Integrated Computational Materials Engineering

Summary Presentation
6/1/08

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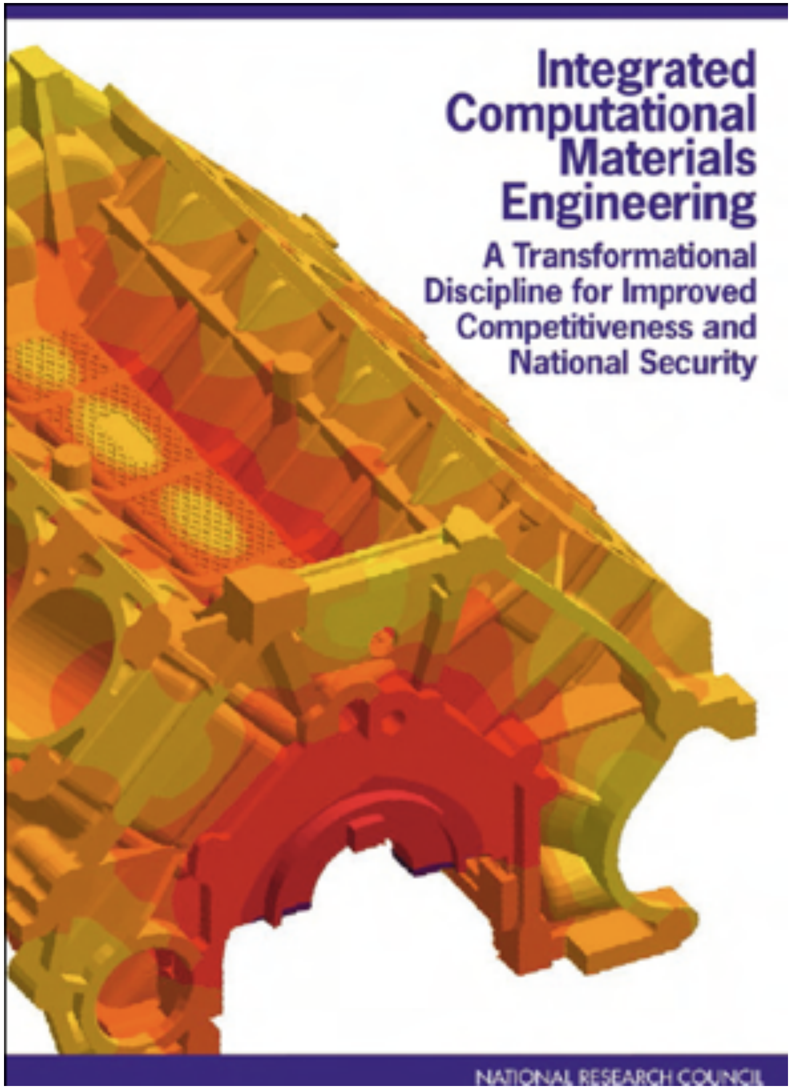

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The Vision

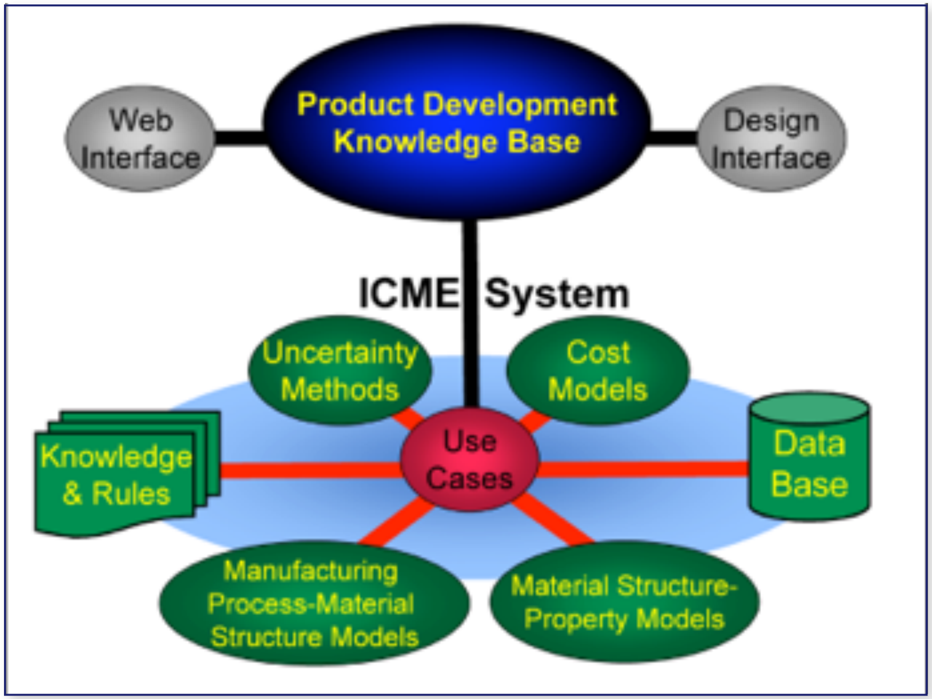
Computationally-driven materials development will be a core activity of materials professionals in the upcoming decades, uniting materials science with materials engineering and integrating materials more holistically and computationally with product development.

