material implementation and joint stress state (joints, interfaces, multiaxial loading failures, etc.) are inadequately understood				✓		

Recommended Actions

The following recommended actions lie within nine of the roadmap's 10 crosscutting streams, with the most actions (including high priority) under **Data Analytics and Visualization, Benchmarking and Business Case,** and **Input/Output Confidence and Reliability.** The Data Analytics Stream also contains the critical gap for this Key Element. These recommended actions focus primarily on developing new methods for decision making and UQ and improving existing ones. The recommended actions have the strongest ties to the **robust**, **traceable**, and **user-friendly** characteristics of the 2040 end state.

TABLE 4.2 DECISION MAKING AND UNCERTAINTY QUANTIFICATION AND MANAGEMENT RECOMMENDED ACTIONS AND METRICS

FUNDING: $ <0.5M/year $$ 0.5-2M/year $$$ 2-5M/year $$$$ >5M/year

AC Accessible   **AD** Adaptive   **IN** Interoperable   **RB** Robust   **TR** Traceable   **UF** User Friendly   ✱ High Priority

ACTION	2040 CHARACTERISTICS						TIMEFRAME FOR COMPLETION			FUNDING
	AC	AD	IN	RB	TR	UF	NEAR 2017-2022	MID 2022-2035	LONG 2035+	
DATA ANALYTICS AND VISUALIZATION										
✱ (4.1) 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				RB	TR	UF	■	■		$$$
✱ (4.2) Devise novel UQ methods that use low-fidelity physics based surrogate models to balance computational efficiency with convergence accuracy		AD					■	■	■	$$
(4.3) Devise novel methods for interpreting large uncertainties that are intrinsically generated by computationally inexpensive surrogate-based models		AD		RB			■	■		$$$
(4.4) Investigate creative approaches (e.g., machine learning) for interpreting, visualizing, and summarizing quantified uncertainties and decision-making processes		AD			TR	UF	■	■		$$$
INFORMATION SHARING AND REUSABILITY										
(4.5) Consider establishing requirements to quantify and disclose uncertainty levels for particular applications (e.g., FAA regulations) • Requires highly controlled protocols for disclosing information	AC				TR			■		$$
MULTIDISCIPLINARY COLLABORATION										
(4.6) Coordinate with existing standards committees (DoD, national labs, professional societies, academia, etc.) to establish standards and methods of communicating uncertainty among various multiscale modeling approaches including molecular dynamics (MD), computational fluid dynamics (CFD), and structural mechanics	AC		IN			UF	■	■		$$

ACTION	2040 CHARACTERISTICS AC	AD	IN	RB	TR	UF	TIMEFRAME FOR COMPLETION NEAR 2017-2022	MID 2022-2035	LONG 2035+	FUNDING
MULTIDISCIPLINARY COLLABORATION, CONTINUED										
(4.7) Convene representatives across industry, government, and academia to adapt/modernize engineering educational curricula and training modules to strengthen workforce expertise in decision-making/UQ approaches • Seek alternative pathways—outside of curricula—to teach UQ approaches	✓					✓	✓			$$
INSTITUTIONAL PARADIGMS										
(4.8) Integrate methods into materials science and engineering curricula to teach lifetime predictive approaches to minimize maintenance errors and risks			✓	✓		✓	✓	✓		$$
(4.9) Coordinate and execute a plan to incorporate advanced statistics into university curricula to establish UQ and error propagation as standardized workflow components	✓		✓			✓		✓		$$
BENCHMARKING AND BUSINESS CASE										
(4.10) Leverage existing efforts to develop open standards for documenting and presenting the decision-making process	✓				✓	✓	✓	✓		$$
(4.11) Identify key uncertainties that are missing from design considerations but are present—or arise—in manufacturing environment (e.g., variability of hole size/placement/ovality in design versus manufacturing)			✓	✓	✓		✓	✓		$$
(4.12) Generate a set of publicly available benchmark UQ problems with varying levels of fidelity and make accessible to the broad modeling and simulation communities	✓				✓	✓	✓			$$
(4.13) Conduct a technoeconomic analysis for integrating common UQ issues into product design and develop training modules to encourage adoption of methods/approaches: • Provides risk assessments, return on investment (ROI), and cost estimates based on failure probabilities • Define minimum acceptable levels of UQ within reasonable cost levels	✓		✓		✓	✓	✓			$$
SCALABILITY AND COMPUTATIONAL INFRASTRUCTURE										
* (4.14) Establish a framework for developing numerical UQ approaches that appropriately scale with advanced parallel HPC architectures		✓					✓	✓	✓	$$
(4.15) Develop techniques to build well-trained surrogate models for large-scale optimization of materials/components for novel applications	✓	✓		✓			✓	✓	✓	$$$

ACTION	2040 CHARACTERISTICS						TIMEFRAME FOR COMPLETION			FUNDING
	AC	AD	IN	RB	TR	UF	NEAR 2017-2022	MID 2022-2035	LONG 2035+	
LINKAGE AND INTEGRATION										
✱ (4.16) Develop decision/UQ tools that link experiments with corresponding simulations • Apply existing UQ approaches to complex multiscale simulations for conducting risk assessments • Create a platform that incentivizes the integration of novel UQ methods in production software packages			✓		✓	✓	✓	✓		$$$
(4.17) Develop inverse UQ toolsets that identify unknown/influential input parameters and calibrate their values to match simulations to experimental datasets			✓	✓		✓	✓	✓		$$
INPUT/OUTPUT CONFIDENCE AND RELIABILITY										
✱ (4.18) Advance existing UQ computational tools to enable automated determination of required experiments to reach target levels of uncertainty with respect to model's predictive capability • E.g., Determining the number of additional data points required to have enough quantified uncertainty needed to make a decision		✓		✓				✓	✓	$$
✱ (4.19) Improve methods for analyzing the sensitivity of various UQ sources across length and time scales and throughout the product lifecycle			✓	✓			✓	✓	✓	$$$
✱ (4.20) Develop new design of experiments (DoE) approaches that improve data yield and usability to increase UQ confidence for multiscale modeling approaches				✓	✓		✓	✓		$$$
(4.21) Develop criteria to support screening of bad/undesirable experimental test results (caused by errors, impurities, etc.) • Start by collecting/generation base sets of data to build screening methods					✓		✓	✓		$$
(4.22) Define multi-parameter decision making objectives	✓				✓		✓			$
BEHAVIOR OF MATERIALS AND STRUCTURES										
(4.23) Create physics-based stochastic multiscale models to inform the development of advanced UQ algorithms • Model-generated outputs provide distributions of materials behavior and service conditions				✓				✓	✓	$$$$

Relationships with Other Key Elements

The Decision Making and Uncertainty Quantification and Management Key Element will serve the future ecosystem by facilitating the transition from deterministic to probabilistic modeling methods, providing frameworks for error and uncertainty propagation across scales, improving the process of decision making, and simplifying regulatory compliance.

TABLE 4.3 EXAMPLE INTERRELATIONSHIPS OF KE4 (DECISION MAKING AND UNCERTAINTY QUANTIFICATION AND MANAGEMENT) AND OTHER KEY ELEMENTS

Note: Interrelationships among KEs vary. Equal weight should not be inferred.

OTHER KEY ELEMENTS	INTERRELATIONSHIP	THIS KEY ELEMENT
KE1 Models and Methodologies	Illuminate errors, bound error propagation, and enable model-based material and probabilistic component definitions	KE4 Decision Making and Uncertainty Quantification & Management
	Forward modeling of 3D/4D characterization tools to bound measurement uncertainty and error	
KE2 Multiscale Measurement and Characterization Tools and Methods	Introduce probabilistic methods for structural characterization and component analysis	
	Deliver data for model input sensitivity assessments, efficient experimental designs, and enhanced model UQ	
KE3 Optimization and Optimization Methodologies	Provide manufacturing constraints with integrated uncertainties for readily manufacturable solutions	
	Support optimization algorithms with integrated UQ information for enhanced decision making	
KE5 Verification and Validation	Establish probabilistic methods for quantifying errors between simulation and experimental data	
	Inform V&V/UQ tools to assess linkages and approaches for enhanced experimental design	
KE6 Data, Informatics, and Visualization	Employ feedback systems to provide data quality markers, substantiate data quality, or identify data generation needs	
	Provide automated uncertainty prediction tools and novel visualizations of uncertainty	
KE7 Workflows and Collaboration Frameworks	Streamline automated workflow tools via common standards and protocols for uncertainty quantification, management, and reporting	
	Employ characterization, uncertainty prediction, and activity-tracking tools for autonomous decision making	
KE8 Education and Training	Offer academic courses on V&V experimental testing and evaluation grounds	
	Train graduates in probabilistic methods for uncertainty quantification and propagation	
KE9 Computational Infrastructure	Investigate computationally efficient and cost-effective methods for achieving sufficient design accuracies	
	Exploit parallel software frameworks and computer architectures for uncertainty quantification and propagation	

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Key Element 5:

Verification and Validation

Definition

This Key Element encompasses methods/practices associated with verification of algorithms and validation of models.

1 **Verification** can be defined as finding and eliminating errors in numerical algorithms/codes and evaluating the solution accuracy of numerical methods against design requirements by comparing with highly accurate or closed-form benchmark solutions.

2 **Validation** is the process of determining the degree to which a model accurately represents reality (the experiment) within the range of intended use.

Current State of the Art

Role

Verification ensures that a model is correctly numerically implemented and is conducted by checking model inputs and outputs with simplified or benchmark example cases. Verification is followed by validation, in which the physics implemented in the model is assessed by checking accuracy of predictions against experimental measurements. For integrated systems with multiple linked models or sub-models, each model is verified and validated to the required level using a hierarchical approach. Uncertainty in model inputs, boundary conditions, and outputs, along with experimental errors, are assessed to the accuracy level required by a given organization.

Today, modeling applications are migrating from being strictly deterministic to probabilistic in nature, requiring increased use of formalized verification and validation (V&V) tools and frameworks. V&V is a common "language" among engineering disciplines that deploy computational methods and as such is a requirement for material and system modeling acceptance and multidisciplinary application.

V&V tools and methods are currently critically under-used across industry, from suppliers of raw materials through the OEMs. Of the companies surveyed as part of this initiative, only 12.5% used what they would describe as a "defined" process for V&V. The remainder of those surveyed all indicated that some verification and validation work occurs, at least irregularly, in their organizations but none of it was consistently performed or formally defined.

Summary

V&V STANDARDS/PROTOCOLS

To date, the Institute of Electrical and Electronics Engineers (IEEE) has published a standard for System and Software Verification and Validation, initially published in 1998 and revised in 2004 and again in 2012 [1,2]. Similarly, the American Institute of Aeronautics and Astronautics (AIAA) developed guidelines for the V&V of computational fluid dynamics (CFD) simulations in 1998 [3,4], which subsequently led to the development of the V&V guide published in 2006 by The American Society of

Mechanical Engineers (ASME) for solid-mechanics models [3,4]. The U.S. Air Force sponsored an assessment of V&V activities between 2010 and 2012, which led to the development and publication of V&V guidelines and recommendations for the materials community [2]. However, this publication was only known to one in four of the participants in the Vision 2040 V&V workshop. The American Welding Society (AWS) proposed standardization for V&V of computer code-based welding models [5], which referenced the much more generic ASME work. Among the Vision 2040 V&V workshop participants, only one in three were aware of the ASME and Air Force guidelines. In short, these existing guidelines were completely unknown to the majority of the Vision 2040 workshop participants before they deliberately researched V&V methods in general industries.

Within the broader community of model developers and users there has been an overall lag in the implementation of existing V&V methods and protocols. Unlike established material testing and characterization methods, found as ASTM standards embraced throughout the world, V&V standards have not been extensively adopted.

Although some V&V tools, methods, and guidelines exist, new ones are needed that are suitable for emerging multiscale/multiphysics models. Engineers have an immediate need to use these models and to have them fully verified and validated. This means new V&V practices and technologies need to be created, verified and validated themselves, and taught to workers, all in parallel with multiscale/multiphysics model development.

V&V SOFTWARE TOOLS & METHODS

Methods for model validation/calibration have developed rapidly in both academia and industry over the last 10 years. Many industries have called for rigorous, probabilistic methods that can quantify the bias(es) between models and real-world observed data, as well as calibrate the sets of possible input values to a model that best align to the real-world data [6]. Work at the University of Sheffield in the UK [7] and by Sandia National Laboratories [8,9] in the United States in particular have shaped these methods and created early-adopter tools for applying them. Now, professional software developers like SmartUQ are creating more powerful tools to apply these methods across industry [4] in the wake of successes such as Southwest Research Institute's DARWIN suite [10] for probabilistic analysis and application of models.

Additionally, some recent initiatives have demonstrated the extensive use of V&V in solving foundational engineering problems (FEPs). One example is the U.S. Air Force's FEP program [11], which focused on developing and demonstrating ICME infrastructure to incorporate bulk residual stress into manufacturing, design, and structural analysis of aeroengine disks. Methodologies were developed and demonstrated for verifying and validating OEM process models linked with supplier materials and structural analysis tools.

2040 End State

By 2040, V&V will wrap around the entire simulation infrastructure, including experimental methods and characterization tools. A widely accepted V&V framework will be fully established with standards and protocols for multiscale modeling. The framework will necessitate the use of V&V tools is not only a standard but also a requirement for all simulations. V&V will thus be encoded into modeling and simulation processes directly, such that only validated models/methods will be used to make predictions. As a result, next-generation aerospace platforms will be designed, validated, manufactured, and certified in far fewer years.

Gaps

The following gaps lie within five of the roadmap's 10 crosscutting streams, with the **Benchmarking and Business Case** stream containing the largest number of gaps. The central challenge to establishing a community-wide framework for verifying and validating models, software, and systems is a lack of widely accepted guidelines and benchmarks to facilitate the adoption of new and existing multiscale/multiphysics V&V practices. These gaps have the strongest tie to the **accessible** characteristic of the 2040 end state. Without an accessible V&V framework, the 2040 end state cannot be achieved.

TABLE 5.1 VERIFICATION AND VALIDATION GAPS AND IMPACTED 2040 CHARACTERISTICS

AC Accessible **AD** Adaptive **IN** Interoperable **RB** Robust **TR** Traceable **UF** User Friendly ❖ Critical

GAPS	2040 CHARACTERISTICS					
	AC	AD	IN	RB	TR	UF
INFORMATION SHARING AND REUSABILITY						
Lack of readily available training on existing V&V tools and methods for multiple experience levels	✓					
MULTIDISCIPLINARY COLLABORATION						
Insufficient communication pathways between modelers and experimentalists (e.g., communication via metadata)			✓			✓
INSTITUTIONAL PARADIGMS						
Lack of graduates trained in ICME and V&V entering the workforce, and lack of opportunities to apply their knowledge • Limited university courses covering V&V	✓					
BENCHMARKING AND BUSINESS CASE						
Absence of publications containing quantitative data on the savings potential of applied V&V	✓				✓	
Lack of V&V risk assessment and UQ for ICME models				✓		
Inaccurate perception of V&V—and collection of experimental data—as a too time-consuming and resource-intensive to be value-added	✓					
Lack of standard benchmark problems and example V&V approaches • E.g., End-to-end example problem provided by ASME V&V committee	✓					✓
INPUT/OUTPUT CONFIDENCE AND RELIABILITY						
❖ Lack of guidelines and practitioner aids for multiscale/multiphysics (e.g., ICME) V&V • V&V methods are not well known among the materials science and engineering community, and engineers do not know how to use them in the context of single and multiscale materials modeling • Experiments performed for model validation are not well understood	✓					✓
Emerging V&V methodologies/ approaches are immature and underdeveloped • Lack of application-specific V&V methods				✓		

Recommended Actions

The following recommended actions lie within six of the roadmap's 10 crosscutting streams, with the most actions affecting **Input/Output Confidence and Reliability**. Quantifying and assessing confidence and reliability in models and data is the main purpose of V&V during product design and deployment. Many of the recommended actions call for establishing community-wide practices and approaches for building out the V&V framework. The recommended actions have the strongest ties to the **accessible**, **robust,** and **user-friendly** characteristics of the 2040 end state.

TABLE 5.2 VERIFICATION AND VALIDATION RECOMMENDED ACTIONS AND METRICS

FUNDING: $ <0.5M/year $$ 0.5-2M/year $$$ 2-5M/year $$$$ >5M/year

AC Accessible **AD** Adaptive **IN** Interoperable **RB** Robust **TR** Traceable **UF** User Friendly ✱ High Priority

ACTION	2040 CHARACTERISTICS						TIMEFRAME FOR COMPLETION			FUNDING
	AC	AD	IN	RB	TR	UF	NEAR 2017-2022	MID 2022-2035	LONG 2035+	
DATA MANAGEMENT										
✱ (5.1) Develop, approve, and actively support the development of V&V standards for hierarchical and/or complex models • Establish minimum requirements and definitions for V&V of multiscale materials models	AC				TR	UF	■	■		$$$$
INSTITUTIONAL PARADIGMS										
✱ (5.2) Develop training modules to teach V&V approaches throughout the design process (i.e., structural component to materials & processes to model development) • Teach systems paradigm that integrates theory and experiments for concurrent model development and validation	AC		IN			UF	■	■	■	$$$
BENCHMARKING AND BUSINESS CASE										
(5.3) Create a web-based platform to host code verification benchmarking activities	AC					UF	■	■		$$
SCALABILITY AND COMPUTATIONAL EFFICIENCY										
✱ (5.4) Develop V&V-friendly model formats and/or surrogate model structures so V&V can be "designed in" from the start	AC	AD	IN				■	■		$
LINKAGE AND INTEGRATION										
(5.5) Accelerate multiscale V&V data collection efforts starting at lower length scales			IN	RB	TR		■	■		$$$
(5.6) Explore multiscale-compatible V&V approaches capable of comparing small samples to larger parts			IN	RB			■	■		$$$

ACTION	2040 CHARACTERISTICS						TIMEFRAME FOR COMPLETION			FUNDING
	AC	AD	IN	RB	TR	UF	NEAR 2017-2022	MID 2022-2035	LONG 2035+	
INPUT/OUTPUT CONFIDENCE AND RELIABILITY										
✱ (5.7) Establish best practices for data collection techniques for high quality model emulation and/or calibration data	✓			✓	✓	✓	✓			$
(5.8) Establish best practices for mathematical/statistical approaches to calibrating models against experimental data and available analytical solutions	✓			✓		✓	✓			$
(5.9) Develop best practices for generating and validating flexible parametric models and surrogate models for complex geometries		✓		✓		✓	✓	✓		$
(5.10) Determine best practices for screening the quality of V&V repository data	✓			✓	✓	✓	✓			$$
(5.11) Enable a "backward simulation" validation capability				✓			✓	✓		$$

Relationships with Other Key Elements

Verification and validation practices are vitally important to establishing suitability of algorithms and prediction accuracy of models. Serving as an essential conduit for experimental methods, characterization tools, and models, this Key Element will pervade data collection techniques and automated workflow tools, enabling an industry-wide ICME framework that streamlines product certification and boosts overall adoption of computational models.

TABLE 5.3 EXAMPLE INTERRELATIONSHIPS OF KE5 (VERIFICATION AND VALIDATION) AND OTHER KEY ELEMENTS

Note: Interrelationships among KEs vary. Equal weight should not be inferred.

OTHER KEY ELEMENTS	INTERRELATIONSHIP	THIS KEY ELEMENT
KE1 Models and Methodologies	Validate models via concurrent companion modeling	KE5 Verification & Validation
	Create industry-wide standards, protocols, and model formats to enable V&V tool and method applications	
KE2 Multiscale Measurement and Characterization Tools and Methods	Assess physical and computational method linkages, and optimize experimental plans to support V&V	
	Enable integrated parameter sensitives and error propagation studies for enhanced model validation	
KE3 Optimization and Optimization Methodologies	Calibrate and validate estimated uncertainty in optimization routines	
	Foster model-based optimization routines for V&V activity planning and selection	
KE4 Decision Making and Uncertainty Quantification and Management	Inform V&V/UQ tools to assess linkages and approaches for enhanced experimental design	
	Establish probabilistic methods for quantifying errors between simulation and experimental data	
KE6 Data, Informatics, and Visualization	Employ feedback systems to provide data quality markers, substantiate data quality, or identify data generation needs	
	Establish minimum requirements, common definitions, and readily accessible high-pedigree datasets for model validation	
KE7 Workflows and Collaboration Frameworks	Establish widely accepted V&V standards and protocols to streamline automated workflow tools	
	Automate workflow tools to incorporate and simplify V&V practices	
KE8 Education and Training	Offer academic courses at V&V experimental testing and evaluation facilities	
	Increase total graduates trained in ICME model validation	
KE9 Computational Infrastructure	Verify peta- and exascale computing algorithms	
	Provide hardware/software frameworks for managing/accessing experimental datasets for V&V	

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Key Element 6:

Data, Informatics, and Visualization

Definition

This Key Element encompasses the following:

1 **Data and Informatics**
All aspects associated with the electronic capture, analysis, archival, maintenance, and dissemination of material data* related to experiments, simulation, and applications:
- Methods and technology for gathering, manipulating, storing, retrieving, mining, and analyzing data to extract new knowledge from existing information (i.e., data analytics)
- Technologies for accessing, aggregating, and sharing structured/unstructured data from geographically disparate locations
- Information and knowledge management systems required to seamlessly and automatically connect 1) experimental, simulation, and manufacturing materials and structural data at different length scales; and 2) toolsets and best practices within and across users, organizations, data sources, and structural applications

2 **Visualization**
Technologies for representing/displaying data and analytical results across time and length scales to enable the comprehension of information, gain new insights, and inform decision-making

Current State of the Art

Role

Information management (in the form of material property data and simulation management) plays a key role in today's design paradigm, particularly in highly regulated industries like aerospace, where the need to establish a "gold standard" for material data is paramount. Although data repositories (experimental, material property, simulation) exist, they are often siloed and company/department specific: connection within a given organization—and most assuredly along the supply chain—is limited at best. Companies that have established a digital thread and accompanying digital culture are reporting high payoff in terms of efficiency increases and cost savings; however, to date progress has occurred on either the material or structures side of the house with only limited connection between the two. Visualization goes hand-in-hand with information management, transforming raw data into a form interpretable by designers, engineers, and decision makers. In today's world, icons, graphical user interfaces, and smart devices are exploding in use around the globe.

