Integrated Computational Materials Engineering (ICME):

Implementing ICME in the Aerospace, Automotive, and Maritime Industries

TMS A Study Organized by The Minerals, Metals & Materials Society

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Warrendale, PA 15086

www.tms.org

Cover: Representation of the industrial sectors and the three main toolset arenas: properties, microstructures, and processing. Microstructure image used with permission from the article titled “Two-Dimensional and Three-Dimensional Analyses of Sigma Precipitates and Porosity in a Superaustenitic Stainless Steel,” published in the November 2007 issue of *Metallurgical and Materials Transactions A*, Figure 2 (a). Cover design by Dave Rasel.

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Acknowledgments

Integrated Computational Materials Engineering (ICME): Implementing ICME in the Aerospace, Automotive, and Maritime Industries draws on the contributions of almost 50 technical experts from industry, academia, and government, who donated significant time and effort to this study. These experts worked in five teams focused on the aerospace, automotive, and maritime industries, pervasive ICME implementation issues, and a careful review of a draft of the final report. The dedication and active involvement of all of the experts (complete list in appendix B) has been the major foundation of this effort. The information enclosed in this report represents the collective compilation of their efforts, and in no way represents the specific views of any of the individuals who contributed to this report, or any of their employers and/or affiliated organizations.

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with TMS as Materials Innovations Director). Nexight LLC staff members who were heavily involved and contributed mightily to this effort included Ross Brindle (Executive Vice President), Jared Kosters (Research Analyst), and Emily Maffett (Communications Specialist).

In the spirit of the "I" in ICME, this was truly an integrated, team effort in which all of the individuals named above worked together in a strongly cohesive, collaborative, and congenial manner.

John Allison, Automotive Team Leader
Brad Cowles, Cross-Cutting Team Leader
John DeLoach, Maritime Team Leader
Tresa Pollock, Aerospace Team Leader
George Spanos, Project Leader

Preface: Who Should Read This Report

This report will be of use to a variety of individuals within and beyond the materials community. It is not written solely for materials scientists or engineers, but rather for a range of stakeholders within industry, academia, and government, and across the spectrum of integrated product development teams and professional disciplines. Those who will particularly benefit from reading this report include the following:

- Professionals and leaders in the aerospace, automotive, and maritime industries
- Professionals and leaders in other materials-intensive industries
- University professors, researchers, students, and higher level managers
- Government scientists and engineers, program officers, and policy makers

Professionals and Leaders in the Aerospace, Automotive, and Maritime Industries

In part, the audience for this report includes a wide-ranging group of professionals in the aerospace, automotive, and maritime industries. This includes materials scientists or engineers, engineers from disciplines that work with materials in integrated product development teams (e.g., mechanical, civil, and electrical engineers), designers, ICME integrators (with experience leading ICME efforts), project managers, department heads, chief engineers, and chief executive officers (CEOs) who are interested in taking advantage of the great potential of ICME. Many company types within the supply chain are likely to benefit from this report including: raw material suppliers, primary material manufacturers, original equipment manufacturers (OEMs), tier 1 and tier 2 suppliers, and software companies.

Professionals in Other Materials-Intensive Industries

Engineers and managers in other materials-intensive industries also stand to benefit from reading this report. Although the case studies, frameworks, and recommendations presented here are primarily oriented toward the aerospace, automotive, and maritime industries, these concepts may be easily adapted to other sectors, including those with a focus on electronics, biomedical components, and a vast array of other materials types (e.g., semiconducting materials and magnetic materials). Additionally, the consumer products and infrastructure industries (e.g., bridges, buildings, and highways) and other energy and environmental sectors could all likely benefit from the ICME implementation strategies outlined in this report.

University Professors, Researchers, Students, and Higher-Level Managers

A wide spectrum of individuals within the academic community would also benefit from this report, including professors, graduate students, research engineers and technicians, undergraduate students, department heads, deans, and research vice presidents. The research groups themselves (professors, graduate students, engineers, and technicians) can contribute directly to the computational modeling, codes, and experimental validation needed to implement ICME by teaming with industry, and could thus benefit from a more detailed read of this report. Undergraduate students represent the ICME workforce pool in both the near and long terms; this report can provide them with knowledge of what ICME is and how it can be implemented. Higher-level university administrators could benefit from the executive summary of the report to gain a sense of how universities might engage ICME as an interdisciplinary endeavor across departments and as a platform for development of university–industry–government collaborations.

Government Scientists and Engineers, Program Officers, and Policy Makers

Technical experts and managers at national laboratories can use the knowledge provided here as a base from which to engage both industry and academia and contribute to ICME infrastructure and implementation. Government program officers and policy makers can use this report to help enhance government-supported ICME programs, and efforts related to the Materials Genome Initiative (MGI).

I. Executive Summary

Background and Motivation

The 2008 National Research Council (of the National Academies) study, *Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security,*[1] stated: "A new and promising engineering approach known as integrated computational materials engineering (ICME) has recently emerged. Its goal is to enable the optimization of the materials, manufacturing processes, and component design, long before components are fabricated, by integrating the computational processes involved into a holistic system." It was acknowledged even in its early stages that developing ICME represented a grand challenge but, if successful, would "provide significant economic benefit and accelerate innovation in the engineering of materials and manufactured products." In the context of the present report, ICME can be considered to encompass: *the integration of personnel (e.g., engineers, designers, etc.), computational models, experiments, design, and manufacturing processes across the product development cycle, for the purpose of accelerating and reducing the cost of development of a materials system or manufacturing process.*

Now that ICME is recognized as a nascent discipline and awareness is growing worldwide, the science and engineering community is at a critical juncture. In order to unlock the great potential of ICME and begin to realize this vision in an accelerated timeframe, the pathways to rapid implementation for practical engineering problems need to be defined in a more focused manner and within specific industrial sectors. This report identifies, prioritizes, and makes detailed recommendations for the frameworks and key steps needed to implement ICME in the near term in three critical industrial sectors: automotive, aerospace, and maritime. In addition, the report also addresses pervasive ICME issues that apply across all three sectors. This study also supports the Materials Genome Initiative (MGI) announced in June 2011 by President Barack Obama. In particular, this report makes specific recommendations on ICME implementation that, if undertaken, would support the MGI goal to discover, develop, manufacture, and deploy advanced materials at least twice as fast as possible today (at a fraction of the cost), and would support development of the MGI materials innovation infrastructure. Finally, the knowledge and recommendations in this final report, as well as the interactions and work performed on this project among members of the integrated working groups (referred to hereafter as ICME Implementation Teams), provide the basis for initiating, in the near-term, ICME-accelerated product development programs, primarily centered about structural light-weighting and propulsion applications.

Study Process, Utility, and ICME Implementation Team Composition

The ICME Implementation Teams were assembled to define the key steps needed for rapid implementation of ICME in the automotive industry, the aerospace/aircraft industry, and the maritime industry. In addition to identifying and analyzing ICME frameworks, key technical needs or gaps, and solutions to barriers to implementing ICME in the near term in these industrial sectors, a fourth key element of this study was to make recommendations for addressing pervasive issues that cut across all three industrial sectors. Therefore, a fourth team was engaged—the "crosscutting team." A fifth group, the "review team" reviewed a complete draft of the report and made significant contributions to its ultimate form and content.

Throughout this report, "near-term" ICME implementation is used to connote *starting* an ICME-accelerated product development program within 3 years (*not* producing a new product within the three-year timeframe). As such, the current report is intended to serve as a "field manual" for ICME implementation in the near term.

The detailed frameworks, actions, and recommendations provided here are to be viewed as building blocks, or templates for implementing specific ICME-accelerated product development programs (IAPDPs) within individual organizations. Adjustments will be required to tailor these frameworks and recommendations to a particular organization, and the specific product or materials system under consideration. The knowledge and recommendations provided here can also be used to make additions and/or adjustments to the structure/organization within individual companies and other organizations, to whatever extent they are feasible, as they are needed to enable much more rapid (and lower-risk) implementation of IAPDPs than would otherwise be possible.

Critical to the success of this project was the formation of teams with the proper blend of knowledge and experience across the integrated product development cycle. The five ICME Implementation Teams were composed of roughly 10 members each with experience in areas including: engineering, design, ICME implementation, primary material manufacturing, software development, and materials science and engineering. Although the majority of the team members were from industry, experts from government and academia were included on each team. Teams also included members with expertise in various structural materials categories, including steel, aluminum, polymer matrix composites, ceramics, magnesium, and titanium. Each of the three industrial ICME Implementation Teams focused on the following four tasks, as documented in the automotive, aerospace, and maritime chapters:

- Evaluating the current state of the art of ICME
- Defining frameworks for implementing ICME (in the form of integrated flow diagrams and tables that include actions and personnel required for implementing ICME)
- Identifying current barriers to ICME implementation, as well as recommendations for overcoming or circumventing these barriers in the near term
- Identifying application opportunities for implementing ICME in the near term

Current State of ICME in the Three Industrial Sectors

Case studies demonstrating the ability of ICME to reduce manufacturing costs and accelerate the development and deployment of materials in an integrated way have been identified in the aerospace and automotive industries. Examples include the development of a new corrosion-resistant alloy for landing gear by QuesTek, LLC; the insertion of low-rhenium alloys in aircraft engine turbine components by GE; and the Virtual Aluminum Castings (VAC) program by Ford Motor Company. Though the maritime industry may not have any such flagship application, this sector has made important contributions to building the ICME foundation and infrastructure of computational and experimental tools. Despite a few demonstrations of the great success of ICME in accelerating the development and deployment of new materials and manufacturing solutions in developing new products, ICME has not yet been implemented extensively in any of these industrial sectors.

Frameworks for Implementing ICME

In this study, frameworks have been developed for the automotive, aerospace, and maritime sectors to provide basic guidelines for companies seeking to integrate computational materials engineering approaches into their product development cycles and begin to establish ICME-accelerated product development programs within the next 3 years. These frameworks include flow diagrams and extensive tables that provide detailed actions needed at each of the many steps in the product development cycle, entry and exit points of the ICME portions of the cycle, suggestions for computational models and tools to use at various steps, skillsets and personnel needed at each step, and key decision points. These frameworks also include the flow of information and data within not only the computational materials engineering portions of the cycle, but across the existing upstream (beginning with the identification of customer needs) and downstream (ending with the serial production and in-service component/platform lifetime) portions of the full product development cycle. Each framework thus consists of three major items: (1) a general structure that depicts the entire product development cycle and includes the flow arrows of information and data, (see Fig. 1 as example) (2) a figure representing the ICME portion of the product development cycle, including some of the tools typically employed within each major tool suite, and the flow of information and data between these tool suites and, (3) an extensive table that lists the specific actions needed at each step within the ICME implementation framework.

Current Needs and Barriers to Implementing ICME

Although ICME has the potential to significantly reduce the costs and accelerate the introduction of new products in these three industries, challenges remain that must be addressed to better enable the widespread adoption of ICME within the next 3 years. This report considers these challenges and provides many recommendations for specific actions to either address or circumvent each issue in the near term. Although the detailed recommendations are far too lengthy to provide in this summary, general categories of these issues addressed by each ICME Implementation Team are summarized in Table I. There was significant overlap in the types of issues discussed by each of the three industrial ICME Implementation Teams. Key overlapping issues are addressed in the Pervasive Issues chapter, whereas the industrial chapters focus primarily on the issues that are specific to the corresponding industry.

Table I. Current Needs/Barriers and Their Solutions for Implementing ICME in the Near Term

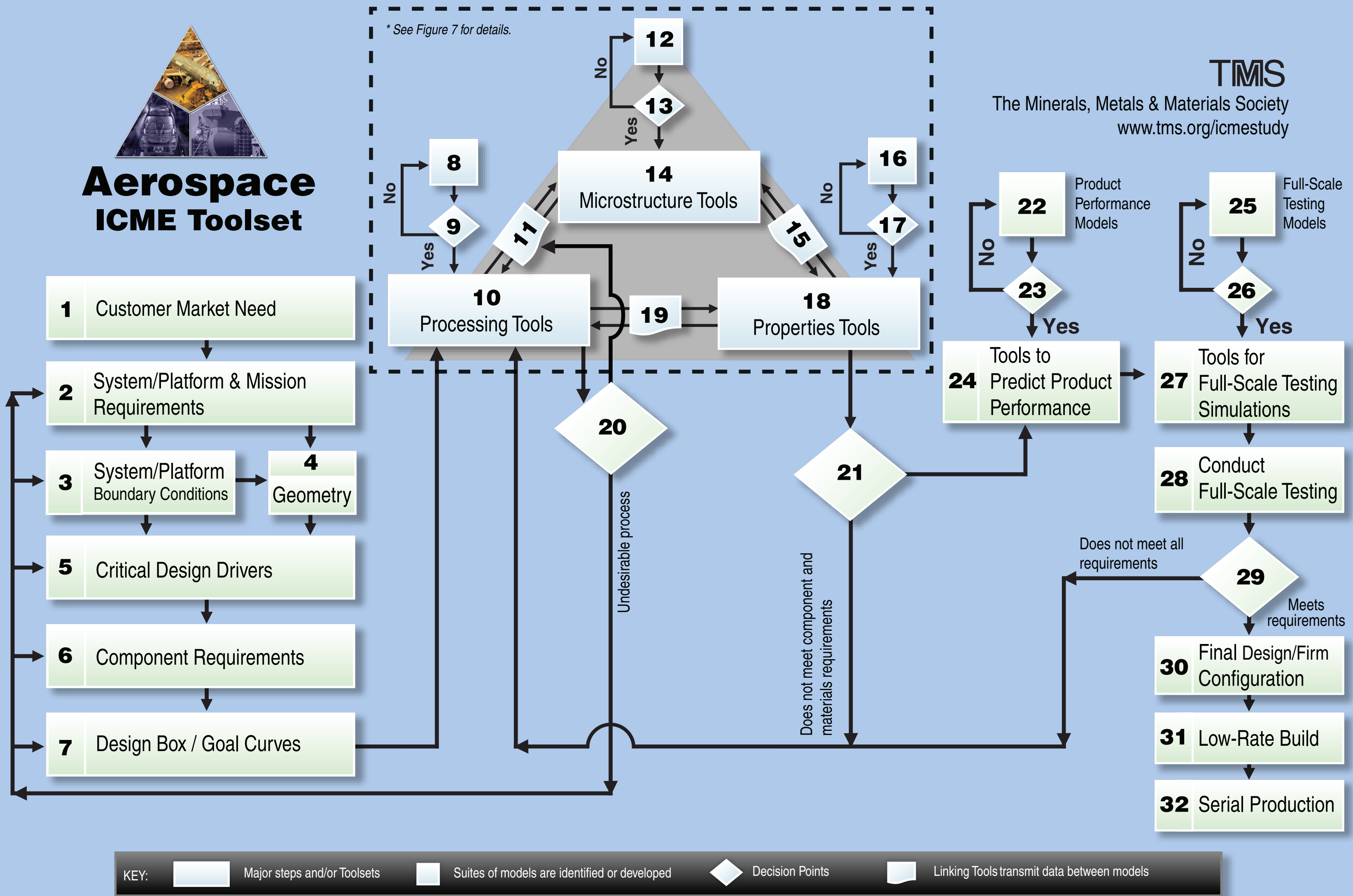
	Automotive	Aerospace	Maritime
Improved Quantitative Modeling Tools	x	x	x
Cultural Barriers and/or Intellectual Property Issues	x	x	x
Establishing a Business Case for ICME	x	x	x
Workforce Development	x	x	x
Lack of Past Experience in Implementing ICME		x	x
ICME Standards		x	x
Linkage Software and Tools	x		x
Regulations and Certification		x	

Near-Term Application Opportunities for ICME Implementation

While many new products could benefit from ICME approaches, each of the three teams identified specific near-term ICME opportunities. These recommendations included a wide range of ideas on how ICME can be used to accelerate the advancement of the respective industries. The full lists of recommended near-term application opportunities (a total of more than 50) for ICME Implementation in the Automotive, Aerospace, and Maritime Industries can be found starting on pages 53, 83, and 106, respectively.

Fig. 1. Aerospace ICME implementation framework. Specific instructions, personnel, and tools for each step are presented in more detailed frameworks and extensive tables within the chapters.

(Full details of actions and personnel at each step are provided in Table VII.)



Selected recommendations for near-term applications, for illustrative purposes only, include the following:

- High-performance alloy development for cast wheels
- Expanded use of cast or wrought magnesium for aircraft interiors, using better models to address concerns regarding the flammability of magnesium.
- Lightweight, low-cost watertight doors for maritime applications
- Out-of-autoclave composites processing (e.g., for seat structures, structural components)
- Development of weld sequencing protocols for structure optimization

Pervasive ICME Implementation Issues across Industrial Sectors

The highest-priority pervasive issues across all three industrial sectors, and the steps that can be taken to effectively address or circumvent those issues in the near term, were identified and analyzed by the crosscutting team. Detailed approaches to address or circumvent these issues were developed. A summary of those issues and the recommended approaches to address them is provided in Table II, with specific tactics for each recommendation/approach detailed in the full text of chapter III.

Table II. Summary of Pervasive ICME Implementation Issues Across Industrial Sectors *(Detailed recommendations for each issue are provided in chapter III)*
1: Creating a Business Case for ICME
A) Develop a quantitative economic case B) Document case studies and lessons learned C) Identify, pursue and support funded ICME efforts D) Develop tools that support concept development for new products E) Address patent, intellectual property, and export control issues up front F) Explore existing physics-based modeling tools
2: Implement Effective Verification and Validation, Risk Mitigation, and Tolerance of Models and Linking Tools
A) Use benchmark cases to assess and validate models, software, IT systems B) Identify required level of verification and validation (V&V) C) Identify minimum number of experiments needed to validate models D) Identify and apply practices for V&V consistent with some other disciplines

3: Establish Adequate Standards, Data, and Integration, Particularly in Manufacturing Supply Chains
A) Set data standards and classifications B) Develop data/workflow strategies C) Increase communication efforts between ICME stakeholders
4: Encourage Integration among Product Design, Structures, Materials, and Manufacturing
A) Initiate collaboration and team efforts B) Create education and training opportunities C) Develop techniques and programs that incentivize cross-pollination D) Enhance manufacturing process models E) Implement ICME enablers
5: Address Need for Personnel with ICME Expertise
A) Collaborate with other companies that have ICME experience B) Increase hiring efforts C) Create training and continuing education programs D) Develop new academic programs and curricula
6: Manage and Mitigate Uncertainty Quantification and Risk
A) Establish maturity level assessments B) Determine Uncertainty Quantification (UQ) methods and approaches C) Execute UQ techniques
7: Some Longer-Term Actions for Addressing Pervasive Issues and Advancing ICME
A) Support education and workforce development B) Fund ICME R&D efforts C) Develop new ICME tools D) Drive widespread acceptance of ICME by advocacy of ICME champions

Call to Action and Benefits of This Report

Professionals within the three industrial sectors addressed here (automotive, aerospace, and maritime) can use the knowledge base, frameworks, actions, required personnel types, needs and recommended solutions, and application opportunities provided in this report to tap into the great potential benefits of ICME, and consider initiating an ICME-accelerated product development program (IAPDP) within their organizations within the next 3 years. Readers in other industries can also take advantage of this report to provide templates for innovative ICME implementation activities within their companies. Such industries could include (but would not be limited to) those focused on non-structural applications such as electronics, functional biomedical components, and a vast array of other materials types (e.g., semiconducting materials and magnetic materials).

A number of groups outside of industry have clear calls to action in response to this report that could provide great benefits to not only their organizations, but to society as a whole, by tapping into the great potential of ICME to reduce the time to market and costs of developing new products and manufacturing processes. Stakeholders in academia could seek to apply the tenets of this report in the development of undergraduate and graduate curricula. In addition, researchers within academia and national laboratories can use the specific recommendations provided here to guide their efforts in partnering with and supporting the efforts of industry, such as building the computational models and codes needed to implement specific IAPDPs. Government agency personnel and policy makers can also use this report to help build and enhance government-supported innovative efforts in ICME and the MGI. Professional societies can play a key role in convening stakeholders in industry, government, and academia toward implementation of ICME in the near term by taking advantage of the knowledge gained from this report, as well as acting upon relevant recommendations.

As discussed in detail throughout this report and in the closing comments (section VII), this study thus offers benefits to a variety of different stakeholders in industry, academia, government, and professional societies. Due to the strong development of ICME-related experimental and computational tools, the growing worldwide recognition of ICME and its value, and the promising (yet limited) ICME success stories to date, it is now an opportune time for these stakeholders (i.e., the readers of this document) to act upon the recommendations provided here in order to help implement ICME much more broadly and begin to take advantage of its great potential benefits within the next 3 years.

II. Introduction

Integrated Computational Materials Engineering (ICME) is a relatively new discipline that has begun to show great promise in reducing the cost and time to design and deploy new materials and manufacturing technologies, while contributing to the creation of superior products. Although ICME has been successfully utilized in some product development programs to date, the industrial community has yet to move forward with broad implementation of ICME. This report presents detailed frameworks and recommendations that will guide implementation of ICME in the near term in the aerospace, automotive, and maritime industries. These frameworks can be adapted in a straightforward manner but also include crosscutting issues and ideas that have broader applicability to other industries. These frameworks and recommendations include detailed descriptions of the steps, actions, and decision points, as well as the personnel required at each step, throughout ICME-accelerated product development programs (IAPDPs). This report also considers some needs and associated recommendations, some immediate application opportunities for implementing ICME, and pervasive ICME issues across industries.

Integrated Computational Materials Engineering

ICME is growing in recognition and acceptance in science and engineering circles worldwide. In a 2008 report of the National Research Council of the National Academies,[1] ICME was described as "the integration of materials information, captured in computational tools, with engineering product performance analysis and manufacturing-process simulation." Although there has been some variation in the descriptions of ICME,[1–7] the most distinguishing characteristics that set it apart from other materials-related sub-disciplines are the "I" and "E" in ICME. That is, ICME involves the integration of personnel (e.g., engineers, designers, scientists, analysts, etc.), models, computational tools, experiments, tests, analyses, design, and manufacturing processes across the entire product development program. In a fully developed ICME approach, computational models and codes, informed and tested by targeted experimental verification and validation and integrated into the full product development and engineering cycle, accelerate the process and reduce the cost of developing a material or manufacturing process. This approach also allows engineers and designers to examine a larger design space more thoroughly and in a much shorter time than provided for by traditional empirical or experimental approaches. In the context of the present report, ICME encompasses: *the integration of personnel (e.g., engineers, designers, etc.), computational models, experiments, design, and manufacturing processes across the product development cycle, for the purpose of accelerating and reducing the cost of development of a materials system or manufacturing process.*

Integrated Computational Materials Engineering

In the context of the present report, ICME encompasses:

the integration of personnel (e.g., engineers, designers, etc.), computational models, experiments, design, and manufacturing processes across the product development cycle, for the purpose of accelerating and reducing the cost of development of a materials system or manufacturing process.

Value and Impact of ICME

ICME is oriented toward reducing the time and cost of developing a materials system or manufacturing process in order to support the development of advanced products. As outlined in the June 2011 Materials Genome Initiative (MGI) whitepaper,[8] approaches such as these offer strong promise to contribute to national goals including clean energy, national security, and general human welfare. At this time, there are relatively few ICME case studies or examples of implementation. ICME has just begun to demonstrate its potential to accelerate product development processes, yield improved returns-on-investments (ROIs), and improve the quality of life of consumers. Industry is poised for widespread ICME implementation, and the main goal of this study and report is to facilitate such implementation in the near term (≤ 3 years).

Early industrial demonstrations of the potential of ICME include a project led by Ford Motor Company that has, for some time, served as a flagship example of the potential benefits of ICME in the automotive industry. The Ford Virtual Aluminum Castings project (explored in more detail in the automotive chapter) is reported to have yielded a 7:1 ROI and a corresponding 15%–25% reduction in development time and led to a lighter engine design.[1,6] A second successful program, led by GE Aviation and explored in more detail in the aerospace chapter, led to a reduction of the rhenium (a rare and expensive element) in superalloys for aircraft engine turbine airfoil components.

The ICME approach taken resulted in the introduction of a new alloy in two years rather than the typical six years historically required for such a new alloy.[9] Another well-known ICME case study (described in more detail in the aerospace chapter) was the development of the corrosion-resistant Ferrium S53 advanced high-strength steel alloy by QuesTek Innovations for landing gear and other applications.[10] In this case, the use of ICME tools and principles resulted in significant reductions in alloy development time and an estimated development cost savings of nearly $50 million.[11]

Goal of This Study

The major goal of this report is to serve as a "field manual" for implementation of ICME on a much broader scale, in the near term. Throughout this report, the phrase "near-term" is used to connote starting an ICME-accelerated product development program within 3 years (as opposed to actually producing a new product or process within 3 years).[a]

Process of This Study: Five ICME Implementation Teams

Integrated working groups, referred to hereafter as the "ICME Implementation Teams," were assembled to define the key steps needed for rapid implementation of ICME in (1) the automotive industry, (2) the aerospace/aircraft industry, and (3) the maritime industry. Each of the first three teams addressed the following issues in their industrial sector:

- The current state of the art of ICME
- Frameworks for implementing ICME
- Current needs and barriers to ICME implementation, as well as recommendations for overcoming or circumventing these issues in the near term
- Application opportunities for implementing ICME in the near term

Although there were many unique issues and differences in the frameworks and approaches amongst the three industrial sectors, there were also common elements. Some areas of redundancy or overlap across the three industrial sector chapters were intentionally left in the individual chapters, so as not to inhibit a reader interested in a specific industry from missing important details. But, a fourth, key element of this study was also to make recommendations on the most significant pervasive issues that cut across all three industrial sectors. Therefore, a "crosscutting team" was engaged to provide foundational results and recommendations that can be applied more broadly to not only the three industrial sectors considered here, but to other industries as well.

Finally, a fifth team, the "review team," was assembled to review a draft of the final report and make detailed suggestions and edits.

a. 3 years was chosen in the present context to define "near term" for initiation of an ICME-accelerated product development program for two reasons: (1) to provide a quantitative reference point from which to focus the frameworks and recommendations for near-term ICME implementation (as opposed to focusing on long term infrastructure issues), and (2) because the team leaders and members reached a consensus that based on the current state of ICME, as well as their experience with product and manufacturing development in these industries, 3 years was an achievable goal.

Teams were assembled with systematic consideration of the required combination of expertise and experience across integrated product development cycles. The five teams were composed of roughly 10 members each and included engineers, designers, individuals with ICME project experience, primary material manufacturers, experts from software companies, and materials scientists and engineers. Although the majority of the team members were from industry, key members from the government and academia were also present on each team. The teams' expertise covered a range of structural materials categories including steel, aluminum, polymer matrix composites, ceramics, magnesium, and titanium.

Outputs and Limitations of This Study

The output of this study is an up-to-date summary of issues, opportunities, and recommendations that are intended to guide industry toward implementation of ICME much more broadly, rapidly, and with less risk in the near term. This output has been provided in the following specific forms:

- Frameworks for implementing ICME in three industrial sectors, in the form of integrated flow diagrams and related tables that include actions and types of personnel required at each step
- Current needs and barriers to ICME implementation, and specific recommendations for overcoming or circumventing these issues in the near term
- More than 50 near-term application opportunities for implementing ICME in the aerospace, automotive, and maritime industries
- Pervasive ICME issues and recommendations that apply across these and potentially other industrial sectors

It is very important to note that, although significant effort was given to composing the detailed frameworks, steps, actions, parties involved, and recommendations for the three industrial sectors in a way that would make them as comprehensive as possible, the entries in the tables and frameworks are to be viewed primarily as building blocks, or templates for these and/or other industries. For specific product development programs within individual companies or organizations, adjustments will be required to fit this methodology into the "boundary conditions" (e.g., facilities, personnel, and culture) imposed by that organization, as well as to the specific product under consideration. Although the ideas and recommendations provided here were centered about structural lightweighting (and to a lesser extent propulsion) applications, they can also be used more broadly to make relevant additions and/or adjustments to other ICME efforts within individual organizations (companies, universities, government institutions, and/or professional societies). In any case, it could be highly advantageous for integrated product development teams (IPDTs) to begin with these "templates" and make modifications, specific to the constraints within their companies. Similarly, the examples of codes, models, and experimental tests provided in the "actions" column of the framework tables are in no way all-inclusive or recommended for specific applications. They are instead meant to serve as inspiration to help organizations wishing to implement ICME, develop an understanding of the computational, experimental, and personnel resources needed, and adjust to their particular situation, to enable more rapid, lower-risk implementation of ICME-accelerated product development programs than would otherwise be possible.

III. Pervasive ICME Issues

Introduction to Pervasive Issues

Common issues arise for any engineering approach that uses computational approaches to accelerate the product development cycle. ICME is no exception to this rule. For ICME, many of the needs and potential obstacles to broad implementation within the science and engineering community will likely not be solved in a complete fashion in the near future. However, significant strides can be made toward overcoming or circumventing a number of these issues in the near term. This chapter contains a review of some of the most significant needs and barriers facing ICME implementers across the three industrial sectors considered here (and possibly others), and provides suggestions on how they may be overcome or circumvented to allow for the successful execution of ICME projects. One overarching concept that will provide context for most of the specific pathways recommended in this chapter is that increased communication and collaboration among stakeholders throughout the product development cycle can make a strong contribution to the development of effective strategies for the near term, and are a key to establishing effective solutions in the long term.

ICME requires the active engagement of multiple parties and necessitates a robust team structure and efficient methodology. The success of the IPDTs (integrated product development teams) described in this study will rely fundamentally upon the expertise and collaboration of the materials engineers, project managers, component designers, and other stakeholders in the projects. The personnel in these projects should have the ability to merge the use of computational methods with practical, established engineering applications and achieve outcomes within acceptable degrees of certainty. The initial adoption of these approaches within an organization can present significant risk and requires a substantial, ongoing financial commitment. The maturity level of ICME-accelerated product development projects is currently relatively low for the majority of the science and engineering community. In addition, teams interested in carrying out an ICME project generally do not have comprehensive standards for sharing and maintaining computational tools and databases. This includes a lack of protocols for managing error and uncertainty and for verifying and validating modeling tools with experimental results. The ICME community recognizes many of these issues, which they can address through both near-term strategies and longer-term cultural shifts to ensure the widespread adoption of ICME by the science and engineering community. Therefore, this chapter will describe the following issues in more detail and provide proactive strategies and specific recommendations for addressing the needs listed in Table III. Following treatment of near-term strategies, the Pervasive Issues chapter also presents a number of longer term strategies for overcoming barriers to broader uptake and adoption of ICME approaches.

