Materials Genome Initiative

&

Integrated Computational Materials Science and Engineering

Dr. Charles Ward

ICMSE Lead

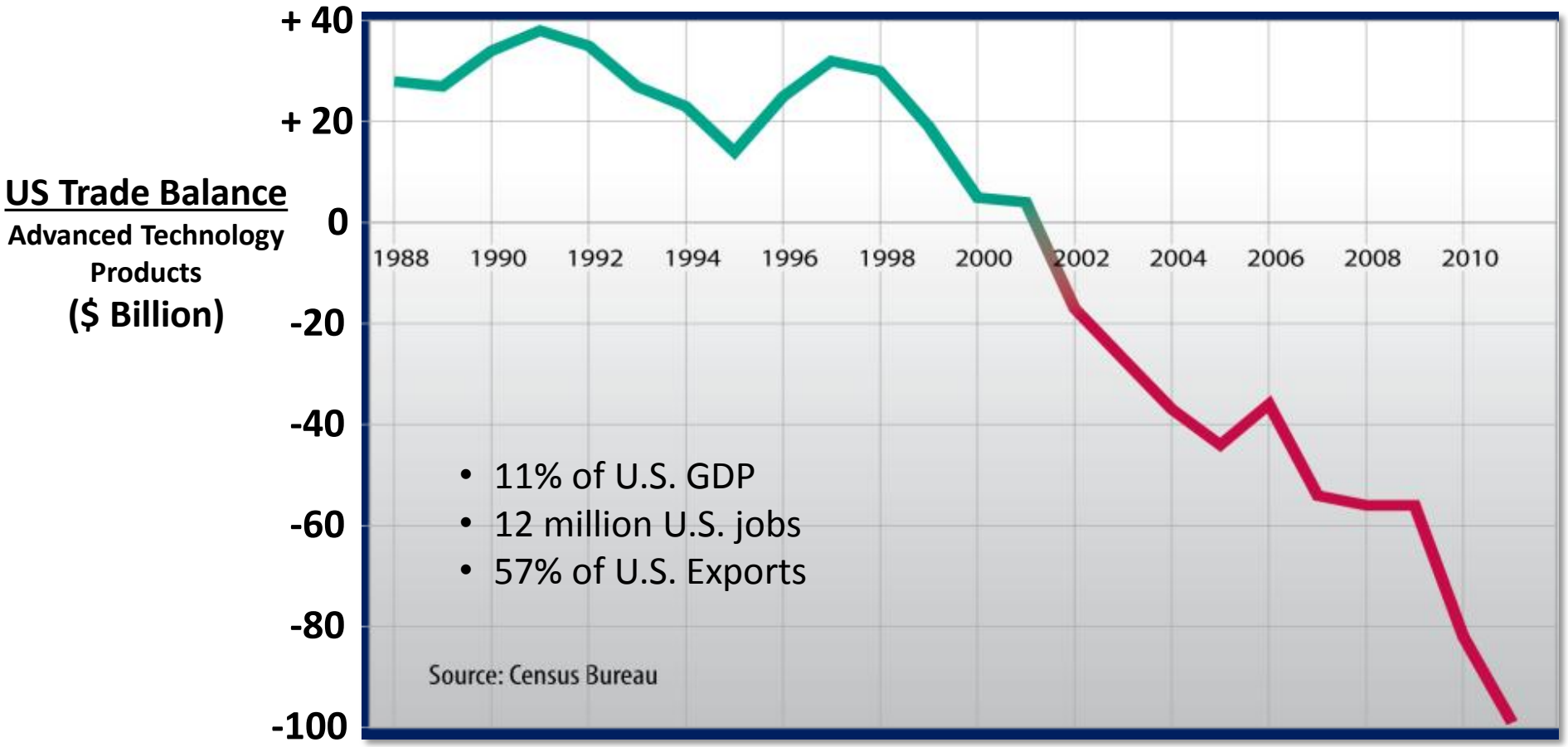
Materials & Manufacturing Directorate

Integrity ★ Service ★ Excellence

Approved for public release, distribution is unlimited (88ABW-2014-5912)