Summary

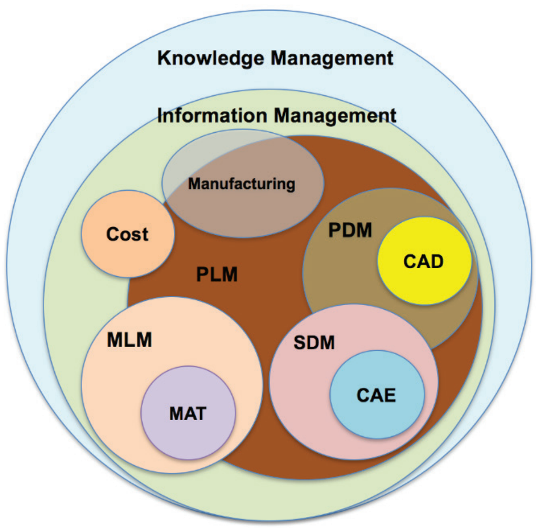
JOURNEY OF DATA MANAGEMENT

Transitioning from "paper" to digital representation has been ongoing for decades, with some technical communities being earlier adopters of the various technologies than others (e.g., system design and simulation vs. materials), with software evolving to manage this digital footprint. For example, early on disparate collections of structured data associated

*Material data includes both data and metadata. **Data** are the outputs from a physical experiment, computer simulation, or analytical model. **Metadata** is "data of data" that describes the data resource, format of the data resource, and the administrative rights associated with the data.

with specific topic areas like cost, manufacturing, computer-aided design (CAD), computer-aided engineering (CAE), material properties (MAT), etc. appeared (Figure 6.1), yet this data was largely unmanaged and had minimal associated metadata, traceability, and searchability. Then product data management (PDM) software designed to manage CAD data and simulation data management (SDM) designed to manage CAE data emerged, followed

FIGURE 6.1 INFLUENCE AND INTERACTION OF VARIOUS MATERIALS AND SYSTEM ENGINEERING SOFTWARE PRODUCTS.



by Product Lifecycle Management (PLM) for managing and integrating engineering data and processes as well as business and manufacturing processes from cradle to grave. Soon after that came Material Lifecycle Management (MLM) systems designed to manage MAT data with their own unique requirements. Now the generalization to information management – associated with explicit data (know what) – and the even more challenging area of knowledge management – associated with tacit, or hidden, data (know how) – is underway. Note that knowledge is defined as information with intrinsic value, implications, or connections (e.g., insight, intuition, skills); experience; and other knowledge that has not been formally shared. The design, implementation, and deployment of these broadly termed information/knowledge management systems remain today the focal point of on-going research and development efforts. The supporting methods, tools, and approaches for these types of data infrastructures all fall under an emerging discipline called Data Science and Informatics [1,2].

Because no one-size-fits-all solution is anticipated, the concept of creating a digital ecosystem of federated (highly interconnected) components is advancing, a recent example being the Industrial Internet of Things (IIoT) [3]. It is this desire to share and interact with data/information/knowledge within and among varied and often times disparate disciplines and skill sets, throughout the entire supply chain, which makes the development and deployment of such an ecosystem challenging. This is particularly true for the materials and structural modeling and simulation communities, in which the interaction of complex physics over multiple length and time scales makes the absorption, comprehension, utilization, and retention of this multifaceted data/information/knowledge problematic. Furthermore, in highly regulated industries, such as aerospace and defense, in which certification and liability issues are prominent, additional complications arise associated with traceability and version and access control. For example, aerospace companies must maintain the supporting information used to certify an aircraft for operation throughout its lifetime, as well as the manufacturing records of flight critical components.

Significant government-sponsored initiatives/projects (both national [4-6] and international [7-9]) and private/public consortia [10-14] have been established over the past 15 years in an attempt to accelerate the creation of this "digital tapestry" [15] for materials and structural engineering:

- The objective of the **LOTAR International Consortium** [10] is to develop, test, publish, and maintain standards for long-term archiving (LTA) of digital data, such as 3D CAD and PDM data. These standards will define auditable archiving and retrieval processes. LOTAR International's membership includes leading OEMs and suppliers from the aerospace and defense industry from the EU and the Americas.
- The **Materials Data Management Consortium** (MDMC) [11] has been working for over 15 years to develop tools and methods to support material data management and retrieval for use in engineering design and structures. The

consortium is focused on building and continuously enhancing data management systems and applications, establishing best practices in material data information management, and developing community-accepted data schemas for the Granta family of materials data products [20].

- **FIBERS** [12] is an industry-led polymer composites consortium, funded by NIST, to develop a technology roadmap that identifies shared technical obstacles and defines pathways toward manufacturing advances to enable scale-up of cost-effective, high-volume production processes.
- **TOICA** [13] is the latest in a series of EU-funded projects, coordinated by Airbus, consisting of 32 partners from eight countries to understand the evolution of behavioral Digital Aircraft dataset from concept to certification. TOICA focuses on the thermal behavior of the whole aircraft.
- The **SimBest** project [14], funded by Innovate UK, is focusing on gathering and disseminating best practice in the use of simulation and modeling tools for engineering design simulation in high value-added manufacturing.

One critical outcome of these initiatives has been the engagement and focus of professional societies (AIAA, ASM, ASME, NAFEMS, and TMS), associations (ASD-STNN, AIA, PDIES, ProSTEP), standardization bodies (NIST, ISO, ASTM, ASD-SSG), and regulatory bodies (FAA, EASA) on this development process, resulting in a number of published studies (see [16-19]).

DATABASES AND DATA INFRASTRUCTURE

Currently, a number of materials-oriented databases and infrastructures, both open and commercial, exist. These databases span various length scales, from atomic to macroscale, and provide essential input to material models, whether atomic potentials or material properties. For example, at the atomic scale, several new databases/repositories have been established to house interatomic potentials and the output of *ab initio* calculations [21-25]. Combined, the three databases [23-25] contain fundamental material property information for over 1 million compounds based on primarily 0 K (zero Kelvin) calculations. CALPHAD [26] is an approach to develop multicomponent descriptions for a variety of phase-based properties including the Gibbs energy (allowing phase equilibria calculations), diffusion mobilities, molar volume, and elastic constants [27]. This approach has been used to develop a variety of open-source and commercial multicomponent thermodynamic and diffusion mobility databases that are frequently used by industry to integrate materials design approaches. More recently, database efforts have expanded to include molar volume data. Citrine Informatics has developed a public platform that supports data-driven materials and chemistry research [28]. There are also a number of engineering property databases, such as MatWeb [29], Granta Design [30], MatNavi [31], and MAPTIS [32]. A key feature missing, however, in these property-centered databases, as well as most proprietary in-house databases, is a rigorous description of the associated material microstructure and the connection to associated processing parameters, making processing-microstructure-property relations difficult to establish. Such relationships (information) are extremely important, as they enable cost-effective, fit-for-purpose modification of these materials as well as provide crucial insight for material innovation. An attempt to link simple measures of microstructure features (data and metadata) with mechanical material properties and performance response as well as enable multiscale modeling within an information management workflow and toolset was demonstrated by NASA GRC with the Granta MI installation [20] and has since been adopted by the MDMC [11] and incorporated into its ICME schema (see Case Study 4, Appendix B). Also, while some tools for tracking and creating detailed digital microstructures now exist (e.g., DREAM3D [33]; see Case Study 3, Appendix B), the resulting detailed digital descriptions have yet to be tightly incorporated within commonly available data infrastructures.

Open data repositories for experimentally obtained data are also emerging, driven by efforts such as the Materials Genome Initiative (MGI) [34] which calls for platforms to exchange materials data as well as a decentralized infrastructure. Notable examples are the NIST Repositories [35], the Materials Data Facility at the University of Illinois [36], the Materials Commons at the University of Michigan [37], and the Computational Materials Data Network hosted by ASM International [38], and the HyperThought system at AFRL [39]. Efforts to capture, document, and share transient/dynamic material properties during processing are just beginning to emerge. For example, Worcester Polytechnic Institute (WPI), University of Connecticut, SUNY Buffalo, and ASM International are establishing the Center for Materials, Modeling, and Manufacturing Data aimed at generating transient materials property data that is applicable for manufacturing process simulation. The commercial Granta data management products are generally, but not exclusively, intended for internal organizational use and enable the establishment of corporate in-house material data information warehouses with both access and version control. By contrast, the AFRL-sponsored Metals Affordability Initiative has developed and launched an access-controlled, cloud-based data management and sharing repository called MAIhub [40], which is only accessible to member organizations but can house export controlled materials data. This first-of-its-kind repository for aerospace materials data paves the way for secure sharing of materials data among industrial, academic, and government collaborators.

Whether for internal data management systems or global data infrastructures, an important emerging paradigm in best practices for the management of technical data is the FAIR principles [41], guidelines that define what it means to make data Findable, Accessible, Interoperable, and Reusable to help technologists be good stewards of scientific and engineering data.

- **Findable** has two key components: unambiguous identification of data through a Universal Resource Identifier, such as a digital object identifier (DOI), and discoverability of data through a search function such as with natural language. NIST has been at the forefront of providing guidance and technology that support the FAIR principles in materials and is currently piloting a web-based tool, the Material Resource Registry (MRR) [42], that will provide a means of discovering coarse-grained data-oriented resources. This tool uses relatively simple standards by which users can expose their data resources to the MRR and make them discoverable through the internet. NASA is also piloting similar functionality with a system called Digital World, which provides registries of domain-specific resources (datasets, code, etc.).
- **Accessible** is relatively self-explanatory, while **Interoperable** denotes readability by both human and machine and compatibility with other data formats. Currently, the HDF5 file format [43] appears to be the leading candidate for encoding complex material data due to its open and hierarchical structure [44].
- **Reusable** means that data contains sufficient metadata to be contextually well-defined for a specific purpose. Here, NIST's Materials Data Curation System (MDCS) provides a structured means for capturing, describing, sharing, and transforming material data into a structured format that is XML-based, which is both human and machine readable. The data is organized using user-selected templates encoded in XML Schema [45]. While data schemata are emergent within the materials community, they are still relatively rare.

At present, most devices used to characterize or measure a material produce a proprietary or manufacturer-unique data format, replete with non-standard terms to describe the data and metadata fields. Much effort is still required to simplify and speed the workflow to take data from experiment or simulation through storage, discovery, and reuse. The development and adoption of open data standards and formats, starting with characterization, testing, and processing equipment, is an essential first step in creating these workflows. Manufacturers encountered this same issue in extracting data in a common, readable format from manufacturing equipment. NIST sponsored and established a consortium called MTConnect [46] to develop common standards for interfacing with manufacturing equipment.

Capture of the relevant data and the metadata associated with a given part through its lifecycle ("data provenance"), including material, design, manufacture and use data, provides a complete "digital thread" that describes and defines a component in a reusable digital format. This holistic approach to data capture is emerging as the new philosophy for materials data management and control. As data is collected on a given material and component and is analyzed relative to other components with a common material type, increased knowledge and understanding about the behavior of the underlying material can be developed. This data-driven "cradle-to-cradle" design system approach to data capture and reuse is enabling materials and manufacturing models to be created and validated that support current and future component and systems designs.

No centralized standards for the communication or storage of materials information currently exist. In terms of data storage, no clear community standards have developed to store materials data, like the Flexible Image Transport System (FITS) in astronomy [47]. Common file formats enable easier data sharing but must also contain proper access controls, in the case of proprietary data. Significant cultural challenges also exist, most notably the lack of a community-accepted ontology for the communication of materials information. The lack of a common language is driven by the diversity of materials systems. Defining common ontologies would allow researchers from disparate materials fields to more easily communicate across materials problem spaces [48]. Numerous other technical communities such as biology, biomedicine, astronomy, and earth sciences are in various stages of developing and adopting ontologies as a way of fully describing the potential data within a domain. Ontologies provide organization to the concepts in a domain by formally naming and defining the types, properties, and interrelationships of entities. By building these interrelationships through a network graph, the data become interpretable by a computer, allowing complex relationships between data to be discovered. In addition, ontological approaches to data management allow much greater discovery and interoperability between platforms, making traditional rigidly structured databases redundant. As a component of semantic-based technologies, ontologies can be described through a Resource Description Framework (RDF), enabling the concept of “linked data” across a network. AFRL has sponsored development of a semantic tool called MatOnto [49] to tie data, processes, and concepts together. Further investigation of the various applications of semantic database tools and methods will help provide insight into the future direction of this technology.

Lastly, government-sponsored research programs have begun to require development of Data Management Plans (DMP). DMPs are intended to promote good data stewardship during and after a research program by defining the types of data to be generated, the required metadata, and the formats used to capture and transmit data, as well as storage, access, and security strategies and policies. These practices help ensure a program runs smoothly by clearly communicating the why, what, when, who, and how of data and its transfer within a program. Additionally, DMPs can help ensure the long-term preservation of data for reuse in other programs. Furthermore, the practice of presenting valuable digital data through a peer-reviewed journal article, which is already commonplace in some technical disciplines, is gaining traction in materials science and engineering (e.g., Integrating Materials and Manufacturing Innovation, Scientific Data, Data in Brief). The key issues – how technical publications and their supporting research data must be bound together in a rational fashion – that need to be considered as the community develops an approach to data archiving supporting publications, were recently discussed by Ward et al. [50].

MATERIAL INFORMATICS (DATA ANALYTICS)

Performing physics-based analytical models on materials systems is a classic way to apply understanding of materials behavior for the acceleration of design. This approach involves using existing physical understanding or approximation to extract new, useful information concerning materials systems. A complementary method involves deriving new knowledge from the structure of existing information. This approach, which is fueled by the widespread adoption of computational systems, is often termed informatics. This approach to extracting new knowledge about materials represents a new paradigm compared to historical methods, expanding upon the foundation of experiments and physics-based models and simulations [51]. Informatics, due to its nature, involves significant computation and understanding of the theory behind communication of information [51-53].

Advances in networked communications and search algorithms have led to remarkable opportunities for the discovery and sharing of materials data. In particular, increasing the availability and accessibility of high-quality materials data across different length and time scales is an essential requirement for multiscale materials and structural modeling [54]. It is critical to be able to discover, manipulate, mine, manage, analyze, and share scientific and engineering data in an easy and efficient way [55]. Unfortunately, there has been only limited utilization of this data, due to the lack of suitable data repositories [27], standards, and incentives for sharing.

The primary objective of materials data analytics is to extract high-value information (e.g., processing-microstructure-property-performance relationships) from available compilations of materials datasets. This information can be particularly difficult to obtain; for example, a materials microstructure and evolution can span a multitude of length and time scales and have a variety of complex details (e.g., random defects and disorders). As an added complication, microstructural details often only exist as micrograph images, requiring conversion into some form of digital signature in order to use modern image-analysis tools [56]. These conversion methods (i.e., identification of key descriptors) are still an active area of research [57-59]. The reconstructing of full 3D representations from the typical 2D images that most measurement techniques provide is another challenge area. Data analytic and data mining tools and techniques [60] (e.g., noise filtering, uncertainty quantification, patter recognition, regression analysis, and machine learning) exist in various commercial packages as well as software repositories [61-63]. However, adopting/transforming these techniques as well as other big data technologies [64,65] to aggressively interrogate material datasets and the associated material simulation results to glean the required processing-microstructure, microstructure-property relationships will be a major challenge in building the 2040 ecosystem. Kalidindi and De Graef [1] provide a description on how material data corresponds to the five Vs (volume, velocity, variety, veracity, and value) of big data and how practitioners in material data science and informatics can interact with it.

The Materials Data Facility (MDF) provides a flexible data storage and sharing platform with control over content access [66]. While MDF provides a needed function for data sharing, it does not currently extend strongly into data mining for knowledge discovery. The Materials Project is attempting to bridge this gap by providing open-source workflow management for generation and manipulation of materials property data, especially those associated with molecular compound search and discovery [67]. However, the Materials Project is far from spanning the required breadth and scope of multiscale materials and structures modeling. Alternatively, some small businesses, such as Citrine Informatics and selected development aspects of the Granta database system, have also attempted to bridge this gap by providing forward-facing databases that enable materials informatics driven by machine learning [68]. The Citrine approach involves ingesting generally unstructured data, such as patents and publications, and extracting unitary measures [68]. A crucial gap in current approaches is the lack of inclusion of spatially defined materials data (akin to the Google Maps concept). Current implementations for approaching materials informatics generally focus on thermomechanical or structure measurements, such as tensile strength, melting point, or band structure. The spectrum of materials data is generally far broader, however, with significant amounts of data, especially evaluation and inspection data, being spatially located on a part geometry. Finally, it is not currently common practice to upload or access research or industrial data on a decentralized storage network. Since the strength of the informatics framework should scale with the information it ingests, obtaining community involvement is critical.

VISUALIZATION

Data visualization aims to communicate data clearly and effectively through graphical representation. Data visualization techniques are also utilized to discover data relationships that are otherwise not easily observable by looking at raw data. Han et al. [60] review the basic concepts of data visualization and in particular discuss several representative approaches, including pixel-oriented techniques, geometric projection techniques, icon-based techniques, and hierarchical and graph-based techniques.

In consumer markets (internet, video games, and entertainment), technologies are being developed to provide increasingly immersive virtual experiences. Some examples include the advent of WEBGL [69-71], consumer televisions with 3D capabilities [72], holographic and volumetric displays that allow 3D projections from any viewing angle [73], augmented reality applications for mobile devices [74], and user interfaces with voice commands (e.g., Siri and Cortana).

FIGURE 6.2 EXAMPLE OF SOA VISUALIZATION TECHNOLOGY: ESI'S IC.IDO VIRTUAL REALITY SOFTWARE WITH HTC VIVE HEAD-MOUNTED DISPLAY.

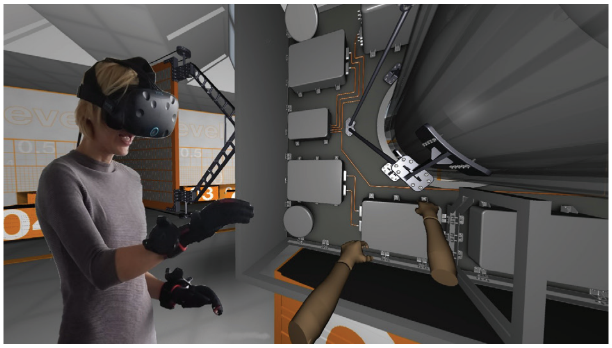


Figure 6.2 shows an example of state-of-the-art visualization technology. Here, an ESI software engineer uses a head-mounted display and virtual reality gloves to evaluate satellite assembly. Many open-source visualization and commercial tools are also available today and play an important role in communicating complex (often high-dimensional) data. Open-source tools such as

- ParaView [75] (and the variant TomViz [76]), Avizo [77], and MeshLab [78], used for interactive exploration of gridded or meshed volumetric data
- Commercial simulation software such as Abaqus [79] and ANSYS [80]
- Analysis software such as MATLAB [63] and Mathematica [81]

have built-in capabilities to generate rich visualizations for volumetric data, as well as a wide array of plots and graphs.

These visualization tools and methods are being embraced by the aerospace design, manufacturing, and maintenance communities, relative to the study of ergonomic aspects of human-machine or human activity assessment. Similarly, research efforts are ongoing to apply visualization tools and methods to system operation, such as the ability of an engineer to enter into the computed flow-path of a turbine engine to visualize geometry, flow, and boundary-layer interactions during a simulated operating condition. The multiscale and multi-dimensional aspects of material, structures, and system design and optimization make it challenging for humans to visualize by historical static snapshots.

The materials community is rapidly embracing 3D structure characterization. Tools, such as DREAM3D [33], are supporting visualization of SERVE and other hierarchical and multimodal data in a concurrent fashion. The hierarchical nature of those tools is expanding as they become more akin to the Google Maps analogy (see Key Element 2, Multiscale Measurement and Characterization Tools and Methods). This approach of representing and visualizing microstructures enables engineers to assess wide ranges of statistically equivalent structures not possible in other methods. These tools are allowing new and extreme microstructures to be visualized and assessed relative to modeled performance.

Data fusion methods are emerging to allow visualization of data from disparate sources and can support zoning or categorizing materials within a component volume with unique combinations of statistically equivalent characteristics. Microstructural analysis in 2D/3D is a crucial part of the current visualization paradigm. Image analysis techniques are necessary to turn 2D/3D information into data that can be used to test or validate microstructure-sensitive models. A multitude of image analysis software codes currently exists, with ImageJ [82] being one of the most common in the materials community, notwithstanding its biology-focused inception. However, one of the greatest challenges is the segmentation of images for any further post-processing because human intervention in the segmentation of 2D/3D images for analysis provides a large source of error and inconsistency. Adaptive image-analysis techniques are only emerging, as characterization methods become higher and higher "resolution." Additionally, multimodal data (e.g., chemical, crystallographic, and structural) collected by multiple detectors with different sampling volumes and inherent distortions poses some unique problems for visualization of materials data that often do not exist in other fields. These challenges limit the current quantitative visualization of materials and their usefulness in the chain of multiscale modeling.