Table III. Pervasive Issues
1: Create a business case for ICME
2: Implement effective verification and validation, risk mitigation, and tolerance of models and linking tools
3: Establish adequate standards, data, and integration, particularly in manufacturing supply chains
4: Encourage integration among product design, structures, materials, and manufacturing
5: Address need for personnel with ICME expertise
6: Manage and mitigate uncertainty quantification and risk
7. Some long-term actions for addressing pervasive issues and advancing ICME

Process Overview

Following the meetings of the individual sectors, members of the crosscutting group convened to discuss the pervasive issues facing ICME implementation across the automotive, aerospace, and maritime sectors. With the aid of liaisons from the three industrially focused teams, the crosscutting team was able to evaluate the state of ICME across the three sectors. Prior to the meeting, participants created a list of the most common pervasive issues in launching ICME-accelerated product development programs and provided some potential ways to deal with the issues. During the workshop, the group used these ideas as a basis to identify and define the highest-priority issues (shown in Table I) that all ICME implementation programs need to address and the steps to take in the near term (within 3 years) to implement an ICME-accelerated product development cycle that effectively addresses or circumvents those issues.

1: Create a Business Case for ICME

Convincing stakeholders to adopt ICME methods as a way to discover, develop, and deploy advanced materials cheaper and faster can be a challenge. The modeling software, supporting databases, and qualified personnel are significant investments to begin an ICME-accelerated product development program (IAPDP), and are often viewed as a substantial business risk from the perspective of management. Typically, stakeholders rely on numerous relevant case studies to develop a plan with a sound business structure and fiscal strategy to ensure they achieve their expected return on investment (ROI), but these are still in limited supply for ICME. This section identifies issues that companies new to ICME will inevitably encounter and lays out sound tactics to construct a business case and successfully adopt ICME-accelerated product development methods.

How to Address the Issue

Actions that can contribute to making a business case for ICME within a company within 3 years are presented within the following categories:

A. Develop a quantitative economic case
B. Document case studies and lessons learned
C. Identify, pursue, and support funded ICME efforts
D. Develop tools that support concept development for new products
E. Address patent, intellectual property, and export control issues up front
F. Explore existing physics-based modeling tools

A: Develop a Quantitative Economic Case

To develop a strong economic case favoring the implementation of ICME, it is important for companies to provide a sound quantitative analysis that details the benefits. Specifically, supporters of ICME need to define how an ICME-accelerated product development program can reduce the risks, costs, and/or time expenditures associated with technology development and insertion into a project. Contributions to such reductions include decreased testing requirements; reduced risk, time, and iterations for the materials and process development; and the elimination or reduction of costly traditional product iterations. To assess substitute material costs, business case developers should consider the complete manufacturing chain of that particular material or component rather than just the cost of the raw material, so as to demonstrate reduced cost or time expenditures in order to substantiate any material or process substitutions. Since different materials have different characteristics, limitations, and design constraints, the aspects of the product design can vary in order to take advantage of the unique properties of the materials considered. As a result, when assessing material substitution, cost models should utilize an overall systems approach wherever possible.

B: Document Case Studies and Lessons Learned

Successful case studies can demonstrate the benefits of ICME to stakeholders and potential adopters. Examining how competitors are using ICME and finding examples that have resulted

Develop a Quantitative Economic Case

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in time savings, decreases in the number of experiments needed, and/or reduced risk may support the internal case for ICME implementation. Some successful ICME case studies are included in publications such as the 2008 NRC ICME Study,[1] *Integrative Computational Materials Engineering*, edited by Georg Schmitz and Ulrich Prahl,[2] and *Integrated Computational Materials Engineering (ICME) for Metals* by Mark Horstemeyer.[4]

Whenever possible, once they have obtained the necessary information to proceed with a business case, companies can utilize case studies of ICME cycle-time compressions to provide quantitative information that can be used to verify and document the potential ROI for an IAPDP. A convincing, quantitative business case will include, if possible, case studies of developing and improving materials systems with maturity levels that were previously lower than ideal; this would demonstrate the capacity for ICME-accelerated methods to improve materials systems. The complete quantitative assessment may also include an examination of non-ICME product development programs that experienced problems and explanations of how ICME could have eliminated or helped to identify the problems earlier in the development process.

C: Identify, Pursue, and Support Funded ICME Efforts

To create a successful business case for ICME, it is important for companies to demonstrate that there is a trained workforce capable of developing and launching an IAPDP. One way to stimulate growth within the ICME space is for companies to partner with small businesses and fund projects at universities that have multidisciplinary innovation centers and ICME research and development (R&D) programs that can help companies develop appropriate models and tools. Later, hiring university students who have been supported through these programs could serve as an effective ancillary strategy for preparing a company to implement and make the case for future ICME endeavors.

D: Develop Tools that Support Concept Development and Optimization for New Products

A method for demonstrating the potential impact of ICME is for companies to construct "what if" scenarios and propose potential materials property combinations to develop virtual products that can be used to develop a persuasive business case. Advocates of ICME can execute these "mock" scenarios and make assumptions on the accuracy of ICME tools[b] to establish a value proposition for ICME approaches. In addition, companies can propose and pursue internal efforts to conduct periodic, system-level concept studies and identify existing and low technology readiness level (TRL) technologies that are suitable candidates for applying ICME methods.

E: Address Patent, Intellectual Property, and Export Control Issues Up Front

Companies should address issues involving patents, intellectual property rights, or export control early on in the development process to identify and avoid potential problems and time delays further downstream. They can scan the intellectual property and export control documentation and resources and identify the product and manufacturing opportunities which are available for their company, and in parallel use ICME to establish parameters for a broad range of new products, processes, and/or patents. Additionally, certain computational software has been used to guide patent development and has even demonstrated the ability to reverse-engineer product patents from existing products. Although intellectual property issues are a reality in a competitive manufacturing economy, there is much to be gained by leveraging collaborations and information sharing in the pre-proprietary space. Companies should determine the furthest extent of their pre-proprietary threshold for a given product or manufacturing development program in advance, and in making the business case include taking full advantage of leveraging existing or past efforts by others, rather than considering unnecessary expenditures of time and money for "reinventing the wheel."

F: Explore Existing Physics-Based Modeling Tools

An exploration of existing physics-based predictive modeling tools, including codes that are not commonly used in current design efforts, is an important step in determining the overall parameters of an ICME project. The use and demonstration of multiple physics-based computational codes can help integrated product development teams (IPDTs) make a more compelling case for adopting

b. In the present context, "ICME tools" refers to computational (or experimental) tools that are used within the ICME portions of the product development cycle. These tools compose the "ICME toolset" but do not have to be exclusive to that toolset. For example, many computational tools such as DEFORM, phase field codes, etc. might be employed only within the ICME toolset; whereas, experimental tensile testing can be used to validate ICME models and would thus be considered part of the ICME toolset in this context, even though it is often used throughout other parts of the product development cycle as well.

ICME and help them arrive at powerful solutions that are representative of real-world conditions. By working to assemble these existing predictive tools together into an ICME-accelerated framework, companies can develop out-of-the-box solutions that would not be possible under traditional product development programs and can provide a competitive advantage in the marketplace. Efforts can be made to combine these modeling tools, such as coupling microstructure models with materials processing models and linking manufacturing procedures with materials development procedures.

2: Implement Effective Verification and Validation, Risk Mitigation, and Tolerance of Models and Linking Tools

Whether a business is focused on initial implementation or long-term sustainment of ICME approaches, it is essential for the IPDT leading the ICME project to ensure that their model tools and simulation results are accurate and representative of real-world conditions. Verification of computational codes confirms the proper execution of physics formulas and code, and validation utilizes targeted experiments to confirm that the simulations are grounded in physical reality and within an acceptable degree of confidence. To minimize error, extensive experimentation has to be conducted to verify and validate the computational models. Not only can these experiments be costly, but there are no established standards for different types of model validation. Evaluating the maturity and functionality of modeling tools and determining the parties responsible and procedures for verifying computational codes and validating these tools all add complexity to the verification and validation processes, but there are certainly steps that can be taken, even in the near term, to address these issues.

How to Address the Issue

While the introduction of ICME methods into product development cycles can reduce cost and deployment times, teams need to follow guidelines to ensure that modeling predictions are accurate and reliable. Actions that have the potential to overcome or circumvent issues with the effective verification and validation (V&V)[c] of models and linking tools within 3 years are detailed below.

Wherever possible the relevant personnel involved in an ICME project might define or use benchmark cases to assess model capability and validate the model, software, and IT systems. Some software firms have standard benchmark cases for this purpose while others can obtain a third-party benchmark study.

To effectively verify and validate models, the IPDT needs to first identify a required level of V&V for the design phase and define standards for the types of model validation. After identifying the varied components involved in a given problem that would be addressed computationally versus experimentally (e.g., thermodynamics, continuum, microstructure, strength, casting, and joining), the team can conduct a cost-benefit analysis to assess which approach is most beneficial.

Next, they could identify the minimum number of experiments needed to validate the models

c. Verification here refers to demonstration that a computer code provides an accurate mathematical representation of the fundamental engineering principles and relationships that it is designed to represent; Validation here refers to demonstration that the model provides accurate predictions of some materials-related property or behavior within a defined domain, accomplished via comparison of model outputs with the results of controlled experiments.

(e.g., high-throughput measurements) and determine who should validate a commercial model or code (e.g., end user, supplier, etc.) and how the parties can work together. To update the model's V&V process based on the experimental data, software users will need to develop standards to compare experiments and models in a statistical framework. Verifying the mathematical operations within computational codes, and experimentally validating modeling results with quantified uncertainties will help convince decision makers to trust the ICME results for that specific application.

To validate models for a certain set of calibrated input data, the IPDT can identify and apply a recommended practice for ICME V&V that is consistent with other disciplines and assess the level of V&V needed based on the ICME application and risk/consequences to a specific system or product. This assessment should align with Technology Readiness Level/Tool Maturity Level (TRL/TML) ratings of systems and known IPD processes. It is recommended that the team apply TML concepts or equivalent methods to assess, improve, and communicate the capability of the ICME tools, and to plan ICME V&V activities.[12] They could then also employ risk and consequence information to identify risk mitigation plans for specific applications and across the product development cycle.

Once they have met V&V requirements and used validation to quantify the confidence in the prediction, the IPDT members can use this process as a framework for future ICME-accelerated product development cycles. It is important that they understand the level to which the model and experimental results are in agreement and identify any potential reasons for disagreement; organizations may choose to alter V&V procedures during the next ICME-accelerated project so that the model is more useful. When completed at one stage, V&V can also provide clues for how to improve models downstream before they become linked, allowing ICME to be implemented more efficiently across the complete system or supply chain.

Finally, it is important that whenever possible the people working within the ICME portions of the integrated product development team communicate and collaborate with relevant software vendors. It takes a critical mass of users in order to get new models developed and implemented into commercial (or even public domain) software. Software vendors are customer oriented and do not often have the resources to undertake the development of constitutive models and robust experimental validation.

3: Establish Adequate Standards, Data, and Integration, Particularly in Manufacturing Supply Chains

As ICME is a relatively new approach to materials and process development, few established standards exist for constructing and maintaining database structures with accessible, exchangeable information. Software codes and modeling tools require large databases to ensure accurate prediction of materials processes, structures, and properties. Additionally, the integration of these tools among ICME-accelerated organizations requires strategies for efficient communication and workflow.

How to Address the Issue

Sharing advanced data and tools within teams and across organizations can enhance computational efforts and help cultivate a culture of ICME. Actions that have the potential to make progress toward overcoming or circumventing problems with inadequate or unusable data structures and/or content within 3 years are presented within the following categories:

A. Set data standards and classifications
B. Develop data/workflow strategies
C. Increase communication efforts between ICME stakeholders

A: Set Data Standards and Classifications

To set effective data standards, a first step for companies and other organizations in the manufacturing or ICME chain is to catalog information on available standards and collect case studies that provide the reasoning behind standards selection. It is also important that teams working on ICME projects clearly define taxonomies (i.e., classifications into categories or related groups) for materials-related data, in the same fashion that has been done more robustly in biology, for example. Refining assessments of proprietary data and putting contract requirements in place to deliver the data could also represent important steps in developing these taxonomies and standards, especially for government-supported data generation, since government does not always require documentation and delivery of data. Professional societies can set precedents by helping develop data content and format standards for information related to ICME (e.g., microstructure and materials pedigree) and for materials processing details beyond approximate or nominal values. Once data of interest is acquired in a standardized format, and includes the "metadata" related to the details and history of how the data was acquired, the data users should consider developing a system interface that is well defined in terms of the transfer of data and information. Such an interface could employ systems engineering approaches that include the development of requirements, interface control, and configuration management plan documents to manipulate and transfer the data.

B: Develop Data/Workflow Strategies

An effective data management strategy (e.g., for storage, access) will document the workflow through all data analysis steps. Systems developing in support of this strategy must be flexible and enable automatic updates, as standards evolve and change, and should allow for easy translation of published data into the format required by the computational tools used. Within these databases, it is best to keep the data in its rawest form possible for archival purposes rather than storing only the manipulated data, as some data (e.g., Gibbs energy functions) cannot be derived backwards easily or without a loss of resolution. It is also important for the storage and sharing of metadata[d] along the manufacturing chain to be automated in these databases. If the process of storing raw data is automated with ICME modeling and linking tools, it will ensure that the data is retrievable and reusable. In the event that any relevant attributes are missing from the stored data sets, the IPDT can assume or estimate values from given data distributions and follow with uncertainty quantification (UQ) and management strategies. Incomplete data sets may limit the use of certain modeling tools; therefore, wherever possible to would be best if modeling tools could be flexible in this regard.

d. Metadata refers to the attributes (or "data") that describe some specific data content. For example, the metadata for properties data, such as yield strength, might include (but is not limited to) the material composition, the material processing conditions, the specimen geometry, the test standard, the test temperature, and the date of the test to determine the yield strength.

Following the development of these protocols, it is very beneficial to establish, document, and enforce an internal standards policy within an organization and data supply chain and document and publish the necessary data formats and storage protocols, both internally and with data suppliers.

C: Increase Communication Efforts Between ICME Stakeholders

Building a collaborative environment for a cross-disciplinary ICME team to share data, tools, and concepts is a critical part of increasing communication among stakeholder groups and encouraging active engagement. Although the "language" barrier can occasionally present a challenge to convening individuals from varied backgrounds and disciplines to work together on data issues, online systems and special interfaces could be extremely useful (some are currently available in basic forms) to exchange information, and concepts for discussion sessions. A standing technical committee within a professional society could simultaneously facilitate the exchange of information regarding ICME projects and identify pressing issues while defining the data attributes needed in those particular applications.

4: Encourage Integration among Product Design, Structures, Materials, and Manufacturing

The traditional integrated product development team arrangement has not typically included materials scientists and engineers working in concert with designers and manufacturing engineers, except in a support role. The power of integrated design/manufacturing groups that include materials experts to develop and implement new technologies was recognized in a 2004 National Research Council study focused on accelerating technology transfer in the defense industry.[13] To realize the true potential of a multi-disciplinary approach to product development, it is essential that materials engineering be integrated seamlessly with product design and manufacturing—which requires a heavy reliance on computational as well as traditional, experimental, and testing approaches to materials engineering. Once this is achieved, predicted benefits include significant reductions in the cost and time to deploy new products, which will ultimately increase manufacturing competitiveness. However, until clear pathways are defined toward this integration, there remains a significant impediment to forming and engaging the most effective IPDTs in the ICME process.

How to Address the Issue

Actions that have the potential to begin overcoming or circumventing the lack of integration among product design, materials, and manufacturing processes within 3 years are presented within the following categories:

A. Initiate collaboration and team efforts
B. Create internal education and training opportunities
C. Develop techniques and programs that incentivize "cross-pollination"
D. Enhance manufacturing process models
E. Implement ICME enablers

A: Initiate Collaboration and Team Efforts

A first step toward integration would be developing a cross-functional team comprised of members from design, materials, and manufacturing teams. This would initiate inter-organizational conversations regarding the incremental integration of procedures and, ultimately, the inception of an ICME-accelerated product development cycle through its launch and execution. Regular meetings between team leaders from the various disciplines or organizations to review the status of integrated design and manufacturing and identify ways to leverage each other's efforts can serve an important role in advancing ICME and other interdisciplinary efforts. In many companies, this may be most effective when focused on the conceptual development and optimization stages of product development where the impact of new materials or manufacturing processes may be greatest.

B: Create Education and Training Opportunities

Internal training programs taught by internal or external experts in ICME can bring together staff needed to drive implementation and motivate them to work together. In addition, specialized training can demonstrate the value of an ICME-accelerated product development program (IAPDP) to employees as well as the needs and requirements of such a program. Educating employees, specifically senior management, on the need to adjust the organization and internal processes to make ICME happen is a critical step in obtaining employee support and inspiring change. Senior management would particularly benefit from being educated on the potential ROI as well as the multi-year commitment required to achieve it. Another possible focus area would be the education of materials and process engineers in the use of computational tools for product design and structural

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analysis. Such cross-disciplinary skill training would facilitate better understanding, communication, and appreciation for computational methods that are currently used in product development (see also “Create training and continuing education programs” on page 25).

C: Develop Techniques and Programs that Incentivize “Cross Pollination”

It is critical that companies and other organizations implementing ICME tools devise ways to use such tools to incentivize team members to integrate design, ICME-enabled materials engineering, and manufacturing into product development programs. This needs to be done across departments within a given organization, as well as across multiple organizations. Web portals that encourage collaboration and the exchange of ideas, data, tools, and concepts (e.g., Purdue’s nanoHUB[e] and social networking and collaboration sites such as the MGI Digital Data Community[f]) can strengthen communication among team members and encourage collaboration across companies, professional societies, national laboratories, and academia. Companies interested in adopting ICME could work with small businesses, software companies, and universities to transition their theoretical approaches and research tools to practical approaches and validated engineering tools. As part of the “ICME supply-chain” described in a 2011 *JOM* article,[14] universities, national laboratories, and software companies can play a critical role in providing computational resources to teams engaged in ICME accelerated projects. Holding internal workshops on these topics can help stakeholders within companies identify opportunities for ICME, agree on data structures and interfaces, and establish sensitivity rankings and accuracy targets for the purposes of highlighting quantifiable goals in materials predictions. Progress toward ICME model development and implementation may be incremental and will likely require the effort of many personnel across varying disciplines within a company. Having a forum for presenting progress and issues will also benefit ICME integrators and other members of IPDTs working on ICME projects across many companies, as well as advancing the discipline as a whole.

D: Enhance Manufacturing Process Models

Process models require a wide range of physical and kinetic material data which necessitates the use of user-defined material (UMAT) subroutines, in the case that materials model libraries do not accurately represent materials behavior. To advance these manufacturing process models, developers can determine the high-priority requirements for design and materials property inputs, and identify generally used manufacturing process models that are in a format capable of integrating more specific predictive models related to ICME. Then the specific models, such as response surface methodologies (e.g., via *ab initio* calculations), can be explored, developed, and subsequently integrated into the manufacturing process models. Additionally, most advanced manufacturing process models could be made to work with parametric geometry software tools (some examples are shown in Appendix C), which allow for easier modification of the size and shape of a component of interest. Enhancing manufacturing process models in this way could be a critical element in early materials-related quantification of manufacturing process capability and limits, which today is largely empirically based.

e. Available at https://nanohub.org/.

f. Available at http://www.mgidata.org/Home/.

E: Implement ICME Enablers

In order to speed the adoption of ICME approaches, organizations could assess predictive manufacturing tools (especially for process modeling) and work with in-house "ICME integrators" or outside contractors to determine how to integrate them into specific applications. This includes collecting or defining manufacturing process variables for use in ICME evaluations and identifying scenarios and potential capabilities that are believed to be possible or achievable through ICME. Companies could also benefit in this regard from reviewing any publicly available information on government ICME implementation programs such as government efforts that have integrated design, structures, materials, and manufacturing processes, as a model for government agency leadership in ICME implementation and acceptance. Prior to developing more fully integrated tools, IPDTs may also wish to identify and mitigate internal organizational barriers that may limit the use of software licenses (e.g., cost, IT, and policy) across departments and sites and thus impede ICME acceptance and implementation. The teams might also consider leveraging current practices from other disciplines, such as quality-of-information-driven uncertainty quantification (UQ) techniques based in the information sciences.

5: Address Need for Personnel with ICME Expertise

ICME is a relatively new paradigm in the development of materials and components that requires integrated product development teams (IPDTs) to bring a knowledge base of traditional processes to bear on computational approaches. As recognized, for instance, by the leaders of a GE Aviation program utilizing ICME, though the utilization of linked models connecting processing, microstructure and properties can accomplish a great deal, the true framework for such activities is the knowledge base and expertise of the users.[15] In the ideal scenario, the personnel leading ICME projects (referred to in this report as ICME integrators) would be professionally trained in both experimental materials science and modeling or computational methods. However, ICME curricula are not fully integrated into academia, necessitating industrial stakeholders to assist in defining the educational needs and providing the expertise to accomplish this. Because these cutting-edge product development processes lack standards and relevant case studies to guide new ICME Integrators, adoption of these processes requires that companies employ or have access to significant staff resources from experts trained in ICME. The current workforce of materials scientists and engineers also lacks sufficient proficiency in overall computational engineering methods, creating a gap which calls for both a short and long-term increases in available computational engineering and ICME training and professional development programs.

How to Address the Issue

Many concerted efforts have the potential to provide necessary training for the current workforce, offer near and/or long-term solutions to increase the number of professionals in the field, and boost the competitiveness of materials manufacturing industries. Actions that have the potential to begin overcoming or circumventing the barrier to ICME implementation imposed by the lack of skilled ICME integrators within 3 years are presented within the following categories:

A. Collaborate with other companies that have ICME experience
B. Increase hiring efforts

C. Create training and continuing education programs
D. Develop new academic programs and curricula

A: Collaborate with Other Companies that Have ICME Experience

ICME-accelerated product development approaches require significant investment from companies that are new to these approaches. These companies are under pressure to achieve initial success and help encourage the continued adoption and sustained use of ICME. While case studies are an excellent resource for illustrating the successful application of modeling tools in materials development, there are so few well known case studies that they do not provide sufficient information to encourage broad emulation. However, partnering with a company that is mature in its use of ICME can provide these new adopters with the guidance and support they need to achieve success. As ICME is still a new way of doing business, such partnerships benefit both parties by helping them identify and establish best practices and effective approaches for implementing more integrated computational methods. Owing to the competitive landscape, this could be done either amongst companies that already work together (e.g., a materials supplier and platform/component manufacturer, such as a steel company and a shipbuilder), or companies that work in the same competitive space but can leverage each other to provide precompetitive advantage for both.

B: Increase Hiring Efforts

Hiring experts or skilled ICME integrators can help companies establish a strong foundation for launching a successful IAPDP. A strategy to help management make smart hiring decisions and build an effective team with the necessary expertise is to form a panel of product designers, materials engineers, data analysts, and others to assess internal capabilities and identify areas where additional help is needed to support and provide leadership for non-ICME personnel in new integrated computational methods. Hiring need not require large numbers of new personnel but rather, can entail a very selective and focused search for ICME leadership and other highly skilled members of an ICME oriented IPDT (such as skilled software users, test engineers etc.). Once new personnel are in place, organizations can establish an internal ICME crosscutting team that features members from different disciplines. While this internal support group does not necessarily need to be rigorously structured within the organization, members should view team interactions as opportunities to share knowledge and ideas while fostering the integrative culture of ICME within the company.

C: Create Training and Continuing Education Programs

Customized online training and traditional hands-on education courses can help employees and students gain critical skills and reduce the proficiency gap among members of an industrial product development team. To develop and launch successful training and continuing education programs, companies can first determine their overall needs with regard to applications that could benefit from an ICME-accelerated approach. Instructors could use real-world, industry-specific scenarios as much as possible when designing the course content, structure, and modules, as this approach may be more useful than training employees in general software use.

The effort to further education and training in ICME needs to be driven by collaboration to achieve optimum results. Academics working together with industry engineering experts will typically combine technical and pedagogical expertise to achieve maximal results. Professional societies could play an important role in supporting the networking needed to make this happen, utilizing their memberships to help define the skills needed to meet specific ICME needs, and in some cases directly organizing and providing the continuing education courses. In addition to current efforts to provide support for cross-disciplinary training and badge or certification courses, companies might consider dedicating funding to retraining current workforce employees in emerging technical areas associated with ICME via the approach described above.

D: Develop New Academic Programs and Curricula

Providing a strong educational foundation for students will be instrumental in building a workforce that has the skills required to launch effective ICME-accelerated programs. This can be approached in a number of different ways, almost all of which will require educational innovation, computational resources, and support for faculty to develop these new resources. Any curriculum changes will also have to be made in coordination with the university's accrediting body (e.g., ABET).

A first step could be to introduce ICME skills into existing Materials programs, particularly in capstone design courses. Perhaps a more challenging endeavor is to establish five-year Bachelor's/Master's interdisciplinary degree programs that combine traditional academics with hands-on industrial experience and perspective to allow degree-seeking students to join programs that offer academic credit while giving them the opportunity to work closely with members of industry. This type of approach requires synergy between universities and companies, and is currently underway at Northwestern University.

A longer range plan for companies and members of the academic community to develop the ICME workforce is to establish collaborative ICME "university centers" to encourage training and hiring of M.S. and Ph.D. ICME students. In addition to developing relationships with students who are pursuing their degrees, enacting a 1-year residency or internship within industry would provide opportunities for these students to apply theoretical coursework under the supervision of a company mentor; such integration of real industrial issues into the academic program is regarded as extremely useful.

Leveraging U.S. Department of Energy (DOE), Department of Defense (DoD), National Science Foundtion (NSF), and other agency funding in the field can be another successful way to generate discussion about ICME and engage outside talent. Industry-academia consortia can also be developed to offer student fellowships that have a computational component to the students' thesis and emphasize, for instance, maritime-relevant technologies such as welding. A funded ICME Center of Excellence hub funded by DOE, DoD, or NSF could house experts in particular topics and provide a pathway to establish best practices and offer industry members the chance to contract experts to address specific problems. A computational mechanics subset, or discipline, could potentially reside within the Center of Excellence, training ICME integrators who are proficient in merging traditional engineering product development processes with new computational methods and tools. Such approaches could be taken by various agencies and programs, such as the NSF

Industry & University Cooperative Research Center (I/UCRC) program, DOE Energy Innovation Hubs, or DoD ManTech Centers of Excellence.

In the absence of a new degree program dedicated to ICME, colleges and universities could move to require materials science and engineering students to graduate with at least basic ICME knowledge and the ability to apply their engineering and design experience to ICME problems. Amending the current educational requirements, though, is a difficult, longer-term solution, which will require changes to course materials and curricula and persistent ongoing demand from industry. Any changes in requirements would also have to be made within the context of ABET requirements, and such planning would benefit from universities collaborating with the relevant ABET professional/technical societies working in ICME-related areas. Through industrial partnerships with select universities, companies could encourage faculty to teach ICME skills while utilizing an outreach network to attract highly qualified students. Taken together with the recommendations above, this is essentially a call to industry to become more involved and invest in education of the domestic ICME workforce in order to support near-term and future successes in this area. Likewise, faculty members would benefit from a better understanding of industrial needs by developing strong relationships with appropriate industrial members of IPDTs including scientists, engineers, designers, and managers.

6: Manage and Mitigate Uncertainty Quantification and Risk

There is often skepticism associated with modeling results that predict materials processes, structures, and properties. In addition to the error quantified in computational simulations, skeptics associate additional uncertainties with ICME programs. For example, the integrated product development teams leading ICME projects are not always involved in producing the starting materials for a component, instead relying on suppliers who have to fabricate materials that ultimately play a leading role in meeting final component property and performance requirements. The fact that materials processing is often spread across multiple teams or organizations introduces difficulties relating to the passing of materials data and models, especially in regard to quantifying the uncertainty associated with such information. Integrated product development teams must ascertain whether all modeling tools and data utilized—those generated in-house or elsewhere—are reliable and functional and the associated uncertainty is quantified for their specified uses across the overall IAPDP.

How to Address the Issue

Determining maturity levels to rate the abilities of ICME staff, methodologies, and computational tools is a new concept and part of an effort to address uncertainty when adopting ICME-accelerated methods. Teams conscious of these issues have the potential to effectively quantify and mitigate uncertainty when adopting ICME-accelerated methods. Actions that have the potential to overcome or circumvent issues with managing the risk and uncertainty quantification for ICME within 3 years are presented here within the following categories:

A. Establish maturity level assessments
B. Determine Uncertainty Quantification (UQ) methods and approaches
C. Execute UQ techniques

A: Establish Maturity Level Assessments

As maturity levels and protocols are not known or established for ICME modeling tools, companies could consider instituting a standardized, ubiquitous system to measure the maturity level of tools and databases that are being used for their intended application. They can assess the level of overall uncertainty relative to the intended application and determine whether it is acceptable, using metrics, benchmarks, and known readiness levels for computational codes. Tool Maturity Levels (TMLs)[12] are most useful when compatible with and related to protocols surrounding the use of Technology Readiness Levels (TRLs), the latter already being commonly used to evaluate the maturity of evolving materials, components, and products. Taking into account the skills and experience of staff members in their application of ICME tools may provide an additional system for establishing maturity level.

B: Determine Uncertainty Quantification (UQ) Methods and Approaches

To manage uncertainty and error in quantitative predictive modeling approaches, teams involved in ICME could begin by conducting a gap analysis between state-of-the-art UQ methods[16] and the level of uncertainty required for specific applications. Once this is complete, performing a high-level analysis of the relationship between uncertainty in a product and uncertainty in a process is important to assessing the integrated design of a material and the overall product or component. Within the hierarchy of the model, companies can explore and use protocols to reduce uncertainty at a fundamental database/model level of the project and linear transformation methods at the final summary level. Professional societies can help assemble the experts required to develop guidelines for managing the propagated uncertainty in a product development process chain and/or establish the experimental test problem standards needed to verify a design method or process. To define any additional risk mitigation actions, teams could then complete any additional testing and analysis necessary for their specific project and assess the risk in comparison to the potential consequences or outcomes.