Integrated Computational Materials Engineering

- What is it?
- Origins and Approach of NRC Study
- Selected Findings
- Case Studies
  - Example of ICME (Virtual Aluminum Castings)
- Recommendations and the Way Forward

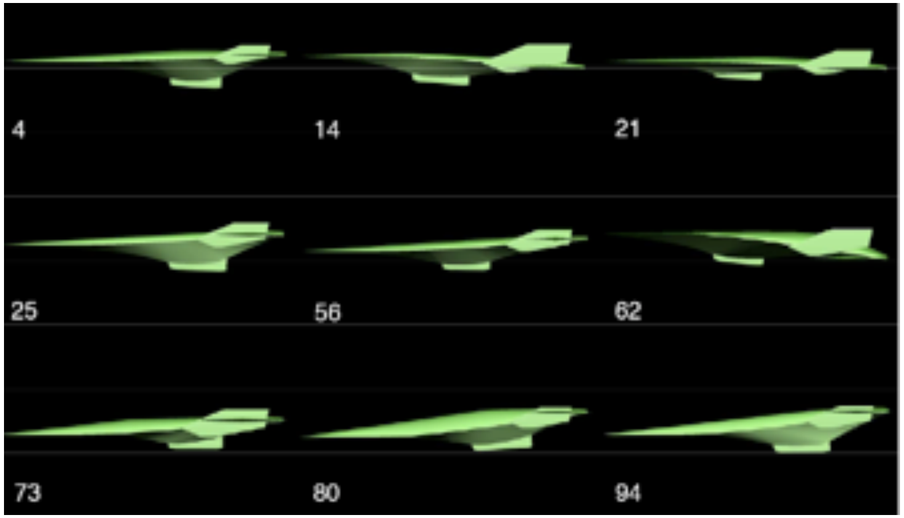
What is ICME?

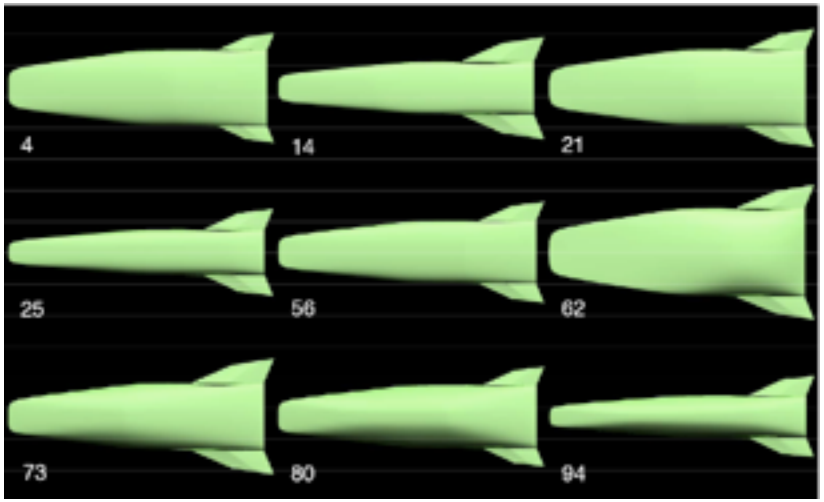
Integrated Computational Materials Engineering (ICME) is the integration of materials information, captured in computational tools, with engineering product performance analysis and manufacturing-process simulation.



Emphasis on "I" and "E"

The "I" and "E" Challenge
Example: Shape Optimization of Hypersonic Vehicles





Using advanced computational techniques, designs can be studied and optimized in matters of hours or days. Optimization of new materials must be done experimentally and can take 10-20 years.

Source: K. Bowcutt, Boeing

Changing the Role of the Materials Engineer

- A materials engineer on an Integrated Product Development Team (IPDT) is generally used to provide a certified material whose properties match those needed in the design: materials selection not materials design

- Development of new materials is slow and cumbersome so materials are generally not optimized to enable more advanced designs

- Example: use of composites in aircraft: "black aluminum"

- ICME offers the chance to optimize materials design and properties along with product design

Study initially proposed by the National Materials Advisory Board
Sponsored by the Department of Defense and Department of Energy