Despite the relative prevalence of advanced dynamic visualization technologies in the consumer market, these technologies have not yet taken hold in the aerospace materials industries, in which analysis and interaction with software technologies is mostly done on two-dimensional displays (e.g., flat monitor screen and part prints). Modern computer-aided design (CAD) systems represent geometries in three dimensions but are still limited by two-dimensional displays. There are opportunities for the materials and structures communities to learn from other engineering disciplines how to visualize materials mechanisms, such as dislocation generation and damage generation as a function of material chemistry, structure, component geometry, and application loading paths.

Computer agents and assistances are in their infancy and will need to be improved, personalized, and standardized by the community. As data is linked, the favored set of commands for data and representation will need to be stored, reviewed, shared, and built upon in an easy to use/reuse way. Agents can be thought of as a detective, gathering information for you and sometimes taking action. Assistances can be thought of as butlers, mostly handling your own things and information.

Harnessing the promise of advanced materials design concepts such as Integrated Computational Materials Engineering requires the design practitioner to be comfortable with manipulating, analyzing, and mining large amounts of material data. Unlike current databases which are largely textual and tabulated, materials databases in the near future will also contain spatial and temporally resolved microstructure information (potentially from multiple imaging modalities), local (spatial) and global property data, thermodynamic data, and metadata detailing the history of the sample, etc. In addition, this is likely to be a blend of experimental characterization and testing as well as modeling and simulation data. Because human designers, unlike machine learning algorithms, are not adept at developing correlations and recognizing patterns in complex, high-dimensional data environments, they will require new visualization tools that can work along with the data science tools to provide abstractions of data that may be viewed in a small number of dimensions (3 spatial plus temporal evolution).

Historic analogues in materials science are thermodynamic abstractions such as phase diagrams, continuous cooling curves, and Ellingham diagrams, as well as the well-known Ashby plots [83] for materials selection. The general idea behind these diagrams is the presentation of multidimensional data projected into some intuitive (with a little training) space defined by key design variables, which allows a designer to explore complex data relationships in a simple visual environment. The challenge in developing general abstractions for future material design applications is the heterogeneous nature of the material data and the extreme dimensionality of the datasets. Unlike the historical examples given above, where the form of the correlation in the data is *a priori* specified by the governing physics and the axes of the diagrams have a physical meaning, we will be relying on correlations developed through machine learning to extract a physical understanding of the system. This presents challenges for visualization, as the tools must be general and flexible while reducing the data down to a small set of essential correlations.

Work in this area is still largely in the nascent stages. Work from Fullwood et al. [84] on microstructure sensitive design advanced the idea of a microstructure design space and a microstructure hull, which spanned the space of possible material states. However, this work was limited to material descriptors that had a well-defined compact spectral representation (such as the generalized spherical harmonic description of crystallographic texture in polycrystalline materials). More recently Sundararaghavan and Zabaras [85-87] and Niezgoda and Kalidindi [88,89] explored dimensionality reduction approaches such as kernel principal component analysis to define a general materials design space, develop property relationships in this space, and visualize microstructure data. Such digital representation of the material microstructure will be a key feature of the 2040 vision ecosystem.

2040 End State

By 2040, automated workflows will feed the data infrastructure, in which pedigree, provenance, and quality metadata is attached to all data. The FAIR principles of data stewardship will be practiced throughout the community, facilitated by community-developed vocabularies, schemata, and ontologies, as well as open data standards and formats, publicly accessible data-translation tools, and modern and open APIs. The infrastructure will accommodate all types of materials (metals, ceramics, polymers, biomaterials, etc.) and composites of each. Mining this wealth of data collected throughout the lifecycle will reveal new materials knowledge. Additionally, data-transfer protocols and encryption technologies will allow visibility and easy sharing without compromising proprietary information.

Visualization of multidimensional data using immersive 3D displays, which can be manipulated with audio commands and motion feedback, will be commonplace. It will be possible to “zoom in and out” to visualize phenomena across scales, such as crack propagation simulation all the way down to the grain scale. Visualization will be more collaborative, allowing engineers and scientists to interact with their data and each other in the same visual space.

Gaps

The following gaps lie within seven of the roadmap's 10 crosscutting streams, with the **Data Analytics and Visualization** stream containing the largest number of gaps. Analyzing and representing data is a major part of this Key Element, and many emerging capabilities need to be incorporated into the modeling and simulation framework. These gaps have the strongest ties to the **traceable**, **accessible,** and **user-friendly** characteristics of the 2040 end state. Accessibility and user-friendliness depend largely on the ease with which people interact with their data, while information traceability is at the heart of an interconnected cyber-physical-social ecosystem.

TABLE 6.1 DATA, INFORMATICS, AND VISUALIZATION GAPS AND IMPACTED 2040 CHARACTERISTICS

AC Accessible **AD** Adaptive **IN** Interoperable **RB** Robust **TR** Traceable **UF** User Friendly ❖ Critical

GAPS	2040 CHARACTERISTICS					
	AC	AD	IN	RB	TR	UF
INFORMATION SHARING AND REUSABILITY						
❖ No widely accepted community standards or schema for materials information storage and communication methods	AC		IN		TR	UF
No consensus on how to define comprehensive material pedigree short of tabular or key-value structures					TR	UF
Insufficient descriptions of materials compositions (e.g., impurity levels, defect evolution)				RB		
Approaches for tracking metadata and data pedigree are not widely available	AC				TR	
Poor data storage, transfer, and retrieval times prevent ability to conduct real-time/remote multiscale visualization			IN		TR	UF
Tool and code obsolescence threatens the integrity of the digital thread • Difficult to ensure old versions are maintained or updated	AC			RB	TR	
DATA ANALYTICS AND VISUALIZATION						
Lack of community-accepted practices or standards for mining and quantifying complex materials information and datasets between experiments and models	AC				TR	UF
Many materials information frameworks are not sufficiently developed for compatibility with state-of-the-art data analysis and management technology			IN	RB	TR	
Human involvement in thresholding and segmentation limits the suitability of 2D/3D/4D images for analysis						UF
Limited ability to capture and represent time dependent data (4D)				RB	TR	UF
Limited ability to represent translucency among multiple layers of data				RB		UF
Deep Learning and Machine Learning (ML) techniques are not implemented across MS&E disciplines, and across length scales				RB		
Workforce not sufficiently trained in data science, machine learning, programming, and analysis • Not yet accepted as vital aspect of materials and structures engineering disciplines	AC					

GAPS	2040 CHARACTERISTICS					
	AC	AD	IN	RB	TR	UF
INFORMATION SHARING AND REUSABILITY						
Need for decentralized, accessible data storage network • Lack of approaches for dealing with data ownership issues (e.g., IP and legal)	✓		✓			
Lack of user-friendly (i.e., user can easily retrieve correct information in correct format at correct time) infrastructure that accommodates linkage between relational and non-relational databases for storing both disparate and wide-ranging material geometries and information types • Lack of sufficient security access controls	✓		✓		✓	✓
Lack of easy access to data precludes the appreciation, use, and adoption of data-driven models (e.g., fast acting surrogates) over physics based models within the materials community • Volume and variety of datasets makes them difficult to move	✓	✓				
MULTIDISCIPLINARY COLLABORATION						
Lack of data/nomenclature translators for more effective interaction between different communities • Limited dissemination of existing translators	✓		✓			
INSTITUTIONAL PARADIGMS						
User-friendly, interactive visualization used in other communities have not yet been adopted in materials science and engineering						✓
BENCHMARKING AND BUSINESS CASE						
No sustained funding or stewardship model for ensuring the continuity of the computing hardware infrastructure (upload, storage, communication, etc. of materials data) within a materials information infrastructure					✓	
Rewards/incentives for better management of data are nearly non-existent					✓	
LINKAGE AND INTEGRATION						
Insufficient inclusion of spatially-defined materials data throughout material lifecycle, including evaluation and inspection data (i.e., spatial location on part geometry)			✓	✓		

Recommended Actions

The following recommended actions lie within seven of the roadmap's 10 crosscutting streams, with the most actions under **Data Management** and **Data Analytics and Reliability.** These recommended actions aim to build an interconnected data and informatics infrastructure through common databases, formats, data management practices, and enhanced visualization capabilities. As with the gaps for this Key Element, the recommended actions have strong ties to the **accessible** and **traceable** characteristics of the 2040 end state.

TABLE 6.2 DATA, INFORMATICS, AND VISUALIZATION RECOMMENDED ACTIONS AND METRICS

FUNDING: $ <0.5M/year $$ 0.5-2M/year $$$ 2-5M/year $$$$ >5M/year

AC Accessible **AD** Adaptive **IN** Interoperable **RB** Robust **TR** Traceable **UF** User Friendly * High Priority

ACTION	2040 CHARACTERISTICS						TIMEFRAME FOR COMPLETION			FUNDING
	AC	AD	IN	RB	TR	UF	NEAR 2017-2022	MID 2022-2035	LONG 2035+	
DATA MANAGEMENT										
* (6.1) Establish schema standards and protocols to enable federated data infrastructure comprising both public and private sources • E.g., open architectures, APIs, semi/unstructured data formats, and microservice development	AC				TR	UF	■	■		$$
* (6.2) Establish/recommend common, open, and adaptive file formats with proper access controls to enable easier data retrieval, sharing, and archival	AC	AD			TR	UF	■	■		$$
(6.3) Define a structured approach to building ontologies, and define common ontologies/semantics to permit communication across materials-related disciplines • Assure the approach represents the spatiotemporal hierarchy innate to materials and structures engineering practices	AC			RB	TR	UF		■		$$
(6.4) Implement standardized data collection modalities for a given metric of interest with bounded uncertainty	AC		IN		TR	UF	■	■		$$
(6.5) Develop tools and templates for guiding the building of robust data management plans	AC				TR	UF	■			$
(6.6) Create a meaningful definition and representation of "pedigree" both structurally and visually	AC				TR		■			$
(6.7) Create a set of benchmark datasets to better define microstructures and facilitate more quantitative results	AC			RB	TR		■	■		$
(6.8) Develop data/nomenclature translators	AC		IN		TR			■		$$

ACTION	2040 CHARACTERISTICS						TIMEFRAME FOR COMPLETION			FUNDING
	AC	AD	IN	RB	TR	UF	NEAR 2017-2022	MID 2022-2035	LONG 2035+	
DATA ANALYTICS AND VISUALIZATION										
✱ (6.9) 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										$$
(6.10) Develop methods to quantify the quality of data										$$
(6.11) Develop adaptive 2D/3D/4D microstructural segmentation techniques to reduce human error and boost quantitative visualization of materials and structures										$$
(6.12) Enhance the accuracy and speed of visualization of unstructured, high dimensional data (e.g., through translucency) to show relationships between multiple layers of data										$$
(6.13) Design immersive 3D displays for increased data interaction • Significant potential in additive manufacturing design										$$
(6.14) Create user-friendly, easy to learn interfaces using the latest in natural user interface technology (voice, gestural, etc.)										$$
(6.15) Develop real-time visualization (e.g., "auto-pilot") for condition-based real-time monitoring of experiments										$$
INFORMATION SHARING AND REUSABILITY										
✱ (6.16) Establish specific community (e.g., academic, government, industry) incentives for contributing data and models to public databases										$$
(6.17) Fill in missing experimental data (basic thermodynamic and kinetic properties)										$$$$
(6.18) Encourage community acceptance of decentralized storage and transfer of materials information										$

ACTION	2040 CHARACTERISTICS						TIMEFRAME FOR COMPLETION			FUNDING
	AC	AD	IN	RB	TR	UF	NEAR 2017-2022	MID 2022-2035	LONG 2035+	
MULTIDISCIPLINARY COLLABORATION										
(6.19) Seek inputs and lessons learned from other communities (e.g., biology, astronomy, etc.) for developing a large-scale cyberinfrastructure	●	●	●	●	●	●	■			$
INSTITUTIONAL PARADIGMS										
* (6.20) Require all NASA contractors, staff, and grantees to engage in best practice data management	●				●		■			$
* (6.21) Teach the current and emerging workforce how to properly interpret information from the materials informatics framework, and integrate the information into the research and design processes			●	●	●		■	■		$$$
INSTITUTIONAL PARADIGMS										
* (6.22) Adopt and increase use of advanced visualization techniques, whether they are physical displays (e.g., powerwalls) or virtual displays (VR or AR headsets) • Demonstrate best-in-class nD techniques and document benefits to build business case for adoption	●						■	■		$$
LINKAGE AND INTEGRATION										
* (6.23) Automate the ingestion and storage of materials lifecycle data • Automatic direct uploading of materials data and associated metadata from characterization equipment and simulations (integrate with equipment and vendor formats)			●		●	●	■	■		$$$
(6.24) Enable the automatic co-registry and co-sampling of hierarchical materials data (to enable fusion of spatiotemporal data) from corresponding topologies to drive correlative analyses			●	●	●		■	■		$$
(6.25) Advance characterization techniques and experimental methods to collect high-throughput experimental data across length and time scales and enable merging of multimodal data for visualization	●	●	●		●		■	■	■	$$$

Relationships with Other Key Elements

Data, Informatics, and Visualization is a broad yet vital Key Element that operates as the focal point for data stewardship, comprehension, and knowledge extraction. This technical area contributes to other Key Elements by focusing on the capture and management of lifecycle data, autonomy of data ingestion methods, ease and security of data transfer, and all efforts that increase the value, maintainability, reusability, interoperability, and accessibility of data.

TABLE 6.3 EXAMPLE INTERRELATIONSHIPS OF KE6 (DATA, INFORMATICS, AND VISUALIZATION) AND OTHER KEY ELEMENTS

Note: Interrelationships among KEs vary. Equal weight should not be inferred.

OTHER KEY ELEMENTS	INTERRELATIONSHIP	THIS KEY ELEMENT
KE1 Models and Methodologies	Define materials structures; enable capture, analysis, and dissemination of all relevant data; and integrate data-driven models via informatics framework	KE6 Data, Informatics, & Visualization
	Provide model-based material hierarchies that define data structures	
KE2 Multiscale Measurement and Characterization Tools and Methods	Provide informatics framework to house characterization and response data to facilitate integration and application of machine learning tools	
	Provide experimental/characterization model-based material hierarchies that define data structures	
KE3 Optimization and Optimization Methodologies	Build common data infrastructure, standardized data formats, and multidimensional visualizations for improved optimization routines	
	Deliver optimization algorithms that retain and expand knowledge of previously solved problems	
KE4 Decision Making and Uncertainty Quantification and Management	Provide automated uncertainty prediction tools and novel visualizations of uncertainty	
	Employ feedback systems to provide data quality markers, substantiate data quality, or identify data generation needs	
KE5 Verification and Validation	Establish minimum requirements, common definitions, and readily accessible high-pedigree datasets for model validation	
	Employ feedback systems to provide data quality markers, substantiate data quality, or identify data generation needs	
KE7 Workflows and Collaboration Frameworks	Provide knowledge capture framework to support data modeling tools for automated workflow data recognition and capture	
	Facilitate cross-organizational/cross-sector low-cost rapid data generation	
KE8 Education and Training	Automate software conversion of formats, provenance, and database building for robust data generation across research instrumentation	
	Offer educational modules in image processing, machine learning, and statistical methods	
KE9 Computational Infrastructure	Incorporate machine learning methods into high-level HPC programming frameworks for hardware interoperability	
	Supply HPC programming tools and frameworks for transferring/accessing large distributed datasets	

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Key Element 7:

Workflows and Collaboration Frameworks

Definition

This Key Element encompasses technologies associated with workflows and collaboration functions.

1 **Workflows** refer to the flow of physical and/or computational activities and associated data/information through a linked string of functions/steps.

- A workflow is a plan or schedule of operational steps to perform an overall activity which informs how and when data, instructions, and input/output requirements must be handed off to subsequent operations. This includes a focus on usability and interoperability requirements toward smooth, seamless operations.

2 **Collaboration frameworks** refer to the flow of information, analysis results, or shared tools between internal or external individuals/organizations.

- Collaboration frameworks are the platforms or organizational structures that help inform human interaction, enable the creation of extended workflows, and help people, groups, and organizations achieve clearly defined outcomes. These frameworks facilitate the integration of models and simulation infrastructure with the performance of experiments, characterization process, and data infrastructures through workflow developments.

Current State of the Art

Role

Workflows and collaboration frameworks are highly interrelated and critical to aerospace discovery, design, and development. Currently, workflow frameworks establish a methodical path for the execution of individual steps toward the accomplishment of a particular task. The task can be of limited complexity—like the execution of a single test or computational activity—or it can be extremely complicated, such as the development of an entire aerospace system. It is useful to consider a workflow framework as a knowledge capture and transfer mechanism that establishes best practices for a particular task. Workflows are critical for physical characterization processes where multiple, complex testing and analysis functions are performed, as well as for computational methods where data, models, and analysis tools are linked together for a specific sequence of operations. Workflows can and should evolve as better processes are discovered and improved tools become available.

Collaboration frameworks define how human capital is organized and establishes the basis for how people, teams, and organizations interact, sometimes including other collaboration tools and practices. Collaboration frameworks today include intra-organizational networks (e.g., design groups, project and product teams) and inter-organizational networks (e.g., government-industry consortia, industry-based consortia, industrial supply chains). The tendency toward formally established collaborative frameworks increases as the scope and complexity of an entity's mission increases. Alternatively, smaller, more focused organizations seeking maximum agility might favor an informal/ad-hoc collaborative framework. A collaboration framework can provide the organizational underpinning for the execution of increasingly complicated workflows.

Summary

WORKFLOWS

Most existing workflows do not encompass the complete development and verification/validation process for a material, system, or subelement. Similarly, many workflows do not integrate computational and physical aspects particularly well. Computational and physical workflows currently support the iterative experimentally intensive workflow for materials development and implementation. Computational workflows, where they exist, are largely limited to individual modeling and analysis tools employed at specific points along the timeline from research to preliminary design, process scale up, detail design, or component/system lifing. Similarly, physical workflows for characterization of materials and manufacturing of components or systems are largely manually developed virtual or hardcopy routers that direct and track the operational steps within a series of operations. Workflows that combine physical (experimental) and computational aspects are not as common but do exist, often within organizational design and engineering practices.

Workflows support identification, tracking, and capture of generated data from each operational step. There are many tools that support automated generation, execution, and tracking of workflows, including commercial and proprietary laboratory information management systems (LIMS), software that facilitates workflows for a particular string of experiment and/or analysis (e.g., LabVIEW [1], SIMULINK [2]), and software that enables linkage of other models and tools (e.g., Isight [3]).

Database and optimization software is being established with certain post-processing workflows embedded into the code functionality, such as the GRANTA MI software suite. Database software companies have recognized the need to link material characterization workflows with data collection and archival activities. These linked functions and the associated pedigree/provenance information are bringing the “no cost of data capture” and “no data loss” goals closer to reality. Many optimization software tools and codes developed for specific model simulation efforts are expanding to include optimization functions as automated internal workflow capabilities.

The generation of effective workflows is often facilitated by the existence of and reference to standards established by professional standards development bodies or government organizations such as ASTM [4], ISO [5], ASME, SIE, NIST, and others. These standards document specific practices, terminology, and more, providing valuable building blocks for complex workflows. Although the majority of these established standards reference physical/experimental procedures, standards that establish computational procedures exist, as do standards that connect physical and computational procedures.

COLLABORATIVE ENVIRONMENTS

Intra-organizational collaboration across design, materials, manufacturing, and quality disciplines within organizations can be readily accomplished today. However, the community has yet to truly recognize the value and benefits from collaboration and the formal linkage of tools and methods. While grassroots collaborative efforts can be quite successful, faster, more meaningful progress is realized when senior leadership recognizes the value of collaborative environments and provides resources and prioritization for these activities. Leadership can advocate for and invest more heavily in collaborative environments when results are demonstrated in a quantitative way. Well-defined demonstration efforts that can demonstrate quantitative business and technical benefits can be quite useful in winning organizational support, while poorly defined or overly ambitious collaboration demonstration efforts can produce ambiguous results or fail entirely.

Incentives are required to encourage sharing of resources, data, and methods among individuals and/or organizations. This incentive is often cost savings from cost-sharing development efforts across consortia. Through collaboration efforts, data, tools, and methods will become available to the members of consortia. The most effective collaborations are found where the targeted topics are pre-competitive or when different organizations partner to take on critical problems that are beyond the resources of any single organization. The benefits from the collaboration of groups of organizations are substantially based on cost sharing from the shared development efforts performed with a collaboration network. There are also other tangible benefits that arise from disparate organizations coming together for a common purpose where one organization is specialized in one element of the collaboration goal and other organizations are specialized in others. There may be proprietary information and intellectual property constraints, but the benefits and ability to collaborate can override these challenges.

Industrial and government-sponsored consortia have been successful in the organization of these collaborations. One notable aerospace example is the Metals Affordability Initiative (MAI). The MAI consortium comprises 16 aerospace original equipment manufacturers (OEMs), component manufacturers, and metals producers. This consortium has achieved a tremendous record of technology transfer and cost-reduction impact. The MAI infrastructure can serve as a model for collaboration of competing entities where project-related experimental and computational data and methods development can be shared. A digital framework for efficient collaboration, called the MAI-Hub, has been developed and deployed successfully within this consortium program and the Vision 2040 end state expects that analogous frameworks will be available throughout aerospace engineering. However, what is not clear at the present time is the longer-term viability and sustainability of such networks, especially for those that span organizations. Just as for the data and informatics infrastructures or the call for open software and model building, there are no established business models or government commitments for sustaining such enterprises.