Conducting an inventory of computational and experimental tools and identifying the tools needed to implement an ICME-accelerated program (without overcommitting resources) is important to measuring and mitigating technical and financial risk. In addition, it is important that enough of an accurate, physically realistic approach be utilized in the modeling tools to achieve the level of accuracy and predictability required for a specific product. For example, if semi-empirical models are working for the application with acceptable levels of quantifiable error/uncertainty, they may or may not need to be more predictive or physics based.

C: Execute UQ Techniques

Structured hybrid modeling and standard UQ methods can be employed to better mitigate and manage modeling uncertainty, beginning with an assessment of the intended application and the identification of potential consequences of using ICME and the associated levels of uncertainly for the specific application. This approach will reduce the number of experiments necessary and allow for the ongoing management and reduction of risk over the course of a project. Some models may require new experiments; therefore, IPDTs should be prepared to conduct tests tailored to their models. For example, if the mechanistic model can predict the correct shape of the distribution function, they may need to employ linear transformation methods to shift the curve in order to validate experimentally the model for a specific material and product, as opposed to for general purposes. Comparing multiple models, approaches and databases using the same materials system can help identify outliers among the various tools or approaches and help the teams challenge the results of individual models.

It is important to consider using strategies that will allow experimenters and modelers on the integrated product development team to inform each other and quantify the information gained within each activity to reduce testing efforts. The team can track how much information is gained between experimental and modeling results to determine when to stop gathering and generating information, and use it as a robust metric to measure progress within the product development cycle and reduce the number of experiments required. In addition, implementing a statistical framework to quantify the variance in microstructure and propagate it from the prediction of the processing approach to the prediction of performance should further reduce testing.

7: Some Longer-Term Actions for Addressing Pervasive Issues and Advancing ICME

In addition to near-term solutions, there are opportunities for industry leaders, universities, and government agencies to make long-term investments in the future of ICME that can help ensure its sustainment and enduring success. These actions are presented in detail within the following categories:

A. Support education and workforce development
B. Fund ICME R&D efforts
C. Develop new ICME tools
D. Drive widespread acceptance of ICME by advocacy of ICME champions

A: Support Education and Workforce Development

In addition to some of the nearer-term efforts described in section 5, sustained adoption of ICME will require long-term effort dedicated to revising undergraduate and graduate-level education as well as internal training and development programs. This will require developing an overall systems engineering integration methodology that is designed with sufficient flexibility that different disciplines are able to follow the same methodology. Colleges and universities might consider incorporating systems engineering into their undergraduate and graduate programs, teaching specifically about strategic systems engineering where design of materials, manufacturing, and products is possible. In addition, incorporating ICME tools into science-based applications within graduate-level curricula can help integrate and promote the value of engineering in science-dominated materials science and engineering programs, and with faculty. Engaging bachelor's-level materials science and engineering graduates who are more computationally proficient in ICME tools can help to encourage the broad, pervasive integration of ICME proficiency at moderate skill levels. Ultimately, the use of ICME tools in the context of design within materials science and engineering programs might become second nature for graduating students.

In addition to revising and augmenting current curricula, industry can drive or support the development of new interdisciplinary degree programs, such as a 5-year Bachelor's/Master's degree program or collaborative Ph.D., in which students work closely with professors and industry members. To help design and establish these programs, industry could place support staff at universities for approximately 3 years to assist faculty with integrating ICME tools into their curricula.

B: Fund ICME R&D Efforts

Funding R&D efforts in ICME is critical to establishing a strong foundation for ICME. However, many of these opportunities will require a long-term investment from industry and government partnerships dedicated to the advancement of the field. Within federal agencies, establishing significant funding programs (e.g., leadership programs) that focus on injecting ICME R&D in industrially relevant problems can help strengthen partnerships between government and industry and promote ICME R&D, education, and adoption. Such partnerships could lead to the creation of ICME hubs (similar to the nanoHUB at Purdue University or the DOE energy hubs) as well as the funding of new small businesses in the ICME supply chain, both of which could increase the exposure of ICME in industry and academia and lead to further innovation and advancement in the field. Existing examples of venues for such ICME government industrial partnerships are the NSF Industry & University Cooperative Research Center (I/UCRC) Program (such as the Center for Computational Materials Design of Pennsylvania State University and the Georgia Institute of Technology, or the Center for Advanced Non-Ferrous Alloys of the Colorado School of Mines and University of North Texas), and/or NSF's Grant Opportunities for Academic Liaison with Industry (GOALI) program.

Government and industry leaders who control R&D funding in the field could also consider initiating a series of grand challenges for funding consideration that would require teams to integrate ICME methods and models with design for product development. Government and industry partners could also dedicate funding toward establishing cross-disciplinary research teams to develop ICME tools and generating ICME pull from the product or system developers at the concept development and optimization phases.

C: Develop New ICME Tools

Sufficient ICME tools—both computational and experimental—are not available in all fields. Government, industry, and academia can focus on developing new tools with predictive capabilities that have the potential to bring about the largest advances. For example, this could include new tools relevant to composites and lightweight materials, and/or tools for functional (rather than just structural) applications. Suites of models could be built using "what if" materials and processes to illustrate, analytically, the "celestial limits" of various materials classes (e.g., nickel superalloys, titanium, etc.). Consulting designers could help to determine materials capabilities and place boundaries on the Ashby materials selection limits[17] for structural materials, as well as similar limits for functional materials (e.g., electronic, magnetic). In addition, developers could create an equivalent to the ASME *Guide for Verification and Validation in Computational Solid Mechanics* for computational materials engineering in order to better support the development and recognized confidence of new models.[18]

D: Drive Widespread Acceptance of ICME by Advocacy of ICME Champions

To encourage and achieve the widespread adoption of ICME in industry and government product development programs, champions of ICME should encourage senior management buy-in and enlist high-profile CEOs to provide public support for ICME, both in the near term and the long term. New product concepts are difficult to advance through various levels of decision making. Therefore, in addition to engaging high-level industry personnel, ICME supporters might consider publishing papers on the value of ICME in well-respected business publications (e.g.*, Harvard Business Review*) and commissioning independent business case reviews that demonstrate the value of ICME from a neutral third-party point of view.

Successful case studies must be available in order to obtain buy-in from senior management and motivate industry leaders to champion ICME implementation. Therefore, advocates of ICME need to establish rigorous, documented case studies in relevant technical journals (e.g., *Integrating Materials and Manufacturing Innovation*[g]) and feature detailed accounts of ICME implementation and case studies that include a well-grounded, quantitative ROI. Although within the next 3 years multiple studies could be published that focus on teaming, management, cross-functional teams, and other critical elements of a successful ICME program, the number of such case studies published could increase (possibly exponentially) as ICME grows rapidly in the next decade. Because ICME is not broadly implemented at this time, the current case studies should take a strategic approach to presenting the value of ICME. By the same token, broad strategic analyses aimed at showing business leaders the risks and opportunities of greater usage of ICME approaches, in the style of the McKinsey study on market penetration of materials and chemicals,[19] could have a significant impact on driving a wider acceptance of ICME.

Closing Comments on Pervasive Issues

The potential benefits of ICME-accelerated product development programs are enormous. Realizing the potential of ICME to facilitate the rapid conception, development, and insertion of new materials and processes into products, and especially to influence the very nature and capability of new products, will require both near-term action and investment, and long-term commitment, from skilled leaders and ICME Integrators. Widespread development and implementation of ICME may be incremental, but significant progress can be made within the next 3 years. The pervasive and crosscutting needs and recommendations discussed here are believed to include some of the key issues that need to be recognized and addressed to enable such successful implementation of ICME in the near term. The result will be a culture in which ICME is integrated into the entire materials, manufacturing, engineering, and product development cycle.

g. Available at www.immijournal.com.

IV. Industrial Sector Focus: Automotive

Process Overview

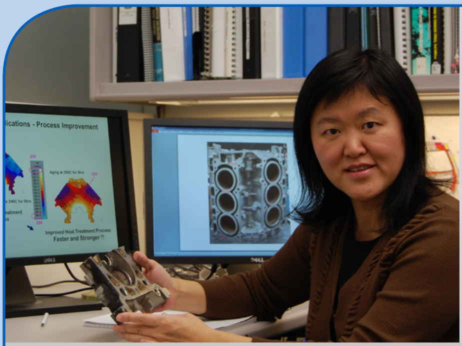
The Automotive ICME Implementation Team consisted of experts from primary metals manufacturers (steel and aluminum), a polymer matrix composites expert, and materials engineers and designers from two large automotive companies. The team also included individuals with experience in developing and/or using computational and experimental tools and applying them to ICME problems within the automotive industry. Although the majority of the team members were from the automotive industry, key members from government and academia made substantial contributions to this report. For a complete list of automotive team members, please see Appendix B.

Current State of ICME in the Automotive Sector

A small but growing number of case studies or success stories demonstrate the ability of ICME to accelerate and reduce costs of manufacturing a large-scale component or platform in the automotive industry. Although there have been some significantly robust ICME-type programs in various companies within the automotive industry, many may not have been specifically referred to as "ICME" and/or may not have been widely publicized due to proprietary concerns. The most widely known case study in which ICME has been implemented within at least a substantial portion of the product development cycle is the Virtual Aluminum Castings (VAC) program by Ford Motor Company. In this ICME-accelerated product development program, computational modeling was used to simulate the linkages between thermal processing and the resulting microstructure of an aluminum alloy, and in turn, make accurate predictions of the material's local mechanical properties and the durability of cast engine components composed of the alloy. The engineers, led by John Allison (now at the University of Michigan), utilized a combination of commercially supported codes and in-house codes.[6] Notably, more than 50% of the effort was dedicated to experiments—demonstrating that ICME approaches rely heavily on experimental data to inform and validate modeling approaches.[1] The Ford VAC project resulted in a reported ROI of over 7:1,[1] an estimated $120 million in savings, and product and process development time reduction of 15%–25%, as detailed in the accompanying case study excerpt.[11]

Although corporations such as Ford and GM are now investing in ICME, most companies in the industry have been reluctant to implement ICME broadly, for a variety of reasons. For instance, predictive computational efforts are only now being applied to lightweight magnesium (Mg) applications, since up to this point computational models available for Mg were too limited to undertake such an effort. Recently however, the Department of Energy (DOE) sponsored a program led by the U.S. Automotive Manufacturing Partnership (USAMP) to develop Mg alloys for automotive front-end applications, which included an ICME element,[20,21] as shown in Fig. 2.

In 2012, the DOE Office of Energy Efficiency and Renewable Energy (EERE) Vehicle Technologies Program also supported three important new programs focused on ICME in automotive applications: (1) ICME Development of Advanced High-Strength Steels, (2) Predictive Engineering Tools for Injection-Molded Long Carbon Fiber Composites, and (3) Advanced Alloy Development for Automotive and Heavy-Duty Engines.[21] Nevertheless, ICME has still not been implemented very broadly across the automotive industry, despite some demonstrations of its contributions to accelerating the development and deployment of new materials and manufacturing solutions in



ICME Case Study: Ford Motor Company Virtual Aluminum Castings

Excerpted from

Materials: Foundation for the Clean Energy Age[11]

Mei Li, Ford Research and Advanced Engineering Laboratory, holds a section of the cylinder head designed using Ford's Virtual Aluminum Castings process.

Automotive manufacturers are pushing aluminum alloys and other advanced lightweight materials to the furthest boundaries of their capabilities. Strategies to decrease the weight of a vehicle component for the sake of fuel efficiency can potentially compromise its strength, while certain operating conditions stress the wear and corrosion tolerance of many lightweight materials. Success in deploying a new lightweight material is often measured in microns—a minute adjustment in the design or manufacturing process can make all the difference between bringing a quality, cost-effective product to market or having to shoulder the expense and competitive disadvantage of "going back to the drawing board."

Changing the shape of the drawing board to reduce time and costs, while also achieving an optimal outcome, is an approach that Ford Motor Company has used with great success through its Virtual Aluminum Castings (VAC) project. Initially developed for cast aluminum cylinder heads and engine blocks, VAC replaces the traditional product development process focused on building and testing a series of expensive physical prototypes. These test results are often analyzed without knowing what impact the manufacturing processes had on the component. Therefore, subsequent retooling of the design is more of a "best guess," often resulting in failure of the component in later, more costly phases of development.

By combining a vast knowledge base on cast aluminum research with readily available computer-aided engineering (CAE) tools, VAC enables Ford engineers to design, cast, heat treat, and test specific aspects of vehicle parts in a virtual manufacturing environment, often quickly revealing microstructural issues that could otherwise set the process back by months. Rather than having team members work separately within their areas of expertise, the VAC approach serves to bring these realms together to work simultaneously on problems, saving time and facilitating the exchange of information and ideas.

A significant benefit of VAC is its ability to take some of the guesswork out of identifying the optimum manufacturing process for a given component. By modeling different processes, engineers can determine long before a prototype is cast how a material will perform within a particular design under certain conditions. Engineers can address micro-scale differences in factors affecting component integrity at the workstation until they define the process that potentially yields the highest-quality product in the most cost-effective manner.

Ford's investment in "redrawing the drawing board" has provided a significant return to its bottom line while making more durable, higher-performing products available to its customers. Reducing product and process development time by 15% to 25%, the system has saved Ford more than $120 million in development costs for powertrain components. Ford's success has been widely noticed, earning it a place as a benchmark example of the power of ICME—an emerging discipline in materials science—in a study released by the National Academies in 2008.

VAC is now fully integrated on a global scale into Ford Powertrain Operations and, according to Mei Li, technical expert and group leader of Light Metals Research and ICME, Ford Research and Advanced Engineering Laboratory, work is underway to introduce this approach to other aspects of Ford product development. "The knowledge gained in metallurgy, physics, mechanics and the computational models developed for microstructural evolution and property predictions have been extended to other materials and processes," said Li. "This includes the development of computational tools for gear steels during the heat treatment process, and high-pressure die casting of aluminum alloys for additional powertrain and body applications." Li noted that her group is also developing tools based on the VAC approach for magnesium alloys and advanced heat-resistant alloys, as Ford continues to seek the competitive advantage in manufacturing lightweight, durable, energy-efficient vehicles.

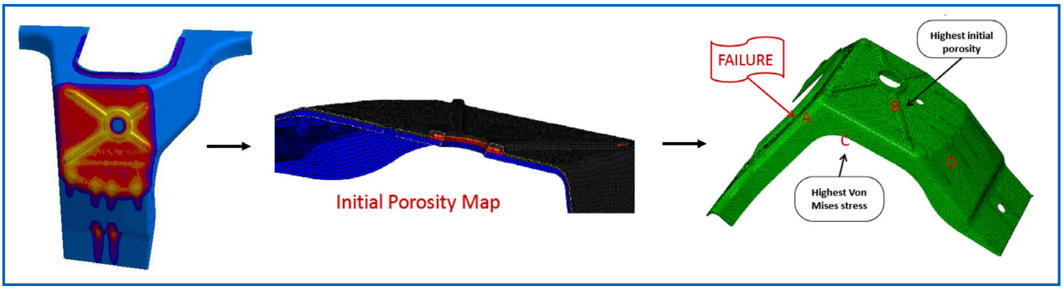


Fig. 2. Results are displayed from the ICME for Mg Project, sponsored by DOE VTP and led by USAMP and partners.

developing new products. A framework and detailed guidance to help implement ICME in the automotive industry in the near term will be presented in this chapter.

Framework for Implementing ICME

(See pages 38-49 for automotive ICME implementation framework)

Companies in the automotive industry represent a wide range of materials suppliers and product manufacturers who are developing components such as engine blocks, transmission components, and automobile frames. The framework depicted in Fig. 3 represents basic guidelines to implement computational materials engineering approaches in automotive companies in order to begin an ICME-accelerated product development program within 3 years.[h] Parties involved with the implementation framework are listed in Table IV. The full framework is a combination of Figs. 3 and 4 and Table V, which taken together contain detailed descriptions of each step, suggestions for computational models and tools[i] to use, types of skillsets and personnel needed, key decision points, and flow of data and information dictating the direction of the product development process. This framework should be considered the starting point, or foundational building block or template, for implementing ICME in a company in the automotive industry. They will of course have to be adapted, and full details filled in, for a specific company, product, and manufacturing process.

Arrows in Fig. 3 represent the sequence and flow of information between steps. As can be seen, the framework does not contain a direct linear sequence of steps, but instead illustrates the many feedback loops that can take IPDTs (integrated product development teams) back to earlier/other stages of development if needed, depending on the outcome of the steps. The second framework diagram (Fig. 4) provides examples of how companies in the automotive industry can use modeling tools to implement ICME. Examples of some specific tools within each of the modules are provided

h. As mentioned in the introduction, 3 years was specifically chosen to provide a quantitative reference point from which to focus the frameworks and recommendations for near-term ICME implementation after a consensus was reached that 3 years was an achievable goal (based on the current state of ICME and the experience of the team members).

i. Here, “models” refers to the fundamental physics/materials-based models (e.g., a crystal plasticity model) while “tools” refers to computational codes (e.g., Deform®) that have been properly validated and verified and can be used in a quantitative fashion to implement ICME. The tools are often commercial codes, but can be freeware as well.

below (Fig. 4 and Table V); a more comprehensive list of available computational tools is available in Appendix C. These specific computational tools and databases are all also accessible via the TMS Cyberinfrastructure Portal, at www.tms.org/cyberPortal.

Specific Actions for Implementing ICME into the Product Development Cycle

Table V provides detailed information at the various steps within the framework represented in Figs. 3 and 4 to assist with the development and launch of an IAPDP. Although all required actions should be completed before moving on to the next step, the ICME framework involves an iterative process that enables integrated product development teams to revisit individual steps and/or revise the flow direction as necessary. At certain stages throughout the product development cycle, the relevant experts on the IPDT may need to return to a different step (and even alter how that step is done) if the desired outcomes are not being met. In addition to specific actions and examples of tools that can be used to complete each step, the parties involved at each stage in the framework are provided in Table IV.

Table IV. Key Personnel Involved in Traditional and ICME-Accelerated Product Development Processes in the Automotive Industry *

- **Customer** (person paying for the product)
- **Design and release engineer** (engineer with the responsibility for product design and approving and releasing products for manufacturing)
- **ICME integrator** (engineer tasked with coordinating ICME elements of the project)
- **Information scientist/data management** (tasked with handling data transfer and storage issues)
- **Manufacturing engineer** (engineer tasked with developing and optimizing manufacturing approaches)
- **Materials engineer** (engineer with the expertise and responsibility for development of new materials, as well as selection and deployment of existing materials)
- **Production analyst** (plans and analyzes production activities and schedules)
- **Research experimentalist** (engineer and scientist who oversee and carry out experiments supporting research and development efforts including model verification and validation)
- **Research modeler/scientist** (engineer or scientist who build and execute computational models and simulations)
- **Test engineer** (engineer tasked with testing the performance of and developing use specifications for finished products)

* See “Parties Involved” sections of Table V for placement within framework.

Current Barriers/Needs, and Recommendations for Addressing Them, in order to Implement ICME in the Automotive Sector

Although ICME has the potential to significantly reduce the costs and accelerate the introduction of new products in the automotive industry, some potential barriers need to be addressed to better enable the widespread adoption of ICME within the industry.

Need for Improved Quantitative Modeling Tools

Modeling tools for predicting materials microstructures are often not robust or reliable enough for the development of complex new materials systems. Therefore, it is recommended that computational methods experts work together in workshops or other venues to advance quantitative microstructure prediction models and address foundational engineering problems via projects funded by different organizations. More specifically, they could use these opportunities to develop and/or enhance the following:[j]

- Predictive precipitation kinetics models/tools for cast and wrought aluminum alloys during aging that include type, volume fraction, and morphology
- Predictive models/tools for high-pressure die casting aluminum and magnesium alloys that include volume fraction and morphology of porosity and eutectic phases
- Predictive solution treatment models/tools for aluminum and magnesium alloys
- Accurate kinetics databases for aluminum and magnesium alloys
- Predictive models/tools for phase transformation kinetics in gear steels
- Predictive models/tools for texture evolution, including recovery, recrystallization, and grain growth, during rolling and extrusion processes for aluminum and aluminum alloys
- Predictive models and tools for forming/welding induced geometric/property changes in subsequent crash and noise-vibration-harshness (NVH) simulations
- Microstructure-based models and tools for fracture and fatigue that take the extremes in distributions of microstructure and defects into consideration. In particular, minima in defect sensitive properties (e.g., low and high cycle fatigue) will require that ICME can predict both the size distribution and details of both microstructural and exogenous defects, and accurately calculate life distributions via crack growth analysis.
- Microstructure-dependent model/tool for quench-cracking in automotive components

It is also vital to understand how the molecular structure and microstructure of materials affect properties such as corrosion, strength, and electrochemistry. In this regard, structure-property relationships are relatively immature in terms of their mathematical representation, as is the ability of current software tools to predict these characteristics quantitatively in computational approaches.

continued on page 50.

j. In this context, "models" are considered more fundamental and typically developed by universities or national laboratories. Computational "tools" are seen as being developed primarily by software companies.

Fig. 3. Automotive ICME Implementation Framework: Incorporating an ICME Toolset into the ICME-Accelerated Product Development Program (IAPDP)

(Full details of actions and personnel at each step are provided in Table V.)

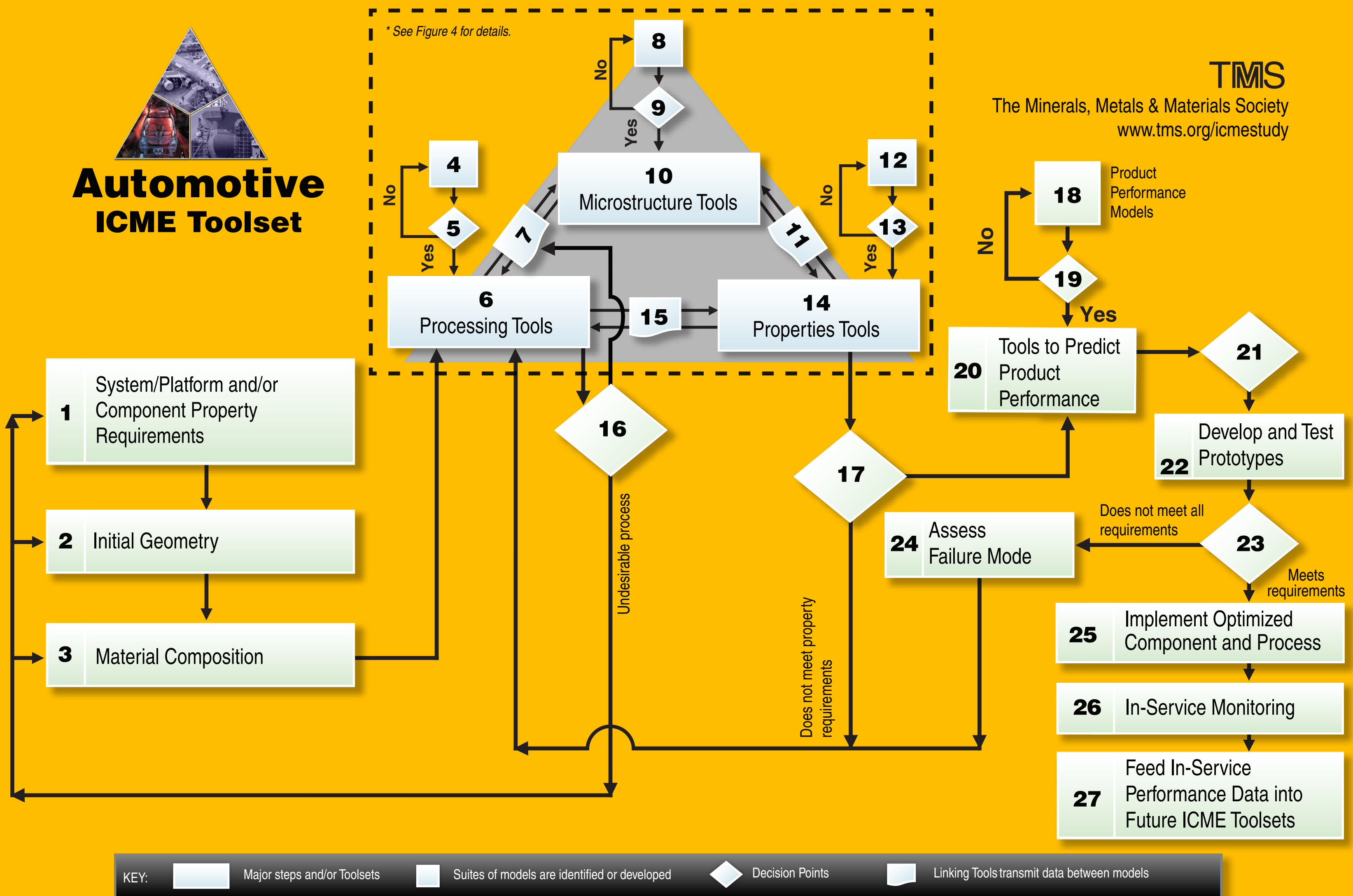


Fig. 4. Automotive ICME Toolset

(Full details of actions and personnel at each step are provided in Table V.)

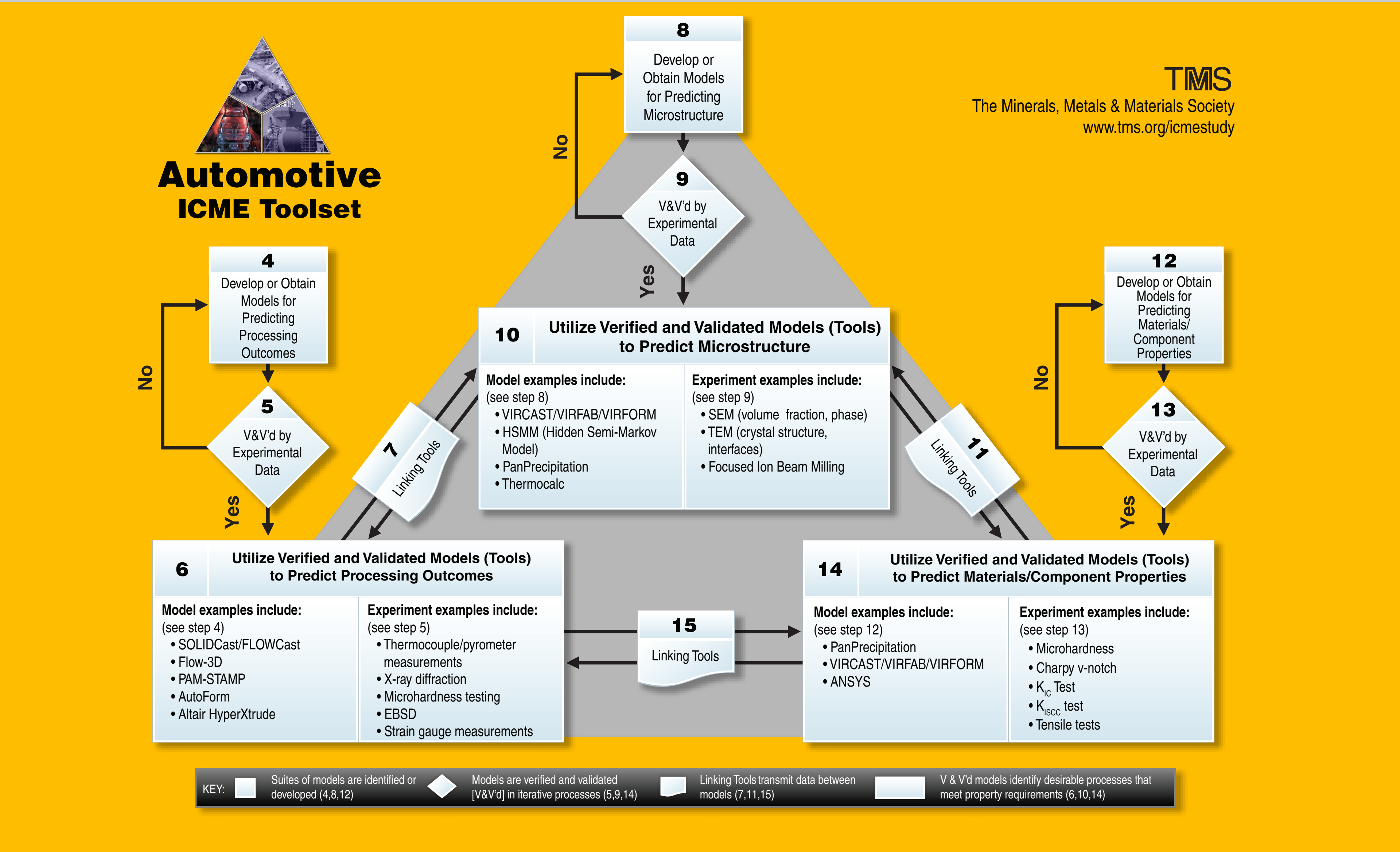


Table V. Detailed Steps for Implementing ICME Within the Automotive Industry
(See figures 3 and 4 for illustrated automotive ICME framework)

1. System/Platform and/or Component Property Requirements

Parties Involved: Customer; design and release engineer

- Determine the key requirements of a given system or component within the product (e.g., mass, cost, stiffness, vibration characteristics, durability, corrosion and environmental durability, dimensional tolerances, and relevant crash energy management).
  - » Determine how the overall system requirements, or purpose of the product (e.g., specifications, predicted loads, environmental/corrosive environments), may affect the property requirements.

2. Initial Geometry

Parties Involved: Design and release engineer

- Determine the geometry/dimensions of the product component using basic topology optimization software (e.g., use computational fluid dynamics (CFD) codes to optimize aerodynamic characteristics).
- Consider the effects of product geometry on the final packaging of the product.
- Incorporate structural health monitoring (SHM) systems into the design early, if they are used.
- Create a component shape that conforms to styling and packaging requirements based on customer needs.
- Consider whether geometry affects other component characteristics (e.g., does geometry affect environmental/lubrication temperatures or debris resistances?).
- Consider the effects of product geometry on manufacturability (such as casting).

3. Material Composition

Parties Involved: Research experimentalist; manufacturing engineer; design and release engineer; materials engineer: research modeler; ICME integrator

- Identify a short list of candidate (approximately 2–3) materials compositions.
- Use thermodynamic/kinetic/thermo-physical modeling suites and databases to determine the component property data and feasibility of the material composition in a product.
  - » Note: Modeling tools used include Thermo-Calc, Pandat, PanPrecipitation, FactSage, and JMatPro.
- Down-select an appropriate material composition to be inserted into the ICME toolset.