Committee on Integrated Computational Materials Engineering

Tresa M. Pollock, University of Michigan, *Chair*
John Allison, Ford Research Laboratory, *Vice Chair*
Daniel Backman, Worcester Polytechnic Institute
Mary Boyce, Massachusetts Institute of Technology
Mark Gersh, Lockheed Martin Space Systems Company
Elizabeth A. Holm, Sandia National Laboratories
Richard LeSar, Iowa State University
Mike Long, Linux Networx Inc
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Deborah DeMania Whitis, GE Aviation
Christopher Woodward, Air Force Research Laboratory

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The committee is grateful to the NRC appointed reviewers

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David J. Srolovitz, Yeshiva University
Patrice E.A. Turchi, Lawrence Livermore National Laboratory
James C. Williams, Ohio State University
Mark Verbrugge, General Motors

Committee Charge

1. The exploration of the benefits and promise of integrated computational materials engineering (ICME) to materials research through a series of case studies of compelling materials research themes that are enabled by recent advances and accomplishments in the field of computational materials.

2. An assessment of the benefits of a comprehensive ICME capability to the national priorities.

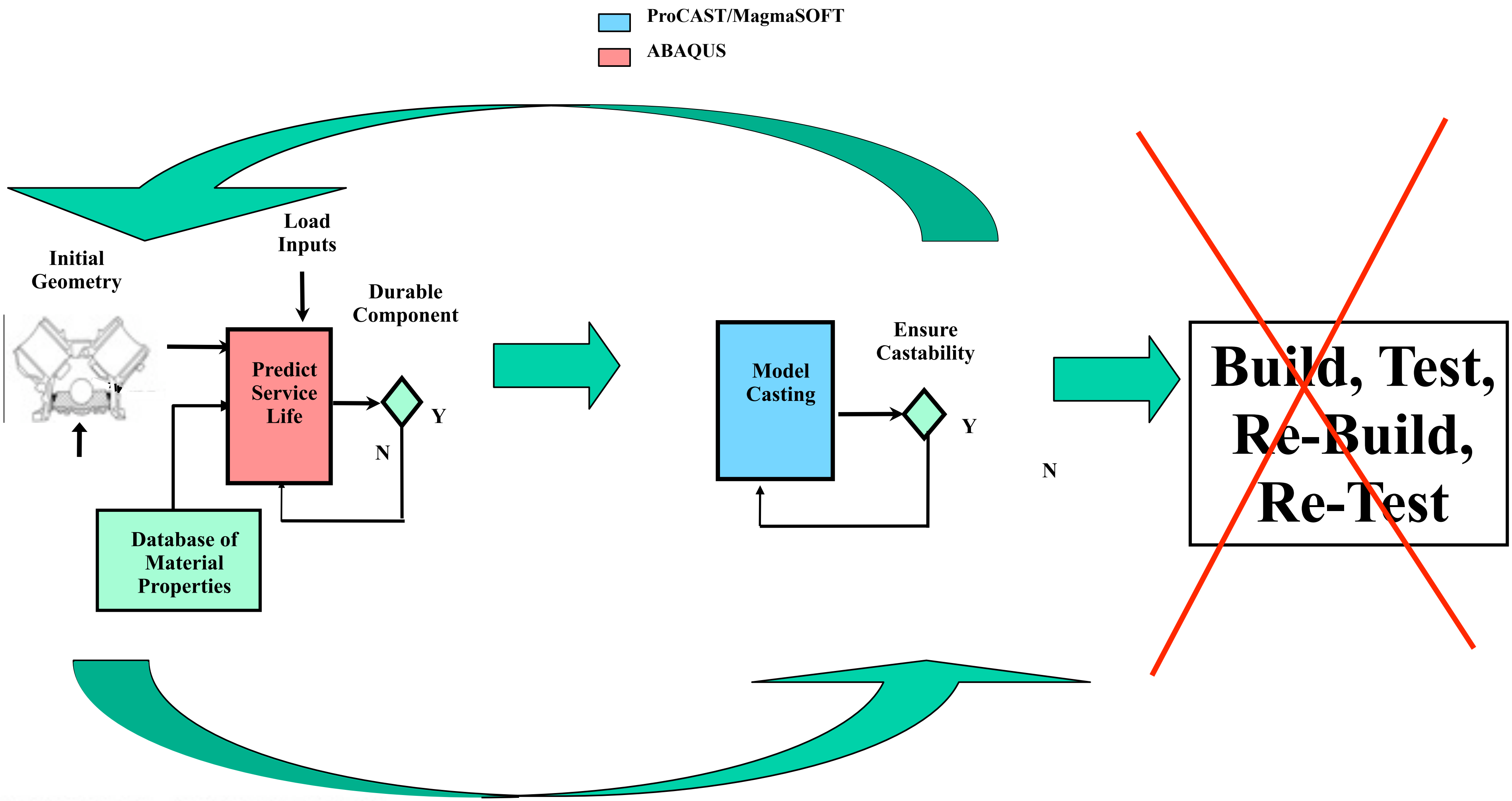
3. The establishment of a strategy for the development and maintenance of an ICME infrastructure, including databases and model integration activities. This should include both near-term and long-range goals, likely participants and responsible agents of change.