Technologies are continuing to evolve to support safe and effective collaboration throughout the supply chain, for both hardware (components) and computational collaboration networks. Supply-chain-type collaboration networks that enable transmission and sharing of digital data, tools, and methods are starting to emerge. Historical methods for collaboration within a supply chain were defined by direct human interaction in a "concurrent engineering" approach. Commercial business solutions offered by companies such as SAP and its competitors can offer significant automation for routine supply chain/logistical collaborations. In many organizations, routine purchase of established materials and defined components is entirely automated based on a "demand signal" that is manually triggered or automated, allowing for efficient supply chain collaboration to support systems during their lifecycle. Digital security and protection of intellectual property and sensitive information (e.g., classified, export controlled) are also critical concerns inside collaborative networks. Advanced encryption technologies are readily available (if export controlled), as are permissions frameworks that allow people and systems collaborative access to only appropriate information. Methods to safely share digital information and interact virtually between organizations are emerging and continuing to advance, as evidenced by tools like Vanderbilt-Forge or Semantic Web [6], though there are some limitations based on organization-specific issues of network security relative to IP and export control.

Establishing collaborative environments in which fundamental data can be jointly developed and cost-shared will enable rapid, cost-effective databases that the entire community or set of collaborating organizations (consortium) can use equally. This approach enables competitors, suppliers, and customers to work together in a way that is mutually beneficial and not directly product related or product competitive in nature. One example of an emerging collaborative network relevant to the 2040 roadmap goals is the Center for Materials Processing Data (CMPD). In the CMPD, Worcester Polytechnic Institute (WPI), along with the University of Connecticut, the University of Buffalo, and ASM International, is leading an effort to create a consortium for the generation of materials data required for manufacturing process model development, calibration and validation. Processing-space-relevant data, such as diffusivity, reaction rates, flow stress, viscosity, and thermo-physical properties, is very difficult to generate and locate in the open literature. This unique type of data center will provide a way for organizations to collaborate to generate dynamic data that supports foundational materials models and not final properties for unique proprietary components and product forms. Publishing companies and technical journals are moving toward models of open data with DOI identifiers, though platforms for storing and sharing large datasets have yet to be developed.

COLLABORATION TECHNOLOGIES

A large number of technologies already exist to facilitate collaboration, many of which are used routinely, yet their collaborative value is taken for granted (e-mail, shared calendars, texting, web meetings, social media). Other examples include platforms for multi-user editing of documents (Wikipedia/wikis) and platforms for crowd-sourcing for information (Reddit, Quora, chat groups, etc.) and technology solutions (InnoCentive).

Semantic technologies are another family of emerging approaches that have the potential to dramatically improve the collaboration between humans and machines. Semantic approaches utilize communications frameworks that define entities and their relationships in a way that allows reuse of properly coded information in unanticipated ways, sometimes well beyond the original intended use or purpose. Semantic approaches are particularly powerful because the discovery and reuse can be done by computers working semi-autonomously.

Another emerging collaboration technology relevant to the Vision 2040 scope is multi-user CAD, in which a single computational model can be open and worked on by many engineers from disparate disciplines at the same time. This enabling technology is being applied to next- generation turbine engine designs and has the ability to link multiscale materials and structural models to a single component/system model within a fully digital collaboration environment. This technology, like visualization technology (see Key Element 4), is largely based in multi-user gaming systems, in which game users across the globe can interact at the same time in a single model environment. Over time these technologies should extend across the multiscale systems framework, permitting detailed hierarchical materials and manufacturing information, represented in models, to influence designs (see Case Study 3, Appendix B).

Multi-user CAD will continue to evolve into an environment where design, structures, materials, and manufacturing engineers can simultaneously add discipline-specific models that can be executed in a self-assembling optimization configuration. This system will enable continuous analysis and enhancement of one set of linked models that can then drive the re-application of other linked models. An example may be the linkage of a lifing model to a component parametric solid model. Simultaneously, a materials engineer can attach a model-based material definition and a manufacturing engineer can attach a model-based process definition. Upon execution of a parametric optimization process by a design or systems engineer, the multi-user CAD model will pull from the geometry model, process model, materials model, and structural analysis model to establish the optimal component geometry for the specific objective function. If an engineer modifies any of the attached models, the defined optimization functions can be automatically initiated. This multi-user, multidisciplinary model environment will be fully established and part of daily functions in the year 2040.

There are examples of limited capability inter-organizational infrastructures for collaboration, such as the MAI (Metals Affordability Initiative) MAI-Hub [7]. Inter-organizational collaboration begets additional challenges since protection of IP and linking very different standards of practice add complexity.

2040 End State

Tools will automate the generation, maintenance, and execution of coupled physical and computational workflows to support fast and efficient material characterization and model verification and validation. Workflows will be an integral part of all processes, embedded into the code functionality of information/knowledge management systems and optimization software. Linked workflows will bring the goals of “no cost of data capture” and “no data loss” closer to reality.

Collaboration frameworks will be the standard workspaces that manage the outputs of research, development, and engineering enterprise. These frameworks will leverage and share the collective capabilities and resources within the aerospace community (OEMs, suppliers, government, and academia). They will be fully integrated with informatics and machine-learning tools to facilitate engineering design. Multi-user, multidisciplinary model environments will be fully established with optimization functions that automatically initiate when models are changed.

Gaps

The following gaps lie within six of the roadmap's 10 crosscutting streams, with the **Data Management** stream containing the largest number of gaps, including the most critical gap. Similar to the Data, Informatics, and Visualization Key Element (KE6), improving data management is a major challenge for developing workflows and collaboration frameworks. The proposed gaps have the strongest ties to the **traceable** and **accessible** characteristics of the 2040 end state. Traceability and accessibility are the primary goals of this Key Element, with workflows and collaboration frameworks aiming to connect people, organizations, and the information they need.

TABLE 7.1 WORKFLOWS AND COLLABORATION FRAMEWORKS GAPS AND IMPACTED 2040 CHARACTERISTICS

AC Accessible **AD** Adaptive **IN** Interoperable **RB** Robust **TR** Traceable **UF** User Friendly ❖ Critical

GAPS	2040 CHARACTERISTICS					
	AC	AD	IN	RB	TR	UF
DATA MANAGEMENT						
❖ Lack of open, community/industry standards defining inputs/outputs, needed functionality, data quality, model maturity levels, etc. for smooth operation in the envisioned ecosystem	AC		IN		TR	UF
Limited ability to automate the identification and collection of workflow-generated data (e.g., context-based data tagging and application)			IN		TR	UF
Difficulty in knowing what data is required at different modeling scales	AC	AD			TR	UF
INFORMATION SHARING AND REUSABILITY						
Adoption of collaboration tools is constrained by fear of loss of IP (i.e., typically by the vendor), liability, and/or export controls	AC				TR	
Limited availability of good pedigreed data and models from published journal papers and industry/supplier-focused studies	AC				TR	
MULTIDISCIPLINARY COLLABORATION						
Lack of consistent material data (composition, microstructure, processing, precursor materials, etc.) from material manufacturers	AC		IN		TR	
BENCHMARKING AND BUSINESS CASE						
Insufficient understanding among organizations of ROI for external collaborative network participation	AC					UF
LINKAGE AND INTEGRATION						
Inability to automate the linking and execution of disparate models and computational methods with data from federated databases			IN			
INPUT/OUTPUT CONFIDENCE AND RELIABILITY						
Lack of error handling and failure recovery tools inhibits workflow resiliency				RB	TR	UF

Recommended Actions

The following recommended actions lie within eight of the roadmap's 10 crosscutting streams, with the most actions (including high priority) under the **Data Management** and **Information Sharing and Reusability** streams. These recommended actions deal with improving methods to track data throughout the workflow, while allowing for secure information sharing throughout the product lifecycle and supply chain. The recommended actions have the strongest ties to the **accessible, user-friendly,** and **interoperable** characteristics of the 2040 end state.

TABLE 7.2 WORKFLOWS AND COLLABORATION FRAMEWORKS RECOMMENDED ACTIONS AND METRICS

FUNDING: **$** <0.5M/year **$$** 0.5-2M/year **$$$** 2-5M/year **$$$$** >5M/year

AC Accessible **AD** Adaptive **IN** Interoperable **RB** Robust **TR** Traceable **UF** User Friendly * High Priority

ACTION	2040 CHARACTERISTICS						TIMEFRAME FOR COMPLETION			FUNDING
	AC	AD	IN	RB	TR	UF	NEAR 2017-2022	MID 2022-2035	LONG 2035+	
DATA MANAGEMENT										
* (7.1) Enhance existing ontological and semantic tools and standards and/or create a data modeling technology to support workflow automatic analysis, recognition, and tagging of broad set of materials/workflow datasets		AD	IN		TR	UF	X			$
(7.2) Enable automatic capture and archival of physical and computational process workflow data • E.g., Simulation process data management			IN		TR		X			$
(7.3) Boost traceability and reusability of data through automated pedigree and provenance assignments for various materials data/metadata types • Must be tamper-proof and likely involve revision control and cryptographic technologies	AC				TR	UF	X			$
(7.4) Develop standard APIs and standards for compliant APIs			IN		TR	UF	X			$
(7.5) Develop, enhance, and use interface standards • E.g., functional mockup interfaces					TR	UF	X			$
DATA ANALYTICS AND VISUALIZATION										
(7.6) Incorporate informatics and machine-learning tools into collaboration networks to facilitate engineering design and optimization of collaborative tools and networks	AC	AD	IN			UF	X			$
INFORMATION SHARING AND REUSABILITY										
* (7.7) Develop access controls (built into workflows and collaboration frameworks) to protect vendor data; use specific computations to limit exposure to risks associated with competitive datasets	AC						X			$

ACTION	2040 CHARACTERISTICS						TIMEFRAME FOR COMPLETION			FUNDING
	AC	AD	IN	RB	TR	UF	NEAR 2017-2022	MID 2022-2035	LONG 2035+	
INFORMATION SHARING AND REUSABILITY, CONTINUED										
✱ (7.8) Provide access to modeling codes, data analysis tools, machine learning tools, HPC resources, automated workflow linkage tools, and simulation tools	✓	✓	✓				✓	✓	✓	$$
(7.9) Provide access to example datasets, workflows, and analysis results for initial tool and standard development	✓			✓		✓	✓			$
(7.10) Deliver effective tools for inputting project data into complex models or analyses (as simply as possible)	✓		✓			✓	✓	✓	✓	$$
(7.11) Provide example frameworks for data sharing and trading within collaborative partnerships and markets	✓					✓	✓			$
MULTIDISCIPLINARY COLLABORATION										
✱ (7.12) Establish a collaborative initiative to develop, demonstrate, and deploy automated computational tools that link computational workflows together	✓	✓	✓				✓			$$$$
(7.13) Develop best practices (testing, continuous integration, etc.) for developing and using the collaboration framework	✓		✓			✓		✓		$
(7.14) Establish a collaborative initiative to develop standards for modular architectures to enhance workflow computational tools	✓		✓	✓		✓		✓		$$
INSTITUTIONAL PARADIGMS										
(7.15) Push materials manufacturers to adhere to material data reporting standards (provided by federal agencies, professional organizations, etc.)	✓				✓				✓	$$$
BENCHMARKING AND BUSINESS CASE										
✱ (7.16) Select a few real-world problems from different technical domains to tackle in an open, demonstrational fashion using workflows and collaboration frameworks, and present the ROI metrics to build business case	✓			✓			✓			$$
(7.17) Conduct a benchmarking study and develop an associated analytical tool to quantify the benefits of participating in a collaborative network	✓						✓			$
(7.18) Develop financial analysis tools to support objective analyses of collaboration framework benefits	✓						✓			$

ACTION	2040 CHARACTERISTICS						TIMEFRAME FOR COMPLETION			FUNDING
	AC	AD	IN	RB	TR	UF	NEAR 2017-2022	MID 2022-2035	LONG 2035+	
LINKAGE AND INTEGRATION										
(7.19) Integrate workflow with UQ tools so the workflow is informed by the uncertainty (i.e., feedback loop)										$
(7.20) Enable automatic linking of disparate models and federated databases										$
INPUT/OUTPUT CONFIDENCE AND STABILITY										
(7.21) Develop and implement standards for data quality and model maturity levels										$
(7.22) Develop error management systems										$

Relationships with Other Key Elements

This Key Element focuses on the management and execution of physical and computational activities among Key Elements, across disciplines, and throughout the supply chain. Workflows and collaboration frameworks align with two of the fundamental pillars of ICME: integration of processes and tools and engineering ingenuity.

TABLE 7.3 EXAMPLE INTERRELATIONSHIPS OF KE7 (WORKFLOWS AND COLLABORATION FRAMEWORKS) AND OTHER KEY ELEMENTS

Note: Interrelationships among KEs vary. Equal weight should not be inferred.

OTHER KEY ELEMENTS	INTERRELATIONSHIP	THIS KEY ELEMENT
KE1 Models and Methodologies	Use collaboration frameworks for joint development and validation of models, and automate linking and execution of disparate models	KE7 Workflows & Collaboration Frameworks
	Generate cost-benefit models for collaborative activities	
KE2 Multiscale Measurement and Characterization Tools and Methods	Accelerate materials characterization via automated generation and execution of coupled physical/computational workflows	
	Provide systems-based materials structure paradigms that define local workflow connections	
KE3 Optimization and Optimization Methodologies	Develop interdisciplinary collaboration tools for holistic multiscale systems-level optimization	
	Link design problems for efficient workflow construction	
KE4 Decision Making and Uncertainty Quantification and Management	Employ characterization, uncertainty prediction, and activity-tracking tools for autonomous decision making	
	Streamline automated workflow tools via common standards and protocols for uncertainty quantification, management, and reporting	
KE5 Verification and Validation	Automate workflow tools to incorporate and simplify V&V practices	
	Establish widely accepted V&V standards and protocols to streamline automated workflow tools	
KE6 Data, Informatics, and Visualization	Facilitate cross-organizational/cross-sector low-cost rapid data generation	
	Provide knowledge capture framework to support data modeling tools for automated workflow data recognition and capture	
KE8 Education and Training	Provide advanced university instrumentation with collaborative frameworks for materials data sharing and virtual materials processing	
	Deliver systems-based training in computational tools and methods, and interdisciplinary programs/degrees	
KE9 Computational Infrastructure	Supply HPC-ready multiscale collaboration frameworks	
	Enable simultaneous access for global collaboration via high bandwidth networks and software platforms	

References

[1] LabVIEW - http://www.ni.com/en-us/shop/labview.html, accessed November 30, 2017.

[2] SIMULINK - https://www.mathworks.com/products/simulink.html, accessed November 30, 2017

[3] Isight - https://www.3ds.com/products-services/simulia/products/isight-simulia-execution-engine/, accessed November 30, 2017.

[4] ASTM F2996 - 13 Standard Practice for Finite Element Analysis (FEA) of Non-Modular Metallic Orthopaedic Hip Femoral Stems.

[5] ISO 7206-4:2010 - Implants for surgery -- Partial and total hip joint prostheses -- Part 4: Determination of endurance properties and performance of stemmed femoral components.

[6] T. Berners-Lee, et al., *The Semantic Web: A new form of Web content that is meaningful to computers will unleash a revolution of new possibilities* Scientific American, May 2001.

[7] Naik, R. A. “Metals Affordability Initiative (MAI),” Private communication, Pratt & Whitney, 2016.

Key Element 8:

Education and Training

Definition

This Key Element encompasses 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.

1 Seamless linkages and common language between disparate engineering disciplines through multidisciplinary teams and systems-oriented approaches to integrated, multiscale materials and structures modeling/engineering

2 Acquiring fundamental science and engineering knowledge and multidisciplinary core competencies such as critical thinking, gap identification, and decision making to name a few

3 Building understanding of current and emerging computational methods, modern coding practices and experience, collaborative development and version control, quality assurance practices, image processing, data and machine learning tools, statistical methods, and familiarity with standard software packages used by industry

4 Identifying and defining industry-relevant skills and certification requirements for performing specific job functions and bridging across disciplines (e.g., experimentation and simulation) to develop the existing workforce

Current State of the Art

Role

The role of education and training is to prepare the workforce with the fundamental engineering and scientific knowledge, computational skills, and experimental testing experience for the discovery, design, and development of materials, structures, and systems. In addition to technical knowledge and skills, the current work environment requires multidisciplinary teamwork; therefore, education and training must also prepare the workforce to communicate and effectively collaborate with teammates from disparate disciplines. To better prepare students for the workforce, current engineering education paradigms are increasingly moving away from traditional lecture-based learning and toward experience-based learning. The experiential learning approach focuses on providing students hands-on training in applying concepts to real-world applications and results in improved understanding and retention of new material. Through teaching techniques and methods such as flipped classrooms, multidisciplinary senior design projects, and undergraduate research, education and training is trending towards an immersive experience learning environment in which students from varying majors and concentration areas work together to solve problems, create and test designs, and analyze results using the software, first principle methods, and experimental testing techniques used in the workplace. Additionally, education does not end at graduation. Given the rapid advancement of technology, lifelong learning via training throughout an entire career is essential to maintaining a workforce that is prepared to solve emerging challenges.

Summary

UNDERGRADUATE LEVEL

Over the past few decades, unlike many other engineering disciplines, the undergraduate curriculum in materials has undergone significant evolution as the field broadened from its origins in metals and ceramics to include electronic and photonic, magnetic, macromolecular, biological, soft matter, and other classes of functional materials (e.g., sensors, smart materials, coatings, shape memory alloys). This historical trend for continued evolution is promising from the point of view that modified sets of skills and perspectives are a familiar element of the materials field. Most curricula consist of core courses that cover the fundamentals of materials science and engineering across materials classes, including structure, properties, processing, and performance. Specialty classes on individual material types (e.g., metals, ceramics, polymers, semiconductors) come later in the curriculum.

The addition of new topics in any curriculum requires displacement of others. For example, the classical quantum mechanics course, often taught by physics departments for engineering students, has been replaced by a course on electronic materials in many U.S. departments, with some loss of mathematical depth. The classic first-year chemistry course has in many programs been replaced with a “materials chemistry” course, making the chemistry content more materials relevant. Senior capstone design courses with a significant component of communication are now a requirement that has displaced the senior research thesis. There are notable efforts to integrate computation into the curriculum in the context of design and the capstone course [1], but these are not yet pervasive. Further, there is some sense that the need for software and data skills at the undergraduate level is growing, although the degree to which this needs to affect curricula and the means by which to do so remain unclear.

Undergraduate programs are subject to accreditation by the Accreditation Board for Engineering and Technology (ABET) in a process that matches objectives and outcomes with course content. Major curriculum change is slow and difficult, not only due to accreditation but also because changes require a four-year time period for a single class of students to complete before the first impact data can be gathered. Because aspects of this may affect realization of the Vision 2040 end state, alternative educational schemes need to be evaluated.

There are typically several technical electives in most undergraduate materials programs in which new computationally oriented courses may be implemented. Until very recently, textbooks appropriate for upper-division undergraduate or introductory graduate computational materials science and engineering courses have been completely lacking. Some textbooks are beginning to emerge; for example, a recent book [2] used in a number of programs is organized to cover the following topics: electronic structure methods, interatomic potentials, molecular dynamics, the Monte Carlo method, random walks, kinetic Monte Carlo, cellular automata, phase field methods, and mesoscale dynamics. The emphasis is on basic principles rather than commercial packages that employ these approaches for solving materials problems.

Given the lack of space in the undergraduate curriculum, new topics in computation, data, and instrumentation are most easily implemented through integration with existing core topics. For example, it is increasingly common that CALPHAD-type software and calculations on phase equilibria are integrated with courses on thermodynamics [1]. Figure 8.1 reports the results of a 2008 survey of a large number of universities (mostly in the United States) on the software packages used in undergraduate programs [3], and a small survey at Pratt & Whitney in 2016. Examinations of analogous data from across the multiscale engineering domain would be fruitful for not only updating the data but also providing indicators of the rate of change and commonality of tools across the design-materials and manufacturing enterprise.

FIGURE 8.1 EXAMPLES OF REPORTED PACKAGES USED IN UNDERGRADUATE ENGINEERING AND MATERIALS-FOCUSED EDUCATION

SOFTWARE CATEGORIES	EXAMPLE PACKAGES	MATERIALS-FOCUSED	MECHANICAL/ AEROSPACE ENGINEERING	REFERENCE
CAD	SolidWorks	●	●	http://www.Solidworks.com/
	Inventor		●	http://www.autodesk.com/products/inventor/overview
Computational Thermodynamics	Thermo-Calc	●		http://www.thermocalc.com
Crystallography	CaRine	●		http://pagespro-orange.fr/carine.crystallography/
Density Functional Theory	ABINIT	●		http://www.abinit.org
	PWSCF	●		http://www.pwscf.org/home.htm
	VASP	●		http://crns.mpi.univie.ac.at/vasp
Finite Element	ANSYS		●	http://www.ansys.com/
	ABAQUS		●	https://www.3ds.com/products-services/simulia/products/abaqus/
	LS-DYNA		●	http://www.lstc.com/products/ls-dyna
	Marc		●	http://www.mscsoftware.com/product/marc
High-Level Programming Language	MATLAB	●	●	http://www.mathworks.com/
	Python		●	http://www.python.org/
Materials Properties	CES Materials Sector	●		http://www.granatadesign.com/products/ces
Molecular Dynamics	LAMMPS	●		http://lammps.sandia.gov/
	NAMD	●		http://www.ks.uiuc.edu/research/namd
Quantum Chemistry	Gaussian	●		http://www.gaussian.com
Spreadsheet	Excel	●	●	http://office.microsoft.com/excel
Symbolic Mathematics	Mathematica	●	●	http://www.wolfram.com
	MathCAD		●	http://www.ptc.com/engineering-math-software/mathcad
Visualization (data)	Minitab	●		http://www.minitab.com
	JMP		●	http://www.jmp.com/en_us/software.html

GRADUATE LEVEL

Given the scope of potential topics in the areas of modeling and simulation, uncertainty quantification, data, informatics, and optimization, M.S. degrees with an emphasis in these areas may be a better approach. A certificate with an ICME emphasis within an M.S. program has recently been established [4] that requires five units of core courses (Analytical and Statistical Thermodynamics, Phase Transformations, Materials Design, Computational Materials, and an ICME seminar) plus seven units of electives; to date only two or three students per year have elected to pursue this academic track. If such certificates are oriented more toward manufacturing or to structures design and mechanics, both integral to ICME, the participation would be higher. Also, if one introduced topics such as data analytics/informatics, image processing, etc., the participation may be higher from further interdisciplinary activities.