4. Develop or Obtain Models for Predicting Processing Outcomes

Parties Involved: Research modeler; research experimentalist; materials engineer; ICME integrator; manufacturing engineer; production analyst

- Assemble and assess a suite of modeling tools to predict the processing outcomes. Examples of computational codes include the following:*
  - SOLIDCast/FLOWCast: Cast design, solidification/melt modeling and optimization
  - MAGMASOFT: Cast design, mold-filling, solidification/melt modeling and optimization
  - ProCAST/QuikCAST: Cast design with processing including core blowing, semi-solid modeling, centrifugal casting, lost foam and continuous casting
  - FLOW-3D: CFD simulation software for modeling high-pressure die-casting processes, solidification/melting, lost foam casting
  - CAP: Thermal and solidification simulation, sand casting, high pressure die casting (HPDC), semi-permanent mold, investing casting, other processes
  - PAM-STAMP: Simulation of stamping process
  - AutoForm: Simulation of sheet metal forming
  - LS-DYNA: Simulation of stamping process
  - Autoform: Sheet metal forming
  - Altair HyperForm: Simulation of stamping process
  - Altair HyperXtrude: Virtually develop and validate extrusion dies
  - Deform: Modeling of extrusion and rolling processes
  - COMSOL Multiphysics: modeling and simulation of any physics-based system.

5. Verify and Validate Processing Models with Experimental Data

Parties Involved: Research modeler; research experimentalist; materials engineer; ICME integrator; manufacturing engineer; production analyst

- Conduct a series of experiments to validate that the modeling results are representative of real-world conditions. Design experiments specifically to work within the bounds of the model to confirm validity. Experimental tests could include the following:
  - Casting experiments with embedded thermocouples (or some other mechanism) to measure temperature profiles in order to validate casting models
  - Experiments to characterize (qualitatively) the preliminary microstructure (and defects) resulting for the processing cycle to test generally overall validity of the model. These could include optical microscopy, electron-backscatter diffraction

(EBSD), scanning electron microscopy (SEM), electron-probe micro-analyzer (EPMA) and transmission electron microscopy (TEM).
  - Experiments to measure texture and/or strain to compare to output of mechanical process models: EBSD, X-ray diffraction (XRD) techniques, strain gauge measurements
  - Experiments to characterize (qualitatively) the preliminary local properties (and profiles) resulting from the processing cycle to test generally overall validity of the model. These could include microhardness mapping.
- Conduct tests to verify that the modeling codes are executing computations properly and providing an accurate mathematical representation of the fundamental engineering principles and relationships that they are designed to represent.
- Note: These tasks may require several iterations of the experiments and/or tweaks to the modeling tools to ensure validity and robustness.

6.

6. Utilize Verified and Validated Models (Tools) to Predict Processing Outcomes

Parties Involved: Research modeler; research experimentalist; materials engineer; ICME integrator; manufacturing engineer; production analyst

- Move forward and utilize suite of verified & validated models that is representative of the particular process used to modify the material

7.

7. Linking Tools

Parties Involved: ICME integrator; information scientist/data management; research modeler

- Use special software packages to link computational models for ICME-enabled product development and automate the process of data entry between steps.
  - Note: Tools that link the input and output parameters of model simulations to predict processing, microstructure, and properties are commercially quite limited, but would otherwise reduce errors and accelerate computationally driven steps of the product development cycle.
  - Isight and Model Center are examples of tools used to chain simulation process flows between suites of models.
  - Note: In this case, the output parameters are those developed by the materials processing models/tools, and the input parameters are those required by the microstructural models/tools.

8.

8. Develop or Obtain Models for Predicting Microstructure †

Parties Involved: Research modeler; research experimentalist; materials engineer; ICME integrator

- Assemble and assess a suite of modeling tools to predict the microstructure (or other length scale structure) of the material. Examples of computational codes include the following:
  - » Hidden Semi-Markov Model (HSMM): Linked statistical model to simulate thermo-mechanical and microstructural evolution of steel
  - » VIRCAST/VIRFAB/VIRFORM: As-cast microstructure modeling of grain size/growth/morphology and precipitation physics prediction; used for both microstructure and property prediction
  - » PanPrecipitation: Simulation of precipitation kinetics during heat treatment process
- Identify the key microstructural properties for automotive applications.
- Note: Microstructural properties include (but are not limited to) texture, grain size, intermetallic composition, precipitate distributions, dislocation structure, interstitial and other crystallographic defects.

9.

9. Verify and Validate Microstructure Models with Experimental Data

Parties Involved: Research modeler; research experimentalist; materials engineer; ICME integrator

- Conduct series of experiments to validate that the modeling results are representative of real-world conditions; design experiments to work specifically within the bounds of the model to confirm validity. Experimental tests could include the following:
  - » Experiments to characterize first the qualitative nature of the microstructure, to ensure the models are making predictions that are in the right regime. These could include optical microscopy, EBSD, SEM, TEM, and XRD.
  - » Higher-level quantitative validation of the models and the model parameters used. These could include:
    - ◊ Two-dimensional (2-D) quantitative techniques such as optical microscopy (e.g., volume fraction, average particle size), EBSD (e.g., texture, interface types), SEM (e.g., volume fraction, phase), TEM (e.g., phases present, crystallography, interface character and types, defects), and XRD methods (phases present, texture)

        ◊ Three-dimensional (3-D) techniques such as: serial sectioning, X-ray tomography, 3-D atom probe, and focused ion beam (FIB) milling, in conjunction with 3-D reconstruction, visualization, and quantitative analysis techniques to measure quantities (and their distributions) such as 3-D morphology, interfaces, particle size distributions, and defects in 3-D
    - » Note: Experimental validation of empirical models of the microstructure can be difficult in certain materials (e.g., currently difficult to quantify martensite structures versus bainite structures in low carbon steels).
- Conduct tests to verify that the modeling codes are executing computations properly and providing an accurate mathematical representation of the fundamental engineering principles and relationships that they are designed to represent.
- Note: These tasks may require several iterations of the experiments and/or tweaks to the modeling tools to ensure validity and robustness.

10. **10. Utilize Verified and Validated Models (Tools) to Predict Microstructure**

Parties Involved: Research modeler; research experimentalist; materials engineer; ICME integrator

- Move forward and utilize suite of verified & validated models that is representative of the microstructure (or other relevant length scale) of the desired final component.

11. **11. Linking Tools**

Parties Involved: ICME integrator; information scientist/data management; research modeler

- Use special software packages to link computational models for ICME-enabled product development and automate the process of data entry between steps.
    - » Note: Tools that link the input and output parameters of model simulations to predict processing, microstructure, and properties are commercially limited, but would otherwise reduce errors and accelerate computationally driven steps of the product development process.
    - » Isight and Model Center are examples of tools used to chain simulation process flows between suites of models.
    - » Note: In this case, the output parameters are those developed by the microstructure models/tools, and the input parameters are those required by the processing models/tools.

12. **12. Develop or Obtain Models for Predicting Materials/Component Properties**

Parties Involved: Research modeler; research experimentalist; materials engineer; ICME integrator

- Assemble and assess a suite of modeling tools to predict materials properties such as thermodynamic properties (phase boundaries, etc.) and mechanical properties (hardness, toughness, fatigue, strength, ductility). Examples of computational codes include the following:*
  - ANSYS: Standard finite element method (FEM) stress prediction analysis; key for post-heat treatment analysis
  - PanPrecipitation: Simulation of precipitation kinetics during heat treatment process; use for microstructure and property prediction
  - Thermo-Calc: CALPHAD (calculation of phase diagrams) method-based software Thermodynamic and phase diagram calculations
  - VIRCAST/VIRFAB/VIRFORM: As-cast microstructure modeling of grain size/growth/ morphology and precipitation physics prediction; used for both microstructure and property prediction

13. Verify and Validate Property-Prediction Models with Experimental Data

Parties Involved: Research modeler; research experimentalist; materials engineer; ICME integrator

- Conduct a series of experiments to validate that the modeling results represent real-world conditions. Design experiments specifically to work within the bounds of the model to confirm validity. Experimental tests could include the following:
  - Experiments to validate the thermodynamics (phase diagram) results, which could include isothermal and/or continuous cooling heat treatments in combination with microstructural characterization, heat treatment facilities, optical microscopy, EBSD, SEM, EPMA and/or TEM
  - Experiments to measure mechanical and other physical properties, including: Microhardness; Charpy v-notch (toughness); K_{IC} Test (Plane-strain fracture toughness); Fatigue testing; Corrosion test, including corrosion fatigue and K_{ISCC} (Threshold stress-intensity factor for stress-corrosion cracking); Tensile tests (yield and ultimate strength, ductility, elongation/reduction in area); Density measurements
- Conduct tests to verify that the modeling codes are executing computations properly and providing an accurate mathematical representation of the fundamental engineering principles and relationships that they are designed to represent.
- Note: These tasks may require several iterations of the experiments and/or tweaks to the modeling tools to ensure validity and robustness.

14.

14. Utilize Verified and Validated Models (Tools) to Predict Materials/ Component Properties

Parties Involved: Research modeler; research experimentalist; materials engineer; ICME integrator

- Move forward and utilize suite of verified & validated models that is representative of the desired materials or component properties.

15.

15. Linking Tools

Parties Involved: ICME integrator; information scientist/data management; research modeler

- Use special software packages to link computational models for ICME-enabled product development and automate the process of data entry between steps.
  - » Note: Tools that link the input and output parameters of model simulations to predict processing, microstructure, and properties are commercially limited, but would otherwise reduce errors and accelerate computationally driven steps of the product development cycle.
  - » Isight and Model Center are examples of tools used to chain simulation process flows between suites of models.
  - » Note: In this case, the output parameters are those developed by the materials properties models/tools, and the input parameters are those required by the product performance models/tools.

16.

16. Decision Point: Is the Processing Approach Feasible and Desirable?

Parties Involved: Production analyst; manufacturing engineer; design and release engineer; materials engineer; ICME integrator

- Assess the technical feasibility and cost-effectiveness of the processing approach.
- Evaluate other factors including appropriate machine size, control, robustness, cost, production rate, materials supplier abilities, environmental performance.
- Determine how processing is affected by certain geometric features (e.g., overflow wells, chill blocks)

17.

17. Decision Point: Does the Product Meet Component and Materials Requirements?

Parties Involved: Production analyst; Manufacturing engineer; design and release engineer; materials engineer; ICME integrator

- Assess the confidence in modeling results and move forward if results are found to be feasible and validated.
- Re-enter the ICME toolset iteration loop for additional simulation or reconsider the requirements, drivers, and geometry of the component if the product does not meet component and materials requirements.

18.

18. Develop or Obtain Models for Predicting Product Performance

Parties Involved: Research modeler; research experimentalist; materials engineer; ICME integrator; test engineer

- Assemble and assess a suite of modeling tools to use the output of the optimized materials structure/properties/processing approach to predict the product performance.
  - » ABAQUS software linkage tools are advancing to be able to chain modeling results from the ICME toolset to the simulation tools used in prediction of product performance.
- Use largely with commercial finite element analysis (FEA) and other structural tools to model the assembly, producability, and crash testing, using scale-up experiments as validation. Examples of computational codes include the following:
  - » PAM-CRASH: Simulation of crash dynamics testing
  - » LS-DYNA: Simulation of crash dynamics testing
- Conduct fewer iterations in this set of steps as the ICME Toolset and associated models become more advanced.

19.

19. Verify and Validate Performance-Prediction Models with Experimental Data

Parties Involved: Research modeler; research experimentalist; materials engineer; ICME integrator; test engineer

- Determine whether modeling results are representative of real-world conditions and/or whether the modeling software executes computations properly.
- Examples of experimental tests include the following:
  - » Crash testing
  - » Machinability tests

20.

20. Utilize Verified and Validated Models (Tools) to Predict Product Performance

Parties Involved: Research modeler; research experimentalist; materials engineer; ICME integrator; test engineer

- Move forward and utilize suite of verified & validated models for predicting the product performance.

21.

21. Decision Point: Does the Predicted Component Performance Meet Requirements?

Parties Involved: Customer (person paying for the product); design and release engineer; test engineer

- Assess the predictive modeling results.
- Consider changes to the processing approach, materials composition, and/or geometry if the integrated component does not pass performance requirements.
    - » Note: A common current practice in the automotive industry is to only make changes to the geometry based on conclusions of the performance modeling predictions.

22.

22. Develop and Test Prototypes

Parties Involved: Design and release engineer; test engineer (product)

- Conduct specific, targeted full-scale experiments on the ICME-optimized prototype.
- Try to “break things” often using combined testing methods (e.g., crash, fatigue)
- Test SHM systems for integrity and for their ability to report non-destructive evaluation data output

23.

23. Decision Point: Does the Component Meet All Requirements?

Parties Involved: Customer (person paying for the product); design and release engineer; test engineer

- Assess the results of the prototype tests. If the component passes, consider the design final, and begin to develop final component/product specifications.

24.

24. Assess Failure Mode if Component Fails Test

Parties Involved: Materials engineer; test engineer (product); research modeler; research experimentalist; production analyst

- Conduct failure analysis methods on the prototype to properly diagnose the root cause of the failure.
- Feed results into structured databases and use them as input for ICME modeling tools for future product development efforts.
- Examples of failure analysis methods include X-ray microstructure analysis, SEM, scanning acoustic microscopy, and various other spectroscopy methods.

25.

25. Implement Optimized Component and Process

Parties Involved: Design and release engineer; materials engineer; ICME integrator; production analyst; manufacturing engineer

- Create a complete manual and set of specifications for the product.
- Do not conduct additional ICME iterations at this point, as design properties have been established.

26.

26. In-Service Monitoring

Parties Involved: Customer (person paying for the product); design and release engineer

- Feed information output from SHM systems into structured databases and analyze the output for statistical significances.

27.

27. Feed In-Service Performance Data into Future ICME Toolsets

Parties Involved: Materials engineer; research modeler/scientist; research experimentalist;

- Use SHM databases as input for ICME modeling tools for future product development efforts.
- Use this information to advance and verify computational codes and validate modeling results.

* See Appendix C for a list of additional computational tools.

† Although the term microstructure is generally used only in reference to metals and other crystalline materials, in this context it is used to denote the meso-, micro-, or nano-scale structure of the material class undergoing ICME including metals, ceramics, and composites.

continued from page 37.

Experts in the materials science community can contribute to increased understanding of these relationships by taking the following actions:

- Offer a two-day working group or workshop with representatives from industry and academia, and publish the results.
- Establish best practices for evaluating the maturity and predictive capability of different software tools and models.
- Establish foundational engineering problems of properties models that are explicitly linked to microstructures or linked through internal state variables (e.g., damage parameters).
- Establish foundational engineering problems between industry and academia to develop microstructure-based models that can capture the extreme distributions in microstructure in failure predictions.
- Bring corrosion experts into the ICME community.
- Evaluate the state of the art of microstructure-based electrochemical property predictions (e.g., in a workshop).
- Develop mechanistic-based corrosion models that can be used to understand and predict corrosion behavior (e.g., for an foundational engineering problem).

Additionally, funding and support from the National Science Foundation (NSF) could be used to foster partnerships between industry and academia (e.g., the NSF Industry & University Cooperative Research Center Program), which could contribute computational experience for implementing ICME tools and methods.

The effective implementation of ICME tools and methods also requires a broad set of materials databases, which are currently limited by availability and maturity. As one example, it is specifically recommended that databases that house robust thermal and/or mass diffusivity data, including data on a variety of ferrous materials systems, be developed and made available since they are critical to ICME implementation in the automotive industry.

Lack of Acceptable Linkage Software and Tools

Although there are some available integration tools such as Isight and Model Center, smooth, efficient links between codes for processes such as casting and stamping and those designed to model noise, vibration, and harshness (NVH), crash, and durability are still seriously lacking. This lack of versatile, user-friendly linking tools prevents the effective transmission of information between models from various length scales. In addition, there is a need for professionally supported, integrated software tools with state variables that incorporate microstructure.

Integration of Models into Existing Software Tools

To incentivize software developers to improve the way models can be incorporated into their computational tools, the community needs to identify translators to integrate user-developed models into commercial tools in a way that would allow software users to rank and rate their integration friendliness and transmit communications back to the developer. Such a process would, for example, make it easier to put texture evolution code into a numerical method and integrate it into DEFORM software tools.

Cultural Barriers and Intellectual Property Issues

The sharing of knowledge and proprietary data presents a significant challenge for businesses and research organizations that expend significant time and funds generating data for internal use. The current lack of incentives and fully developed platforms for sharing information without intellectual property concerns perpetuates this concern and creates organizational barriers to understanding the links between processes (e.g., casting, stamping) and performance metrics such as crash characteristics. Additionally, materials suppliers may be reluctant to reveal how they develop materials with desired properties, which further limits effective data sharing.

To address some of these issues, trailblazing stakeholders in industry, university, and/or government can convince their management of the benefits of reaching beyond current organizational barriers to obtain and also make more available such data and tools, in order to lavage multiple organizations and expand the reach and potential impact of ICME in the pre-proprietary stage. Additionally, teams from organizations who rely on modeling of microstructure-property relationships could work together to determine and establish a set of key state variables that can be shared across multiple organizations without having to share proprietary information.

Sharing of Pre-competitive Data and Tools

Developing open-source tools for sharing information will require that funding agencies and universities provide incentives for data and information sharing and agree that the outcomes will become publically available or open source, after a period of time. This could be accomplished through the creation of a cooperative model (via a platform such as SharePoint) for sharing materials and tools, models, and data. Contributors would have access to not-yet-published data and tools shared by others (e.g., a company shares one data set on boron steel and is able to collect three other data sets) within a platform that would give project teams the ability to share and track data and models[k] (e.g., the nanoHUB model by Purdue). Input and publications would be traceable and citable, which would promote data sharing among universities, national laboratories, and industry and help companies gain widespread recognition within the industry. This could only be accomplished for "pre-competitive" tools and data, but it is in the best interest of companies and our manufacturing base to leverage such knowledge and push that precompetitive edge to accelerate product development. Government agencies could also require government-funded principle investigators to open up their data to the public after some specified time (and in fact such plans are currently being considered). Finally, journal publishers could play a large role here with open access models of publication and electronic publishing forms which include links to large datasets and/or computational tools.

k. Here, "models" refers to the fundamental physics/materials-based models (e.g., a crystal plasticity model) while "tools" refers to computational codes (e.g., Deform®) that have been properly verified and validated and can be used in a quantitative fashion to implement ICME. The tools are often commercial codes, but can be freeware as well.

Establishing a Business Case for ICME

Although it is often difficult to define the value of ICME and estimate its impact on product weight, cost, and development time, demonstrating successful ICME implementation is necessary to establish and build management support. Considering the current lack of sufficient funding available to solve some of the foundational engineering problems and drive customer demand and influence, ICME currently has a somewhat unclear place in the product development process, including in initial concept design.

One method of communicating the value of ICME is for advocates to more clearly define the potential uses and benefits of emerging models (e.g., casting) to higher management. Additionally, performing a DOE-funded "reengineering" study to demonstrate the value of predictive ICME tools on completed, non-ICME accelerated projects could be instrumental in obtaining management support. Reengineering a component or subsystem (e.g., engine cradle) using ICME and comparing the characteristics of the final products (e.g., cost, weight, performance) would be an opportunity to develop data, reports, papers, and proceedings that could be used to encourage upper management to accept and adopt ICME. For more thoughts on how to establish a business case for ICME, see Chapter III. Pervasive Issues (p. 13).

Performing a DOE-funded "reengineering" study to demonstrate the value of predictive ICME tools on completed, non-ICME accelerated projects could be instrumental in obtaining management support. Reengineering a component or subsystem (e.g., engine cradle) using ICME and comparing the characteristics of the final products (e.g., cost, weight, performance) would be an opportunity to develop data, reports, papers, and proceedings that could be used to encourage upper management to accept and adopt ICME.

Workforce Needs

There is likely to be a high demand for skilled ICME integrators and other essential ICME personnel such as expert software developers and users as adoption and implementation of the approach grows. The existing workforce typically does not have the necessary skills to integrate computational methods into current product development processes, and undergraduates are not being sufficiently trained in ICME or receiving the appropriate combination of theoretical, computational, and hands-on experience in the classroom. Currently, there is limited engagement not only from the academic community, but also from national laboratories and suppliers of ICME tools, as well as a lack of multidisciplinary support from teams with experience in materials, mechanics, software, and information technology to make a strong impact on the workforce needs.

Programs and classes have recently emerged at such schools as Northwestern University, which offers an ICME certificate, and Mississippi State University, which offers a class on ICME. However, broader involvement from the academic communities will be necessary to support large numbers of ICME projects. As ICME becomes more widespread, it will thus be beneficial for significantly more universities to initiate ICME courses and degrees.

Another aspect of workforce preparation in ICME that needs significant attention is the development of the existing workforce. Training and arming the existing workforce with ICME tools and expertise is the most efficient avenue for increasing the uptake of ICME approaches, as existing engineers will be able to leverage their engineering experience and higher positions of authority to successfully drive ICME projects. Many software companies offer training on computational tools (e.g., FLUENT), while other programs (e.g., LAMMPS, VASP, Quantum Espresso) have more limited training offerings. It is recommended that software suppliers make a priority of offering continuing education training to current materials engineers and designers. These companies will in turn benefit from increased knowledge, exposure, and sales of their product.

Near-Term Opportunities for ICME in the Automotive Industry

ICME-accelerated materials and product development is already occurring in the automotive industry, and the approach is well positioned to grow dramatically in use and acceptance in the coming years. While many new automotive products could benefit from ICME approaches, certain applications are poised to benefit in the near term (within the next 3–5 years). The following applications, not in priority order, represent some of the most promising opportunities to apply ICME tools and methods in the automotive industry in the near term:

- Aluminum
  - High-strength, high-ductility extruded parts for body applications
  - High-strength, corrosion-resistant sheet alloys for body applications (using casting, rolling, paint-baking, etc.)
  - Alloys for high-temperature engine applications
  - High-performance alloy development for cast wheels
  - Die-cast alloy with two or more process changes (i.e., heat-treatment and non-heat-treatment) tied to fatigue capacity (e.g., engine cradle application)
  - High-strength non-heat-treated aluminum for die castings
  - Low-cost manufacturing processes for aluminum outer sheets
- Composites
  - Next-generation metal-matrix composites at the micro- and nano-scales (e.g., for brake rotors)
  - Out-of-autoclave composites processing (e.g., for seat structures or various structural components)
- Magnesium

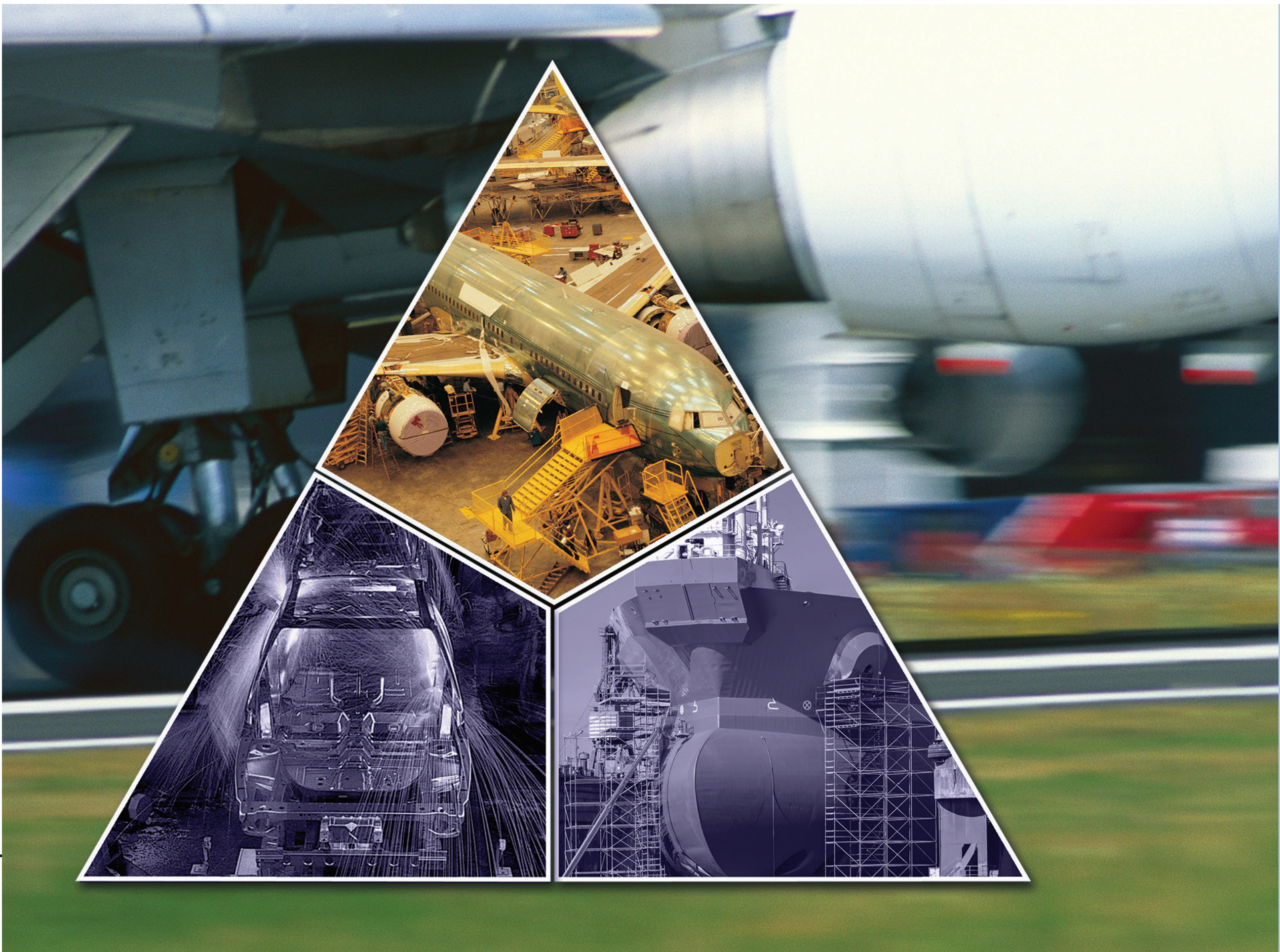
    - High-pressure die-cast alloy with cast holes and machined features for durability, crash, and corrosion characteristics
    - Low-cost, age-hardened magnesium alloys (without rare earth element content)
    - Stamped magnesium alloy doors (inner or roof panels)
- Steel
    - Control of gear distortion from high-pressure quenching
    - High-performance crankshafts
    - Welded body joint steel (or aluminum) staves
    - Alloy development for optimal component manufacturing performance and in-service performance; considering the following property metrics: durability, corrosion, machinability, hardness, strength, and in-service performance
- General recommendations
    - Alloy development for affordable high-temperature exhaust valves
    - Lightweight automotive shafts with an optimal alloy, using an induction-hardening process
    - A multi-material lightweight body structure, including manufacturing steps (e.g., joining of parts is the key focus)

Closing Remarks on Implementing ICME in the Automotive Industry

Although some organizations in the automotive industry have successfully demonstrated large-scale implementation of ICME into the product development process, there is great opportunity in this industrial sector to adopt ICME methods and tools much more widely within the next 3 years. Nevertheless, there still exist barriers and needs that can be overcome or circumvented in the near term in order to encourage such widespread implementation of ICME. Some specific predictive modeling needs in the automotive community are addressed here, including the need for ICME-experienced companies and other organizations (in academia and/or government) to work together on foundational engineering problems through precompetitive efforts, and to develop state-of-the-art linkage tools to better communicate results between modeling tools. Efforts to incentivize the sharing of data and tools will lead to the development of valuable resources that will enable new adopters to utilize computational approaches more easily.

The automotive industry is thus poised to further advance the implementation of ICME into product development cycles and produce innovative modeling tools for the prediction of increasingly complex materials systems. The framework provided in this chapter offers guidelines for implementing ICME-accelerated productive programs (IAPDPs) within the automotive industry and presents details of the personnel and specific actions involved at each step, which can be used to put this framework into practice (see Figs. 3 and 4, and Table V). The specific recommendations, challenges, and opportunities provided here for implementing ICME in the automotive industry can provide significant value to both new and ICME-experienced companies in the automotive industry, as well as members of other organizations who are involved in ICME programs.

V. Industrial Sector Focus: Aerospace



Process Overview

The aerospace ICME Implementation Team members provided expertise on a range of platforms, components and materials. The team included experts in both airframe and engine component applications, as well as people with expertise and experience in the metals, polymers, and composite materials areas. The aerospace team was comprised of experts not only from industry, but also from government and academia, as it will take a coordinated effort from these three groups to sustain the momentum of ICME and accelerate its implementation. More specifically, the development, integration, and implementation of the frameworks, tools, and multidisciplinary teams described in this report will require contributions from among all three of these organizational types. The complete list of aerospace team members and their affiliations is provided in Appendix B.