4. Making recommendations on how best to meet the identified opportunities.

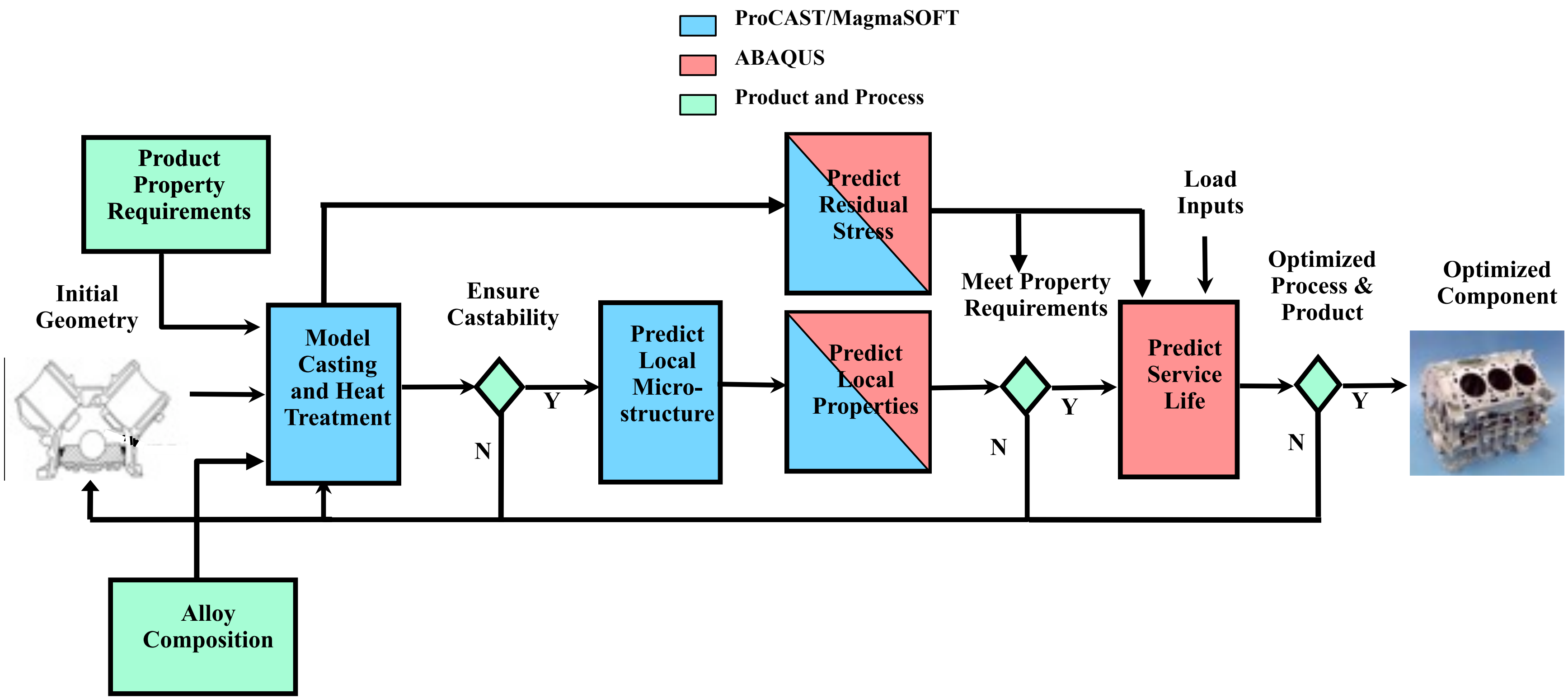
Case Studies

- Early ICME implementations have successfully integrated:
  - Materials, Component Design and Manufacturing Processes $$$$
  - Materials and Prognosis $$$
  - Materials Modeling and Manufacturing Process Development $$
- A series of case studies described in the report demonstrates that application of an ICME infrastructure, even if limited in capability, can result in a significant return on investment.
- The ROI reported to the committee varies from one case to another and is dependent on the class of materials and the expertise required and the situation in which ICME tools are applied.
- Some of the case studies did not result in full realization of potential benefits due to many factors, including lack of investment and cultural issues.
- A ROI in the range of 3:1 to 9:1 can be realized.