Challenge: US losing market lead in Advanced Technology Products

U.S. Trade Balance for Advanced Technology Products



A Widening Valley of Death?
For Materials Transition

Typical Development Times for New Materials (& Processes) for Jet Engines

I. Modification of an existing material for a non-critical component
- Approximately 2-3 years

II. Modification of an existing material for a critical structural component
- Up to 4 years

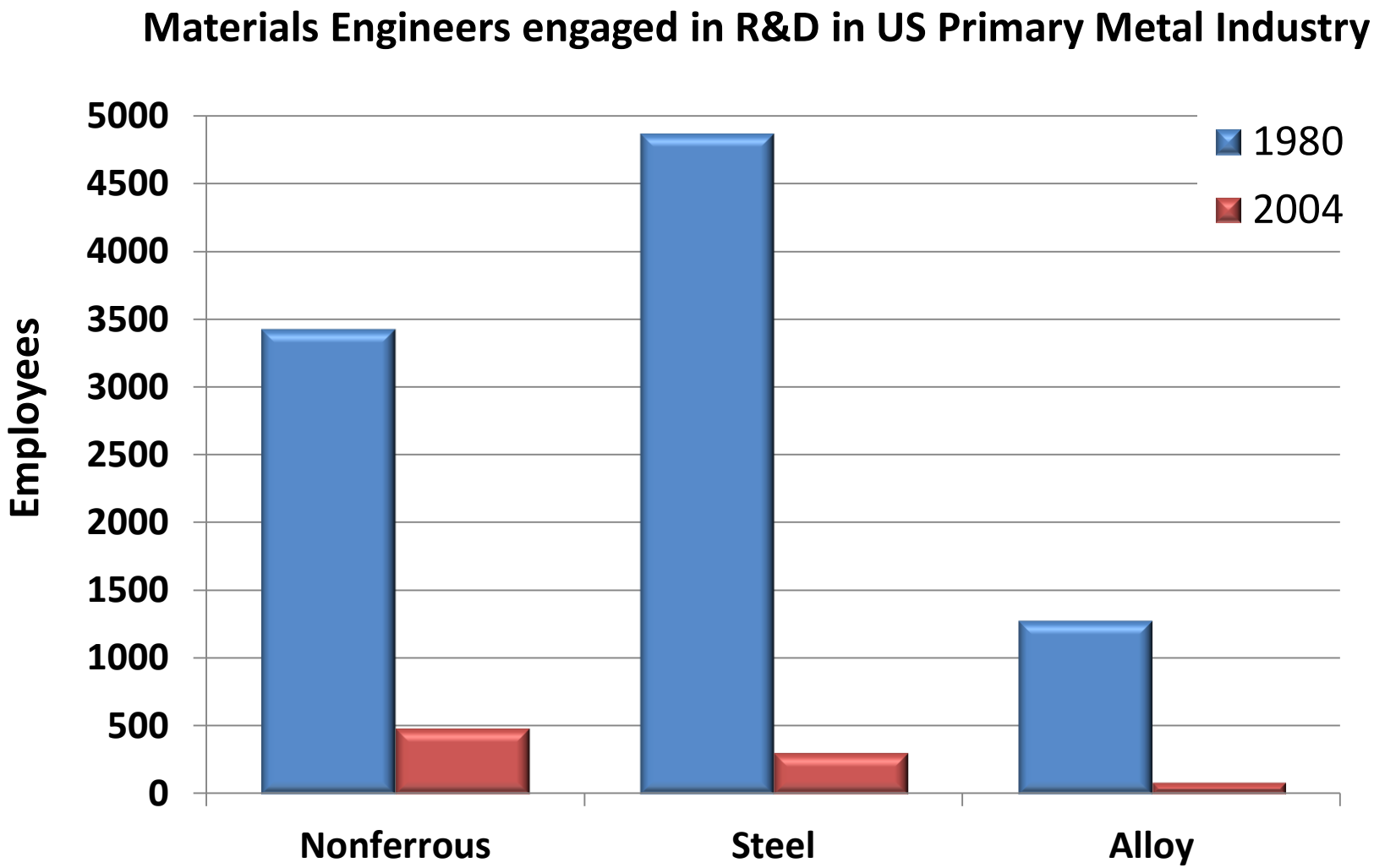
III. New material within a system that we already have experience
- Up to 10 years

IV. New material class
- Up to 20 years, and beyond

However, the jet engine design cycle has decreased by 50% over the past ~10 years