Current State of ICME in the Aerospace Sector

The aerospace industry was engaged in ICME before the 2008 National Academies report labeled this discipline ICME. Nevertheless, there are still relatively few cases of aerospace components in which ICME implementation has occurred throughout the majority of the product development cycle (from inception to deployment) and across an integrated product development team. One successful case in which ICME has been implemented across at least a substantial portion of the product development cycle is the insertion of low-rhenium single-crystal alloy turbine blades in aircraft engines by GE. As part of an effort to reduce their dependence on rhenium in the face of rising costs, GE successfully developed and introduced two new nickel-based superalloys with reduced rhenium content (designated René N515 and N500, respectively) in a fraction of the time usually required for such an effort. The primary enabler of this expedited timeframe was the utilization of a computational modeling approach, which employed a neural net model coupled with an existing GE alloy database to predict the properties of hundreds of alloy chemistries and downselect the most promising compositions, before moving on to large-scale generation of design data and scale-up.[22] According to a presentation by Robert Schafrik of GE Aviation in 2012, this approach enabled the development and insertion into use of the N515 and N500 alloys in a 2-year timeframe rather than the 6 years typically required for such a process, as shown in Fig. 5.[9]

A second successful ICME case study involved the design and deployment of a new landing gear alloy, Ferrium® S53®, developed by QuesTek Innovations LLC (QuesTek). In this and other alloy development efforts, QuesTek has worked in coordination with and/or received support from relevant U.S. government agency programs, such as the U.S. Department of Defense's Strategic Environmental Research and Development Program (SERDP) (executed in partnership with the U.S. Department of Energy and Environmental Protection Agency), and other programs led by the U.S. Navy, the U.S. Air Force, and the Defense Advanced Research Projects Agency. As a part of this particular effort, multiple computational models were utilized to develop this ultra-high-strength steel (Ferrium S53) with superior corrosion resistance, but without environmentally harmful cadmium plating. QuesTek developed S53 with only five prototype alloy compositions (and thermo-mechanical processing methodologies) over a two-year period, resulting in a development cost savings of approximately $50 million.[11] In addition, computational modeling allowed QuesTek alloy designers to consider various manufacturing approaches and integrate them into the design process. This enabled them to achieve the desired properties while constraining the processes to those already employed for similar applications, thus maximizing the material's manufacturability.[10]

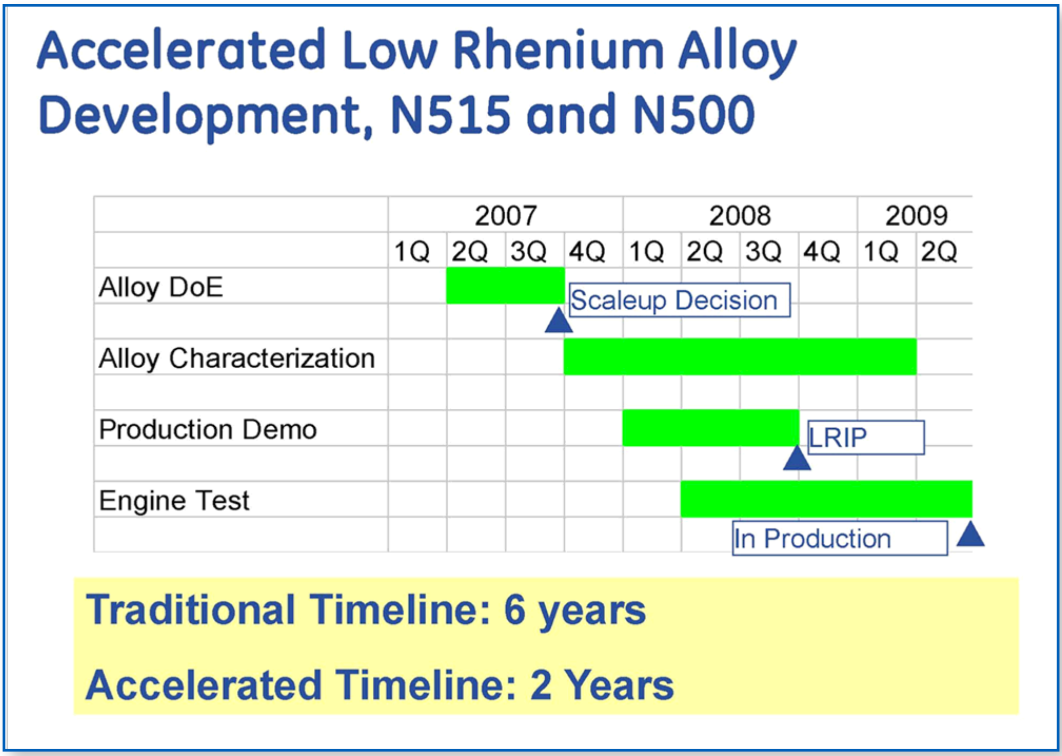


Fig. 5. Accelerated low rhenium alloy development.

Although there are additional ICME case studies in the aerospace industry, to date ICME has not been implemented in a comprehensive way across product development cycles and integrated product development teams (IPDTs) at most corporations within the industry. Predictive computational efforts have assisted very specific parts of component/product development cycles, but that has often occurred only in a qualitative rather than a quantitative way, and not in a fully integrated fashion. There has also been much effort expended in recent years to advance predictive models to assist with advanced materials development, but considerably less success in the proper verification and validation (V&V) of the models to develop them into quantitative computational tools, and implement them into ICME-accelerated product development programs (IAPDPs). An approach to ensuring proper V&V of ICME models was recently proposed by Cowles et al., but community uptake of a consistent and standardized methodology continues to lag behind other engineering disciplines, such as fluid and solid mechanics.[12]

The primary goal of this chapter is to provide a framework and detailed guidance for implementing ICME in the aerospace industry in the near term, which will enable ICME to be adopted much more broadly and quickly by the industry. In the present context, "near term" refers to beginning an ICME-accelerated product development program within 3 years (and not to developing a final product/component within that timeframe).

ICME Case Study: QuesTek Innovations, Ferrium S53

Excerpted from *Materials: Foundation for the Clean Energy Age*[11]

The extraordinary punishment routinely endured by aircraft landing gears has always necessitated high-strength materials to ensure both performance and safety. What has changed over the years are the increasingly stringent environmental impact, cost, and performance goals under which these planes fly.

For instance, because of their exposure to seawater and moisture in the atmosphere, landing gear steels must be both ultra-strong and highly resistant to corrosion to minimize costly repairs and downtime, as well as prevent potentially dangerous equipment failures. What is good for the aircraft, however, can be detrimental to the environment, since commonly used high-strength steels need to be plated with cadmium—a toxic element—in order to achieve acceptable corrosion resistance. Other materials, such as stainless steel, offer corrosion resistance without the need for a cadmium coating, but are lacking in strength. Coupled with these concerns is the ever-mounting imperative to shave weight without compromising performance in order to reduce fuel consumption.

Development of optimum materials to meet these types of specific, evolving needs has generally unfolded over the course of decades—and usually only with incremental improvements. This has compelled aircraft designers to juggle compromises related to strength, corrosion resistance, and weight with materials created for a long past age of aviation.

Change is afoot, however, that could potentially transform how materials are designed, developed, and deployed. As an example, through a project supported by the U.S. Department of Defense's Strategic Environmental Research and Development Program (SERDP), which is planned and executed in partnership with the U.S. Department of Energy and Environmental Protection Agency, QuesTek Innovations, LLC (QuesTek), based in Evanston, Illinois, has presented a solution to the materials dilemma faced by landing gear designers with Ferrium® S53®, an ultra-high-strength steel that offers superior corrosion resistance without harmful cadmium plating. The achievement earned QuesTek the SERDP Pollution Prevention Project of the Year Award in 2002 in recognition of S53's potential to reduce life cycle costs caused by environmental degradation, as well as toxic waste generated by the cadmium plating process. Even more impressive, as noted in SERDP Information Bulletin No. 15, "S53 was developed with only five prototypes over a two-year period, resulting in a development cost savings of approximately $50 million."

QuesTek has made it its business to reconfigure—and significantly accelerate—the materials development process by enabling the designer, from the beginning, to specify what is required of the material. Traditionally, materials development involves making samples of various chemistries that are tested and analyzed, with the process repeating for subsequent samples until a desired result is achieved. By utilizing advanced microstructure and property modeling, computational tools, and extensive databases of material parameters, QuesTek has reduced the need for this time consuming and costly experimentation. Alloy composition and thermal processing precisely targeting design goals and constraints can be calculated and then modeled to identify and address potential issues before an expensive prototype is made for verification.

To date, QuesTek has invented and made four new commercially available ultra-high-performance steels that are improvements over other steels that have been used for decades. They are currently in the process of designing and making commercially available more than 10 other alloys based on other elements such as aluminum, nickel, and molybdenum. Much of the funding for their research has come in the form of Small Business Innovation Research (SBIR) grants from the U.S. government.

QuesTek stresses, though, that its materials design approach goes beyond harnessing computational power. Like other companies pioneering these concepts, QuesTek presents its clients with a new way of thinking about the materials

Charles J. Kuehmann, QuesTek president and chief executive officer (left) with Greg Olson, QuestTek chief science officer and co-founder. (Photo courtesy of Andrew Campbell.)

development process—one that integrates specific design and manufacturing requirements pushing for the next level of technologies, rather than focusing on modifying their needs to fit existing materials limitations.

“Integrated computational materials engineering (ICME) has great potential and the direct savings in alloy development time and cost will help drive adoption,” said Charles J. Kuehmann, QuesTek’s president and chief executive officer. “A much bigger impact will be when computational methods can be integrated all the way upstream into the component design community and downstream fully into the manufacturing and process industry. The new frontier is concurrent design of materials and devices. This will exploit the inherent predictability of designed systems, acknowledging design output as not just a material, but a combined material and information system for rapid adaptability in manufacturing and service.

In 2007, S53® became the first commercially produced, computationally designed alloy, developed by QuesTek’s leveraging its Accelerated Insertion of Materials (AIM) expertise, funded by the U.S. Defense Advanced Research Projects Agency and the U.S. Office of Naval Research. The first deployment of a flight critical part made from a computationally designed alloy occurred in 2010 when a T-38 took off with a Ferrium S53 landing gear. QuesTek continues to learn from and build on these accomplishments to refine its knowledge, expertise, and processes. Its newest landing gear steel, Ferrium® M54™, achieved an SAE Aerospace Material Specification in August 2011, within four years of having its initial design goals established, versus seven years for S53. QuesTek designed M54 to be a lower-cost alternative to an existing ultra-tough, ultra-high-strength steel by reducing the amount of cobalt—the most expensive element in the alloy’s composition—by about half of what is contained in the incumbent material, while computationally adjusting other factors to achieve equivalent or better material properties.

In addition to meeting the particular cost and performance needs of its clients, QuesTek’s new steels have generated an economic ripple effect felt far from Illinois. A very visible testament to that is a 65,000-square-foot, 70-foot-tall specialty steel expansion built by Latrobe Specialty Metals Co. in the Appalachian foothills of western Pennsylvania. The facility houses the world’s largest vacuum induction melting (VIM) furnace. Opened in September 2008, at a time when much of the U.S. economy was struggling, the expansion will serve as Latrobe’s platform for securing its position as one of the world’s leading specialty steel manufacturers, particularly for the high performance alloys demanded by the aerospace and defense industries. Latrobe employs 600 people at its manufacturing headquarters, with nearly 200 more working throughout the United States in support positions.

A factor in Latrobe Specialty Metal’s success has been its ability to offer new solutions that meet the rapidly evolving needs of its customers, thanks in part to QuesTek’s accelerated development process. “During the last four years, we’ve introduced four new high-performance steels to customers worldwide, by licensing Ferrium M54 and S53, as well as C61™ and C64™ from QuesTek,” said Scott Balliett, Latrobe’s director of Technology and Quality. “These new product offerings leverage our state-of-the-art vacuum melting facility and help us continue to expand our business.”

Kuehmann believes that QuesTek’s early successes represent just a glimpse of what the future can hold for the potentially transformative approach to materials design that defines his company. “At some point, all materials will be designed using computational models, and materials modeling will be inherent to component design and manufacturing,” he said. “It may be 10 years from now, 20 years, or 50 years, but it will be done this way. QuesTek will continue to be a leader in this revolution, and when we look back on it, we want people to say that we helped make that happen. We’d also like to come up with some really great alloys in the process, ones that make people say, ‘I didn’t think you could make a material do that!’”

Framework for Implementing ICME

(See pages 62-75 for aerospace ICME implementation framework)

Companies in the aerospace industry represent a wide range of materials suppliers and product manufacturers, including those centered about commercial aircraft and propulsion systems, defense applications, and launch vehicles. The following framework represents basic guidelines for implementing ICME approaches for aerospace companies planning to begin an ICME-accelerated product development program within 3 years. The first diagram of this framework (Fig. 6) demonstrates how ICME can be incorporated within the context of a traditional product development process in the industry, and Table VI indicates the type of personnel involved in this process. This framework is also accompanied by Table VII, which includes descriptions of actions at each step in the implementation process, suggestions of computational models and tools,[l] types of skill sets and personnel needed at each step, and key decision points dictating the direction within the product development cycle. Figure 7 provides examples of how companies in the industry can use tools to implement ICME in the aerospace industry framework presented in Fig. 6. Detailed examples of some other specific tools within each of the modules, or toolset types, are presented in Appendix C. These specific computational tools and databases are all accessible via the TMS Cyberinfrastructure Portal, available at www.tms.org/cyberportal.

Actions for Implementing ICME into the Product Development Cycle

Table VII provides detailed recommendations at the various steps within the framework represented by Figs. 5 and 7 in order to assist with the development and launch of an ICME-accelerated product development program (IAPDP). Typically, the actions within a step should be completed before moving on to the next step; however, the ICME toolset involves an iterative methodology that enables IPDTs (integrated product development teams) to revise the component properties, structures, and processing approach as necessary. At certain stages throughout the product development cycle, engineers are thus encouraged to return to these steps in the event that the desired outcomes have not been met. Table VII includes the recommended actions and parties involved at each stage in the IAPDP framework, as well as some specific examples of actions and tools that can be used to complete these steps. It is important to note that this is not a comprehensive list of all personnel and actions involved at each step of any product development program with the aerospace industry, but instead provides a good starting template from which to set up an IAPDP for a given product or process within a specific company.

l. Here, “models” refers to the fundamental physics/materials-based models (e.g., a crystal plasticity model) while “tools” refers to computational codes (e.g., Deform®) that have been properly verified and validated and can be used in a quantitative fashion to implement ICME. The tools are often commercial codes, but can be freeware as well.

Table VI. Key Personnel Involved in Traditional and ICME-Accelerated Product Development Processes in the Aerospace Industry*

- **Aerodynamics/fluid dynamics/concept designer** (designer specializing in aerodynamics and/or fluid dynamics)
- **Airworthiness representative** (representative authorized by the Federal Aviation Administration to make airworthiness determination (certification) for aircraft, and/or specific components on aircraft)
- **Configurator/ preliminary designer** (performs preliminary configuration/design of a platform)
- **Cost estimator** (estimates the costs (time, resources, labor, and ultimately money) associated with product manufacturing or other programs)
- **Customer** (person paying for the product)
- **Designer** (designs specific components and/or platforms)
- **ICME integrator** (engineer tasked with coordinating the ICME elements of the project)
- **Information scientist/data management** (tasked with handling data transfer and storage issues)
- **Manufacturing engineer** (engineer tasked with developing and optimizing manufacturing approaches)
- **Marketing team** (contacts within the company's marketing department responsible for marketing the specific product to the customer, to maximize sales)
- **Materials engineer** (engineer with the expertise and responsibility for development of new materials, as well as selection and deployment of existing materials)
- **Materials supplier** (key points of contact within materials supplier company)
- **Oversight/chief engineer** (chief engineer within the company, or within a major division/ department in the company)
- **Product engineer/integrated product team lead** (lead engineer for a specific product and/ or integrated product development team)
- **Research experimentalist** (engineer or scientist who oversees and carries out experiments supporting research and development efforts including model verification and validation)
- **Research modeler** (engineer or scientist who builds and executes computational models and simulations)
- **Structures engineer/stress analyst** (responsible for structural behavior and analysis of loads)
- **Supply chain management** (contacts in the supply chain of a product; includes materials supplier)
- **Sustainment engineer & logistician** (performs engineering and logistics investigations and analyses to ensure continued operation and maintenance of a system with managed risk)
- **Systems architect/engineer** (architect and/or engineer for the overall product or system, a opposed to a specific component or material)
- **Test engineer** (engineer tasked with testing the performance of and developing use specifications for finished products)

* See "Parties Involved" sections of Table VII for specific placement within framework.

Fig. 6. Aerospace ICME Implementation Framework: Incorporating an ICME Toolset into the ICME-Accelerated Product Development Program (IAPDP)

(Full details of actions and personnel at each step are provided in Table VII.)

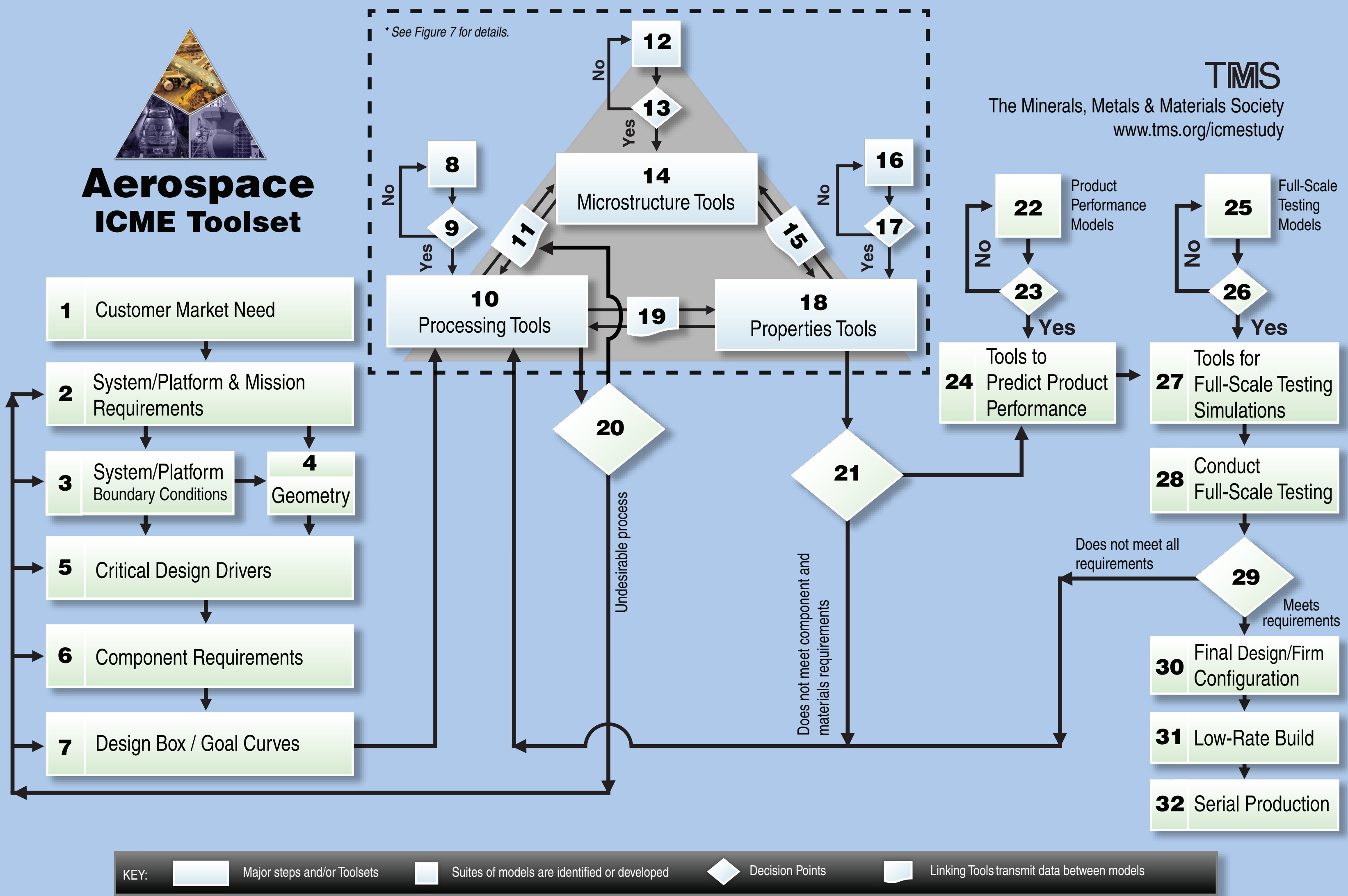


Fig.7. Aerospace ICME Toolset

(Full details of actions and personnel at each step are provided in Table VII.)

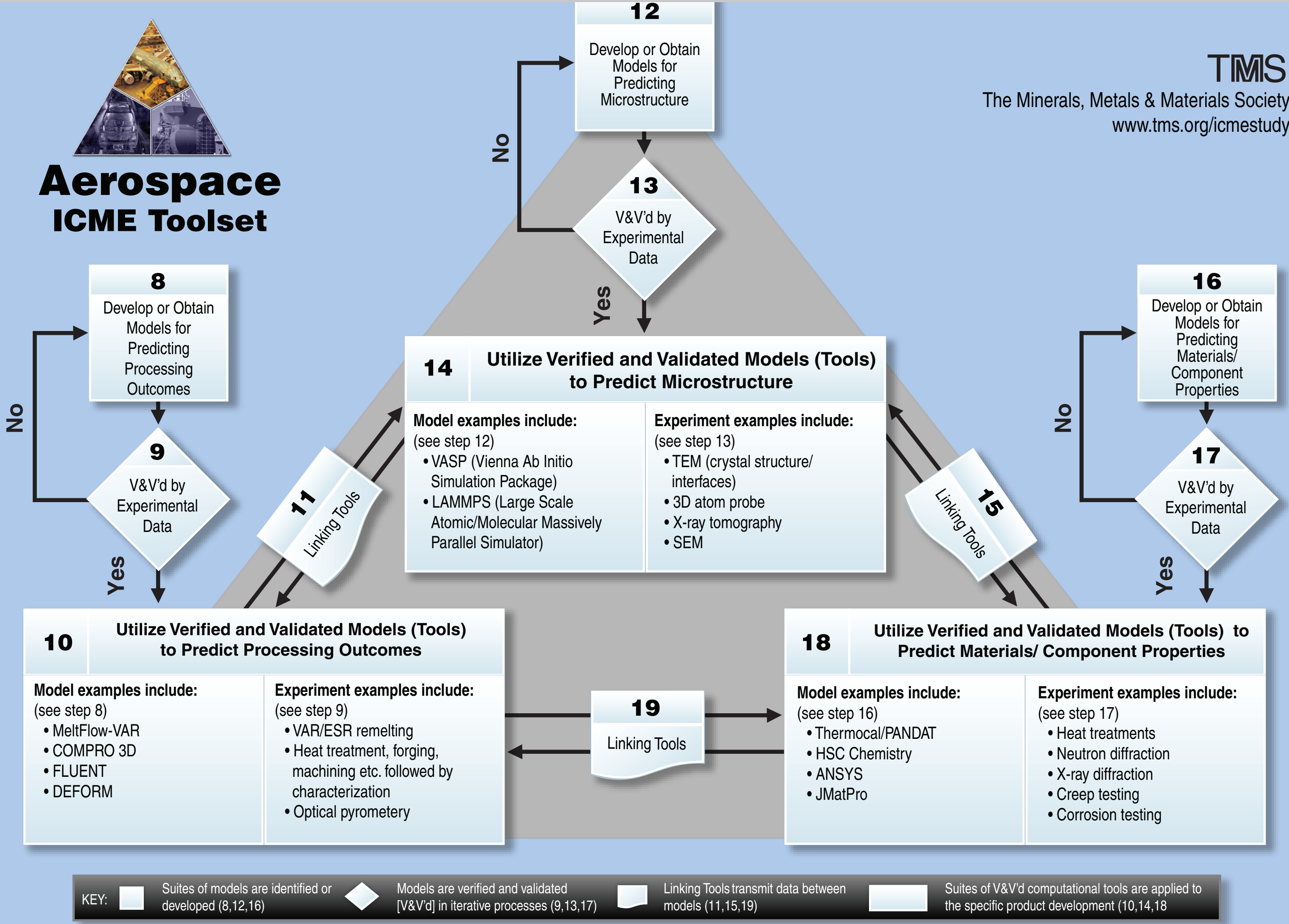


Table VII. Detailed Steps for Implementing ICME Within the Aerospace Sector
(See figures 6 and 7 for illustrated aerospace ICME toolset)

1. Customer Market Need

Parties Involved: Customer; marketing team

- Meet with marketing team (and other relevant groups in the company) to discuss the final product in order to drive the mission requirements.
  - » Example: There is a need for an aircraft that carries X type of cargo, can go Y speed, will last for Z years, and/or is 10% cheaper or lighter than a previous design.

2. System/Platform and Mission Requirements

Parties Involved: Systems architect/engineer; configurator/preliminary designer; aerodynamics/ fluid dynamics/ concept designer

- Identify system/platform and mission requirements based on overall product or system, not solely the component or material you are designing.
- Determine mission requirements such as range, fuel efficiency, top speeds and altitude, aircraft lift, cargo capacity.
  - » Example: Define the most extreme maneuvers of the aircraft, design the ultimate load conditions of those maneuvers.
  - » Note: Consider the initial geometry design before setting mission requirements; these requirements will ultimately drive performance requirements.
- Use platform/mission requirements that will drive the product components, which will have certain property requirements and geometries.

3. System/Platform Boundary Conditions

Parties Involved: Structures engineer/stress analyst; designer

- Identify boundary conditions to which the entire system must conform, including such final design and lifing issues as fatigue, creep, corrosion, etc.
- Use the boundary conditions to drive the geometry/sizing of the component, which will in turn be used to determine the critical design drivers.
- Engage the designer early in this process and increase interactions with the structural engineer to avoid potential conflicts between the geometry and system platform requirements.

4.	**4. Geometry** **Parties Involved:** Designer
	• Enlist the designer to match the geometry to the system platform requirements. • Instruct the designer determining the component geometry to work within a given volume (i.e., the component must logically fit within the system). • Use computational fluid dynamics (CFD) software tools to optimize topology in order to optimize geometry
5.	**5. Critical Design Drivers** **Parties Involved:** Structures engineer/stress analyst; designer; materials engineer
	• Identify boundary conditions with strict constraints. • Determine important drivers, such as density, temperature, producibility, loads, ultimate strength, durability, and damage tolerance. • Identify design drivers and component boundary conditions that will enable the components to achieve overall goals (e.g., know what it takes, specifically, to develop a lighter-weight system). • Use the design drivers to determine component requirements.
6.	**6. Component Requirements (Also known as "Component-Level Performance Requirements")** **Parties Involved:** Airworthiness representative; supply chain management (includes materials supplier); product engineer/integrated product team lead; sustainment engineer & logistician; materials engineer; manufacturing engineer; cost estimator; structures engineer/ stress analyst
	• Dictate requirements at the component level using the system requirements and conditions, such as loads, stresses, or geometries/volumes (as well as cost) to work within. • Focus the team's efforts on comprehensive component requirements, such as structural properties, corrosion, repairability, affordability, manufacturability, trade studies, and risk assessments. » Note: These examples result in the inclusion of more than simple component performance requirements.

7.

7. Design Box / Goal Curves

Parties Involved: Designer; materials engineer; manufacturing engineer; structures engineer/stress analyst

- Obtain or generate (often experimentally) a large, complete property data set for all potential materials/alloys being considered; that includes both new and old materials.
- Establish goal curves based on ideal properties (e.g., plot multiple data sets against goals such as lower weight/cost).
- Do this for multiple materials systems (e.g., various aluminum alloys) or a single system with a range of capabilities that depend on the processing/structure of the material. Identify a materials composition after reviewing large data set for potential materials.
- Use design-allowable specifications to guide goal curves, such as open-hole tension/compression specifications analysis methods or other statistically determined materials property values.
- Enhance this repository of information using ICME and advanced data repositories.
- Iterate with component requirements if needed, as some goal curves or materials requirements may drive component requirements.
- At this point a relationship between the structural design drivers and a material atomistic or molecular structure should be established in order for discrete modeling level ICME tools such as quantum or molecular dynamics to be used in a virtual formulation method.
- Repeat this step as needed until the materials system is narrowed, as ICME methods and output may not initially lead to a desirable prediction of the materials' processing-structure-property relationships.

8.

8. Develop or Obtain Models for Predicting Processing Outcomes

Parties Involved: Manufacturing engineer; materials engineer; research experimentalist; research modeler; materials supplier; ICME integrator

- Assemble and assess a suite of modeling tools to predict the processing outcomes. Examples of computational codes include the following:*
  - » MeltFlow-VAR: Vacuum arc re-melt (VAR) process
  - » MeltFlow-ESR: Electroslag re-melt (ESR) process
  - » DEFORM: Heat treatment, forging, machining, cold forming, etc.

- » COMPRO 3D: Thermal profile modeling; can be used for autoclave modeling for composites
- » FLUENT: ANSYS-based CFD code that can be used to simulate vacuum assisted resin transfer molding (VARTM) in composite systems

9.

9. Verify and Validate Processing Models with Experimental Data

Parties Involved: Manufacturing engineer; materials engineer; research experimentalist; research modeler; materials supplier; ICME integrator

- Conduct a series of experiments to validate that the modeling results represent real-world conditions. Design experiments specifically to work within the bounds of the model to confirm validity. Experimental tests could include the following:
  - » VAR/ESR remelting and subsequent characterization of coupons—both qualitative (to assure that the codes are producing "physically reasonable" results) and more quantitative (to fine tune the model and relevant model input parameters).
  - » Autoclave experiments and characterization of composites processing environment and/or subsequent test coupons
  - » Heat treatments, forging, machining, and/or forming experiments and characterization of resulting microstructure of specimens
  - » Characterization tests for coupons from processing experiments such as above could include:
    - ◊ Qualitative tests: preliminary microstructure resulting from the processing cycle to test generally validity of the model. These could include optical microscopy, electron back-scatter diffraction (EBSD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM) (to provide measurements of phases present, fine scale precipitate morphology, composite fiber morphology, etc.).
    - ◊ Quantitative tests: tests to measure such quantitative data as temperature profiles from processing experiments using, for instance, embedded thermocouples, optical pyrometry, etc.
- Conduct tests to verify that the modeling codes are executing computations properly and providing an accurate mathematical representation of the fundamental engineering principles and relationships that they are designed to represent.
- Note: These tasks may require several iterations of the experiments and/or tweaks to the modeling tools to ensure validity and robustness.

10.

10. Utilize Verified and Validated Models (Tools) to Predict Processing Outcomes

Parties Involved: Manufacturing engineer; materials engineer; research experimentalist; research modeler; materials supplier; ICME integrator

- Move forward and utilize suite of verified & validated models that is representative of the particular processing steps used to modify the material.

11.

11. Linking Tools

Parties Involved: ICME integrator; information scientist/data management; research modeler

- Use the materials or component processing model outputs as input parameters to different microstructure modeling† software packages.
- Link computational models for ICME-accelerated product development and automate the process of data entry between steps.
  - Note: Tools that link the input and output parameters of model simulations to predict processing, microstructure, and properties are commercially limited, but would otherwise reduce error and accelerate computationally driven steps of the product development process.
  - Isight and Model Center are examples of tools used to chain simulation process flows between suites of models.

12.