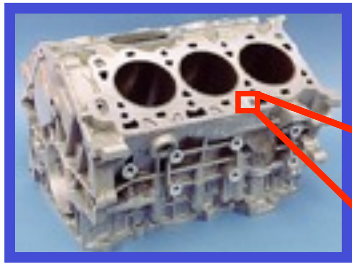
Example Case Study: Ford Motor Company
Traditional Product Development Process



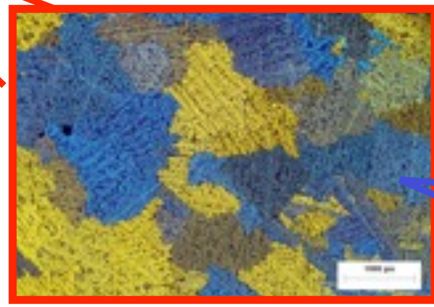
Virtual Aluminum Castings



Materials problems are more complex than other disciplines owing to multiple phenomena across lengthscales

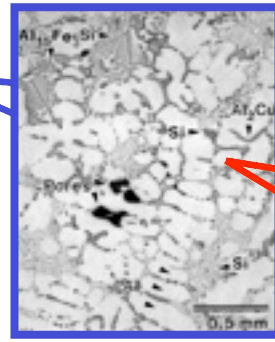


Engine Block
≅ 1 meter



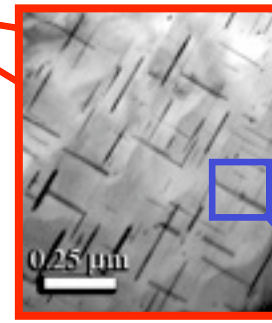
Microstructure
- Grains
≅ 1 – 10 mm

Properties
- High cycle fatigue
- Ductility



Microstructure
- Phases
≅ 100 – 500 microns

Properties
- Yield strength
- Ultimate tensile strength
- High cycle fatigue
- Low cycle fatigue
- Thermal Growth
- Ductility



Microstructure
- Phases
≅ 3-100 nanometers

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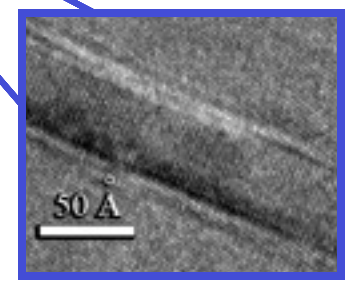

Atoms
≅ 10-100 Angstroms

Properties
- Thermal Growth
- Yield Strength

Models at each scale drive characterization

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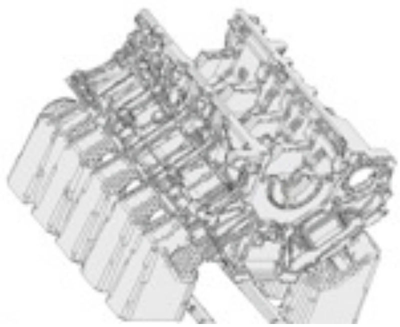
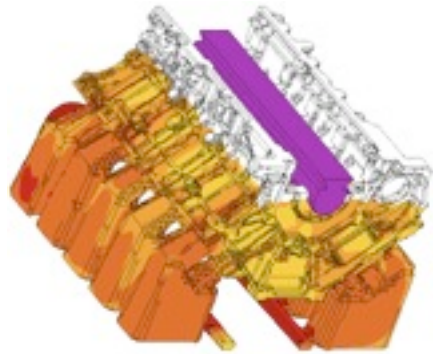
Virtual Aluminum Castings Process Flow

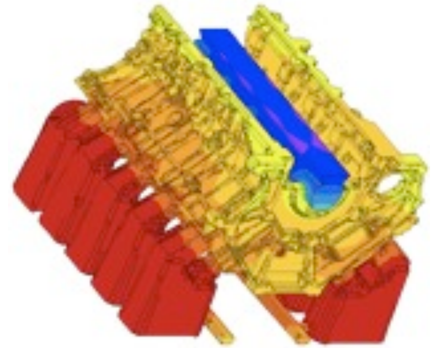
Initial Geometry
- CAD Geometry and Mesh



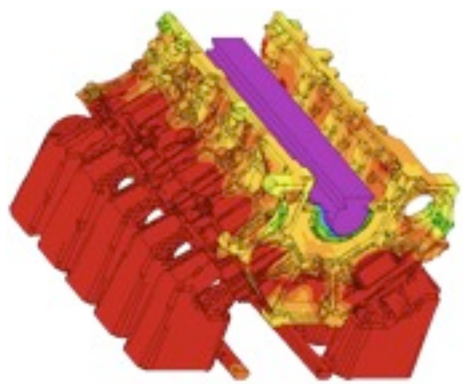
Filling
- Accurate filling Profile (OPTCAST)



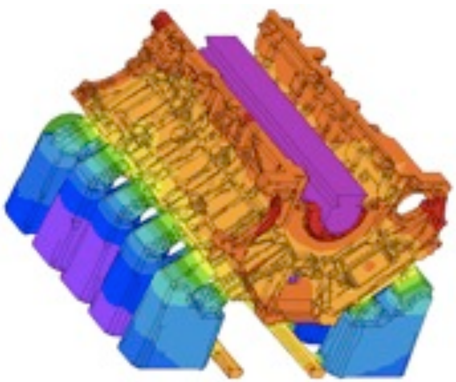
Thermal Analysis
- Boundary Conditions (OPTCAST)
- Fraction solid Curves (ThermoCALC)