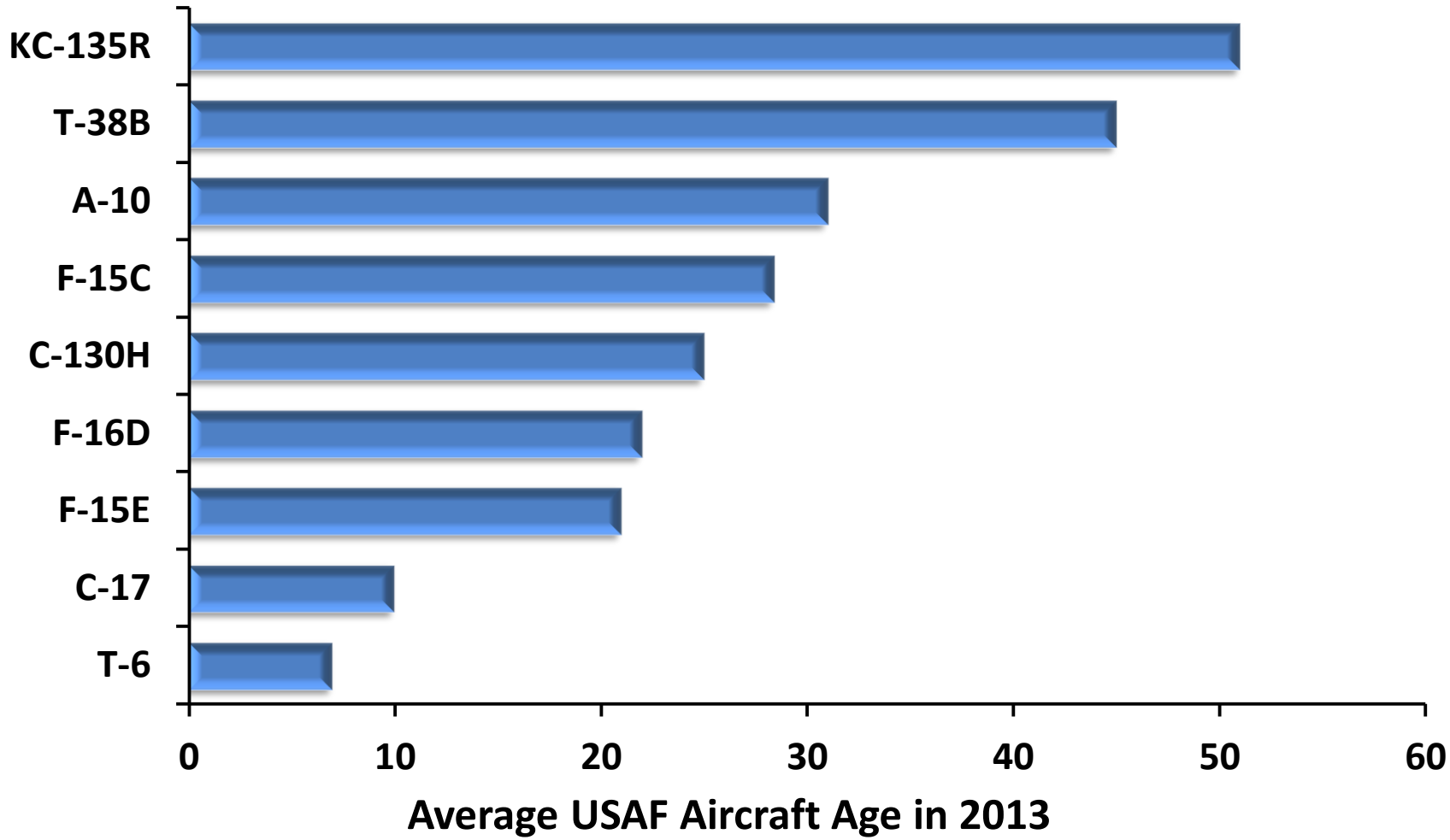
Courtesy C. Haubert & J.C. Williams, GE Aviation, circa 2009

Engineered Materials as a Commodity



Source: *Globalization of Materials R&D: Time for a National Strategy , NRC, 2004*