12. Develop or Obtain Models for Predicting Microstructure †

Parties Involved: Research modeler; research experimentalist; materials engineer; ICME integrator

- Assemble and assess a suite of modeling tools to predict the microstructure (or other length scale structure) of the material. Examples of computational codes include the following: *
  - VASP: Popular electronic structure code using density functional theory calculations to perform ab initio quantum mechanics (QM) and molecular dynamics (MD) operations
  - LAMMPS: Open-source MD simulation code

13.

13. Verify and Validate Microstructure Models with Experimental Data

Parties Involved: Research modeler; research experimentalist; materials engineer; ICME integrator

- Conduct a series of experiments to validate that the modeling results are representative of real-world conditions. Experiments need to be specifically designed to work within the bounds of the model to confirm validity. Experimental tests could include:
  - » Experiments to compare to the results of VASP or LAMMPS codes, including
    - ◊ TEM: e.g., phases present, interface and defect atomic structure, defect character and types
    - ◊ SEM: interface misorientation character and distributions
    - ◊ 3D-atom probe tomography: compositional clusters at the atomic level
  - » Experiments to compare to larger length scale microstructure models, including
    - ◊ Optical microscopy (composites and/or metals)
    - ◊ SEM
    - ◊ X-ray tomography
- Conduct tests to verify that the modeling codes are executing computations properly and providing an accurate mathematical representation of the fundamental principles and relationships that they are designed to represent.
- Note: These tasks may require several iterations of the experiments and/or tweaks to the modeling tools to ensure validity and robustness.

14.

14. Utilize Verified and Validated Models (Tools) to Predict Microstructure

Parties Involved: Research modeler; research experimentalist; materials engineer; ICME integrator

- Move forward and utilize suite of verified & validated models that is representative of the microstructure (or other relevant length scale) of the desired final component.

15.

15. Linking Tools

Parties Involved: ICME integrator; information scientist/data management; research modeler

- Use the materials or component properties model outputs as input parameters to different properties modeling software packages.
- Link computational models for ICME-accelerated product development and automate the process of data entry between steps.

- » Note: Tools that link the input and output parameters of model simulations to predict processing, microstructure, and properties are commercially limited, but would otherwise reduce errors and accelerate computationally driven steps of the product development process.
- » Isight and Model Center are examples of tools used to chain simulation process flows between suites of models.

16.

16. Develop or Obtain Models for Predicting Materials/ Component Properties

Parties Involved: Research modeler; research experimentalist; materials engineer; ICME integrator; structures engineer/ stress analyst

- Assemble and assess a suite of modeling tools to predict materials properties. Examples of computational codes include the following:*
  - » Thermo-Calc and/or PANDAT: CALPHAD (Calculation of Phase Diagrams) method-based software for thermodynamic and phase diagram calculations
  - » JMatPro: CALPHAD method based software; phase equilibria and transformation prediction, solidification behavior, and thermo-physical and physical properties, intended for multi-component alloy systems
  - » HSC Chemistry: Phase equilibria calculations
  - » ANSYS: Standard finite element method (FEM) stress prediction analysis; key for post-heat treatment analysis

17.

17. Verify and Validate Property-Prediction Models with Experimental Data

Parties Involved: Research modeler; research experimentalist; materials engineer; ICME integrator; structures engineer/ stress analyst

- Conduct series of experiments to validate that the modeling results are representative of real-world conditions and design experiments specifically to work within the bounds of the model to confirm validity. Experimental tests could include:
- Experiments to validate the thermodynamics (phase diagram) results, which could include:
  - » Heat treatments (isothermal and/or continuous cooling)
  - » Microscopy: Optical microscopy, SEM/EBSD, and/or TEM to characterize microconstituents resulting from the heat treatments.
  - » DTA (Differential Thermal Analysis)

- Experiments to measure mechanical or other physical or thermo-physical properties (including output of ANSYS), which could include:
  - » Neutron diffraction (residual stress)
  - » X-ray diffraction techniques
  - » Creep testing (engine components)
  - » Corrosion testing
  - » Tensile tests (yield and ultimate strength, ductility/elongation/reduction in area).
- Conduct tests to verify that the modeling codes are executing computations properly and providing an accurate mathematical representation of the fundamental engineering principles and relationships that they are designed to represent.
- Note: These tasks may require several iterations of the experiments and/or tweaks to the modeling tools to ensure validity and robustness.

18.

18. Utilize Verified and Validated Models (Tools) to Predict Materials/ Component Properties

Parties Involved: Research modeler; research experimentalist; materials engineer; ICME integrator; structures engineer/stress analyst

- Move forward and utilize suite of verified & validated models that is representative of the materials or component properties desired.

19.

19. Linking Tools

Parties Involved: ICME Integrator; information scientist/data management; research modeler

- Use the materials or component microstructure model outputs as input parameters to different properties modeling software packages.
- Use special software packages to link computational models for ICME-accelerated product development and automate the process of data entry between steps.
  - » Note: Tools that link the input and output parameters of model simulations to predict processing, microstructure, and properties are commercially limited, but would otherwise reduce error and accelerate computationally driven steps of the product development process.
  - » Isight and Model Center are examples of tools used to chain simulation process flows between suites of models.

20.

20. Decision Point: Is the Processing Approach Feasible?

Parties Involved: Manufacturing engineer; materials engineer; research experimentalist; materials supplier; ICME integrator

- Assess the feasibility of the processing approach.
- Evaluate factors including appropriate machine size, cost, production rate, and materials supplier abilities.

21.

21. Decision Point: Does the Product Meet Component and Materials Requirements?

Parties Involved: Oversight/chief engineer; manufacturing engineer; structures engineer/ stress analyst; product engineer/ integrated product team lead; sustainment engineer and logistician

- Assess the confidence in modeling results and move forward if results are found to be feasible and validated.
- If the product does not meet component and materials requirements, re-enter the ICME toolset iteration loop for additional simulation or reconsider the requirements, drivers, and geometry of the component.
- Conduct product life-cycle assessment, prediction, and monitoring.

22.

22. Develop or Obtain Models for Predicting Product Performance

Parties Involved: Test engineer; manufacturing engineer; structures engineer/ stress analyst; product engineer/ integrated product team lead; supply chain management (includes materials supplier); research modeler; research experimentalist

- Assemble and assess a suite of modeling tools to use the output of the optimized materials processing-structure-properties approach to predict the product performance in terms of scale up.
- Use in conjunction with commercial finite element analysis (FEA) and other structural tools to model the assembly, aerodynamics, failure of large-scale components, etc. using scale-up experiments as validation.
- Conduct fewer iterations in this set of steps as the ICME Toolset and associated models become more advanced.

23.	23. Verify and Validate Performance-Prediction Models with Experimental Data
	Parties Involved: Test engineer; manufacturing engineer; structures engineer/ stress analyst; product engineer/ integrated product team lead; supply chain management (includes materials supplier); research modeler; research experimentalist
	• Determine whether modeling results are representative of real-world conditions and whether the modeling software executes computations properly. Examples of experimental tests include the following: » Air flow/wind tunnel testing (aerodynamics) » Bird impact tests (engine) » Component and airframe static and durability testing
24.	24. Utilize Verified and Validated Models (Tools) to Predict Product Performance
	Parties Involved: Test engineer; manufacturing engineer; structures engineer/ stress analyst; product engineer/ integrated product team lead; supply chain management (includes materials supplier); research modeler; research experimentalist
	• Move forward and utilize suite of verified & validated models for predicting the product performance.
25.	25. Develop or Obtain Models to Simulate Full-Scale Testing
	Parties Involved: Test engineer; manufacturing engineer; structures engineer/ stress analyst; product engineer/ integrated product team lead; supply chain management (includes materials supplier); research modeler; research experimentalist
	• Assemble and assess a suite of modeling tools to use the results of predicted product performance to simulate the full-scale product performance tests. • Note: Full-scale model simulations at this stage are currently immature, but future efforts are in progress. This will help to avoid any potential error when conducting full-scale product tests.

26.

26. Verify and Validate Test Simulation Models with Experimental Data

Parties Involved: Test engineer; manufacturing engineer; structures engineer/ stress analyst; product engineer/ integrated product team lead; supply chain management (includes materials supplier); research modeler; research experimentalist

- Determine whether modeling results are representative of real-world conditions. Examples of experimental tests include the following:
  - » Bird impact tests (engine)
  - » Airframe static and durability testing

27.

27. Utilize Verified and Validated Models (Tools) to Simulate Full-Scale Testing

Parties Involved: Test engineer; manufacturing engineer; structures engineer/ stress analyst; product engineer/ integrated product team lead; supply chain management (includes materials supplier); research modeler; research experimentalist

- Move forward and utilize suite of verified & validated models to simulate full scale testing
- Use basic finite element modeling tools to verify and optimize planned testing for full-scale tests.
- Dictate the models by what the team intends to test at the full-scale testing stage; experiments are not limited by the capabilities or limitations of the model.

28.

28. Conduct Full-Scale Physical Tests

Parties Involved: Structures engineer/ stress analyst; product engineers/ integrated product team lead; test engineer; aerodynamics/ fluid dynamics/ concept designer; supply chain management (includes materials supplier)

- Conduct specific, targeted full-scale experiments and/or physical tests on the ICME-optimized prototype; try to “break things” often using combined testing methods (e.g., crash, fatigue, bird impact)
  - » Note: This is the last step before final design/firm configuration, the point at which a successful full-scale test leads to the building of factories, or commitment to the use of existing factories. Failure to successfully complete full-scale tests can lead to significant setbacks or project termination.
- Conduct model-based testing to assess critical locations

29.

29. Decision Point: Have the Full-Scale Product Tests Passed?

Parties Involved: Oversight/chief engineer

- Assess the results of the full-scale tests. If the tests pass, the design is considered final and the team should begin work on final product specifications

30.

30. Final Design/Firm Configuration

Parties Involved: Oversight/chief engineer; designer; materials engineer; supply chain management (includes materials supplier); structures engineer/ stress analyst; systems architect/engineer

- Do not conduct additional ICME iterations at this point, as design properties have been established.
- Finalize model-based material and product definitions

31.

31. Low-Rate Build

Parties Involved: Product engineer/integrated product team lead; manufacturing engineer; supply chain management (includes materials supplier)

- Produce and inspect a limited number of designs and use the results to confirm that there are no issues present in the design.

32.

32. Serial Production

Parties Involved: Product engineer/integrated product team lead; manufacturing engineer; supply chain management (includes materials supplier)

- Produce the product according to the specifications of firm configuration.

* See Appendix C for a list of additional computational tools.
† Although the term microstructure is generally used only in reference to metals and other crystalline materials, in this context it is used to denote the meso-, micro-, or nano-scale structure of the material class undergoing ICME—including metals, ceramics, and composites.

Current Barriers/Needs, and Recommendations for Addressing Them, in order to Implement ICME in the Aerospace Sector

Although ICME has the potential to significantly reduce the costs and accelerate the introduction of new products in the aerospace industry, some potential barriers need to be addressed to better enable the widespread adoption of ICME within the industry.

Need for Improved Quantitative Modeling Tools

Successful execution of ICME is dependent upon a broad range of tools and methodologies that must be reliable, cost effective, and verified and validated to ensure the accuracy of the results. Many currently available computational models and tools that can be used to support ICME integration are not acceptable for implementation primarily due to the inability to fully or accurately simulate the complexity of materials systems. In addition, the broader community does not fully recognize the potential opportunities and benefits from working with small software vendors, who may be able to provide the necessary tools within an accelerated timeline or at a lower cost to the customer. The following are some specific needs and recommendations regarding available software and modeling tools:

- There is still a lack of sufficient, commercially supported ICME software that predicts salient properties of various materials classes, specifically the properties that those classes are most known for (e.g., ceramics are brittle, strong in compression and weak in tension). There are numerous industry and university in-house software codes with varying capabilities for these purposes, but a much smaller number of formalized, documented, and ICME-adapted codes. Teaming up with small software companies to commercialize some of these codes could be a strong strategy for accelerating verification and validation. Software companies are typically adept at this process, bring the added benefit of commercial technical support for the codes, and have a strong incentive to team with other organizations in such efforts because of the potential to expand their revenue through the development of new products.
- Quantitative physics-based modeling tools for prediction of some critical material design values (e.g., fracture toughness and fatigue crack growth rate) are relatively immature and often expensive to develop. In particular, minima in defect sensitive properties (e.g., low and high cycle fatigue) will require that such models can predict the effect of both microstructural and exogenous defects, and accurately calculate life distributions via crack growth. One recommendation for working around this gap in the short term is for team members to build empirical linear regression models based on targeted experimentation and use these models to define domains in which the physics-based models are applicable. If there are not relevant physics based models to provide accurate, quantitative predictions of the critical material design values, particularly those based on in-service life issues, the linear regression models, coupled with relevant design value data from the experiments, can be used to circumvent this gap. Additionally, rigorous material property models based on first-principles physics are often unavailable and/or unreliable for the needs in a specific

product development program, and should continue to be developed.

- More specifically, there is a need for more quantitative, accurate processing-related models for weldability, formability, and repairability of materials that make the connection from discrete to continuum systems and can be used to identify the materials parameters that drive the properties.
- For composite systems, accurate and general failure theories connecting characteristics from discrete to continuum systems are necessary to enable more predictive analysis capabilities and fill a theoretical gap in the community's current understanding. Additionally, validated computational tools for composite systems, particularly for MD simulations, microstructure prediction, and accurate failure prediction need further development.
- Since modeling every atom is computationally intensive for dense systems, methods to calculate free energy using explicit (atomistic) models need to be pursued.
- Force field development parameters in molecular modeling can be optimized for heterocyclic polymers, metals, and other materials.

An overarching recommendation related to those identified above is that the members of integrated product development teams should support the development of commercially supported software codes that predict salient properties. In order to advance the state of the art of available computational models and tools, potential adopters of ICME could use these codes in foundational engineering problems[1] and consider creating cost-share opportunities between original equipment manufacturers (OEMs) and software companies in applying these tools to such foundational engineering problems. When possible, ICME adopters can also work with small software companies to co-develop and demonstrate the efficacy of codes that predict salient properties to indicate the need for commercial support. Universities and government laboratories could also be excellent potential partners in these efforts, as they are known for developing specific computational codes that are useful yet often not widely implemented. The partnering entities also need to develop linkage tools to facilitate the simple, automated transition of data between models, and integrate these tools into ANSYS or ABAQUS software while conforming to ICME protocols. These recommendations can be implemented in the near-term timeframe for initiation of ICME-accelerated product development programs (within 3 years), and continue to be developed concomitantly with the further implementation of ICME in the product development process.

Cultural Barriers and Intellectual Property Issues

Traditional corporate organizational structures often inhibit the collaboration necessary to fully implement ICME across a large product development program. Acceptance of ICME necessitates that companies, specifically materials developers within companies who have traditionally relied on empirically based design methods, overcome aversion to computational tools and their outputs, and reconsider the way they do business. This includes investing in the methods, tools, and skilled individuals necessary to implement a successful ICME program. Advocates of the ICME approach within the corporation can communicate with more skeptical colleagues to help them understand and become more amenable to considering ICME approaches. Additionally, designers, manufacturers, and materials engineers could communicate better with one another during the product development cycle. It is important to reach out across such lines and consider more structured communication mechanisms within individual organizations. The ability for materials engineers and scientists to communicate with design and structures engineers will be critical for rapid acceptance, and their ability to validate models to the level of accuracy required by customers of model predictions will enable greater acceptance and utilization.

Other cultural barriers include the competing interpretations of ICME and product development procedural flowcharts. This is often a result of different perspectives and is representative of the significant complexity of ICME. This report and some of the references herein can provide some consistency to interpretations of ICME and its implementation in product development procedural flowcharts, for instance by employing the foundational starting framework represented by Figs. 6 and 7 and Table VII, collectively.

Another major cultural barrier to full ICME implementation in the aerospace industry is the intellectual property issue. Inability or unwillingness on the part of industry, academia, and/or government organizations to distribute proprietary information can significantly limit the sharing of data among ICME contributors and OEMs, particularly for areas in which it would be extremely helpful to leverage the strengths of ICME contributors across various organizations. There are few incentives for entities to share proprietary information safely and securely, as they are limited by a sense of ownership of the data and/or the significant cost incurred by generating the data. Consequently, integrated product development teams using ICME must often rely on databases that store information in the public domain, which are often of limited quality and/or use. The importance and the impact of the creation of open-source tools and databases to assist materials and design simulations has been recognized for some time and had a place as a key recommendation of an National Research Council (NRC) study focused on bridging design, materials, and production.[23]

Due to the nature of capitalism and the need for competitive advantage, there will always be proprietary information that companies cannot or are not willing to share; similarly, there will always be national security issues that restrict data within a particular realm. However, actions can be taken to mitigate the impact of these constraints. One of the first recommendations is for each organization, and each ICME integrator within that organization, to determine the furthest limits that differentiate strictly proprietary information from pre-competitive data and computational tools. They can then work toward sharing such pre-competitive data to maximize the significant leveraging opportunities and mutual advantages that ICME integrators across the commercial, government, and academic sectors can take advantage of by working together.

The materials science and engineering community has been aware of data sharing problems for some time, and the government has recently been instrumental in addressing this area through the Materials Genome Initiative (MGI), an interagency government initiative connected to the U.S. Office of Science and Technology Policy.[8] In particular, various government agencies (e.g., the National Science Foundation, U.S. Department of Energy (DOE), U.S. Department of Defense (DoD), National Institute of Standards and Technology (NIST), and U.S. Department of Commerce) are funding programs to help develop the MGI Materials Innovation Infrastructure,[8] across which a major theme is the sharing of digital data. This is a large task that involves people working together to develop appropriate software and hardware platforms and overcome cultural barriers. In this regard, various organizations including NIST, the Air Force Research Laboratory, and professional societies have put together workshops to convene interested parties to address issues with digital data and provide recommendations for sharing data. Potential ICME integrators should consider reading such reports[24,25] and following or getting involved in future MGI efforts by attending appropriate workshops in this arena. Such individuals can also try to stay aware of such events and initiatives through professional societies.

Publications provide another way to share pre-competitive data and, occasionally, computational tools. For example, journals in many fields are increasingly providing access to digital data in their articles, such as *Integrating Materials and Manufacturing Innovation,*[m] *Acta Crystallographica A: Foundations of Crystallography,*[n] and *F: Structural Biology and Crystallization Communications.*[o] Many of the journals that allow uploading of data also follow an "open access" model through which anyone can access the article, and thus any included data, online without having a subscription. Therefore, ICME integrators and other members involved in ICME efforts can use such journals as a source for accessing and publishing data. Notably, although sufficient mechanisms for citing such data and acknowledging intellectual debt are lacking, Thomson Reuters is currently developing an indexing system for published data that will allow data citations to be tracked and acknowledged in a similar fashion as published papers are today.[26] As criteria for publishing and citing data become standard, this will likely provide an incentive for scientists to increasingly share precompetitive data.

Establishing a Business Case for ICME

A business case that demonstrates the value and return on investment (ROI) for stakeholders (e.g., materials suppliers, manufacturers, and designers) is critical to obtaining industry buy-in and sustaining long-term investment in ICME from government, industry, and academia. For instance, software licenses and high performance computing resources often require significant funding, particularly in early stages of development, which can make it difficult to convince stakeholders to provide funding for an investment in ICME, despite the fact that it could save the company significant time and money throughout the entire product development cycle.

To obtain stakeholder buy-in and thus implement ICME, it is therefore important to demonstrate its value through a careful economic analysis of the cost and savings associated with investing in an ICME program. When doing so, testing costs and duration can be quantified in a number of areas. For example, certification costs associated with each product or part are ongoing, yet the volume of certification tests required may diminish significantly because of model simulations. In addition to certification requirements, materials suppliers must meet rigorous qualification standards to prove that they can supply the desired material; this also applies to qualifying existing suppliers if changes are made to the part or product configuration. Although initial investments can be costly, the need for these validation tests will decrease as models become more representative of real-world conditions. Design allowables in the aerospace industry require a significant initial investment to develop new materials specifications and derive their property values from the testing data. However, as computational methods and databases are becoming more advanced regarding

m. Available at http://www.immijournal.com/.

n. Available at http://journals.iucr.org/a/.

o. Available at http://journals.iucr.org/f/.

predictive methods, fewer tests are required to establish the confidence needed to develop new design allowables specifications.

Additional program costs should be considered when quantifying ROI. Passing the quality requirements of the Materials Review Board is time consuming and costly, particularly if temperature, chemistry, or processing costs do not meet certain conditions, when this may otherwise have been avoided by computational methods. Developing statistical or neural net models from relevant materials databases as part of the development of new materials may be easier to achieve with the advancement of robust, physics-based predictive tools. IAPDPs require an IT infrastructure for the generation, capture, and transmission of data, as well as the generation of relevant physics- and experience-based modeling tools, and these should also be taken into consideration when calculating ROI.

Workforce Needs

The availability of skilled users of software and high-performance computing resources are critical to establishing fully operational ICME programs. In current university environments, materials scientists and computer scientists do not typically interact or have cross-training opportunities that could further their knowledge and understanding of ICME. This environment inhibits students from accessing and applying computational methods and tools to materials science and engineering applications, creating a knowledge and experience barrier that can potentially limit entry to the field. However, the current lack of a strong capability in computational materials engineering in many organizations within or supporting industry can be addressed with some near-term tactics.

To address the lack of cross training within universities, increased interaction and collaboration between materials science and engineering and computer science departments can be encouraged and incentivized. Possible tactics include pursuing funding opportunities for such collaborations provided by federal agencies, earning support from university deans and department heads by recognizing the potential for attracting more students to each department by offering a joint or hybrid degree, and utilizing the current “cluster hire” model in which new faculty positions are created across multiple departments.

Establishing a strong capability in computational materials engineering within an organization or industry in the near term may require hiring additional staff with the appropriate capabilities and require supplementary training of existing personnel. Both will involve increasing the number of skilled users of software and high performance computing facilities in the near term and the long term. One suggestion for advocates of ICME within industry to address such a limited workforce trained in ICME is to hire 2–3 interns each year to work on specific problems (e.g., projects requiring computational methods) that are interesting, appropriate, and provide some ROI. Interns could have access to senior management and make presentations to management at the end of their term, with an aim toward a job offer being presented at the end of the internship. This effort can be supported by establishing relationships with universities, primarily person-to-person relationships with a member of academia who is interested in using computational methods to train students and prepare them for entry into the field. Mini-courses, summer schools, and continuing education programs can effectively augment the ICME training of present employees within industry, and professional societies could be considered as potential partners for continuing education opportunities. Finally, industry can consider providing increased funding for university projects that support industry activities in this field.

Within an existing organization, management can also encourage the development of internal ICME leaders and partnerships to leverage traditional industry experience and computational/digital expertise. This can be accomplished through the development of working partnerships between senior, experienced personnel and junior talent with strong computer skills. For example, a senior engineer may work with software that only performs geometry optimization and requires an input script for post-processing. This may require script-writing skills not possessed by the senior staff but readily available from junior staff. Formalizing this type of partnership and making it a part of career development can be an efficient way to produce results and help to bridge the gap between new hires and the aging workforce. If onsite employees do not have the necessary skills to complete ICME projects, organizations can also form partnerships with external parties that possess the desired expertise.

Lack of Past Experience in Implementing ICME

As ICME is an emerging discipline there remain various hurdles for companies interested in adopting the approach. One of the most significant is that launching an IAPDP is a significant effort that requires cost, personnel, and time investments. As with any innovative new methodology, it can be difficult for new adopters to recognize the benefits in time and cost savings of ICME, and commit to the set-up and sustainment of ICME without demonstrations of past performance and fully vetted data within their organization to predict a successful ICME approach more confidently. The first demonstration of a new methodology is a challenge in itself for some large organizations and can equate to a much larger hurdle for smaller organizations interested in implementing an ICME approach. Additionally, both types of companies often lack a full understanding of the metrics for victory associated with ICME.

A suggestion to overcome such challenges within a company is to highlight and study past successes within the industry using this methodology, as well as smaller-scale or partial successes that have been achieved in that company, or others, using ICME methodologies. Studying the implementation of other multidisciplinary technologies, such as computational fluid dynamics modeling tool integration can also help provide background information for an ICME endeavor. Additional experience will be gained by addressing problems that may be ripe for the aerospace industry in the near term, which are explained in the following section. Organizations can also first use ICME approaches to develop a simple component or product, for which successful execution will require a smaller investment of time and money, although it will also have a lower ROI. Once the first ICME-accelerated program is undertaken, whatever the size, the experience will provide the confidence needed to expand ICME implementation to larger programs and other product lines. The past ICME success stories outlined in this report and in other references[p] may be quite helpful in this regard, as will the detailed frameworks and recommendations provided in this study.

p. Additional references are provided in section IX.

Need for ICME Standards

There is a need for the community to more aggressively support not only software development tools but also integration infrastructure, which is supported by software and data standards.

Establishing compatible software tools and communication protocols for an ICME framework is critical to enabling the robust implementation of ICME. To date there is no standard framework for sharing models across a broad user-base or for capturing, formatting, and managing data and metadata across models and steps within the ICME framework. This is important to establish for publishing purposes and will help drive acceptance by the community. Additionally, current software codes are written for central processing units rather than graphics processing units (GPUs), which currently limit the speed at which larger simulation models can be produced. Therefore, software companies and designers can emphasize the need to move toward more standardized GPU compatibility.

Due to a lack of compatibility among tools and established standards, there is also a need for ICME tools with varying levels of maturity to coexist within a framework and still allow teams to have confidence in the tools and successfully quantify uncertainty. One way toward addressing this is to integrate model predictions with associated product test data. Bayesian statistics can support continued uncertainty quantification as additional product data is generated and analyzed.

Another recommendation toward contributing to compatibility between tools is to implement and refine the definition and use of technology readiness levels (TRLs) for software to assess the maturity for ICME implementation. Although the use of TRLs for software is not yet widely spread among DoD organizations, a 2002 report prepared for the Army outlines a path in this direction.[27] Developing consistent criteria for assessing software maturity via a TRL system would assist in uncertainty quantification of model output, information that is particularly critical when linking models in an integrated computational approach.

In addition, models under development can require access to proprietary databases that drive them, but may lack the level of security that would prevent outside entities and those without appropriate clearance from viewing and compromising the models. Due to these security concerns, IPDTs may have limited ability to capture and share valuable data and metadata for the purposes of building databases and models. To the extent possible, the development of models that critically depend on proprietary data should be well secured. A broader group of experts who could strongly contribute to this development could have access to the data, and could sign confidentiality agreements to meet security needs. Additionally, care must be taken to partition or compartmentalize models and required input data features, as models and associated input data can result in unintended export control requirements.

Regulations and Certification Constraints

Gaining acceptance of ICME by regulators (e.g., FAA) is a critical process in enabling ICME. The current system of regulation and certification provides that materials and processes from previous development experiences are acceptable ways of producing a safe, reliable product. However, true innovation often means introducing radically new approaches that do not strictly conform to the previously accepted approach for producing products. Thus, gaining acceptance by certification and regulatory bodies presents a significant challenge for ICME. Therefore, parties interested in implementing ICME within their organizations might reach out to personnel at the necessary regulatory and certification organizations to begin educating them about ICME. This could be done through the same channels as those recommended for creating awareness and understanding of ICME, namely through communicating about ICME, extending invitations to relevant events focused on ICME, and providing reports and literature on ICME.

Near-Term Opportunities for ICME in the Aerospace Industry

Although ICME-accelerated materials and product development is already occurring in the aerospace industry, the approach is well positioned to increase significantly in use and acceptance in the coming years. While many new aerospace products could benefit from ICME approaches, certain applications are poised to benefit in the near term (within the next 3 years). The following applications, not in priority order, represent some of the most promising opportunities to apply ICME tools and methods in the aerospace industry in the near term:

- Identify new alloys in the nickel-cobalt design space for turbine applications using models instead of experimentation
- Conduct a study to predict tool/part interaction of woven composites, modeling reaction kinetics, weaving, mold filling, and residual stress development
- Examine production approaches, repair, integration, and damage tolerance of ceramic exhaust nozzles
- Design improved, high-temperature alloys for nozzle applications using a computational materials design approach
- Expand the use of cast or wrought magnesium for aircraft interiors, using better models to address concerns regarding the flammability of magnesium
- Develop simulation-based assessments to reduce the qualification costs (in terms of destructive tests) of Ti-6Al-4V or Al 750 airframe forgings
- Construct models based on past failures of old materials, to address a Foundational Engineering Problem
- Model the exchange of chemical potential for fluid-polymer interaction to reduce soaking tests that take 1–5 years
- Lower the transition temperature for shape memory alloys using quantum mechanics; the current market is too small to support an experimental approach, but ICME may be justified.
- Create new materials to extend the life of canopy coatings, which are subject to harsh environmental conditions
- Co-design superalloy single crystals along with oxidation and corrosion-resistant coatings to reduce costs or identify new materials
- Create models for prediction of the microstructure, properties, and processing of titanium, nickel-powder, and cobalt-powder components fabricated by emerging laser- and electron

beam-based additive manufacturing processes.

- Use computational approaches to identify possible new high-temperature rotating alloys for jet engine applications, to increase fuel efficiency.