Microstructure (Al_2Cu)
- Micromodel (PanDat)
- Solution treatment (Dictra)
- Aging Model (PanDat)

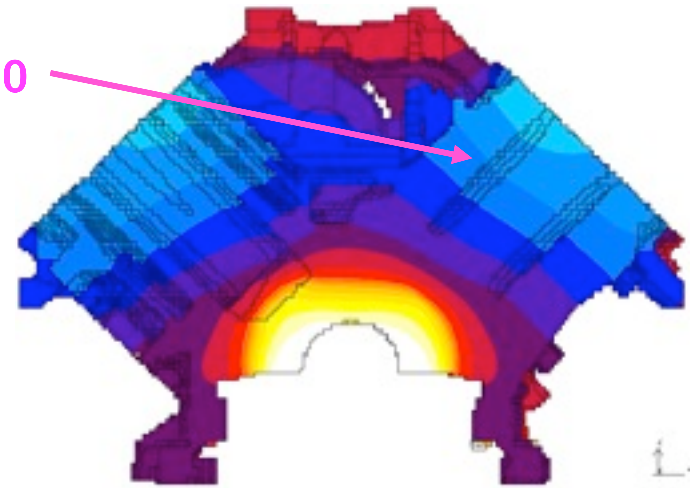


Yield Strength



Using Virtual Aluminum Castings in Product and Process Optimization

210



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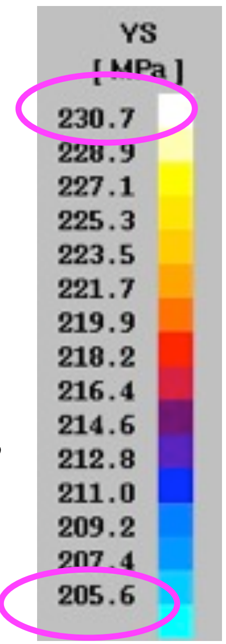

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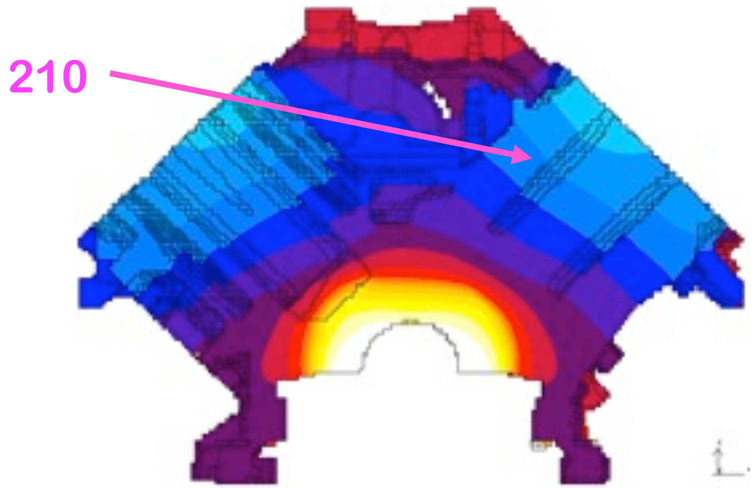
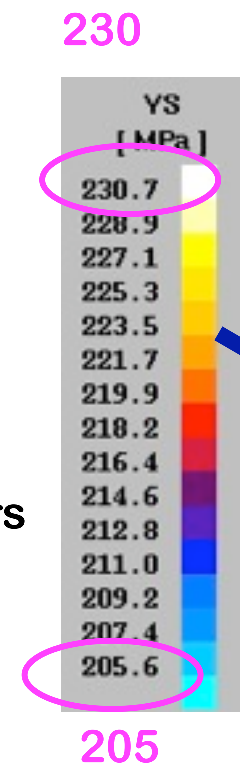
Target Strength = 220 MPa