At the graduate level, many Ph.D. programs admit cohorts of graduate students, more than 50% of whom hold undergraduate degrees in other fields (e.g., physics; chemistry; and electrical, mechanical, chemical, or biomedical engineering [5]). Most graduate programs have core courses at the graduate level that cover the fundamentals of (1) bonding and structure, (2) thermodynamics, and (3) kinetics. Beyond the core courses there is much greater flexibility for the design and implementation of courses that address more specialized aspects of materials modeling and simulation, though these courses compete with specialty courses on specific classes of materials often of interest to students who have already decided on a career path. Courses on computational materials science and engineering, data, optimization, statistics, or uncertainty quantification at the graduate level are often developed by faculty whose research programs have specific needs in these areas. However, the overriding requirement that all courses in the undergraduate curriculum be offered every year often leaves little time for faculty to teach specialized graduate courses.

To identify historical trends in materials science and engineering education, Banerjee and Briber [6] conducted an analysis of the educational background of MSE faculty a function of hire date in their most current position.

External driving forces, such as the Materials Genome Initiative, have motivated the development of an improved infrastructure for integration of theory, simulation, and experimentation at all length scales. This infrastructure largely appears through the research enterprise, through interdisciplinary collaborative programs. For example, the National Science Foundation has recently developed an initiative known as DMREF: Designing Materials to Revolutionize and Engineer our Future. This program addresses the entire spectrum of materials classes and supports collaborative research groups of three to five faculty members, along with similar numbers of graduate students, with the requirement that the research be conducted with a rapid feedback loop between new experimental approaches and new theory/computation. At the graduate level, newly developed tools and codes permeate across research groups as students realize the value of new tools to their own research problems. Emerging software repositories such as GitHub and NanoHub facilitate the propagation of new computational tools.

SPECIALIZED TRAINING/COURSES

In recent years, a wide variety of "summer schools" (e.g., NSF Summer Institute on Nanomechanics, Nanomaterials, and Micro/Nanomanufacturing [7]) have been developed to impart more specialized skills to students and, in some cases, industry personnel. Summer schools are typically two-week sessions with 30 – 60 attendees that combine lectures (for theory) with hands-on instruction in a focused topical area. Examples of summer schools that have been conducted with NSF support from the International Materials Institutes program (recently terminated) include [8]

1. Materials in 3D: Modeling and Imaging at Multiple Length Scales
2. First Principles Calculations for Condensed Matter and Nanoscience
3. Materials and Structures for Hypersonic Flight
4. Techniques of Surface Sciences and Catalysis Nanomaterials
5. Inorganic Materials for Energy Conversion, Storage, and Conservation

6 Computational Materials Science

7 Charged Systems and Solid/Liquid Interfaces

8 Soft Computational Physics and Materials Science: Total Energy and Force Methods

9 Thermal Conductivity and Related Transport Properties of Oxides

10 Materials Modeling from First Principles: Theory and Practice

11 Nanoscale Sciences of Biological Interfaces, Architecture Multifunctional Materials and Structures

12 Material Interfaces and Integrated Computational Materials Education (ICME).

These workshops are largely aimed at senior graduate students, postdoctoral researchers, and junior professionals. Lecturers at the workshops are typically a mix of senior personnel from academia, industry, and government laboratories. In addition to imparting basic skills, these summer schools have the added benefit of developing long-lasting professional networks and collaborations on specific topics [9]. Because no central repository exists for the tools that have been developed for these summer schools, a combined summer school/educational tool development program represents a significant opportunity for the future, enabling web-based delivery of educational modules that have undergone testing in a training environment.

Another area to address includes the training of the current workforce in the aerospace industry. In addition to the aforementioned schools and training sessions, on-site training is often employed by industry to bring advent methods into the workflow. Such training sessions can be days or weeks in duration, covering topics such as process control Six Sigma tools and commercial ICME toolsets (e.g., Thermo-Calc, DEFORM, ProCAST). Such training sessions may cover the basic utilizations of tools into a standard engineering workflow and case studies. Often, experts of such tools in the engineering organizations will aid in the long-term training and troubleshooting of the tools for other employees in the organization.

Continuing education programs for employees in the engineering and scientific workplace is another option that supports long-term education of novel fields of research and tool development. Larger engineering organizations often incentivize the workforce to take additional graduate professional degrees to advance their careers and benefit the organization as well. These degrees are, in most cases, delivered via novel distance-learning tools using custom online software written for specific universities. As an example, with the recent inception of data analytics, machine learning, and advanced algorithms, many engineers in various organizations are enrolling in such programs utilizing their employee benefits of continuing education. Trends such as this will bring an enclave of new tools to aid in the development of the next generation of aerospace products.

INSTRUMENTATION

At the graduate level, materials instrumentation is a key element of the research training mission. Specialized imaging systems (transmission and scanning electron microscopes, atom probes, atomic force microscopes, NMR systems), X-ray systems (including tomography capabilities), material property measurement systems (SQUIDs, mechanical test systems, electrical probes and DMMA), to name only a few, play a central role in the research mission. Students often learn the theory relevant to these systems in graduate courses but also receive “hands-on” training by faculty and technical staff. Because there is rarely any systematic storage or annotation of data from these systems, the raw data from these instruments is effectively lost once students graduate. Advanced instrumentation is both developed by faculty and students and acquired at great expense from equipment manufacturers. Because the instruments are often maintained by expert technical staff, the user base often extends beyond local university users to industry and other academic collaborators. Industry-university collaborative research programs are often motivated by the unique instrumentation capabilities; this is cost effective for industry, as their internal R&D programs cannot justify the long-term expense of housing specialized instruments or supporting the staff to operate them. At present, the cost of acquiring and maintaining advanced materials instrumentation continues to rise at the same time that federal support for instrumentation is rapidly declining.

Internationally, the emergence of multiple synchrotron facilities also highlights a trend toward centralization of instruments. Use of these facilities requires that investigators identify resources for travel to access these opportunities.

2040 End State

By 2040, the workforce will consist of systems-level thinkers, having strong foundations of interdisciplinary fundamentals. Graduating students will have had exposure to “industry-standard” software packages and will be trained to use advanced instrumentation along with data acquisition, processing, and analysis skills. Students will also have access to advanced computational resources via the cloud or other future modes of computing. The workforce as a whole will have a high level of expertise in basic computational methods, image processing, data and machine learning tools, and statistical methods. Workers will be equipped with the understanding to tackle problems at all length and time scales, using any class of existing or newly created material.

Gaps

The following gaps lie within six of the roadmap's 10 crosscutting streams, with the **Institutional Paradigms** stream containing the majority of gaps including the most critical. Creating an educational and training system to supply skilled workers that meet the needs of the future requires making changes to well-established academic institutions. Shifting such a paradigm is no easy task and stands as the largest challenge for this Key Element. The gaps below have the strongest tie to the **accessible** characteristic of the 2040 end state. The cyber-physical-social ecosystem of 2040 will need to be much more accessible than it is today, which starts with adequately training and educating the workforce.

TABLE 8.1 EDUCATION AND TRAINING GAPS AND IMPACTED 2040 CHARACTERISTICS

AC Accessible **AD** Adaptive **IN** Interoperable **RB** Robust **TR** Traceable **UF** User Friendly ❖ Critical

GAPS	2040 CHARACTERISTICS					
	AC	AD	IN	RB	TR	UF
DATA MANAGEMENT						
Substantial discrepancies in the use of key definitions, terminologies, and taxonomies by professionals that employ multiscale modeling and simulation across disciplines • E.g., Physics-based model versus computer simulation model; machine learning versus advanced analytics versus data-driven predictive models	AC					UF
DATA ANALYTICS AND VISUALIZATION						
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	AC					
MULTIDISCIPLINARY COLLABORATION						
Experimental capabilities are highly varied throughout the supply chain, leading to variations in the quality of experiments conducted	AC		IN			
Academic researchers and modeling practitioners do not make effective use of open access data and data sharing • Limited use of collaborative environments (e.g., social networks) to share or disseminate data/practices • Prevents routine use of verification, validation, and benchmarking	AC				TR	
INSTITUTIONAL PARADIGMS						
❖ Education/training does not bridge the gap between "essential" or "fundamental" knowledge and industrially relevant skills • Students lack a complete understanding of the limitations, assumptions, and accuracy level of modeling results when learning how to use software and computational approaches	AC			RB		
Lack of coordination for developing new multidisciplinary graduate-level programs and incorporating multiscale materials engineering into traditional materials disciplines				RB		
No consensus among university faculty regarding the best/appropriate commercially-relevant simulation techniques to teach students how to apply basic computational methods	AC			RB		

GAPS	2040 CHARACTERISTICS					
	AC	AD	IN	RB	TR	UF
INSTITUTIONAL PARADIGMS, CONTINUED						
New courses—including textbooks and computational/data modules—are expensive, difficult to integrate with existing courses, and too community- or sector-specific • Software licensing costs are prohibitive despite academic discounts						
University instruments (e.g., characterization equipment) are often proprietary and inaccessible outside of specific research groups due to a lack of investments in common/standard equipment and codes • Instruments lack common data formats, taxonomies, and metadata structures						
BENCHMARKING AND BUSINESS CASE						
Insufficient business case and/or communication of the educational benefits of multiscale modeling and simulation on competitiveness and career development • Lack of incentives/investment in computationally-focused programs						
BEHAVIOR OF MATERIALS AND STRUCTURES						
Current theories and methods for connecting microstructure and properties of structural materials (to each other and to models) are too phenomenological and empirical • Prevents realization of model-based infrastructure for materials discovery, development, and design						

Recommended Actions

The following recommended actions lie within eight of the roadmap's 10 crosscutting streams, with the most actions (including two high-priority actions) falling under the **Multidisciplinary Collaboration** and **Institutional Paradigms** streams. The only way to enact system-level change in education and training institutions is to bring together experts and stakeholders from various disciplines across industry, academia, and government. Many of these actions focus on developing educational programs tailored to the multidisciplinary skills required in the future multiscale modeling and simulation ecosystem. The recommended actions tie strongly to the **accessible** and **robust** characteristics of the 2040 end state.

TABLE 8.2: EDUCATION AND TRAINING RECOMMENDED ACTIONS AND METRICS

FUNDING: $ <0.5M/year $$ 0.5-2M/year $$$ 2-5M/year $$$$ >5M/year

AC Accessible **AD** Adaptive **IN** Interoperable **RB** Robust **TR** Traceable **UF** User Friendly ✱ High Priority

ACTION	2040 CHARACTERISTICS						TIMEFRAME FOR COMPLETION			FUNDING
	AC	AD	IN	RB	TR	UF	NEAR 2017-2022	MID 2022-2035	LONG 2035+	
DATA MANAGEMENT										
✱ (8.1) 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	AC			RB	TR		■	■	■	$
(8.2) 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	AC			RB	TR		■	■		$
INFORMATION SHARING AND REUSABILITY										
(8.3) Promote use of high quality open source tools as a low-cost alternative to using expensive software suites to teach code writing and computational approaches • Begin with well-documented open source codes to permit faster adoption	AC	AD					■	■		$
(8.4) Launch a portal to aggregate and share university research codes, allowing industry to select codes of interest for transition into commercial software packages	AC				TR		■	■		$$
MULTIDISCIPLINARY COLLABORATION										
✱ (8.5) Foster multidisciplinary classroom activities/ programs (e.g., senior design projects) to help students transition into the workforce and operate effectively across fields/disciplines • Coordinate a small focus group among major universities to identify key interdisciplinary subjects with respect to critically needed competencies in the multiscale modeling and simulation community • Assess the required disciplines that comprise multiscale materials systems (physics, chemistry, materials, etc.) and study their interactions before developing programs and curricula	AC		IN	RB			■	■		$

ACTION	2040 CHARACTERISTICS AC	AD	IN	RB	TR	UF	TIMEFRAME FOR COMPLETION NEAR 2017-2022	MID 2022-2035	LONG 2035+	FUNDING
MULTIDISCIPLINARY COLLABORATION, CONTINUED										
✱ (8.6) Foster academia-industry-national lab partnerships to facilitate student learning opportunities and provide access to equipment, resources, and facilities • Various length internships, coordinated senior design projects, research programs, etc.	●			●			■	■	■	$
(8.7) Create modularized online learning tools and remote/distance learning programs that provide concise courses/training opportunities in multiscale modeling and simulation approaches (e.g., Massive Open Online Courses [MOOCs]) • Develop virtual collaborative learning communities (e.g., through cloud technology combined with technical-social networks)	●			●		●	■	■		$$
(8.8) Coordinate with industry partners to provide prototypical test data (e.g., from outdated/retired programs) to teach students how to use experimental datasets to validate models	●				●		■	■		$
INSTITUTIONAL PARADIGMS										
✱ (8.9) Examine novel approaches to educating effective engineers and fostering competencies in: • Continuous/lifelong learning • Speculation and innovation • Critical thinking • Decision making and management of complexity and uncertainty	●		●	●			■	■		$
(8.10) Develop forward-thinking educational modules that teach the impact of information technology, computational science, and communication technology in terms of the future workforce needs/expectations • Need to convey expectations of future working environments to prepare graduates (e.g., integration of cyber-physical-social systems)	●		●	●			■	■	■	$
(8.11) Promote awareness of materials science and mechanics of materials subject areas as critically important to career development for students in aerospace and other engineering programs	●		●	●			■	■	■	$
(8.12) Organize formal training events for employees on emerging technologies (equipment, software, programming languages, etc.) • Dedicate resources for university professors and government lab researchers to host short workforce training visits	●			●			■			$$

ACTION	2040 CHARACTERISTICS AC	AD	IN	RB	TR	UF	TIMEFRAME FOR COMPLETION NEAR 2017-2022	MID 2022-2035	LONG 2035+	FUNDING
BENCHMARKING AND BUSINESS CASE										
(8.13) Conduct feasibility study to ascertain pathways for new interdisciplinary programs, engineering degrees, and certificates • Solicit feedback from industry on the content and quality of educational curricula and programs to increase the number of well-trained graduates • Disseminate survey to benchmark industry needs and generate interest										$
SCALABILITY AND COMPUTATIONAL EFFICIENCY										
(8.14) Identify new certification programs/tracks to teach industry-relevant computational approaches										$
LINKAGE AND INTEGRATION										
✱ (8.15) Develop a comprehensive course/curriculum on concurrent design of physical and computational experimental methods • Teach methods for multiple length and time scales • Develop courses for multiple scientific/engineering subjects										$
BEHAVIOR OF MATERIALS AND STRUCTURES										
✱ (8.16) Create educational simulation tools with strong theoretical foundations to teach students in methodologies for predicting properties of structural materials with known microstructures • Example topics include: cracking, dislocation accumulation, complex properties such as fracture, yielding, fatigue, corrosion, stress corrosion cracking, oxidation, etc.										$$

Relationships with Other Key Elements

The future ecosystem requires aggressive advancement over the next 25 years to accommodate a considerably different set of skills compared with today's materials and structures engineers, including computational methods, machine learning tools, statistical methods, and image processing. Education and Training will encapsulate critical technological and cultural transformations across the Key Elements to drive curricula change, novel training opportunities, and targeted instrumentation development to help address industry-relevant issues and launch the next generation of modeling and simulation.

TABLE 8.3 EXAMPLE INTERRELATIONSHIPS OF KE8 (EDUCATION AND TRAINING) AND OTHER KEY ELEMENTS
Note: Interrelationships among KEs vary. Equal weight should not be inferred.

OTHER KEY ELEMENTS	INTERRELATIONSHIP	THIS KEY ELEMENT
KE1 Models and Methodologies	Develop and deploy educational modules for multiscale/multiphysics computational methods, industry-relevant ICME models, and methods for government regulator acceptance of ICME approaches Produce multiscale modeling educational platforms, and translation of academic models with interoperability and user-friendly interfaces	KE8 Education & Training
KE2 Multiscale Measurement and Characterization Tools and Methods	Translate systems-based characterization for models approach for classroom curricula and laboratory courses Develop in-line data analysis and reconstruction methods for efficient use of experimental/characterization instruments	
KE3 Optimization and Optimization Methodologies	Create clear education and training modules incorporating best practices in optimization at university and industry level Establish industry criteria and benchmark problems to explicitly describe optimal designs	
KE4 Decision Making and Uncertainty Quantification and Management	Train graduates in probabilistic methods for uncertainty quantification and propagation Offer academic courses at V&V experimental testing and evaluation facilities	
KE5 Verification and Validation	Increase total graduates trained in ICME model validation Offer academic courses at V&V experimental testing and evaluation facilities	
KE6 Data, Informatics, and Visualization	Offer educational modules in image processing, machine learning, and statistical methods Automate software conversion of formats, provenance, and database building for robust data generation across research instrumentation	
KE7 Workflows and Collaboration Frameworks	Deliver systems-based training in computational tools and methods, and interdisciplinary programs/degrees Provide advanced university instrumentation with collaborative frameworks for materials data sharing and virtual materials processing	
KE9 Computational Infrastructure	Build industry-relevant competencies in characterization and simulation code design for current and future computational infrastructure Increase access to government lab HPC resources	

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Key Element 9:

Computational Infrastructure

Definition

This Key Element encompasses the following topics:

1. Computer hardware (storage, CPU, co-processors, memory, backplane), firmware, code base, operating systems, middleware, application software, and the interoperability of these components that enable the numerical simulation of physical phenomena in ways that are useful for engineering purposes
2. High-bandwidth networks and software platforms to support simultaneous access to enable global collaborative engineering
3. HPC architectures and frameworks that use parallel/distributed, neuromorphic, quantum, cloud, machine learning, etc., processing approaches to solve large scale, computationally and data-intensive analysis and/or optimization problems

Current State of the Art

Role

Computational infrastructure is the computer hardware and software ecosystem that enables the numerical simulation of physical phenomena in a way that is useful for engineering purposes. Global collaborative engineering requires high-bandwidth networks and software platforms to support simultaneous access, large data transfer, and management of real and virtual data across geographically disparate organizations.

For ICME to be widely accepted, validated modeling tools will require a degree of fidelity that is beyond the capacity of the current computational resources available to most companies. It is generally expected that the evolution of hardware will enable widespread access to exascale or exa-FLOPS (10^{18} flops) computing by 2040. This is likely to be accomplished with massive parallelization and potentially quantum computing. Simulation software will have to be highly scalable and adaptable to take advantage of this hardware.

Summary

HPC PROGRAMMING TOOLS/FRAMEWORKS

Simulation software is based upon a variety of numerical models of physical phenomena, and is thus related strongly to the Models and Methodologies Key Element (KE1). Modeling codes and suites of the future must be programmed to enable them to adapt to the ever-changing simulation environments. Yet today, only a few modeling codes take advantage of current HPC architectures as there is already a lag between the implementation of multiscale models and simulation infrastructure (see Figure 9.1 for description of five available programming languages/tools).

There are efforts underway at a number of national labs, universities, and companies to develop a higher-level HPC programming language that would automatically take care of the lower-level message passing and multi-threading issues (see Figure 9.2). This approach would free up scientists and engineers to focus on the physics they are trying to model rather than dealing with the often complex coding required to achieve high performance on heterogeneous computing systems. It would also save software companies an enormous amount of development time trying to adapt their codes to changing computer architectures.

FIGURE 9.1 EXAMPLES OF HPC PROGRAMMING TOOLS AND LANGUAGES

PROGRAMMING TOOL	DESCRIPTION
OpenMPI	An open source Message Passing Interface for distributed memory processing (DMP) software [1].
OpenMP	A standard set of compiler directives, or pragmas, for controlling multi-threading, used in shared memory processing (SMP) [2].
OpenACC	A standard set of compiler directives and functions for accessing accelerators, such as the Nvidia Tesla or Intel Xeon Phi. This is likely to be merged with OpenMP [3].
CUDA	A platform consisting of compiler directives and libraries developed by Nvidia to give access to the computing potential of GPU accelerators, like Tesla [4].
OpenCL	Open Computing Language is a programming framework, originated by Apple, to develop code for operating on heterogeneous systems of CPUs and accelerators [5].
CHAPEL, Cray	CHAPEL is an open source parallel programming language that originated at Cray while working on the DARPA funded High Productivity Computing Systems program, from 2002 to 2012. It is designed to support any parallel paradigm, such as data parallelism or task parallelism, on any parallel hardware, including accelerators [6,7].
Cilk Plus, Intel	Cilk was originally developed at MIT and then commercialized as Cilk++ by Cilk Arts. It is now developed by Intel with the name of Cilk Plus. It is an extension to C/C++ that supports efficient multi-threading (SMP) and vectorization [8,9].
Apache Spark, UC Berkeley	Apache Spark is an API for developing applications with data parallelism on clusters. The original impetus was for machine learning and big data analytics. It is being investigated now for managing data movement in HPC simulation software [10,11].