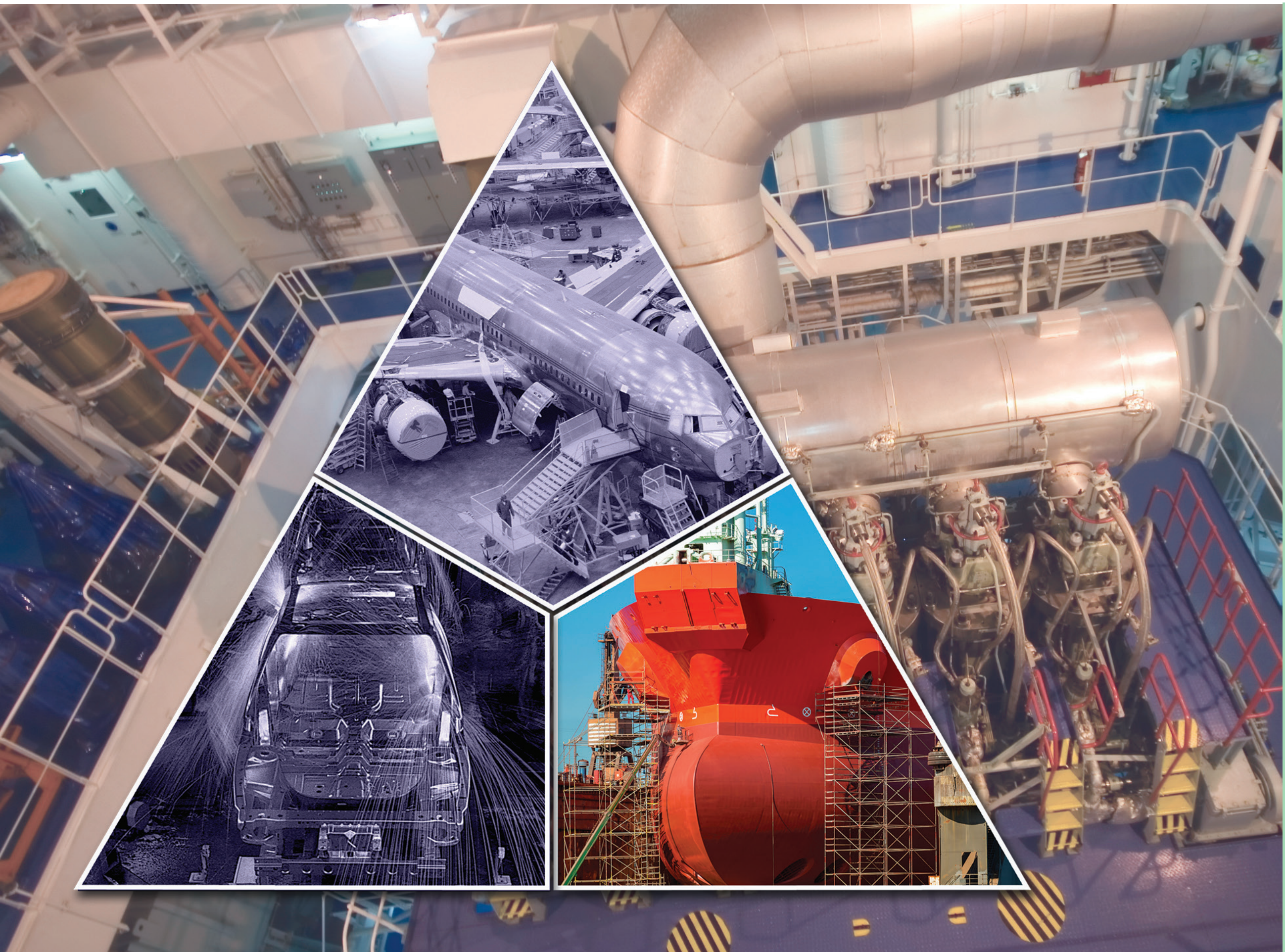
Closing Remarks on Implementing ICME in the Aerospace Industry

This chapter provides a framework that can serve as a template or building block for ICME-accelerated product development programs (IAPDPs) within the aerospace industry as well as details of the personnel and specific actions involved at each step to put this framework into practice (see Figs. 6 and 7). A number of further recommendations, challenges, and opportunities to implementing ICME in the aerospace industry are also provided. For a given product or problem for which ICME can provide value, the integrated product development team (IPDT) within a company can start with the framework and recommendations presented here, and then adapt them and insert much more detail, to address their specific product or problem, before commencing an IAPDP.

Some of the concepts discussed here are unique to the aerospace industry (e.g., the ICME implementation framework and related table of personnel and actions, past success stories, detailed modeling tool needs, recommended near-term opportunities, FAA certification). However, some of the themes elucidated by the aerospace team have applicability across a wide range of industries, such as cultural barriers, intellectual property and data sharing issues, and workforce development needs. In this vein, the most pervasive issues across the three industries considered in this study have been provided in Chapter III. Although this chapter (Chapter V) is written for those interested in implementing ICME in the aerospace industry, it can therefore provide significant value to professionals in other industries who encounter similar circumstances, challenges, and opportunities.

VI.

Industrial Sector Focus: Maritime



Process Overview

The Maritime ICME Implementation Team consisted of materials, mechanical, and structural engineers and designers from two large shipbuilders, experts from U.S. Navy and Department of Defense (DoD) organizations who have worked extensively in platform and product development programs for the navy, individuals who have worked in the development and application of ICME computational and experimental tools associated with maritime applications, and an expert from a steel producer who has worked extensively with Navy shipbuilding programs. For a complete list of the maritime team members, please see Appendix B.

Current State of the Art of ICME in the Maritime Sector

Although the framework presented in this chapter can serve as a starting template for ICME implementation in commercial as well as naval applications, since the maritime industry is largely driven by the interests of the navy, particularly in the United States where the U.S. Navy is by far the largest customer of shipyards,[q] much of this framework was developed from the naval perspective. In this case, product development focuses heavily on tried-and-true methods that follow strict guidelines for manufacturing mission critical components for submarines, aircraft carriers, and other marine vessels. At this time, there are no prominent case studies that demonstrate full ICME implementation in platforms or components throughout the majority of a product development cycle and across an integrated product development team (IPDT). The Office of Naval Research (ONR) and the Defense Advanced Research Projects Agency (DARPA) have invested considerably in the development of ICME tools, such as three-dimensional (3-D) modeling and experimental tools developed in the ONR/DARPA D3-D program discussed in the 2008 National Academies Study on ICME[1]. But these relatively new tools have not yet been implemented in a full ICME-accelerated product development program. Alternatively, there are examples of the application of computational materials engineering techniques to assist, more qualitatively, in specific segments of the product development cycle.[28]

Because of the relative immaturity of ICME implementation in maritime applications, industry stakeholders are often unfamiliar with the use of ICME methods to develop new materials and new processing and manufacturing approaches; therefore, it is challenging for naval designers and engineers to obtain the needed resources, support, and personnel to integrate computational tactics into traditional product development approaches. Due to the wide range of ICME tools developed by the DoD and other industrial, government, and academic organizations, and the ICME experience and successes achieved in other industries, there is a great opportunity to put these tools and this experience base to use in order to implement ICME much more broadly, and in an integrated fashion, across the product development cycle of maritime platforms and components.

Framework for Implementing ICME

(See pages 90-103 for maritime ICME implementation framework)

Companies in the maritime industry represent a wide variety of manufacturers from material

q. For more information visit http://www.shipbuildinghistory.com/today/statistics.htm.

suppliers to product and system manufacturers. Maritime platforms are complex systems that require a wide range of products, from smaller components (e.g., valves, etc.) to entire sub-systems. Shipbuilders have to integrate these products to fabricate hugely complex platforms such as aircraft carriers, submarines, and other platforms to support the needs of the U.S. Navy.

New design projects or programs initiated by the DoD or the navy may require new materials to be developed to meet increasingly demanding performance specifications. The ICME process offers to ease the development of affordable materials with superior properties which may provide a compelling case to naval funding agencies and acquisition offices that would justify investing in such a program. The following framework (represented collectively in Figs. 8 and 9, and Table IX) may provide the representative basic building blocks or blueprints to initiate ICME-accelerated product development programs (IAPDPs) within 3 years. This framework and the related recommendations and opportunities can thus lower the barrier to implementation of these new ICME programs. The framework includes descriptions of each step, computational models and tools,[r] types of skillsets and personnel needed, and key decision points dictating progression within the product development cycle.

In Figs. 8 and 9, arrows represent the sequence and flow of information between steps. The framework does not contain a direct linear sequence of steps, but instead illustrates the many feedback loops that can take IPDTs back to earlier stages of development if needed, depending on the outcome of the steps. Detailed examples of some specific tools within the modules are presented within some of the "Required Actions" entries in the table, with a more comprehensive list available in Appendix C. These specific computational tools and databases are all accessible via the TMS Cyberinfrastructure Portal, available at www.tms.org/cyberPortal.

Actions for Implementing ICME into the Product Development Cycle

Table IX provides detailed information to assist with the development and launch of an ICME-accelerated product development program and Table VIII indicates the type of personnel involved in this process. The corresponding illustrated framework is depicted in figures 8 and 9. Although all required actions should be completed before moving on to the next step, the ICME methodology encompasses an iterative process that enables revision of the component properties, structures, and processing approaches as necessary. At certain stages throughout the product development cycle, members of the integrated product development team (IPDT) are encouraged to return to a given step in the framework in the event that the output is not meeting the desired outcomes. Table IX includes the recommended actions and the parties involved at each stage of the framework represented in figures 8 and 9. Examples of specific tools that can be used at each stage are also included.

r. Here, "models" refers to the fundamental physics/materials-based models (e.g., a crystal plasticity model) while "tools" refers to computational codes (e.g., Deform®) that have been properly validated and verified and can be used in a quantitative fashion to implement ICME. The tools are often commercial codes, but can be freeware as well.

Current Barriers/Needs, and Recommendations for Addressing Them, in order to Implement ICME in the Maritime Sector

Although ICME has the potential to significantly reduce the costs and accelerate the introduction of new products and manufacturing processes in the maritime industry, some potential barriers (or needs) could be addressed to better enable the widespread adoption of ICME within the industry in the near term. Such needs and recommended solutions were determined by the maritime team, and are discussed in this section. Some of these issues were elucidated by the other industrial teams as well (and are thus considered in Chapter III as "Pervasive Issues"), but are considered here in the context of the maritime industry.

Table VIII. Key Personnel Involved in Traditional and ICME-Accelerated Product Development Processes in the Maritime Industry*

- **Academic/university liaison** (contact in academia who provides additional scientific and/or engineering support, in this context, particularly in reference to computational modeling)
- **ICME integrator** (engineer tasked with coordinating the ICME elements of the project)
- **Laboratory technical lead** (individual who carries out certification and documentation testing of materials and products)
- **Materials supplier** (key points of contact within materials supplier including materials engineers)
- **NAVSEA** (Naval Sea Systems Command)
- **Research experimentalist** (engineer or scientist who oversees and carries out experiments supporting research and development efforts including model verification and validation)
- **Research modeler** (engineer or scientist who builds and executes computational models and simulations)
- **Ship design manager** (individual(s) responsible for overall ship design and coordination and integration of individual systems and platforms)
- **Shipyard engineer** (engineer within a shipyard responsible for fabrication of naval vessels)
- **Stakeholder or acquisitions lead of the contract** (e.g, in the navy this would be the Program Executive Officer (PEO) – i.e., the contact within the Navy Acquisition Office responsible for initiating and ensuring fulfillment of technology development projects)
- **Technical warrant holder** (U.S. Navy representative responsible for certifying within their area of expertise - i.e. technical warrant area - that a design for a navy platform is safe, technically feasible, and affordable)

* See "Parties Involved" sections of Table IX for placement within framework.

Improved Quantitative Modeling Tools; Acceptable Linkage Software and Tools; and ICME Standards

The introduction of ICME approaches into the product development process requires robust modeling tools as well as methodologies to ensure that the models and data are effectively used. In the maritime industry, there is a need for microstructural evolution simulation tools and reliable structure-property databases as a key component to enabling ICME. Current ICME Integrators have also identified a lack of analytical tools that could enable the automated acquisition of microstructural information intended as input for modeling tools. Linkage tools designed to integrate data across these models (e.g., the output of model X is input to model Y) are also lacking, immature, or often owned outside of the naval community. Therefore, subsequent to their adoption within a company, specialists have to troubleshoot these software packages frequently to ensure the smooth transmission of input and output data between models. The material properties input data for the models is often limited in its availability and, in cases where data is not proprietary, it is often unpublished or may not be credible, or the data origin or method of collection is unclear. In addition, once data is obtained and used, there is a need for methods to quantitatively verify and validate models faster and more effectively.

Finally, ensuring the availability and cost-effectiveness of relevant materials databases for physics-based models likely will require both near- and long-term investments and actions on the part of the larger maritime community.

Near-term activities recommended

In the near term, members of the community could create an objective method of characterizing and quantifying materials microstructures to assist in the development and validation of physics-based models. Using this method, they can examine the microstructural data, define and quantify the microstructural characteristics, and incorporate the information into the models to simulate/calculate/compute the materials properties. This is best executed on problems for which some microstructure-property relationships are well-known, such as the effect of certain feature sizes or compositions on failure characteristics. The compositional ranges and processing conditions can then be identified for the materials of interest that do not have sufficient data, and experiments can be conducted to generate the empirical data needed to train the models. Once this is complete, the test parameters of the model requirements can be defined and used to enhance the accuracy of the models and identify material property requirements. A key element to the success of this approach is the breadth of compositions, processing parameters, and resulting microstructures that are studied. Characterization of too narrow a range of parameters cannot properly train or inform the computational models rather, sufficient data needs to be collected to quantify structure-property relationships over a significant range.

Collaborative efforts toward the development of standard methodologies and best practices for implementing, linking, and verifying and validating ICME toolsets will enhance the adoption and acceptance of ICME in the maritime industry. This issue could be addressed by holding relevant workshops and/or convening working groups that comprise key stakeholders in industry, the navy,

continued on page 104.

Fig.8. Maritime ICME Implementation Framework: Incorporating an ICME Toolset into the ICME-Accelerated Product Development Program (IAPDP)

(Full details of actions and personnel at each step are provided in Table IX.)

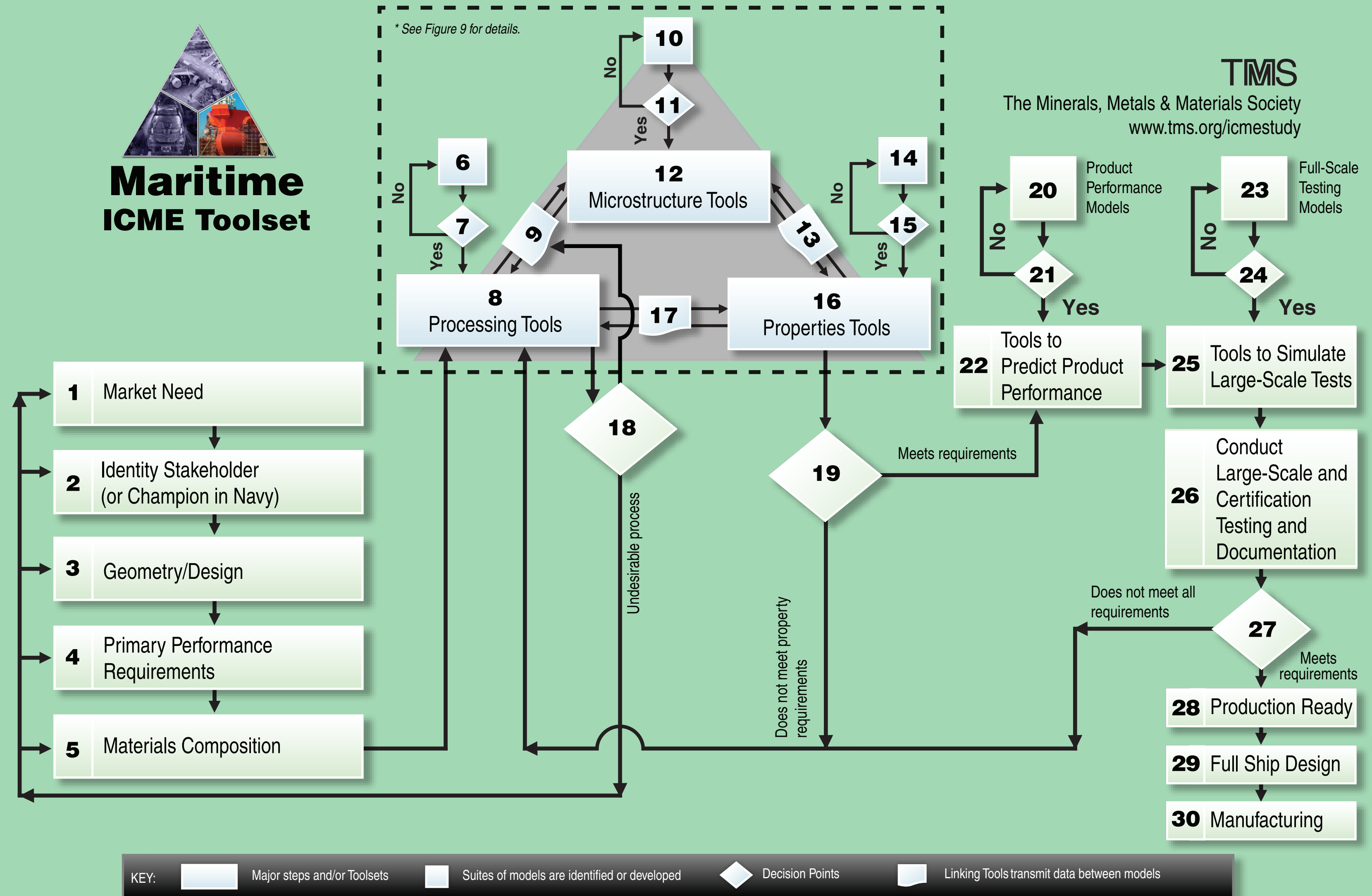


Fig. 9. Maritime ICME Toolset

(Full details of actions and personnel at each step are provided in Table IX.)

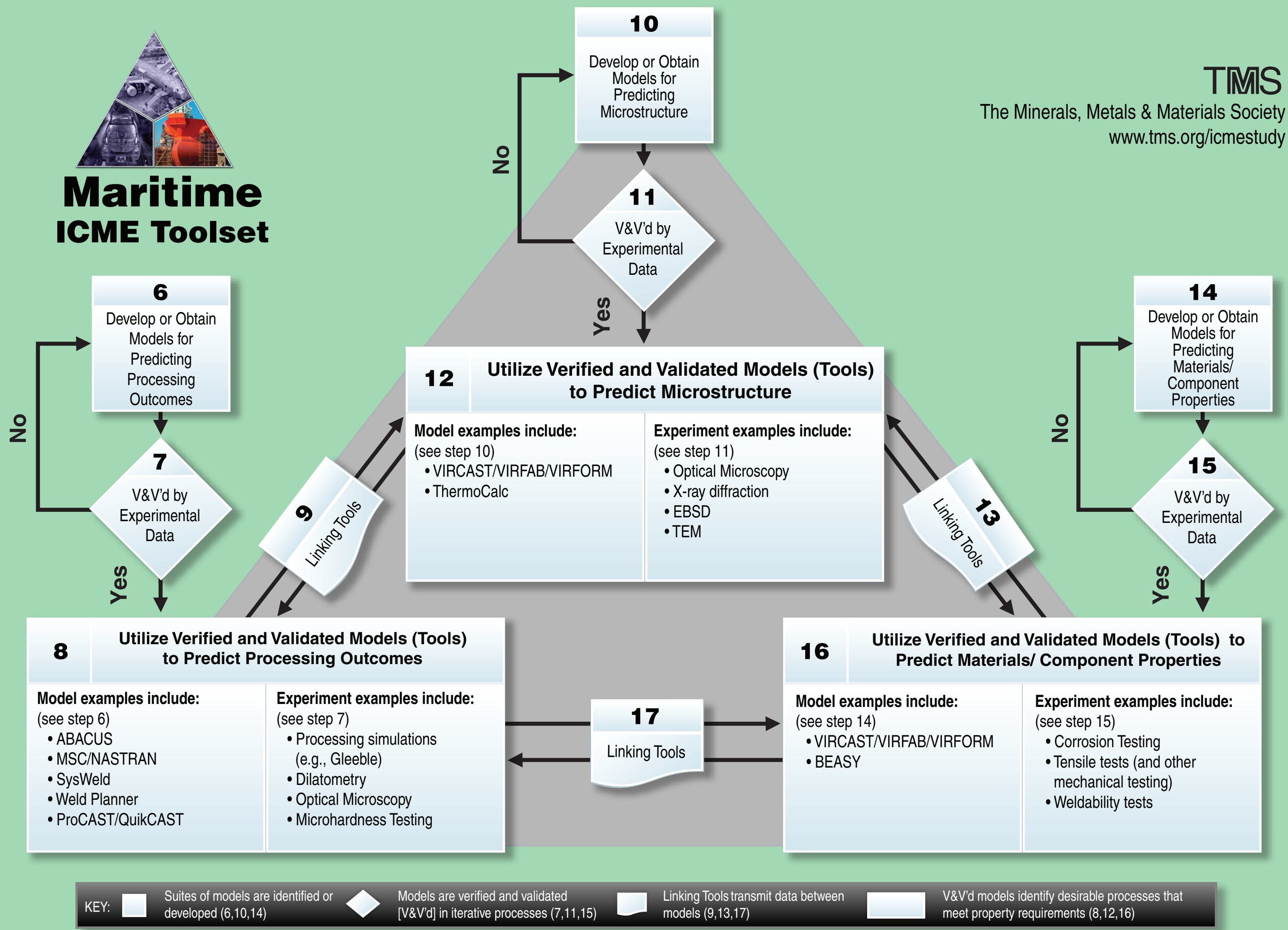


Table IX. Detailed Steps for Implementing ICME Within the Maritime Industry
(See figures 8 and 9 for illustrated maritime ICME toolset)

1.	**1. Market Need**
	Parties Involved: Stakeholder or acquisitions lead of relevant contract; materials supplier
	• Meet with naval and material supplier representatives to discuss the product needs and production capability that will drive mission requirements. • Based on mission requirements; the naval shipbuilding market will determine whether or not the need can be met.
2.	**2. Identify a Stakeholder (or Champion) in the Navy**
	Parties Involved: Technical warrant holder; stakeholder or acquisitions lead of relevant contract
	• Identify a stakeholder or champion within the Navy (e.g., Navy admiral with Navy Laboratory support) to represent the project/program pursuing development of a new product or material. The stakeholder recognizes an opportunity and makes the business case to develop a particular material or materials system and achieve an acceptable level of performance at a significantly reduced cost and schedule. » E.g., a champion may make the case that new a high-strength, low-alloy (HSLA) steel can be developed within a desirable life time cost (taking into account weight reduction benefits and potential reduction in welding costs) and time interval as compared to conventional steel alloys. • Both the technical warrant-holder of the material (e.g., aluminum, steel, titanium) or materials system (e.g., new materials system within a new hull design) and the stakeholder or acquisitions lead of the relevant contract must agree that the cost/time of development is justified by potential savings. If the business case is not sound, one solution would be to pursue negotiations to change the design requirements in order to circumvent the issue causing the market need.
3.	**3. Geometry/Design**
	Parties Involved: Ship design manager; shipyard engineer
	• Determine the geometry/dimensions of the product component using basic topology optimization software. » E.g., use computational fluid dynamics (CFD) codes such as OptiStrut, and HyperStudy to optimize hydrodynamic characteristics

  - » Note: The technical warrant holder may add additional specifications if the new material (or materials system) has widespread implementation possibilities beyond the current need.
  - » It is important to note that geometry determination is part of the iterative design loop of the whole project. As materials property predictions are made later in the system, finite element analysis coupled with the predicted properties may allow geometry modifications (topology optimization) at later stages in the project (in some cases, for light-weighting purposes)
- Some tools for this include Abaqus, OptiStrut, and HyperStudy (Altair Engineering)

4.

4. Primary Performance Requirements for Materials

Parties Involved: Technical warrant holder; materials supplier; ship design manager

- Determine the key performance requirements of the given part or component within a given product (e.g., strength, ductility, weldability, corrosion, environmental durability).
- Establish preliminary fabrication specifications of the material that include the proposed processing approach, testing methods, and basic properties; these specifications may be affected by the outcome of ICME methods and practices.
  - » E.g., to meet deck weight/strength requirements, speed, draft
- Note: It is important to achieve desired performance requirements as a function of lower cost and development time.

5.

5. Material Composition

Parties Involved: Materials supplier; ICME integrator; academic/ university liaison; research experimentalist; research modeler

- Conduct research to investigate materials candidates and alloy compositions, to also include extensive literature review.
- Utilize computational codes such as Thermocalc or Pandat to help determine potential materials compositions.
- Examine compositional design options using a set of trials and screening options on small-scale components (e.g., plates or weld filler wire).
- Define and complete an experimental test matrix; use this matrix to downselect to preferred materials compositions and processing approaches.
- Make changes or additions to fabrication specifications using the performance requirements, geometry, and materials composition.

- Identify and document a list of pertinent material/process characteristics that should be considered based on the intended application and confirm that these are achievable in the planned materials development approach (also part of the structured MSR review process described in step 26).
- Note: From this point through step 26, the materials suppliers are driving the process with metallurgical knowledge, etc.

6.

6. Develop or Obtain Models for Predicting Processing Outcomes

Parties Involved: Materials supplier; academic/ university liaison; ICME integrator; shipyard engineer; research experimentalist; research modeler

- Assemble and assess a suite of modeling tools to predict the processing outcomes. Examples of computational codes include the following:*
- ABAQUS: Standard FEM stress/strain prediction analysis software; can be used for general modeling of forging
- MSC/NASTRAN: Standard FEM stress/strain prediction analysis software; can be used for general modeling of forging
- ProCAST/QuikCAST: Cast design with processing
- MAGMASOFT: Cast design
- SysWeld: Simulation and design optimization of heat treatment, welding, and welding assembly
- Weld Planner: Simulation and design optimization of heat treatment, welding, and welding assembly

7.

7. Verify and Validate Processing Models with Experimental Data

Parties Involved: Materials supplier; academic/ university liaison; ICME integrator; shipyard engineer; research experimentalist; research modeler

- Conduct a series of experiments to validate that the modeling results are representative of real-world conditions. Design experiments specifically to work within the bounds of the model to confirm validity.
- Note: Depending on the cost/availability of the various modeling tools, subcontracting may be used at all stages of modeling
- Note: This may require several iterations of experiments or tweaks to the modeling tools to ensure validity
- Note: All tools must be accepted by the technical warrant holder. Real-world validations will be done by suppliers or subcontractors

- Experiments may include the following:
  - Selected processing (casting, forging, hot rolling and/or welding) to produce representative samples for subsequent characterization
  - Selected processing simulations (e.g. Gleeble heat treatments) to produce representative samples and obtain the stress-strain-microstructure relationship associated with materials processing approaches being utilized
  - Gleeble or dilatometry to determine CCT curves and experimentally simulate weld conditions for comparison to models of continuous cooling and/or welding
  - Experiments to characterize (qualitatively) the preliminary microstructure resulting for the processing cycle coupons (e.g., castings, forgings, hot rolled plate, welds) to test general overall validity of the model. These could include optical microscopy, microhardness testing, X-ray diffraction, EBSD, SEM, and TEM.
  - Experimental measurement of temperature profiles during processing to validate models

8.

8. Utilize Verified and Validated Models (Tools) to Predict Processing Outcomes

Parties Involved: Materials supplier; academic/ university liaison; ICME integrator; shipyard engineer; research experimentalist; research modeler

- Move forward and utilize suite of verified & validated models that is representative of the particular process used to modify the material.

9.

9. Linking Tools

Parties Involved: Academic/ university liaison; ICME integrator; information scientist/data management; research modeler

- Use special software packages to link computational models for ICME-enabled product development and automate the process of data entry between steps.
  - Note: Tools that link the input and output parameters of model simulations to predict processing, microstructure, and properties are commercially limited, but would otherwise reduce errors and accelerate computationally driven steps of the product development process.
  - Isight and Model Center are examples of tools used to chain simulation process flows between suites of models.
- Note: In this case, the input parameters to the linking tools are those developed by the materials processing models/tools, and the output parameters of the linking tools are those parameters required as input to the microstructural models/tools.

10.

10. Develop or Obtain Models for Predicting Microstructure †

Parties Involved: Materials supplier; academic/ university liaison; ICME integrator; research experimentalist; research modeler; laboratory technical lead

- Assemble and assess a suite of modeling tools to predict the microstructure (or other length scale structure) of the material. Examples of computational codes include the following:*
  - » Thermo-Calc: CALPHAD method-based software for prediction of phase formation and phase diagrams
  - » VIRCAST/VIRFAB/VIRFORM: As-cast microstructure modeling of grain size/growth/ morphology and precipitation (used for both microstructure and property prediction)

11.

11. Verify and Validate Microstructure Models with Experimental Data

Parties Involved: Materials supplier; academic/ university liaison; ICME integrator; research experimentalist; research modeler; laboratory technical lead

- Conduct a series of experiments to validate that the modeling results are representative of real-world conditions.
  - » Note: Validation of empirical models of the microstructure can be difficult, particularly in low carbon steels (e.g., quite difficult to differentiate quantitatively and accurately between lath martensite, lath ferrite, and bainite for direct comparison to models)
- Experiments may include the following:
  - » Quantitative microstructural characterization: optical microscopy, X-ray diffraction, microhardness tests, Scanning Electron Microscopy (SEM), Electron-Backscatter Diffraction (EBSD), and Transmission Electron Microscopy (TEM)

12.

12. Utilize Verified and Validated Models (Tools) to Predict Microstructure

Parties Involved: Materials supplier; academic/ university liaison; ICME integrator; research experimentalist; research modeler

- Move forward and utilize suite of verified and validated models that is representative of the microstructure (or other relevant length scale) of the desired final component.

13.

13. Linking Tools

Parties Involved: Academic/ university liaison; ICME Integrator; information scientist/data management; research modeler

- Use special software packages to link computational models for ICME-enabled product development and automate the process of data entry between steps.
- Note: In this case, the input parameters to the linking tools are those developed by the microstructure models/tools, and the output parameters of the linking tools are those parameters required as input to the materials/component properties models/tools.

14.

14. Develop or Obtain Models for Predicting Materials/ Component Properties

Parties Involved: Materials supplier; academic/ university liaison; ICME integrator; research experimentalist; research modeler; technical warrant holder

- Assemble and assess a suite of modeling tools to predict materials properties. Examples of computational codes include the following:*
  - » VIRCAST/VIRFAB/VIRFORM: Used for both microstructure and property prediction
  - » BEASY: Simulation of corrosion phenomena and crack growth associated with corrosion

15.

15. Verify and Validate Property-Prediction Models with Experimental Data

Parties Involved: Materials supplier; academic/ university liaison; ICME integrator; research experimentalist; research modeler; technical warrant holder

- Experiments to validate the modeling results could include the following:
  - » Corrosion testing
  - » Mechanical testing (e.g., tensile testing for yield etc.)
  - » Weldability tests

16.

16. Utilize Verified and Validated Models (Tools) to Predict Materials/ Component Properties

Parties Involved: Materials supplier; academic/ university liaison; ICME integrator; research experimentalist; research modeler; technical warrant holder

- Move forward and utilize suite of verified & validated models that is representative of the desired materials or component properties.