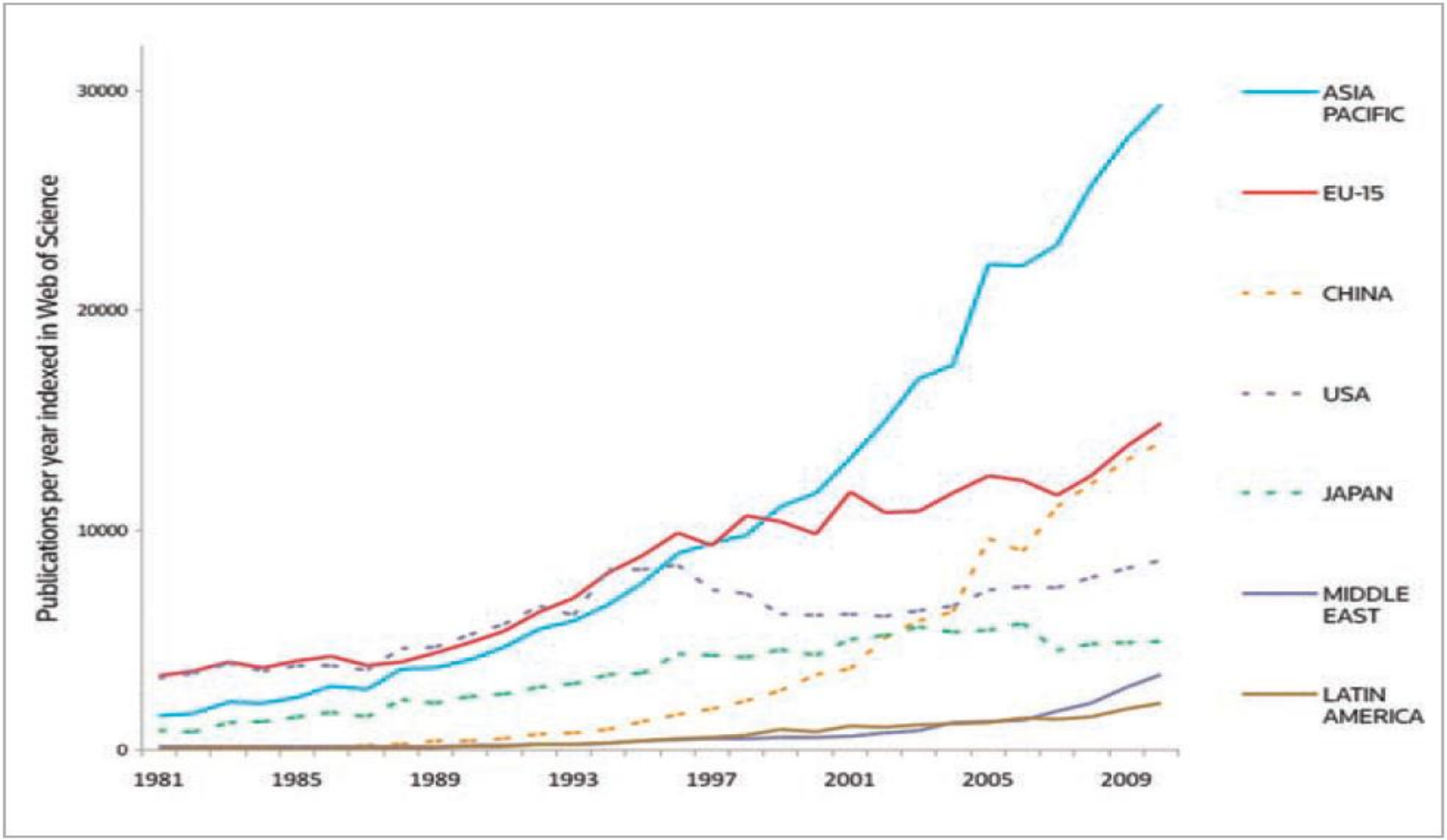
Increased System Expectations



Reduce maintenance costs now; prognostics for future systems

Source: *Air Force Magazine, May 2013*

Growth in Materials Information



Source: *Thomson Reuters Web of Knowledge*SM

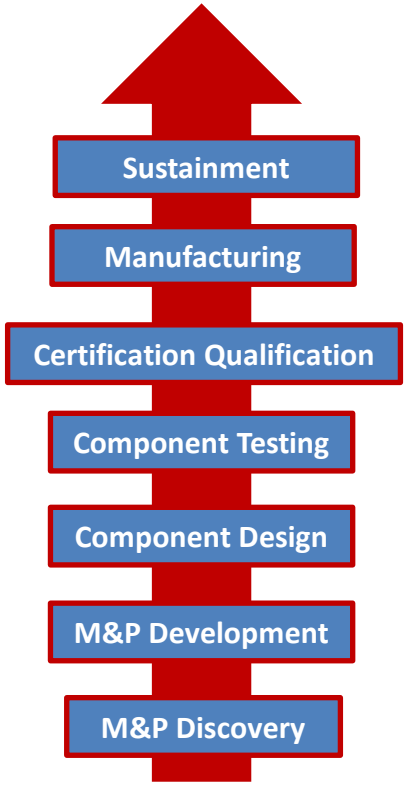
162,000 materials science & engineering journal articles published in 2012