Aging temperature 240C for 5hrs

Initial Heat Treatment Process

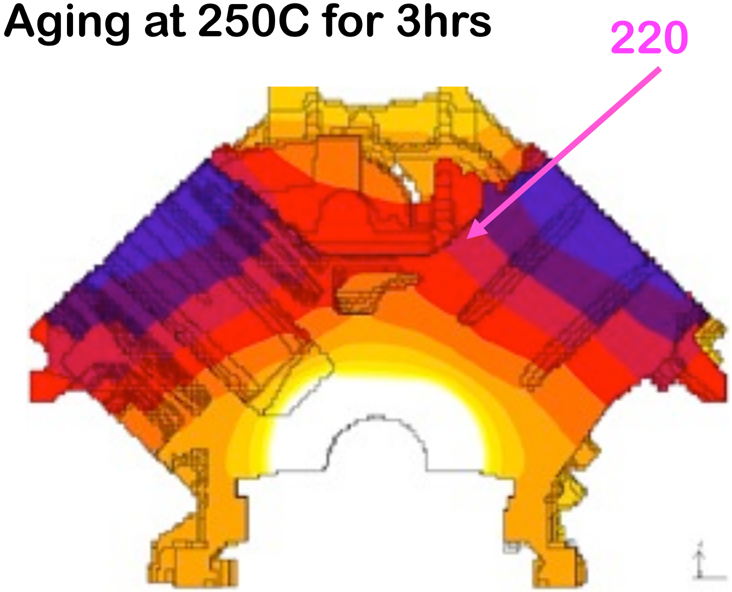
Using Virtual Aluminum Castings in Product and Process Optimization





Target Strength = 220 MPa

Aging at 250C for 3hrs



Aging temperature 240C for 5hrs

Initial Heat Treatment Process

Optimized Heat Treatment Process

Faster and Stronger !!

Ford Virtual Aluminum Castings

Resources

- $15M over 5 years (over 50% experimental work)
- Approximately 25 people involved (15 internal + research at 7 universities)

Return on Investment:

- Over $100M in cost avoidance or cost save (7/1 ROI)
- 15-25% reduction in product development time
- Capability for upgrading and extending at significantly lower cost

Cultural & Organizational Challenges for ICME implementation

- Organizational awareness
- Product development (CAE) work flow
- New job responsibilities
- Supply base information sharing
- Sustained funding

Case Studies - Lessons Learned

- *ICME is an emerging discipline, in its infancy.*
- *ICME can provide a significant positive return on investment.*
- *Achieving the full potential of ICME requires sustained investment.*
- *ICME requires a cultural shift.*
- *Successful model integration involves distilling information at each scale.*
- *Experiments are key to the success of ICME*.
- *Databases are the key to capturing, curating, and archiving critical information required for development of ICME.*
- *ICME activities are enabled by open-access data and integration-friendly software.*
- *Less than a 100% solution may be good enough.*

Barriers to ICME

Technological

- Wide variety of engineering materials and applications
- Multitude of separate mechanisms controlling materials behavior with no single overarching modeling approach (the lengthscale/timescale challenge)
- Targeted, rapid and 3-D materials characterization
- Databases and informatics
- Uncertainty quantification
- Cyberinfrastructure

Barriers to ICME

Cultural and Organizational

- Multi-year investments to realize ROI
- Organizational resistance to change
- Acceptance of "late" materials computational tools by engineering design community
- Demonstrating level of fidelity acceptable to regulatory agencies
- The computational materials science – materials engineering gap
- Collaboration and information sharing
- Education and workforce readiness

Selected Conclusions

- Materials development and optimization cycle does not operate at the rapid pace required by integrated product development teams
- ICME is a technologically sound concept which:
  - Offers a solution to the IPD cycle time dilemma
  - Where successfully applied as a significant ROI
- ICME as a discipline within materials science and engineering does not yet truly exist
- For ICME to succeed, it must be embraced as a discipline by the materials science and engineering community

Conclusions (continued)

- Industrial acceptance of ICME is hindered by the slow conversion of science-based materials computational tools to engineering tools and by the scarcity of materials engineers trained to use them.

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- Although there has been progress in the development of physically based models and simulation tools, for many key areas of application they are inadequate to support the widespread use of ICME.
  - -Near term, ICME can be advanced by use of empirical models that fill the theoretical gaps
  - -Experimental efforts needed to calibrate both empirical and theoretical models and validate ICME capability
  - -Rapid characterization tools alongside new information technology and materials databases are needed

The Vision

Within 10 – 20 year timeframe, **as a result of the coordination and targeted investment by stakeholders in the critical elements of ICME**:

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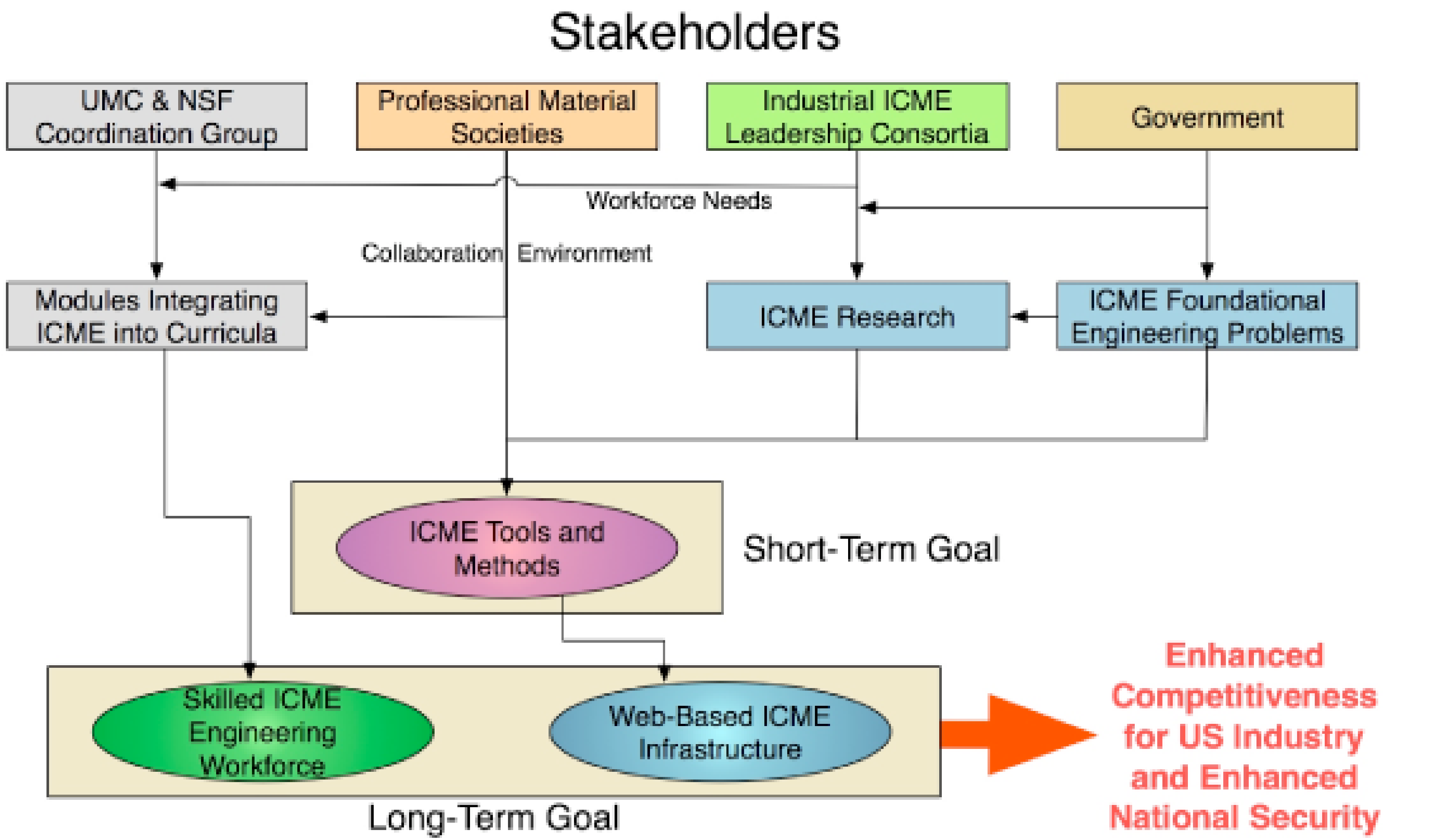
- The materials scientist in academia performing traditional science-based inquiry will benefit from the assembled and networked data and tools. Discoveries will be easier and benchmarking will be standardized.
- Graduating materials science and engineering students will be employed and operate in a multidisciplinary and computationally rich engineering environment.

A Strategy for ICME



Recommendations

Nine recommendations for specific actions for the development, support and national co-ordination of ICME

DOD, DOE, OSTP, NIST, NSF, University Materials Council (UMC), Industry, Professional Materials Societies

Recommendations (continued)

Recommendation 7: **U.S. Industry** should identify high-priority foundational engineering problems that could be addressed by ICME, establish consortia, and secure resources for implementation of ICME into the integrated product development process.

Recommendation 8: The **University Materials Council (UMC**), with support from materials professional societies and the National Science Foundation, should develop a model for incorporating ICME modules into a broad spectrum of materials science and engineering courses. The effectiveness of these additions to the undergraduate curriculum should be assessed using ABET criteria.

Recommendation 9: **Professional Materials Societies** should

- Foster the development of ICME standards (including a taxonomy) and collaborative networks,
- Support ICME-focused programming and publications, and
- Provide continuing education in ICME.

Role of the UMC

- Survey of modeling and simulation is being carried out (Thornton and Garcia)
- As part of a broader discussion on education, the UMC should make specific recommendations about how best to integrate CME into the curriculum
- By bringing ICME to the UMC, our immediate goal is to raise the awareness of the materials education community to this emerging field.

Source: K. Bowcutt, Boeing

One Approach (an opinion)

- The key to ICME is the I and the E
- Our (ISU) plan: (1) introduce computation into curriculum for first year students (MATLAB, …), (2) develop and use MATLAB ICME modules as part of regular curriculum
- Biggest barrier is faculty reluctance
- We are working with MATLAB to provide an introduction and training for faculty based on materials applications

Source: K. Bowcutt, Boeing

Questions?