FIGURE 9.2 EXAMPLES OF HPC FRAMEWORKS

PROGRAMMING TOOL	DESCRIPTION
Trilinos Project, Sandia National Lab	The Trilinos Project encompasses a number of tools and libraries for facilitating the development of parallel capable engineering and scientific programs [12].
	Teuchos "Provides a suite of common tools for many Trilinos packages. These tools include memory management classes such as "smart" pointers and arrays, "parameter lists" for communicating hierarchical lists of parameters between library or application layers, templated wrappers for the BLAS and LAPACK, XML parsers, and other utilities." [13]
	Kokkos "Provides compile time polymorphism via template metaprogramming techniques. Kokkos provides multidimensional array containers, and a set of execution patterns that can operate on these array containers to perform parallel_for, parallel_reduce, and parallel_scan." [14,15] The Kokkos package has a "shared-memory parallel programming model for data structures and computational kernels" which works with OpenMP, POSIX Threads, and CUDA [16].
	Epetra "Provides the fundamental construction routines and services function that are required for serial and parallel linear algebra libraries. Epetra provides the underlying foundation for all Trilinos solvers." [17]
	Tpetra "Implements linear algebra objects. These include sparse graphs, sparse matrices, and dense vectors. Many Trilinos packages and applications produce, modify, or consume Tpetra's linear algebra objects, or depend on Tpetra's parallel data redistribution facilities." [16]

RAJA, Lawrence Livermore National Lab	"Defines a systematic loop encapsulation paradigm that helps insulate application developers from implementation details associated with software and hardware platform choices. Such details include: non-portable compiler and platform-specific directives, parallel programming model usage and constraints, and hardware-specific data management." [18] "No existing programming model is a clear 'best choice' for all architecture considerations. Moreover, each model has unique programming characteristics and models are not easily interchangeable. Yet, interchangeability is necessary to manage performance portability. RAJA enables the use of different programming models in an application without exposing their idiosyncrasies to application scientists and without requiring multiple versions of computational kernels to be coded to different models." [19]
CHARM++, University of Illinois Urbana-Champaign	"Charm++ is a machine independent parallel programming system. Programs written using this system will run unchanged on MIMD machines with or without a shared memory. It provides high-level mechanisms and strategies to facilitate the task of developing even highly complex parallel applications. Charm++ programs are written in C++ with a few library calls and an interface description language for publishing Charm++ objects. Charm++ supports multiple inheritance, late bindings, and polymorphism." [20]
LEGION, Stanford, LLNL, Nvidia	"Legion is a data-centric programming model for writing high-performance applications for distributed heterogeneous architectures." "Legion provides abstractions for programmers to explicitly declare properties of program data including organization, partitioning, privileges, and coherence." "By understanding the structure of program data and how it is used, Legion can implicitly extract parallelism and issue the necessary data movement operations in accordance with the application-specified data properties, thereby removing a significant burden from the programmer." [21]

The National Strategic Computing Initiative (see Figure 9.3 for list of participants) was launched in July 2015 with the objectives of accelerating the creation of an exascale computing system and keeping the United States at the forefront of HPC technology [22-24].

The National Science Foundation is operating a program called Exploiting Parallelism and Scalability (XPS) [25]. This program provides funding for academic institutions that are doing fundamental research on new abstract models and algorithms, new programming models and languages, and new hardware architectures, compilers, operating systems and run-time systems.

HARDWARE

Typical HPC clusters are comprised of rack-mounted nodes containing one to four sockets that support multi-core CPUs. The nodes also contain RAM, interface hardware, usually hard drives, and in some instances video cards (i.e., GPUs). The nodes communicate to each other through interconnects or switches. Standard InfiniBand interconnects between cluster nodes currently operate at 100 Gbit/s for 4X links, with a latency of 0.5 μs. HPC clusters are expected to achieve an order of magnitude speed increase over the next decade. Solid state drives are now available that offer 10x the transfer speeds of traditional hard drives, but at 5 to 10x the current cost.

The latest CPU processors from Intel and AMD are based on 14 nm lithography, which is significant as this determines transistor counts on a single chip, the number of compute cores, and memory sizes. Processor frequencies have plateaued around 3±0.8 GHz because of concerns for power consumption and heat removal. For example, it is estimated that an exascale system built by the early 2020's would likely require 20 to 30 MW of power. Reducing power

FIGURE 9.3 PARTICIPATING AGENCIES IN THE NATIONAL STRATEGIC COMPUTING INITIATIVE

1) Lead Agencies	DOE, Exa-scale Computing Project
	DOD, Big data analytics at NSA
	NSF, Hardware technologies
2) Foundational Research and Development Agencies	IARPA
	NIST
3) Deployment Agencies	NASA
	FBI
	NIH
	DHS
	NOAA

consumption is an important aspect of future chip technologies [26-28]. Consequently, processor manufacturers have attempted to compensate by increasing the number of cores on a processor. For example, the latest Intel Broadwell processor has 22 cores and 55 MB of cache memory. Fabrication facilities for current generation of processors can cost around $7B to construct.

Internet bandwidth affects the usability of remote cloud computers and the ease of distant collaboration. In the United States, it is possible to attain speeds of 500 Mbps with the average being closer to 60 Mbps. This is typical of Western European countries as well. India and China have peaks closer to 20 Mbps [29]. According to Nielsen's "Law of Internet Bandwidth", which has been fairly accurate for the past thirty years, by 2040 a typical bandwidth will be over 1 Tbit/s, which is 2,000 times faster than today. If this holds true, internet bandwidth will not be the potential bottleneck.

Computational methods widely used in the engineering design community today scale poorly on current parallel supercomputers. For example, explicit FEM codes generally scale well to 1,000 cores or more. However, implicit FEM simulations have trouble scaling well past 128 cores because of the need for frequent data exchange between cores. It is not unusual for large simulations to take days or weeks. This class of problem scales best on shared memory architectures, which have fallen out of favor in the last decade. Such simulations provide some of the greatest challenges to realizing multiscale modeling in a standard engineering setting.

The lithography of CPU silicon chips is expected to be reduced from the current 14 nm scale to 5 nm over the next five years. Even at 20 nm, manufacturers are running into the quantum effect of electron tunneling, meaning they can pass through transistors that are supposed to be off. This has led to designs such as the finFET where the channel and gate of the transistors are built up from the die, adding to the manufacturing complexity. There is considerable uncertainty about how much further beyond 5 nm the silicon based technology can be pushed. Also, the costs of fabrication facilities are likely to rise from the current $7B price tag to $20B over the next five years.

There are a number of initiatives currently underway or planned to extend the life of silicon chip technology. One such, previously mentioned, is finFET technology, in which the transistor gate surrounds three sides of the channel. In the future, the gate may surround all four sides, which would give greater control of the current at smaller lithography scales but would be more difficult to manufacture [30,31].

Another concept is the System on a Chip (SOC), where the CPU cores, memory, and accelerators are all built on the same die, which would dramatically increase data transfer rates. There are second generation stacked High Bandwidth Memory (HBM2) units already in production by Nvidia and AMD. This also benefits from much shorter paths over which to transfer data, from centimeters down to millimeters. There are also designs still in the early stages to layer CPUs and memory, which will reduce the data paths to micrometers and result in very high power densities, which has engendered research on using microfluidics both to provide electricity and to extract heat [31,32].

There is research underway on more exotic materials to replace silicon such as graphene, molybdenum disulphide, and black phosphorous in films of one or two atomic layers, as well as carbon nanotube transistors. All these novel materials show promise in the lab, but it is as yet uncertain if they can be manufactured at scale [33-37].

Photonics, or optical computing, and quantum computing still face some daunting technical problems, but, if resolved, there is the possibility for a great increase in processing speed and reduction of power consumption [38, 39].

While it is possible that a breakthrough advancement in computer chip technology could occur in the next 25 years making the current massively parallel paradigm obsolete, it seems unlikely for at least the next decade.

2040 End State

By the year 2040, advances in computational infrastructure will greatly increase the speed and level of detail at which simulations will run. The evolution of hardware will enable widespread access to exascale or exa-FLOPS (10^{18} FLOPS) computing, possibly through massive parallelization and quantum, neuromorphic, or other not-yet-discovered modes of computing. Software will accordingly scale to take advantage of this advanced hardware, with the ability to run on hundreds or thousands of parallel processors.

For industry, user-friendly software toolkits will exist that update and optimize simulation codes to run in the new exascale computing paradigm. Simulations that take weeks to run today will have turnaround times of one day or less, saving time and computational expense. Simulation will augment and even replace experiments in some cases. Other advances in industry and academia will include the following:

- Typical bandwidth will exceed 1Tbit/s.
- Rapid, parallel experimental methods will become widely available as standard lab equipment, designed to specifically inform complex models.
- Error propagation and uncertainty will become a standard practice across the ecosystem (modeling and experiment).

Gaps

The following gaps lie within five of the roadmap's 10 crosscutting streams, with the **Scalability and Computational Efficiency** stream containing the highest number of gaps. The timeless challenge of developing and advancing computational infrastructure is scaling along with the demand of researchers and engineers, while maintaining a reasonable level of computational efficiency. Code compatibility and access to HPC architectures also loom as significant challenges. These gaps have the strongest tie to the **adaptive** characteristic of the 2040 end state. Adaptability (or flexibility) to run codes and simulations on future hardware solutions as they emerge is a crucial aspect of the envisioned ecosystem.

TABLE 9.1 COMPUTATIONAL INFRASTRUCTURE GAPS AND IMPACTED 2040 CHARACTERISTICS

AC Accessible **AD** Adaptive **IN** Interoperable **RB** Robust **TR** Traceable **UF** User Friendly ❖ Critical

GAPS	2040 CHARACTERISTICS					
	AC	AD	IN	RB	TR	UF
DATA ANALYTICS AND VISUALIZATION						
Lack of methods capable of using artificial intelligence/machine learning to improve scalability		AD		RB	TR	
MULTIDISCIPLINARY COLLABORATION						
Disconnect between application domain and computational domain experts inhibits effective collaboration	AC		IN			
BENCHMARKING AND BUSINESS CASE						
❖ Lack of support, or adequate business models, for code development and maintenance, particularly for software used in engineering applications. • Software licensing structure not conducive to massive parallelism	AC	AD			TR	
SCALABILITY AND COMPUTATIONAL EFFICIENCY						
Lack of user-friendly software technology (e.g., new languages, smarter compiler technologies) for accessing peta- and exascale computing resources	AC					UF
Slow transition of application software packages to emerging HPC architectures		AD		RB		
Programming languages (i.e., structure and user interface) are not optimized for scale-up or parallel computational processing		AD				
Inadequate adaptability of software to run on current and future hardware solutions • Commercial vendors are slow to implement changes that take advantage of existing multi-core systems or future hardware advances		AD				
INPUT/OUTPUT CONFIDENCE AND RELIABILITY						
Difficult to match the physics fidelity to the problem at hand, verify the suitability of codes, and account for uncertainty across methods		AD		RB	TR	

Recommended Actions

The following recommended actions lie within five of the roadmap's 10 crosscutting streams, with the most actions (including high priority) under **Benchmarking and Business Case**. Assessing existing and emerging technology through round robin testing and business case analysis will help speed up adoption and development of promising solutions. Many of these recommended actions call for organizing committees or working groups to tackle challenges and align research and development efforts. As with the gaps, the recommended actions have the strongest tie to the **adaptive** characteristic of the 2040 end state.

TABLE 9.2 COMPUTATIONAL INFRASTRUCTURE RECOMMENDED ACTIONS AND METRICS

FUNDING: $ <0.5M/year $$ 0.5-2M/year $$$ 2-5M/year $$$$ >5M/year

AC Accessible **AD** Adaptive **IN** Interoperable **RB** Robust **TR** Traceable **UF** User Friendly ✱ High Priority

ACTION	2040 CHARACTERISTICS						TIMEFRAME FOR COMPLETION			FUNDING
	AC	AD	IN	RB	TR	UF	NEAR 2017-2022	MID 2022-2035	LONG 2035+	
DATA ANALYTICS AND VISUALIZATION										
(9.1) Develop approaches to use technology such as machine learning, AI, and cognitive computing to improve and implement algorithms on new hardware		AD			TR		■	■		$$$
MULTIDISCIPLINARY COLLABORATION										
✱ (9.2) Establish long-term steering/assessment committee to review progress against long-term goals, note incremental advances, and adjust course as computational capabilities change and evolve	AC	AD	IN	RB			■			$
(9.3) Form a multi-year, community working group to develop an open standardized programming model or framework that helps users take advantage of existing and emerging heterogeneous HPC systems	AC	AD				UF		■		$
(9.4) Build cross-functional or collaborative organizations to bring computational expertise to new and ongoing code development early and often		AD					■	■	■	$$$
(9.5) Committees to work with operating system (OS) developers to better integrate software into package deployments and make more OS's compatible with parallel environments and emerging hardware paradigms		AD	IN				■	■	■	$
BENCHMARKING AND BUSINESS CASE										
✱ (9.6) Identify critical and high-quality existing codes to target for modernization	AC	AD		RB			■			$$
✱ (9.7) Develop baseline assessment and conduct round robin testing of existing tools that update and optimize simulation codes for peta- and exascale computing	AC	AD			TR		■			$$$
✱ (9.8) National effort (government and industry) supporting 5-10 key software tools for modeling aerospace materials, processes, structures, and manufacturing; Includes long term (10-20 years) funding and/or a viable business model to maintain the code base		AD		RB	TR		■	■	■	$$$

ACTION	2040 CHARACTERISTICS AC	AD	IN	RB	TR	UF	TIMEFRAME FOR COMPLETION NEAR 2017-2022	MID 2022-2035	LONG 2035+	FUNDING
BENCHMARKING AND BUSINESS CASE, CONTINUED										
(9.9) Sponsor annual roadmapping of pre-competitive research areas, government funding of pre-competitive research and engineering into modeling and computational methods for emerging hardware		✓		✓			■	■		$
(9.10) Host annual round robin testing of key applications to focus development and maximize use of limited resources (e.g., computational methods, parallel experimental measurements)	✓	✓					■	■		$
SCALABILITY AND COMPUTATIONAL EFFICIENCY										
❋ (9.11) Work with hardware suppliers and software OS developers to provide benchmarks and standards to support the ability for an HPC OS to quickly identify and adapt to hardware changes; better "plug and play"	✓	✓			✓	✓	■	■		$$
(9.12) Support for adaptive processor allocation on HPC architectures (e.g., smart schedulers, real-time micro-negotiation)		✓						■		$$
LINKAGE AND INTEGRATION										
(9.13) Programming models that enable migratable work (e.g., Charm++)		✓	✓				■	■		$

Relationships with Other Key Elements

Each Key Element relies on computational hardware platforms, software tools, and programming frames for building and executing simulations, analyzing and sharing data, collaborating across disciplines, and preparing the workforce for the 2040 ecosystem. The Computational Infrastructure Key Element provides a foundation for the ecosystem to improve the scalability, adaptability, interoperability, and efficiency of both computational and physical activities to accelerate the design, optimization, and analysis of aerospace systems and components.

TABLE 9.3 EXAMPLE INTERRELATIONSHIPS OF KE9 (COMPUTATIONAL INFRASTRUCTURE) AND OTHER KEY ELEMENTS

Note: Interrelationships among KEs vary. Equal weight should not be inferred.

OTHER KEY ELEMENTS	INTERRELATIONSHIP	THIS KEY ELEMENT
KE1 Models and Methodologies	Form frameworks for managing/accessing modeling results and governing simulation speed-accuracy tradeoffs	KE9 Computational Infrastructure
	Catalyze scalable computations via reduced order/simplified models	
KE2 Multiscale Measurement and Characterization Tools and Methods	Support linked experimental data generation and computational analysis	
	Support linked experimental data generation and computational analysis	
KE3 Optimization and Optimization Methodologies	Standardize computational environments to enhance multiscale/multiphysics optimization and stimulate collaboration	
	Automate code optimization for optimal performance with computational infrastructure	
KE4 Decision Making and Uncertainty Quantification and Management	Exploit parallel software frameworks and computer architectures for uncertainty quantification and propagation	
	Investigate computationally efficient and cost-effective methods for achieving sufficient design accuracies	
KE5 Verification and Validation	Provide hardware/software frameworks for managing/accessing experimental datasets for V&V	
	Verify peta- and exascale computing algorithms	
KE6 Data, Informatics, and Visualization	Supply HPC programming tools and frameworks for transferring/accessing large distributed datasets	
	Incorporate machine learning methods into high-level HPC programming frameworks for hardware interoperability	
KE7 Workflows and Collaboration Frameworks	Enable simultaneous access for global collaboration via high bandwidth networks and software platforms	
	Supply HPC-ready multiscale collaboration frameworks	
KE8 Education and Training	Increase access to government lab HPC resources	
	Build industry-relevant competencies in characterization and simulation code design for current and future computational infrastructure	

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Appendix A

Multidisciplinary Engineering Challenges (MECs)

Each Key Element contains recommended actions that demonstrate potential approaches for overcoming critical technical and cultural gaps over the next 25 years. To help focus 2040 vision research and development efforts and provide useful engineering solutions at the same time, the roadmap features a series of potential multidisciplinary engineering challenges (MECs). These MECs—which have not been solved by prior efforts and technology applications—represents examples of potential high-impact activities that align with specific roadmap actions across the nine Key Elements.

1

Mitigation of High Temperature Environmental Damage, Oxidation, and Hot Corrosion of High Temperature Turbine Engine Components

One of the critical issues that must be addressed in the aerospace community is the mitigation of environmental attack, oxidation, and corrosion of high-temperature materials exposed to aggressive environments. A continued avenue to increase the efficiencies and capabilities of next-generation gas turbines is to increase gas path and turbine inlet temperatures. Many of the current designs in high-temperature regions of aeronautical vehicles and engines require multi-layer functional materials that can withstand the extreme environments posed upon them. Additionally, space launch vehicle environments offer unique extreme conditions and challenges for today's thermal barrier system materials. As a result of extreme temperatures and environmental contamination, such as dust and dirt, ceramic and metallic coatings can suffer from extensive molten calcia-magnesia-alumino-silicate (CMAS) damage while their substrates (metallic or ceramic matrix composites [CMCs]) fare no better in terms of oxidation and (hot) corrosion attack [1]. The mechanisms of deformation and damage mechanisms in coated superalloys and CMC materials under coupled thermal, mechanical, and environmental (oxidizing and moisture) are not well understood and have not been integrated into a robust system-based analysis and design framework. Specific interaction of CMCs and Environmental Barrier Coatings (EBCs) under the mechanical and environmental conditions must also be realized.

Current efforts to model such phenomena have been piecemeal and challenging [2]. Major milestones in the aforementioned Key Elements must be achieved to implement modeling of damage for high-temperature materials for the year 2040. Databases and data infrastructures must be able to source large amounts of data, such as thermodynamic, kinetic, and mechanical information, for substrates, coatings, and environmental chemistries over a wide range of spatiotemporal domains to build the foundations for predicting attack probabilistically. Advanced experimental methods and testing must be derived to simulate conditions where attack occurs; high-throughput experimental methods should be developed to investigate various substrate-coating-environmental effects. Additionally, novel *in situ* characterization tools and methods must be developed to investigate the effects of these inaccessible and harsh environments. Such methods may even evolve and drive onboard sensors within future aeronautical vehicles for real-time monitoring of component health from prediction of cumulative damage. Fundamentally, current physics-based understanding of oxidation, corrosion, and environmental attack is poor for model systems (e.g., binary and ternary alloys) and nearly non-existent for materials of commercial interest. Extensive physics-based understanding must occur between now and 2040 to support the next generation of gas turbines. The computational framework must include a systems-based approach that integrates multidisciplinary efforts.

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2

Development and Optimization of Polymeric Matrix Composites for Aerospace Applications

Polymeric matrix composites are critical materials for the aerospace industry. Radical changes in this type of material relative to manufacturing capabilities, costs, and component complexity would come from the development of thermoplastic polymeric matrices that deform as thermoplastic polymers. While this has been previously demonstrated, issues regarding environmental stability, processibility, and shelf life have yet to be resolved. Application of advanced modeling tools is needed to develop a polymer system that will fit all performance requirements and be resistant to current manufacturing solvents and environmental attack. This is a multidisciplinary challenge that requires the design of a new material system over many length scales. Models that describe the mechanisms involved in processing, reaction, and behavior are foundationally required, including first principles methods through macro-scale models to support analysis of required structural requirements. This MEC must address the development, validation, and application of molecular dynamics (MD) simulations or other advanced modeling and simulation tools to support polymer design.

Simulation infrastructure efforts will be required to manage the experimental methods to establish and validate the required models. Tools that allow linking of multiscale models and enable use of intrinsic materials properties directly at every length-scale will need to be established and demonstrated. Data to support calibration and validation of each model will be required within a framework of a well-established experimental workflow, data management plan, and database structure.

This MEC would be effectively advanced through collaboration among OEMs, universities, and government laboratories, such as NASA Research Centers. This challenge problem should also be targeted at a future NASA airframe and propulsion system to further advance fuel efficiency and environmental impact.

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

The DARPA AIM program successfully demonstrated the capability of radically reducing weight of critical rotating components through the linking of elements of local microstructure and property prediction and control [1]. However, that program was less successful in establishing full industry-wide acceptance and implementation, substantially due to infrastructural challenges relative to integration of model-based material and process definitions into design optimization and structural analysis methods. The infrastructural issues that hindered full implementation of location-specific design methods for rotors may now be possible with emerging tools and methods. An MEC project that aims to demonstrate model-based materials definitions embedded with design and lifing methods will allow the aerospace community to establish standards that can be applied to many components and systems.