17.

17. Linking Tools

Parties Involved: Academic/ university liaison; ICME integrator; information scientist/data management; research modeler

- Use special software packages to link computational models for ICME-enabled product development and automate the process of data entry between steps.
- Note: In this case, the input parameters to the linking tools are those developed by the materials/component property simulation models/tools, and the output parameters of the linking tools are those parameters required as input to product performance tools.

18.

18. Decision Point: Is the Processing Approach Feasible and Desirable?

Parties Involved: Materials supplier; academic/ university liaison; ICME integrator; technical warrant holder; shipyard engineer

- Assess the technical feasibility and cost-effectiveness of the processing approach.
- Evaluate other factors including appropriate machine size, control, robustness, cost, production rate, materials supplier abilities, environmental performance.
- Determine how processing is affected by certain geometric features (e.g., overflow wells, chill blocks).
- If the processing approach is determined to be both feasible and desirable, then continue iterating between modeling of processing, microstructure, and properties until a processing routine is theoretically optimized.
- If the processing approach is determined to be infeasible or undesirable, then return to consideration and modification of initial parameters such as the geometry, primary performance requirements, or materials composition (steps 3-5).

19. Decision Point: Does the Product Meet Component and Materials Requirements?

Parties Involved: Technical warrant holder; ship design manager; materials supplier; stakeholder or acquisitions lead of relevant contract

- Assess the confidence in modeling results and move forward if results are found to be feasible and validated.
- Re-enter the ICME toolset iteration loop for additional simulation or reconsider the requirements, drivers, and geometry of the component if the product does not meet component and materials requirements.

20. Develop or Obtain Models for Predicting Product Performance

Parties Involved: Materials supplier; academic/ university liaison; ICME integrator; research modeler, laboratory technical lead, research experimentalist

- Assemble and assess a suite of modeling tools to use the output of the optimized materials structure/ processing/properties approach to predict product performance.
  - Note: ABAQUS software linkage tools are advancing to be able to chain modeling results from the ICME toolset to the simulation tools used in the prediction of product performance.
- Use largely with commercial FEA and other structural tools to model items such as assembly, producability, and explosion testing, using scale-up experiments as validation.
- Examples of computational codes include the following:
  - NASTRAN: Simulation for structural reviews
  - ABAQUS: Standard FEM stress/strain prediction analysis software
  - MSC/NASTRAN: Standard FEM stress/strain prediction analysis software
- Conduct less iteration in this set of steps as the ICME toolset and associated models become more advanced.

21. Verify and Validate Performance-Prediction Models with Experimental Data

Parties Involved: Materials supplier; academic/ university liaison; ICME integrator; research modeler, laboratory technical lead, research experimentalist

- Experiments to validate the modeling results could include:
  - Tensile tests (yield and ultimate strength, ductility – elongation/reduction in area).
  - Explosion bulge test for thick plate (blast/ballistics)

22. Utilize Verified and Validated Models (Tools) to Predict Product Performance

Parties Involved: Materials supplier; academic/ university liaison; ICME integrator; research modeler, laboratory technical lead, research experimentalist

- Move forward and utilize suite of verified & validated models for predicting the product performance.

23. Develop or Obtain Simulations for Large-Scale Testing

Parties Involved: Materials supplier; academic/ university liaison; laboratory technical lead; ICME integrator; research modeler; research experimentalist

- Assemble and assess a suite of modeling tools to use the results of predicted product performance to simulate the large-scale product performance tests.
  - Note: Large-scale model simulations at this stage are currently immature, but future efforts are in progress. This will help to avoid any potential error when conducting full-scale product tests.
- Examples of computational codes include the following:
  - ABAQUS: Standard FEM stress/strain prediction analysis software
  - MSC/NASTRAN: Standard FEM stress/strain prediction analysis software

24. Verify and Validate Test Simulation Models with Experimental Data

Parties Involved: Materials supplier; academic/ university liaison; laboratory technical lead; ICME integrator; research modeler; research experimentalist

- Determine whether the modeling results are representative of real-world conditions.

- Conduct tests to verify that the modeling codes are executing computations properly and providing an accurate mathematical representation of the fundamental principles and relationships that they are designed to represent.

25.

25. Utilize Verified and Validated Models (Tools) to Simulate Full-Scale Testing

Parties Involved: Materials supplier; academic/ university liaison; laboratory technical lead; ICME integrator; research modeler; research experimentalist

- Move forward and utilize suite of verified & validated models to simulate large scale tests
- Use basic FEM tools to verify and optimize plans for full-scale tests.
- Dictate the models used based on what the IPDT intends to test at the full-scale testing stage; experiments are not limited by the capabilities or limitations of the model.

26.

26. Conduct Large-Scale and Certification Testing and Documentation

Parties Involved: Materials supplier; laboratory technical lead

- Large-Scale Testing/First Article Testing and Finite Element Modeling
  - » Coordinate with the materials producer to perform large scale and first article testing and ensure that they can supply a product that meets specifications.
  - » Targeted large-scale experiments on the ICME-optimized prototype; may include tests to try to "break things" often using combined testing methods (e.g., tensile, dynamic/explosion, fatigue). This should also include production of mill size components, e.g., plates and then full-scale welding trials.
  - » Conduct explosion bulge tests for structural materials. Note: These tests are typically required for steel, and not aluminum parts. Navy Laboratories, like NSWC-Carderock or similar labs perform large-scale testing.
  - » Request FEM results to accompany test results.
- Materials Selection Requirements (MSR) review
  - » Note: MSR is an example of a structured approach to ensuring that the properties and performance of a new material or process are suitable for the intended application; in naval applications, the MSR document is referred to as TechPub100[29] and a naval representative must audit the review and resulting paperwork. This process begins early in the development of a new material and culminates in final testing and certification of the material.

- » Submit components that are new compositions and intended for critical applications for review, after completing large-scale testing.
- Develop Materials Data Sheet information
  - » Incorporate supplemental materials property information into a Materials Data Sheet.
  - » Note: This information does not necessarily go into the materials specification, but is required (e.g., coefficient of thermal expansion, thermal conductivity).
- Place additional validated materials property output from advanced ICME modeling tools into the Materials Data Sheet specification.

27.

27. Decision Point: Does the Prototype Product Meet All Requirements?

Parties Involved: Technical warrant holder; NAVSEA; materials supplier; laboratory technical lead; stakeholder or acquisitions lead of relevant contract; ship design manager

- Assess the results of the prototype/certification testing by the materials supplier. If the component/material passes, consider the design final and begin to develop final component/product specifications.
- May need to produce additional product sizes and thicknesses to establish full capability of a new product (e.g., first application may be 2″ thick, but what are the properties at 3″ or 3/16″ thick).

28.

28. Final Component Design/ Production Ready

Parties Involved: Materials supplier; technical warrant holder; laboratory technical lead; shipyard engineer; ship design manager

- Create a complete manual and set of specifications for the product.
- Do not conduct additional ICME iterations at this point, as design properties have been established.

29.

29. Integrate Component into Full Platform/Ship Design

Parties Involved: Ship design manager; stakeholder or acquisitions lead of relevant contract; shipyard engineer

- Finalize the design of the completed component and prepare to integrate the component into the intended application.
- Assess the rest of the ship design and address any other issues associated with the integration of the final component.
- Produce and inspect a limited number of component designs and use the results to confirm that there are no issues present in the design.

30.

30. Manufacturing

Parties Involved: Shipyard engineer; materials supplier; ship design manager

- Produce the product according to the specifications of firm configuration.

* See Appendix C for a list of additional computational tools.
† Although the term microstructure is generally used only in reference to metals and other crystalline materials, in this context it is used to denote the meso-, micro-, or nano-scale structure of the material class undergoing ICME including metals, ceramics, and composites.

continued from page 89.

and academia. It is also recommended that maritime-specific ICME literature (e.g., on verification, validation, standards) and conference presentations be developed, as it is critical to the creation of successful maritime-specific ICME-accelerated product development programs. This could be addressed by ICME stakeholders already associated with the maritime and naval communities organizing symposia, special journal issues, and individual articles focused more specifically on the maritime industry.

Development of key material property databases is recommended in order to facilitate rapid implementation of ICME in the maritime industry. In the short term individual organizations or small groups of organizations may work to develop smaller, more targeted databases. In addition to the development of pre-competitive databases, individual organizations or small groups that work together through intellectual property and or national security agreements could develop some maritime-specific databases that may not be publicly available, but that could at least be used by these specific groups in ICME-accelerated product development programs.

Recommended Long-term Activities

In the long term, there is a need for larger databases to store information on microstructures (particularly, phase-based information to ensure that composition and temperature-dependent descriptions can be developed), processing-microstructure relationships, and microstructure-property relationships, in order to support model development and verification. Stakeholders from across the industry and research community—including academia and government agencies—can develop and recommend a standardized format for generating, inputting, sharing, and citing/referencing data in precompetitive databases.

Cultural Barriers to ICME Implementation

Acceptance of ICME requires that maritime community leaders with more conservative design philosophies overcome skepticism of verified computational tools and lack of confidence in validated simulation results. Establishing community support for a process that does not yet have a strong body of proven successes is often difficult. Although ICME has been demonstrated to reduce lifetime product development costs and times, there is limited understanding of ICME costs, benefits, and/or limitations within the naval community.

This lack of common understanding creates competing interpretations and expectations, and, in particular, having separate stakeholders for design and manufacturing steps means that these distinct groups of stakeholders may not fully understand the limitations and requirements in all phases of the product development cycle. This often creates problems such as unrealistic scheduling expectations; in some instances, time is not properly allocated to successfully implement ICME, which has the potential to negatively influence stakeholders who are already impatient with the modeling process. A first step to overcoming some of these cultural barriers could be for designers, materials engineers, and ICME Integrators to work together on a joint project or program that addresses a specific need within a maritime platform, in order to understand better each other's constraints, methodologies, and expectations. To develop a full understanding of the ICME process in the maritime sector, projects could also be carried out over an extended period of time with results being evaluated as they appear. Connecting results and developing state equations and software for such a project will likely involve contributions from academia, industry, and government. Those funding such a project need to be made aware of both the commitments required to make the project successful and the significant potential of such a project to demonstrate holistically the potential of ICME in the maritime sector.

Proponents of ICME associated with the maritime and naval community can also reach out to relevant program managers and builders of potential ICME applications through emails, symposia, and targeted presentations. These stakeholders will also be able to provide examples of ICME successes and failures in the development of materials and components, with a focus on lessons learned, benefits, and limitations of ICME. In order to provide a comprehensive, robust view of best practices for implementing ICME in the maritime industry in the near term, leaders can encourage dialogue among stakeholders and conduct interviews to assess the needs and language of platform acquisition professionals. Engaging an engineering professional society to identify relevant conferences, speak to conference planners, and get stakeholders interested in adopting ICME in the maritime industry also can be a successful way to initiate discussion, cross cultural barriers, and obtain further stakeholder buy-in.

Establishing a Business Case for ICME

In order to encourage stakeholder buy-in and create a community that can support a fully integrated ICME program, it is crucial to develop qualitative or semi-quantitative business case analyses within 3 years. To do so, members of the community could assume ownership of this problem and work toward understanding the inherent cost- and time-reduction benefits obtained through implementation of ICME methodologies. As a first step, this can involve a joint effort among the end-customers of ICME (e.g., shipyards, acquisition warrant-holders, maintenance officers, performance officers, naval officers) to identify the most promising application opportunities or foundational engineering problems as candidates for ICME implementation.

A complete ICME business case analysis will ultimately require the verification and validation history of multiple past components or products. To identify components that could benefit from incorporating ICME methods into their future design and development cycles, members of the community might begin by querying navy maintenance databases, if possible. As an alternative, they could conduct a qualitative analysis to demonstrate the potential benefits of incorporating ICME approaches into the development process for certain products or components. It may also be possible to leverage the Navy ManTech Program or the National Shipbuilding Research Program to conduct a cost-benefit analysis that can be used as a tool to demonstrate the benefits of ICME to companies in this industry.

Workforce Needs

It is also important to create opportunities to increase the number of skilled ICME integrators and ICME-ready integrated product development team members in the workforce in the near term. Building a team with the necessary skills and competencies to apply ICME practices to industrial problems and product development is a critical first step in ensuring proper execution and long-term program success. Establishing a maritime working group to search for students trained in ICME and computational materials and present them with employment and career-building opportunities in the industry is recommended as a strong first step. Leaders in the field can also hold meetings with management to discuss ICME implementation within an organization, and enlist employees that have computational experience to learn the different modules in the company and contribute to the effort.

Lack of Past Experience in Implementing ICME

Overall, ICME does not have a strong presence within the maritime industry. No major U.S. Navy platform/component development program to date has fully utilized ICME, and funding to support such a project has been limited at best. Making the case that sound ICME-enabled product development programs within the maritime community are within reach to such key decision makers in the naval ship-building arena will require further development and advancement of simulation tools as well as skilled software users who are trained to operate and maintain these tools and associated databases. Additionally, high development and usage costs of materials databases and models present challenges for some companies that will need to be overcome or circumvented before ICME can come into its own in the maritime industry. For example, few U.S. facilities are currently producing commercial tools with materials properties based on phase, coefficient of thermal expansion (CTE), modulus of elasticity, and density. Considering the lack of established competition in this particular area, prices may remain high until the community can identify or develop alternatives.

There is also a need for ICME expertise among steelmakers in the field, and the establishment of relationships between ICME experts, steel mills, and foundries. These needs are best addressed at early stages, i.e. when just beginning to consider implementation of ICME into the product development process. ICME requires a non-trivial initial investment in new technology-based infrastructure, including costs associated with purchasing new software packages and hiring skilled ICME integrators.

Near-Term Opportunities for ICME Implementation in the Maritime Industry

The quantitative integration of computational methods into the product development cycle is, to date, relatively immature in the maritime industry. However, there is great potential for ICME implementation to grow within the industry over the next few years and show measurable results in its ability to shorten the overall product development cycle. There are a limited number of available case studies in which ICME has been used, yet several applications can be expected to benefit in the near term. The following applications, not in priority order, represent some of the most promising opportunities to apply ICME tools and methods in the maritime industry in the near term:

- Components
  - » Design high-strength fasteners that avoid potential hydrogen embrittlement and galvanic issues
  - » Design lightweight, low-cost watertight doors
  - » Develop structural components for next-generation ship-to-shore connectors
  - » Develop a durable non-skid surface (heat resistant, lightweight)
  - » Develop revolutionary approaches to integrate non-skid surfaces with ship deck design
  - » Design high-strength, lightweight stiffened panels with increased corrosion resistance, lower cost, and increased processing options
  - » Develop a full ICME approach with materials development for jet blast deflector applications
- Materials
  - » Design low-cost, weldable, fire-resistant materials with a low thermal coefficient and high melting point
  - » Design a duplex stainless steel with minimal number of repair cycles required, and open up the component design space
  - » Design marine-grade aluminum alloys with improved mechanical properties
  - » Design new, improved weld consumables for high-strength steels such as HSLA 100, HSLA 130, and HSLA 150
  - » Design new, "no-preheat" weldable steel plate and welding consumable combinations
  - » Lower the residual stress of HSLA 65 during production to achieve lower weld distortions
  - » Develop tools and establish standards for characterization and prediction of mechanical properties of high-strength steels (e.g., HSLA 170)
  - » Improve predictive capabilities for weldability of high-strength steels (e.g., LE Steel, Granville-Steel)
- Manufacturing
  - » Design for manufacturing to control distortion by incorporating process modeling (welding) with materials knowledge to reduce the need for final dimensional correction of assembled components
  - » Develop weld sequencing protocols for structure optimization
  - » Develop flame straightening optimization
  - » Develop in-place post-weld heat treatment in steam generation
  - » Develop models to predict thermal shrinkage during welding or cutting of panels
  - » Develop reduced-stress "safe end" weld process to eliminate post-weld heat treatment
  - » Design processes for first-time quality welding that integrate automation and non-destructive examination
  - » Improve characterization and prediction of cold forming of high-strength steel plate
- Processing Development
  - » Develop crack repair processes with low residual stress in structural applications
  - » Optimize processes for joining of dissimilar materials (e.g., joining steel to aluminum)
  - » Develop processes for free-form additive manufacturing (e.g., for low-volume parts as temporary replacements).

Closing Remarks on Implementing ICME in the Maritime Industry

Incorporating computational methods (along with critical experiments for model verification and validation) as an integrated component of the product development cycle is a relatively new practice within the maritime industry. Yet it shows great promise for reducing the time and cost investments required for the development of new materials, components, and/or manufacturing processes. The maritime industry typically adheres strictly to the procedures of the Navy, which currently does not account for ICME methods as a regular practice in product development. Experts in integrated computational engineering methods recognize the benefits associated with the use of simulation tools, critical experiments, and advanced materials databases, and are beginning to generate solutions to expand the use of ICME to replace or augment traditional methods. Some of these ICME experts are in a good position to present stakeholders with convincing business cases, including success stories in other industries or in smaller maritime problems, to demonstrate the full capacity of ICME. Collaborative efforts are also underway with industry members, government organizations, academia, and professional societies working together to boost computational proficiency in the workforce. Combined with efforts to develop standards and verification and validation methodologies and activities to increase the number of relevant databases for computational models, the maritime industry stands ready to implement new ICME-accelerated product development programs (IAPDPs) and apply these new methods to several near-term opportunities. To that end, this chapter provides a framework which can be employed as a starting template to begin implementing ICME in the near term (within 3 years) in specific IAPDPs within the maritime industrial sector.

VII.
Call to Action and Closing Remarks:

Who Can Respond to This Report, What Actions Can They Take, and What Benefits Will They Receive?

Industry Stakeholders

Professionals within the three industrial sectors addressed here (automotive, aerospace, and maritime) can use the detailed frameworks, recommendations, and opportunities provided in this report to help initiate ICME-accelerated product development programs (IAPDPs) within 3 years. For a given product or problem for which ICME can provide value, integrated product development teams (IPDTs) assembled to carry out an ICME project could start with the frameworks and recommendations presented here, adapting them and adding detail to address their specific product or problem. Subsequent incorporation of ICME into their product development program could considerably reduce the time and costs of developing and optimizing new or existing products and manufacturing approaches for their companies.

Companies with more experience in ICME may be able to implement such programs more extensively, more quickly, and on a larger scale. The payoff in faster product development and reduced costs could therefore be greater and realized more rapidly. Companies with little to no ICME experience might address smaller problems that represent individual subsets of product development programs or lower-risk endeavors, engage efforts that build ICME capabilities, and/or focus on educating personnel in their companies on the potential benefits and pathways to take regarding ICME implementation. This will result in perhaps fewer short-term benefits in time and cost reduction, but also longer-term benefits in building the expertise and infrastructure within their company to achieve much larger payoffs in the future.

Although this report specifically addresses ICME implementation in the automotive, aerospace, and maritime industries, it can also provide significant value to potential stakeholders in a variety of other industrial sectors, as they will no doubt encounter at least some of the same circumstances, challenges, and opportunities for implementing ICME that have been addressed here. Such industries could include those centered about non-structural (i.e., functional) applications such as electronics, functional biomedical components, and a vast array of other materials types (e.g., semiconducting materials, magnetic materials). The consumer products and civil infrastructure industries and other energy and environmental sectors could also benefit from ICME. The knowledge base, frameworks, actions, required personnel types, and needs and recommended solutions presented here could all be adapted or used as building blocks to create an ICME infrastructure or enhance the existing infrastructure within their company, so as to implement ICME into their product development programs.

In addition to scientists, engineers, and designers, this report could benefit many other stakeholders within industry, including managers at multiple levels within a company, who can then make informed decisions about investing in ICME and its benefits, and provide the necessary leadership and guidance within their departments to assure that ICME programs are well integrated across the company. Another example is that sales and marketing people might use some of the overarching concepts provided here on how ICME accelerates innovation and time to market, and reduces costs, which translate to direct benefits for the customer.

Academic Stakeholders

A wide spectrum of people within the academic community can also play a key role in implementing ICME, and could benefit from applying the strategies described in this report. This includes professors, research engineers, technicians, graduate students, undergraduate students, department heads, deans, and provosts. The research groups at universities (professors, graduate students, engineers, technicians) can and do contribute greatly to building the computational models and codes needed for implementing specific ICME-accelerated product development programs in industry, and thus see their fundamental work transition to application. Additionally, by teaming with industry and government laboratories, they can provide the data content needed for specific IAPDPs and contribute greatly to experimental model validation by working within the frameworks and making use of the detailed recommendations provided here. These transitions to application, and industrial and government collaborations, will also benefit them in at least two other ways: (1) informing their "upstream" fundamental research so that it more fully and more rapidly benefits society and results in additional collaborative publications, and (2) perhaps opening up more doors for research and engineering funding opportunities. Undergraduate students in materials science and other materials-related engineering departments represent a critical lynchpin for the broader success of ICME—they constitute the ICME workforce of the future. This report can provide them with knowledge of what ICME is and how it can be implemented (and possibly be used as a tool in undergraduate and graduate curricula). This added expertise could make a significant difference in a student's ability to procure a job after graduation, particularly in the industrial sector. Higher-level university officials (department heads, deans, and provosts) might read the executive summary or quickly review the report to gain a sense of how their university might engage ICME as an interdisciplinary endeavor across multiple departments (the "I" in ICME), and contribute to strong university-industry collaborations, both of which are of significant value not only to the universities, but also to ICME implementation and to the MGI.

Government Stakeholders

Relevant stakeholders in government agencies are also key enablers of ICME implementation, and can thus respond to and gain benefit from this report in two ways. Technical experts and managers at national laboratories could use the knowledge provided here to help them engage both industry and academia in contributing to ICME infrastructure and its application/implementation, and thus to the MGI materials innovation infrastructure. Thy can also greatly contribute to ICME implementation within individual companies and specific industry-led IAPDPs; in this way government laboratories would be able to more rapidly transition their innovations to provide value to their agencies' "customers" (e.g., societal benefits including national security, employment, standard of living, and energy and sustainability). In addition to those agency benefits, government funding agency personnel might use the strategies outlined in the report to help guide the government's support of ICME and the MGI.

Professional Societies

Relevant professional societies can also contribute significantly to ICME implementation, and can thus respond to and gain benefit from this report. First, they are instrumental in convening the ICME implementers from industry, government, and academia in forums such as conferences, symposia, workshops, etc. which bring these groups together to leverage each other and more rapidly implement ICME into the product and manufacturing development cycle. This is especially important because implementing ICME broadly across many, large product development programs is a significant task that will require coordination of members from all three of these groups. Technical societies can also help implement ICME by assisting ICME stakeholders (i.e. members of their societies) in building the ICME and MGI infrastructure required to implement ICME more broadly, including developing advanced ICME tools, data and database needs, and the ICME workforce. This report can thus benefit professional societies in two ways: (1) providing an overall knowledge base of ICME implementation that can better allow them to convene and work with the relevant communities to address these issues, and (2) helping them assist in execution of some of the specific recommendations within this report. Ultimately this will benefit not only their membership, but the broader science and engineering community, and society, as well.

Closing Comments and Final Charge

Although ICME is now recognized as a discipline and awareness is growing worldwide, we stand at a critical juncture, or tipping point, where the great potential of ICME to significantly reduce the time and cost required for the development of new materials, components, and manufacturing processes is within our grasp. To realize the vision of ICME, though, the detailed pathways to rapid implementation for practical engineering problems need to be elucidated and executed. This report provides industry, as well as other ICME stakeholders and supporters in academia and government, with frameworks and key actions and personnel needed to implement/initiate ICME-accelerated product development programs (IAPDPs) in the near term (within 3 years[s]). It also offers detailed guidance and recommendations for addressing the most critical needs for rapid (and broad) implementation. This report additionally recommends more than 50 specific application opportunities for using ICME to accelerate the development of various new products and innovations in the automotive, aerospace, and maritime industries. Although the study was focused on three industrial sectors (aerospace, automotive, and maritime), it also addresses pervasive ICME issues that apply across these three sectors, and are additionally relevant to other industries. This report has the potential to benefit a variety of different stakeholders in industry, academia, and government. Now is the time for these stakeholders to act upon the frameworks, pathways, and recommendations presented here, in order to help implement ICME much more broadly, and to take advantage of its potential benefits, within the next 3 years.

s. As mentioned in the introduction, 3 years was specifically chosen: (1) to provide a quantitative reference point from which to focus the frameworks and recommendations for near-term ICME implementation, and (2) because a consensus was reached that 3 years was an achievable goal based on the current state of ICME, as well as the experience of the team members with product and manufacturing development in their industries.

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X. Appendices

Appendix A: Acronyms and Abbreviations

Acronym or Abbreviation	Definition
3-D	three-dimensional
AIM	accelerated insertion of materials
CAE	computer-aided engineering
CFD	computational fluid dynamics
CME	computational materials engineering
D3-D	ONR/DARPA D "3-D Digital Structures Program" to develop three-dimensional tools (computational and experimental) and analyses
DoD	U.S. Department of Defense
DOE	U.S. Department of Energy
FEA	finite element analysis
FEM	finite element method or finite element model
GPU	graphics processing unit
HSLA	high-strength, low-alloy
IAPDP	ICME-accelerated product development program
IPDT	integrated product development team
MD	molecular dynamics
Mg	magnesium

MGI	Materials Genome Initiative
MRL	model readiness level
MSE	materials science and engineering
MSR	materials selection requirements
NAVSEA	Naval Sea Systems Command
NIST	National Institute of Standards and Technology
NSWC	Naval Surface Warfare Center
NVH	noise-vibration-harshness
OEM	original equipment manufacturer
R&D	research and development
ROI	return on investment
SERDP	Strategic Environmental Research and Development Program
SHM	structural health monitoring
TML	tool maturity level
TRL	technology readiness level
UM	uncertainty management
UMAT	user-defined material
UQ	uncertainty quantification
USAMP	United States Automotive Manufacturing Partnership
V&V	verification and validation
VAC	virtual aluminum castings
VARTM	vacuum assisted resin transfer molding
VIM	vacuum induction melting

Appendix B: Contributors by Functional Group

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Appendix C: Computational Tools

The following table includes examples of computational resources that can be used to enable an ICME-accelerated product development program. All of the resources listed below are available via the open-access TMS Materials Cyberinfrastructure Portal at www.tms.org/cyberPortal.

Examples of Computational Resources for ICME

(Resources in Bold Font Are Those Explicitly Mentioned in Report)

Abaqus FEA	Granta Design Products
Abaqus/Standard	Helius: Fatigue
Ansys	Helius: MatSim
ANSYS 14	Helius: MCT
ANSYS CFX	**HSC Chemistry**
ANSYS FLUENT	HyperSizer®
AnyCasting	**Isight**
AutoForm	**Jmat Pro**
Avizo® Fire	JSCast
BEASY	**LAMMPS**
Castep	**LS DYNA**
Catia	**MAGMA 5**
COMPRO 3D	Magpar
COMSOL Multiphysics	Materials Project
DACAPO	Matforge
DANTE	MAVIS-FLOW
DEFORM	**MeltFlow**
DICTRA	MICRESS
DMol3	Moldflow
DYNA3D	**MSC NASTRAN**
EKK Inc.	MTDATA
EKK Inc. (CAP)	Nei Nastran
Engineering Virtual Organization for Cyberdesign	**NESSUS**
FactSage	Nmag
FLOW-3D	NX Nastran
FORGE	OOF
Gemini	OOMMF
PAM-CRASH	**SOLIDCast, FLOWCast, OPTICast**

PAM-STAMP 2G
Pandat*
ParaDis
ParaView
Precipi Calc
ProCAST/QuikCAST
SIESTA
SimLAM
Simpleware
SIMTEC
SysWeld
ThermoCalc
uMatIC
VAMP/VASP
VGSTUDIO MAX
VIRCAST/VIRFAB/VIRFORM
VisIt
Welding Simulation Solution
WELD PLANNER
Zencrack

XI.
Key Terms and Definitions

A number of terms are used repeatedly within this report. A few of the most important of these are defined below.

- ***Ab Initio* Model:** A mathematical representation of relationships between materials processing and microstructure and/or materials properties that is built from first-principles assumptions about the way materials behave at the atomic and molecular levels. These models can then be used to quantify requested improvements in the desired structural design drivers and as a basis for the virtual modeling and formulation of new materials.
- **Integrated Product Development Team (IPDT):** The group of stakeholders who are given ownership of and responsibility for the product under development.[1] Integrated Product Development Teams are composed of experts from a variety of disciplines—typically from within the same company—and often include design engineers, materials engineers, productions analysts, experts on product aesthetics, manufacturing engineers, and other key personnel. In an ICME context, an IPDT will also include ICME Integrators, software experts, and anyone else needed to bring an ICME approach to bear on a product development program.
- **ICME-Accelerated Product Development Program (IAPDP):** A Product Development Program that includes ICME tool sets, personnel types, and actions fully integrated into the IPDTs in order to reduce the development time of new (or existing) products.
- **ICME Integrator:** Individual who oversees elements of the ICME approach which may include experimental validation, linkage of computational models, and coordination of the personnel involved.
- **ICME Tools:** In the present context refers to computational (or experimental) tools that are used within the ICME portions of the product development cycle. These tools compose the "ICME toolset" but do not have to be exclusive to that toolset. For example, many computational tools such as DEFORM, phase field codes, etc. might be employed only within the ICME toolset; whereas, experimental tensile testing can be used to validate ICME models and would thus be considered part of the ICME toolset in this context, even though it is often used throughout other parts of the product development cycle as well.
- **ICME Toolset:** A collection of both computational modeling tools and experiments, complete with linkage routines and codes needed to provide predictions of processing outcomes, microstructure, and properties. The definitive aspects of an ICME toolset are the linkage and integration between models and experiments and its use in accelerating product development programs (critical component of an IAPDP).
- **Near Term:** In this report, near term is used to denote a timeframe of 3 years or less.
- **Linking Tools:** Linking tools are software packages or custom codes that translate the format of data output from one set of models into a format suitable for another set of models.
- **Long Term:** In this report, long term is used to denote a timeframe of 5 years or more.
- **Verification of Models:** Demonstration that a computer code provides an accurate mathematical representation of the fundamental engineering principles and relationships that it is designed to represent.
- **Validation of Models:** Demonstration that the model provides accurate predictions of some materials-related property or behavior within a defined domain, accomplished via comparison of model outputs with the results of controlled experiments.

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