An MEC program should establish required model-based material and process definitions for a material, process, and component critical to a future NASA system and mission. This material could be a new material designed with ICME tools and methods to establish the required materials models or a legacy material that requires model development and calibration to describe the mechanisms that control the material's behavior. Similarly, a manufacturing process commensurate with the target component will require model development and validation and could range from forging, casting, or additive manufacturing.

This challenge program would demonstrate and establish critical linkages of materials and process models with structural and design models and methods. System-based optimization processes would be performed to establish an optimal model-based component definition to meet the system requirements and challenge goals. This program would provide a path to industry standard methods for model-based material and process definitions in place of traditional, static, empirically-based specification minima and design curves.

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4

Optimization of Structures for Mitigation of Thermomechanical Fatigue

Thermomechanical fatigue (TMF) is a significant challenge and failure mode within high-temperature aerospace structures. The cyclic nature of high-temperature component and system operation often produces very large thermal gradients and associated stresses during transient stages of repeated mission operation, whether thermal protection systems (TPS) for rockets or turbine airfoils in turbine engines. There is a need for further understanding of the mechanisms that generate material damage during these cyclic processes where thermal and structural loads combine in a complicated spatiotemporal array. Use of multiscale modeling to establish and model the mechanisms for a selected material system will be required. Optimizing microstructures to mitigate damage formation or the rate of damage formation would greatly increase durability and survivability of structural components that experience combined effects of external applied stresses and simultaneous thermal stresses, both in- and out-of-phase.

The design of structures would include optimization of system thermal and stress boundary conditions, component geometry, and material texture, modulus, and strength, all of which can impact the rate of damage generation within a component. Models that can mechanistically predict thermo-mechanical fatigue damage in metallic components are required to enable assessment of arbitrary thermo-mechanical fatigue cycles for future system and component designs. Physics-based fatigue models that enable prediction of damage accumulation as a function of cycles are also needed. These models must include capability of prediction over large time-scales and must be able to incorporate or eliminate mechanisms as the material is cycled through ranges of temperature and stress levels. Modeling methods that enable current computationally expensive calculations to be used in an efficient and accurate manner are required in an updated simulation infrastructure. This MEC will enable needed effort to close critical Vision 2040 gaps and will guide further efforts in the direction of the Vision 2040.

5

Design and Development of Unique Materials Such as Shape Memory Alloys and High-Entropy Alloys in Aerostructures and Components

Emerging materials hold great promise for many applications within the aerospace industry. Unique materials that can support unique behaviors can be enabling for new system architectures and designs. Adaptive structures that respond to surrounding application environments can respond and support the control and optimization of overall system performance. These types of unique "smart" materials can range from shape memory materials or the emerging area of high-entropy alloys.

An MEC program that defines a unique material requirement that would enable new system design or application freedoms is proposed. The unique behavior may be low coefficient of thermal expansion or potential negative coefficient of thermal expansion over a specific range of temperature. The unique behavior could also involve component shape change as a function of temperature exposure for control of airflow or potentially system sealing functions.

This challenge program is aimed at defining and exploiting specific known or emerging physics-based mechanisms that drive unique material behavior. This effort will be required to demonstrate a systematic experimental method that could be standardized for the selection and application of mechanisms and associated models to component and system design optimization. While unique material mechanisms, like shape memory effects, are starting to be used within the aerospace industry [1], this effort would support the development of industry-wide methods for their systematic design and use.

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6

Automated Readaptation 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)

Most HPC software today is written in C/C++ or FORTRAN using MPI routines for DMP and/or OpenMP pragmas for SMP. When a new accelerator comes along (e.g., GPUs or Xeon Phi), a substantial recoding effort is required using a language like CUDA or OpenCL. Efforts are underway at a number of national labs, universities, and companies to develop a higher-level HPC programming language to automatically take care of the lower-level message passing and multi-threading issues. This approach would free up scientists and engineers to focus on the physics they are trying to model rather than dealing with the often complex required coding to achieve high performance on heterogeneous computing systems. It would also save software companies an enormous amount of development time in trying to adapt their codes to changing computer architectures.

This MEC program would target the development of computer software that can write and optimize computer software for a specific function for evolving computational hardware platforms. Ideally, the various efforts currently underway would be consolidated into a new ANSI-standard HPC computer language. A working group or consortium should be established to understand the pros and cons of the HPC paradigms currently under development and come up with a language that combines the best of each. This should be followed by the formation of a standards committee to define and maintain the minimum common elements of such a language. This is a multi-decade undertaking that should be initiated now. Numerical models of physical phenomena that depend on high-performance computing for their utility would certainly be impacted by the availability of an HPC programming language and how it would be applied within a multidisciplinary engineering environment. The tools which encompass such models should be implemented for HPC at the inception rather than at a later stage. Simulation infrastructure must also be up to par. A HPC programming language would depend on the evolution of the computer hardware that it is expected to run on. A programming language is an essential part of the simulation infrastructure. Ultimately, this effort would require the collaboration of the national labs, other government agencies, universities, and software companies across an expansive workflow and collaboration network.

7

Design and Optimization of Ceramic Matrix Composites for Aeronautical Vehicles

Ceramic matrix composites (CMCs) are a class of materials that are beginning to be used in commercial applications, most notably, within the hot sections of gas turbine engines. Interest in CMCs is growing because gas turbine engine efficiency and performance is directly related to the turbine entry temperature where environmentally protected CMCs are expected to replace thermally protected superalloys for certain applications in the future. Higher temperature capability and lower density are the fundamental reasons why SiC/SiC CMCs (silicon-carbide fiber, silicon-carbide matrix composites) offer great potential benefits over metallic components in a gas turbine. As a result of the high cost of raw goods and long duration of manufacturing processes, modeling of manufacturing processes, such as 1) chemical vapor infiltration (CVI), 2) polymer impregnation and pyrolysis (PIP), and 3) melt infiltration (MI), has been an active area of research. Each of the three main processing routes is completed through control of fluid flows and various reaction processes. These processes involve the interaction between microstructure (on the order of micrometers), the part scale (on the order of centimeters) and the equipment scale (on the order of meters). In the case of woven materials, the weave architecture will influence phenomena acting over an intermediate scale between the microstructure and parts (on the order of millimeters).

Despite the fact that there is a high degree of coupling in the flow characteristics at the various scales, most modeling approaches only loosely couple the scales and generally focus at the part scale. Boundary conditions are imposed based on the equipment setup to simulate the effects of the processing environment. Often, these boundary conditions are taken to be uniform based on the assumption that ideal conditions can be achieved in the equipment. Other approaches impose boundary conditions based on models of fluid flow and heat transfer within the equipment. This loose coupling between length scales has hindered the application and advancement of ICME for this class of materials. Key phenomena, such as the dependence of permeability on the flow field or the effects of non-uniform deposition which occurs in industrial scale CVI processes, are not captured which has led to limited applicability of these approaches.

An MEC program is proposed for the development of true multiscale manufacturing modeling of CMCs. The NASA CFD Vision 2030 program highlighted the need for advanced solution methods focused on turbulence modeling in high Reynolds number flows [1]. Such developments, although needed by industry, will not support the processes described above that are dominated by low Reynolds number flows and interactions between length scales separated by several orders of magnitude. Methods should be developed to optimize processing with the goal of minimizing manufacturing time and cost. There is also the need for development of advanced experimental methods for characterizing the reaction kinetics that control the CVI process. The high temperatures and harsh chemicals that exist inside a CVI reactor limit current methods. Additional experimental techniques are needed to properly understand the MI process that is conducted at temperatures above the melting point of silicon (1414 °C). To fully benefit from these developments, processing data will need to be linked to component performance through the use of advanced materials characterization techniques, comprehensive databases, and informatics. Education and training must also be advanced to realize the capabilities of CMCs. There are only a handful of universities in the United States that have active research and educational programs in the area of CMCs and even fewer that are working on coupled multiscale materials modeling with a system-based approach. Similarly, most engineers in the industry still think of designing and analysis of composites without coupling models to drive experimental methods. Significant resources must be devoted to train the current and future workforce to overcome this challenge.

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8

Application of Microstructure Definition Tools and Methods to Enable Model-Based Material and Probabilistic Component Definitions

Models that describe the physics within materials are starting to emerge as the preferred approach to defining material, rather than empirical testing and statistical treatment of results with the assumption that all test results should be the same. Model-based material definitions provide huge potential for advancing component optimization through prediction of properties based on local structure [1]. This opportunity is also accompanied by the challenge of defining local structure from simulation and physical characterization.

To enable prediction of local properties within a component, it is imperative to know the range of structure at the location of interest. The knowledge of the structure must be to a level where the volume and length-scale that interact with controlling physics-based mechanisms are fully defined. For some properties, microstructure features, such as grain size, may be dominant, but for others, features on the submicron level, such as atom clusters or boundary chemistry, may be the controlling feature. Knowledge of the entire range of controlling features within a component volume is needed. The size of the volume that must be predicted or characterized that allows for a statistically valid description of the feature size, volume fraction, and/or spatial distribution is also required.

Determining the critical volume size for a minimum size representation of the material must be based on the physics-based mechanisms involved. The larger the controlling size feature within a material, the larger the critical volume will be. Conversely, the smaller the size of the controlling features, the smaller will be the critical definition volume, which also means that many more critical volumes are within a total volume of a component.

An MEC program is proposed to establish standard methods for defining statistically equivalent representative volume elements (SERVEs) within a material structure, as well as techniques for acquisition of materials information at these representative volumes. This must be accomplished based on mechanism length-scale, knowledge of the component manufacturing method, and component application space. To track and model entire component volumes with respect to mechanism-based length scales would be computationally restrictive with the current state of modeling software and computational hardware, so a near-term, engineering-pragmatic approach is needed, based on zoning of the component volume into smaller number of SERVEs, each with a practical range of structural statistics.

This challenge program is proposed to characterize and define the SERVEs sizes and zones within a titanium component for the purpose of dwell-fatigue optimization and high-cycle fatigue optimization for a system-level component capability. Both material behavior capabilities are driven by structure but at greatly different length scales. The result of this challenge program would be the demonstration of defining and applying a SERVE-based zoned material structure analysis to determine probabilistic behavior at the component level. This program would also provide needed guidance to industry standards for multiscale material structure characterization and statistical descriptions for component structural analysis.

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9

Electrification of Aircraft Propulsion

The aeronautics community has invested 70 years in optimizing tubular fuselage aircraft and podded turbofan engines. While there are still improvements to be made in aircraft and engines, it is clear that those improvements are coming more slowly and are costing more. In the early 2000s, NASA challenged the aeronautics industry to look ahead to future generations of aircraft and predict what technology advancements could have substantial impacts on the metrics of fuel economy, ground and in-flight emissions, and community noise. Electrification of aircraft propulsion was one of the potential solutions identified.

Electrified aircraft propulsion refers to a suite of aircraft configurations that derive all or a portion of the propulsive power from electric machinery, such as a motor-driven propeller. Until recently, the specific power (power/mass) and efficiency of electric machines, along with the supporting control and distribution equipment, was too low for all but the smallest, unmanned aircraft. Rapid advancement in electric machinery, power electronics, and energy storage have changed this value proposition. However, the value of electrified aircraft propulsion does not come from simply replacing a turbine or reciprocating engine but instead from the ability to change propulsion-airframe integration, aircraft functionality, or mission optimization in ways unavailable through traditional propulsion. It is equally important to note that configuration solutions may be different for small versus large aircraft or vertical takeoff/landing versus horizontal takeoff/landing aircraft. The field is exciting yet challenging, because the optimum configurations are far from understood.

Even though aircraft propulsion greatly benefits from rapid advancements in energy storage technologies (batteries, fuel cells, supercapacitors, etc.) and electronics for terrestrial applications, there are unique aviation requirements that will require focused development. Features that make aircraft powertrains different from land vehicle power trains or terrestrial power grids center around specific power (flight weight), efficiency demands (which greatly impact thermal management and overall system weight), dielectric integrity at reduced atmosphere (flight altitude), and system reliability requirements for aircraft safety. Higher voltage electrical transmission is a prime example of a technology challenge which will enable or constrain the implementation of electrified aircraft propulsion. Higher voltage transmission, improved thermal management, higher electrical frequency operation of machines, and higher electrical frequency operation of power electronics are parameters that are crucial in these powertrain subsystems. Likewise, the electric machines and the power electronics are subsystems which need significant and coordinated improvement to achieve powertrains suitable for commuter, regional jet, and larger aircraft. This development is a key system optimization challenge at many levels. At the component level, for example, the electric machine can be optimized by treating the electromagnetic circuit (e.g., conduction coil, soft magnetic laminations, and insulation) as a meso-scale composite. At the subsystem level, the electric machine and controlling power electronics must be optimized together to take advantage of new semiconductor device options in the power electronics and reduce the overall subsystem mass. And at the powertrain system level, choice of operating power, voltage, and protection schemes must be optimized. Each level must be designed with a broad range of new component materials, manufacturing techniques, and integration possibilities in mind. Perhaps most critically, limitations in current energy storage technologies are critical bottlenecks for enabling electric aircraft requiring dramatic improvements relative to the state-of-the-art lithium ion battery technology.

Insulation Examples

One of the key challenges to using electric powertrains for aircraft thrust is the distribution of power (current times voltage). Distribution of high voltage allows lower current ratings but requires significant development insulation systems. Terrestrial high voltage solutions are insufficient since the reduced atmospheric pressure associated with standard flight altitudes can lead to ionization near high voltage components. This ionization both increases the likelihood of partial discharge and accelerates degradation in many ionic materials. Non-traditional combinations of inorganic and organic materials may be required to enable high voltage protection on aircraft. While high voltage insulation development is essential, advancement of insulation materials for electric machines and power electronics will improve specific power and efficiency and enable electrification for larger vehicle classes. In these components, the dielectric breakdown, thermal conductivity, and volume are crucial parameters. An MEC program that addressed these insulation challenges as multi-variable composite systems would greatly accelerate development.

Magnetic Material Examples

Magnetic circuits are the backbone of electric machines and power electronics. Development in hard and soft classes of magnetic materials have direct impacts on specific power through magnetic field strength and efficiency through electrical loses. The highest performance hard magnetic materials rely on high fractions of rare earth metals, the cost and availability of which are strategic concerns. Current research is exploring ways to maintain magnetic performance with smaller fractions of rare earth elements. Future research enabled by advanced materials modeling could explore alloying or microstructure improvement to increase saturation strength, increase magnetic permanence, or maintain these performance parameters with lower fractions of rare earth elements. Current soft magnetic materials research focuses on reducing the energy lost in each magnetic cycle and maintaining performance at high switching frequencies on known classes of alloys. Future research enabled by advanced materials modeling could explore new chemistries to provide greater magnetic saturation strength with tailored permeability, low losses, and good mechanical properties. These material improvements can enable higher performance in electric machines, power electronics, and power quality filtering, directly impacting the upper limits on powertrain performance and aircraft size.

Semiconductor Examples

Wide band gap semiconductors such as SiC and GaN are being applied to an increasing range of electronic devices. These devices provide the ability to switch at higher frequencies, translating into not only processing speed increases but also increased electrical efficiency in many applications. Although wide band gap semiconductors have increased potential over pure Si in many facets, they still require maturation in both processing and applications.

Conductor Examples

Pure aluminum and copper are ubiquitously used for electrical conductors in current aircraft. Advanced conductor systems based on superconductors, graphene, or carbon nanotubes would provide an enormous step change in power management in aircraft. Superconductivity is quite mature in several terrestrial applications but faces specific challenges for application in aviation. Superconducting wires are composite systems which must provide structural support as well as electrical and thermal management. Graphene and carbon nanotubes have unique conduction properties that may provide breakthroughs in specific conductivities. These are high-risk, high-payoff development areas.

Energy Storage Examples

The energy storage requirements of electric aircraft are dramatically higher than most other terrestrial applications including electric cars and consumer electronics. In addition to very high requirements with respect to specific energy and specific power, there are equally challenging requirements regarding cycle life, cost, reliability and safety. For example, the state of the art rechargeable battery technology is based on Lithium Ion chemistry and has a specific energy of approximately 200 Wh/kg. The Boeing SUGAR study however identified 400 Wh/kg as the threshold requirement for General Aviation and 750 Wh/kg for commercial regional service. Meeting these extreme requirements will require breakthrough developments in the basic material science of energy storage component materials (e.g. electrodes, electrolytes, etc.) as well as their interfaces. Such developments will not only address basic material property requirements but will also address how these material respond to these highly reactive and corrosive electrochemical environment. Significant progress in advanced “beyond Lithium ion” battery technologies(e.g. Li-Air, Li-S, silicon based, etc.) as well as advanced fuel cells and supercapacitors will be needed to achieve these goals. System level consideration will also be critical to determine how these potentially very different materials work together in an energy storage device as well as how it interfaces with other aircraft systems.

Appendix B

Case Studies

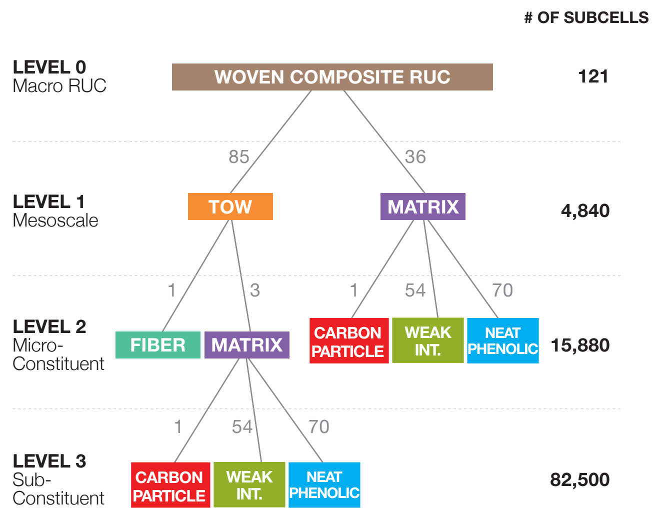
The following case studies illustrate the potential of work currently only being conducted by R&D departments in industry and/or government labs that could be performed regularly once the 2040 vision is realized.

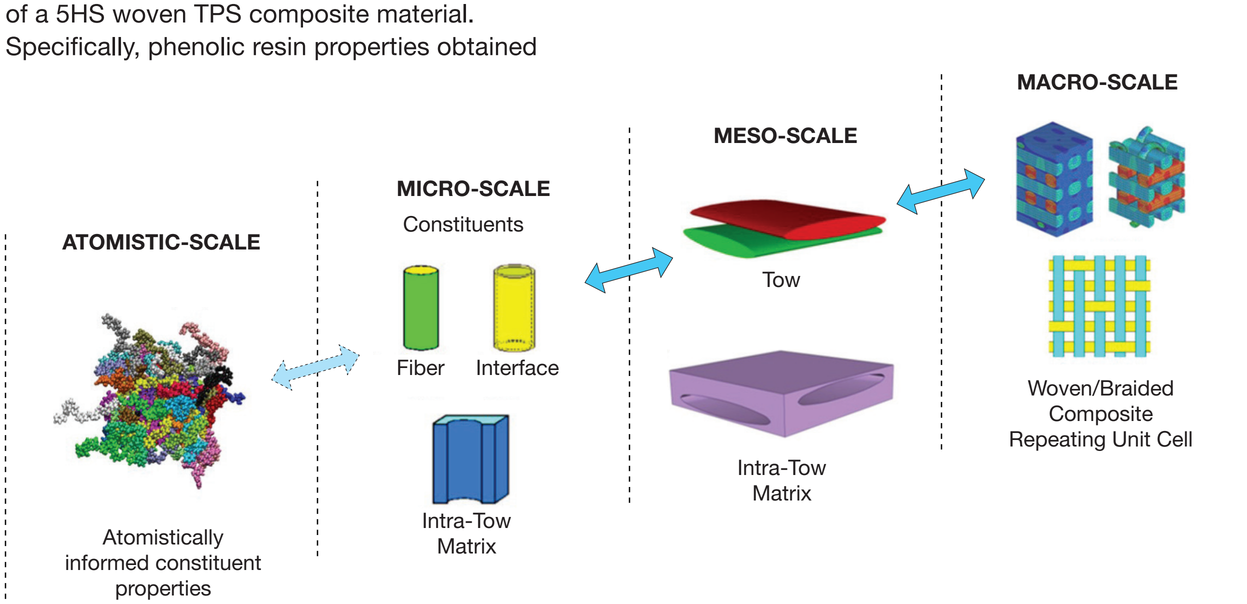
Case Study 1 Multiscale Modeling of Carbon/Phenolic Composite Thermal Protection Materials: Atomistic to Effective Properties

Next-generation ablative thermal protection systems are expected to consist of 3D woven composite architectures. It is well known that composites can be tailored to achieve desired mechanical and thermal properties in various directions and thus can be made fit-for-purpose if the proper combination of constituent materials and microstructures can be realized. Recently, NASA GRC and ARC teamed up to conduct the first multiscale, atomistically informed, computational analysis of mechanical and thermal properties of a present-day Carbon/Phenolic composite Thermal Protection System (TPS) material, wherein micromechanics and molecular dynamics were combined to demonstrate how ultimately the design of new material systems can be achieved.

The Multiscale Generalized Method of Cells (MSGMC) methodology was employed to incorporate atomistically informed constituent properties and detailed microstructural features in a coupled, synergistic multiscale analysis of a 5HS woven TPS composite material. Specifically, phenolic resin properties obtained

Levels of scale included in modeling a woven TPS composite. The macro-, meso-, and micro-scales were considered in a synergistically coupled MSGMC analysis, while the atomistic-scale was included using an uncoupled hierarchical procedure.

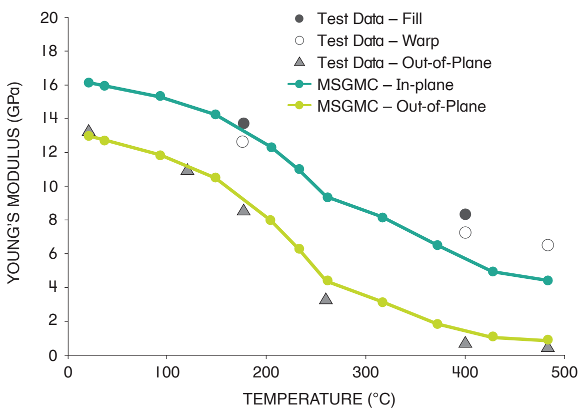


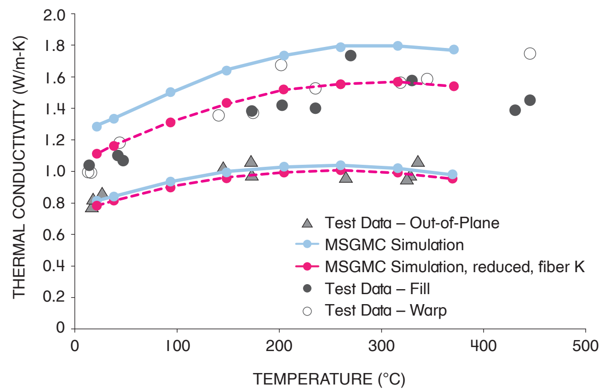


from molecular dynamics (MD) simulations and carbon fiber and carbon black filler materials drawn from experimental literature were used as input for micromechanics computations. Results indicate that given sufficient microstructural fidelity, along with lower-scale, constituent properties derived from molecular dynamics simulations, accurate composite level (effective) thermos-elastic properties can be obtained. This suggests that next-generation TPS properties can be accurately estimated at temperatures below charring via atomistically informed multiscale analysis.

References:

Predicted Thermomechanical properties for a 5HS woven TPS composite





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.

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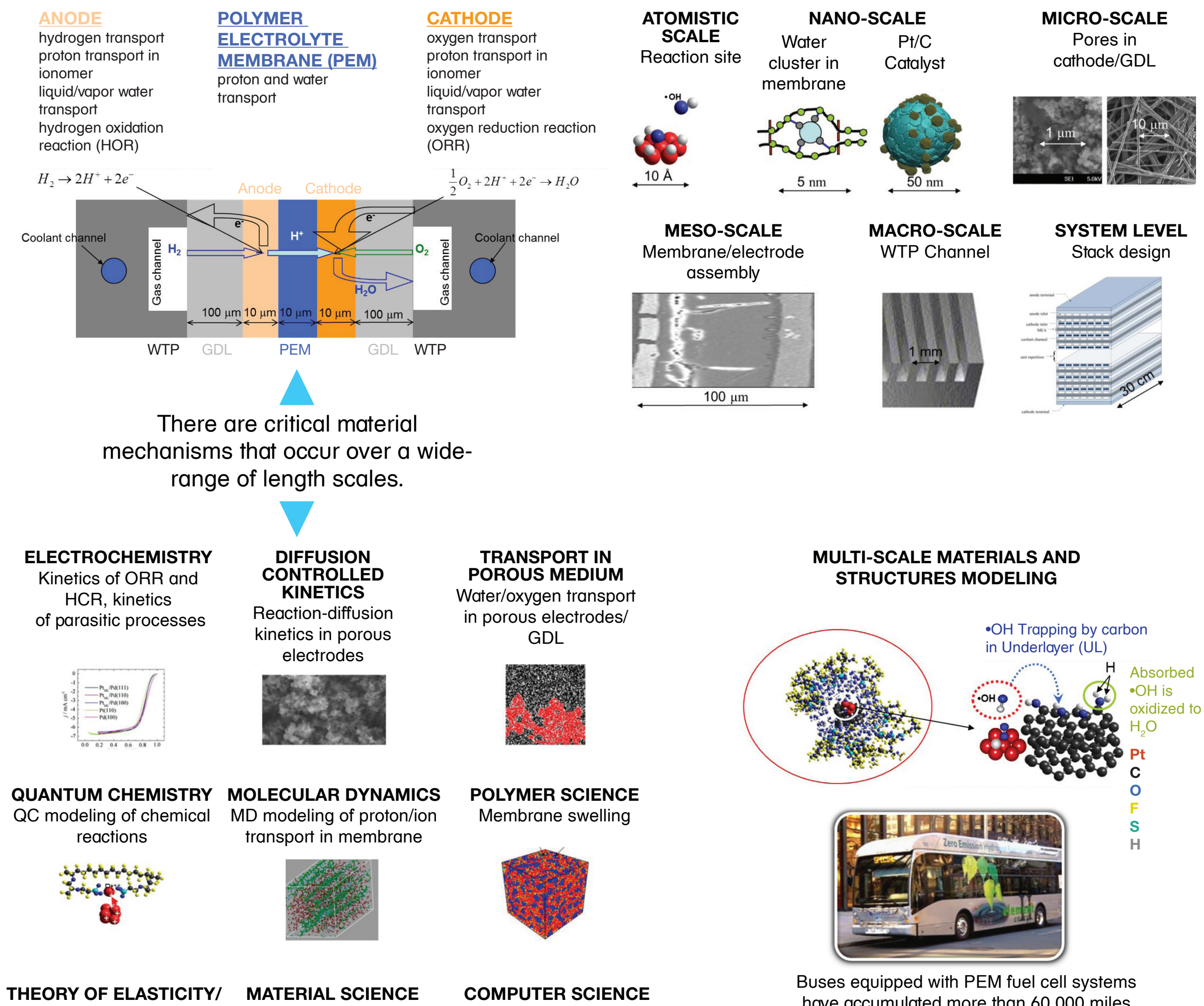
Examples courtesy of NASA

Case Study 2 Multiscale Modeling of Complex Systems: Fuel Cells

Fuel cells are complex systems that convert fuel into electrical energy through controlled sets of chemical reactions. The reactions within these systems provide a harsh environment for the required chemical species separation membranes. Degradation of fuel cell capabilities involves multiple processes subject to a variety of scientific disciplines.



Understanding of the physics-based mechanisms with Polymer Electrolyte Membrane (PEM) fuel cells has enabled optimization of materials and structures for unprecedented durability.

At the Polymer Electrolyte Membrane (PEM) Pt ions diffusion/precipitation occurs, along with oxygen/hydrogen diffusion (crossover) and catalytic reaction at Pt. Free radical generation/quenching at Pt occur and polymer decay progresses by free radical formation (chemical degradation). Mechanical cracking develops under mechanical stress to catastrophic failure. At the cathode, Pt dissolution/diffusion/precipitation occurs with a loss of catalytic activity, leading to polymer decay by free radical formation from loss of proton conductivity. Carbon oxidation occurs followed by cathode flooding and loss of oxygen permeability. At the anode, Pt poisoning by CO results in loss of catalytic activity. Gas Diffusion Layer (GDL) exhibits carbon oxidation with GDL flooding and loss of oxygen permeability.

Understanding of the physics-based mechanisms with PEM fuel cells has enabled optimization of materials and structures for unprecedented durability.

Significance for Vision 2040

MODELS & METHODOLOGIES
An integrated framework linking models and advanced experimental tests will increase accuracies of models that predict materials and structure responses under extreme conditions or harsh environments.

EDUCATION & TRAINING
Interdisciplinary programs and degrees will bridge across disciplines including computer science, materials science, polymer science, and other engineering fields to elucidate critical material mechanisms across scales.

OPTIMIZATION
Novel optimization methods will account for emergent behaviors across scales, and help solve computationally intensive, high-dimensional design problems.

COMPUTATIONAL INFRASTRUCTURE
Programming language frameworks and advanced algorithms will permit large-scale computing of critical material mechanisms over a wide range of length scales.

CHARACTERIZATION
Next-generation characterization methods will systematically link proposed models and experimental results at different hierarchical scales to inform model validation efforts.

WORKFLOWS & COLLABORATION FRAMEWORKS
Computational tools will automate the linking and execution of disparate models.

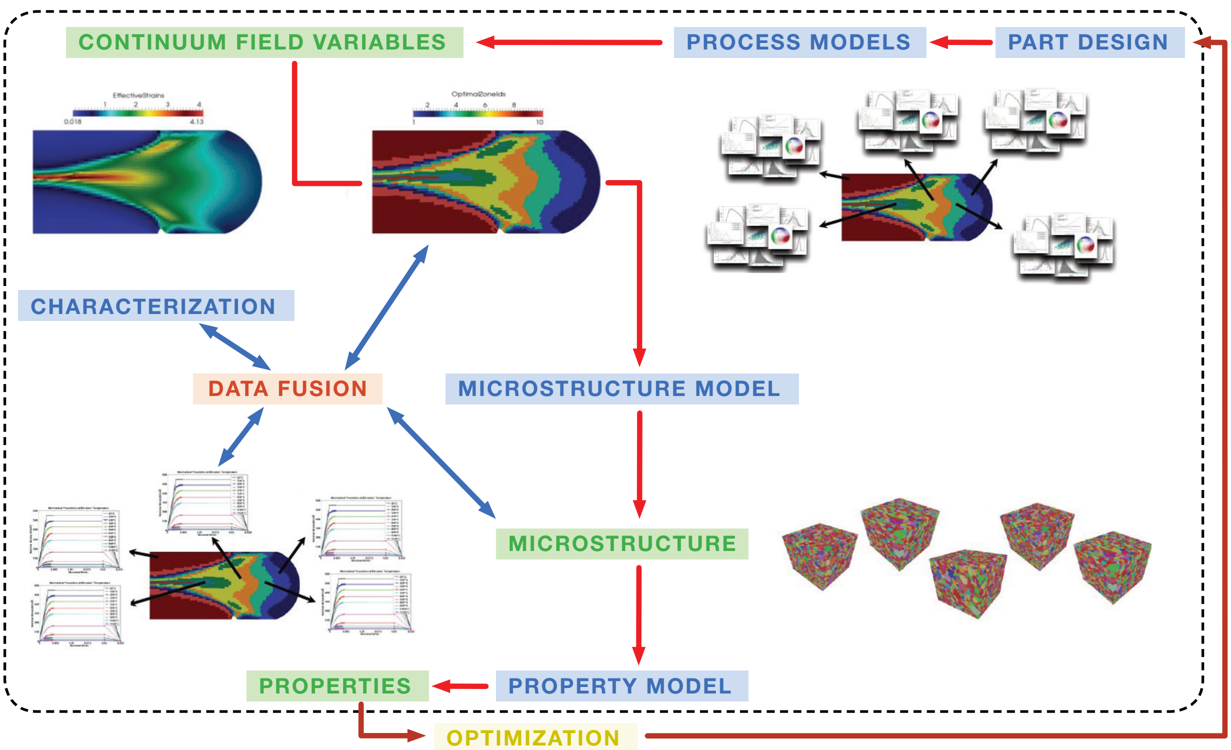
Example courtesy of United Technologies Research Center

Case Study 3 Materials Design in the Digital Age – SIMPL and DREAM.3D

In order to advance the rapid engineering of materials in accordance with the precepts of integrated computational design, the Air Force Research Laboratory sought to develop a unified platform for objectively describing and quantifying materials structure. This project led to the development of DREAM.3D, the Digital Representation Environment for the Analysis of Materials in 3D. DREAM.3D is a comprehensive software suite that enables materials scientists, and increasingly other engineers and data scientists, to manage multidimensional, multimodal materials data in a consistent framework. Underpinning the analysis capabilities and materials knowledge embedded in DREAM.3D is a management library capable of tracking and organizing the complex spectrum of hierarchical data that defines modern engineering materials. This management library is called SIMPL, or the Spatial Information Management Protocol Library. These toolsets are developed and supported in an open fashion by BlueQuartz Software and designed in such a way as to allow additional packages to be plugged into the SIMPL/DREAM.3D ecosystem.

DREAM.3D has been utilized as a framework for enabling local materials structure design driven by process-structure-properties relationships. A particular use case involving the microstructure design of a titanium forging is shown below. In this workflow, a part designer uses industry standard tools to propose a potential overall shape for the given part.

Schematic view of hierarchical design in a titanium forging using DREAM.3D.



With DREAM.3D, both the part geometry and predicted local processing variables can be integrated and managed using SIMPL. The field variables are then “zoned,” defining contiguous regions of material that have undergone similar processing history. This objective definition of structure below the part mold-line begins the process of local microstructure design. The processing histories are used to predict microstructure characteristics for each zone, which DREAM.3D can then use to instantiate virtual instances of the representative microstructures. These virtual structures are then run through a property model, which results in locally-specified mechanical properties throughout the part geometry. At each step, more materials information is generated at different length scales. Through its use of SIMPL, DREAM.3D is capable of organizing this data hierarchy and fusing the information into a common reference frame. The result is a unified view of the material structure, from the part mold-line down to the microstructure, allowing for local optimizations.

The overall philosophy of hierarchical materials designed implemented in DREAM.3D extends beyond classical metallurgical materials problems. DREAM.3D has been used to analyze ceramics, carbon foams, additive manufacturing data. The continuing development of the SIMPL/DREAM.3D ecosystem represents a potential method for opening the concepts of integrated computational design to the broader materials enterprise.

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.

WORKFLOWS & 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.

References:

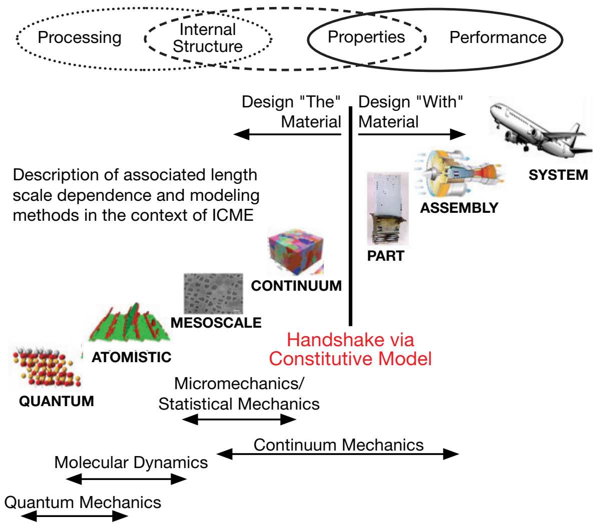
[1] M. Groeber, M. Jackson, *DREAM.3D: a digital representation environment for the analysis of microstructure in 3D*, Integr. Mater. Manuf. Innov. 3 (2014)

Example courtesy of BlueQuartz Software

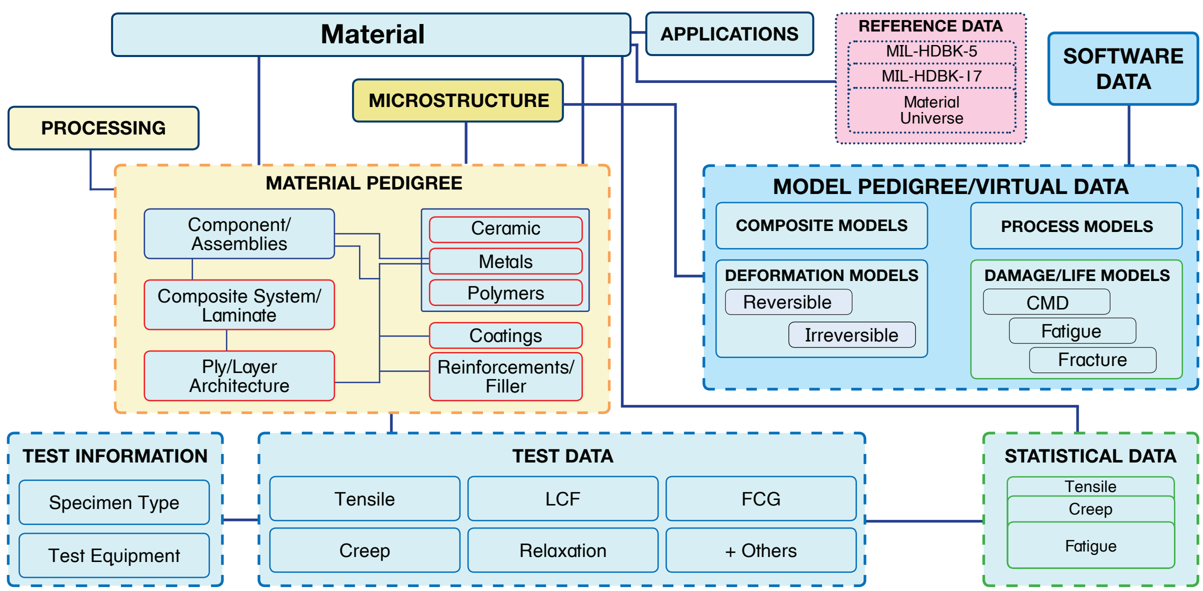
Case Study 4 Information Management Workflow and Tools Enabling Multiscale Modeling Within ICME Paradigm

With the increased emphasis on reducing the cost and time to market of new materials, the need for analytical tools that enable the virtual design and optimization of materials throughout their processing-internal structure-property-performance envelope, along with the capturing and storing of the associated material and model information across its lifecycle, has become critical. This need is also fueled by the demands for higher efficiency in material testing; consistency, quality, and traceability of data; product design; engineering analysis; as well as control of access to proprietary or sensitive information. Consequently, material information management systems and physics-based multiscale modeling methods must keep pace with growing user demands.

Description of associated length scale dependence and modeling methods in the context of ICME

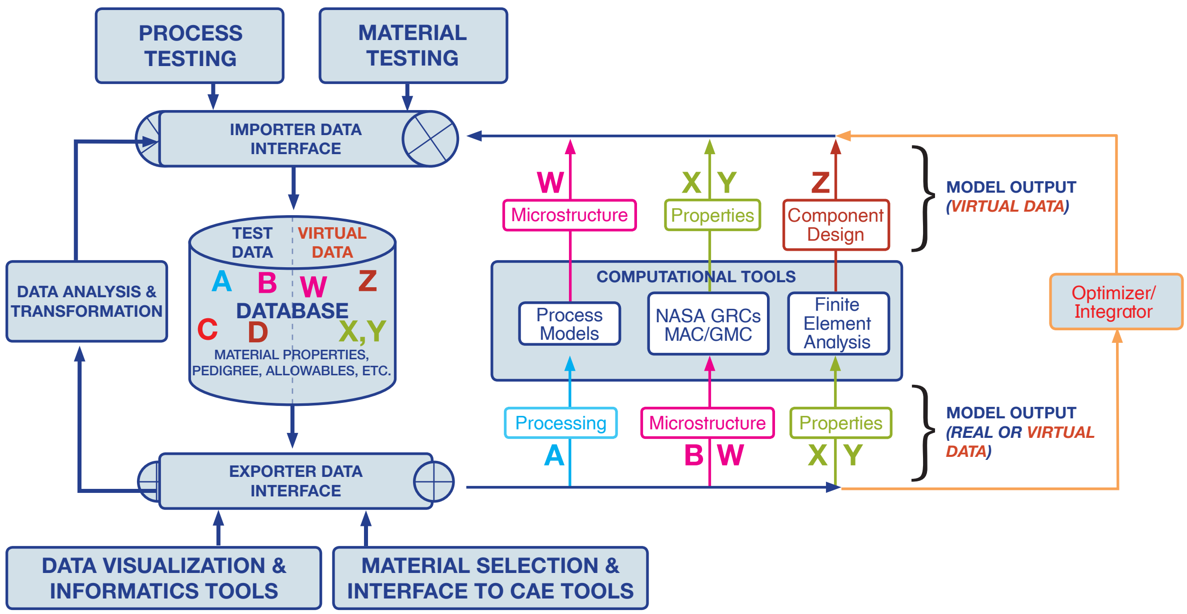


NASA Glenn's Schema Modified to Incorporate Virtual data to enable ICME



Recently, NASA Glenn and Granta Design established a workflow and demonstrated a unique set of web application tools for linking NASA GRC's Integrated Computational Materials Engineering (ICME) Granta MI® database schema and NASA GRC's Integrated multiscale Micromechanics Analysis Code (ImMAC) software toolset. The goal was to enable seamless coupling between both test data and simulation data, which is captured and tracked automatically within Granta MI® with full model pedigree information. These tools, and this type of linkage, are foundational to realizing the full potential of ICME, in which materials processing, microstructure, properties, and performance are coupled to enable application-driven design and optimization of materials and structures.

ICME infrastructure for housing both modeling and testing information



Significance for Vision 2040

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

References:

[1] Arnold, et al.; *"Combining Material and Model Pedigree is Foundational to Making ICME a Reality"*, IMMI, 4:4 DOI 10.1186/s40192-015-0031-2, 2015.

[2] Arnold et al.; *"Information Management Workflow and Tools Enabling Multiscale Modeling Within ICME Paradigm"*, 57th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference, AIAA SciTech 2016, ICME Special Session, Manchester Grand Hyatt, San Diego, California, Jan 4-8, 2016.

Example courtesy of NASA

Appendix C

Contributors

In developing this 2040 vision study, over 450 professionals from industry, government, and academia participated. The 200+ contributors listed in this appendix attended at least one of the four professional society-coordinated 2040 vision workshops and/or participated as panelists; panel participants are indicated by Key Element topic. The remaining 250 participated anonymously via a community-wide survey.

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