Imperatives & Opportunities

Strengthen US Industrial base by:

- **Improve cost, schedule & materials solutions for system design**
- **Enhance capability to develop, manufacture & design systems**
- **Increase fidelity of system life-cycle performance predictions**
- **Leverage global investment in creating materials knowledge**

Changing the Materials Life Cycle



PAST

Sequential
Qualitative
Empirical
Ad Hoc
Fragmented Data (in a drawer)
Disjoint Processes
Material & Process Specifications

FUTURE

Integrated Approach
Digital Data & Processes
Flexible Interfaces across Engineering
Shared Knowledge
Retained Knowledge
Plug & Play Modularity for tools and data

Materials Genome Initiative & Integrated Computational Materials Science and Engineering

"Integrated Computational Materials Engineering (ICME) is the <u>integration of materials information</u>, <u>captured</u> in computational tools, with engineering product performance analysis and manufacturing-process simulation." **…NRC (2008)**

- MGI and ICMSE are a paradigm shift in capability and culture:
  - Quantitative & Predictive Tools
  - Combined Computation and Experiment
  - Addresses complete materials life cycle
  - Integrated with system design framework

Goal: A model-based definition of materials & processes

The Materials Genome Initiative

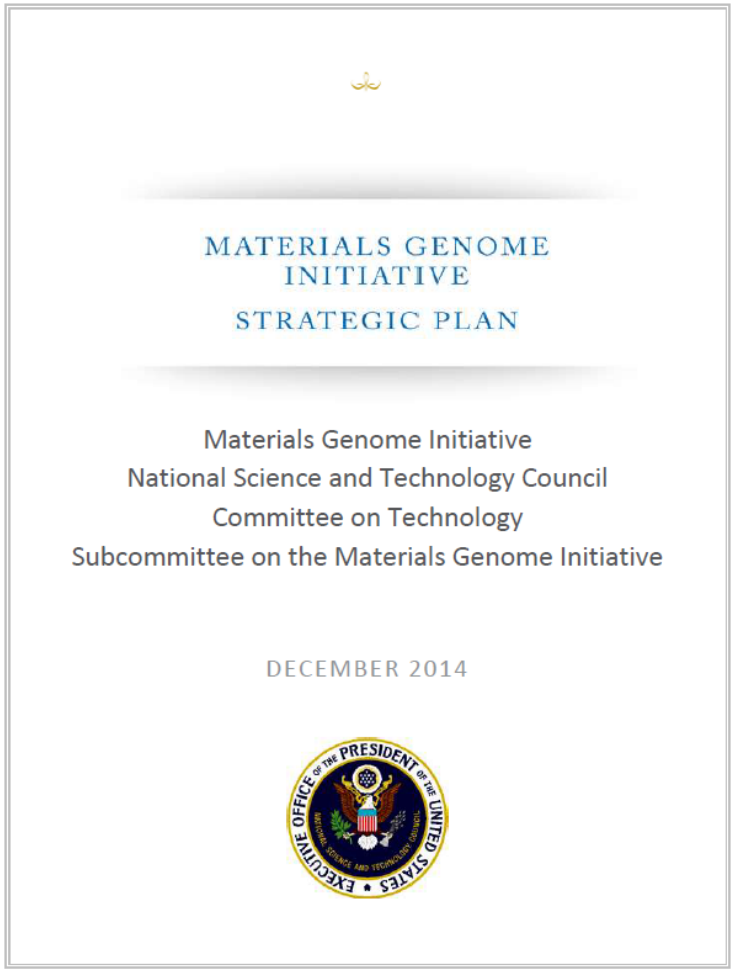
Goal: to decrease the time-to-market by over 50%

1. Develop a Materials Innovation Infrastructure

2. Achieve National goals in energy, security, and human welfare with advanced materials

2. Equipping the next generation materials workforce

MGI Strategic Plan


MATERIALS GENOME INITIATIVE

STRATEGIC PLAN

Materials Genome Initiative
National Science and Technology Council
Committee on Technology
Subcommittee on the Materials Genome Initiative

DECEMBER 2014

1. Enable a Paradigm Shift in Culture
2. Integrate Experiments, Computation, and Theory
3. Facilitate Access to Materials Data
4. Equip the Next-Generation Materials Workforce

http://www.whitehouse.gov/sites/default/files/microsites/ostp/NSTC/mgi_strategic_plan_-_dec_2014.pdf

Elements of the Materials Innovation Infrastructure (MGI)

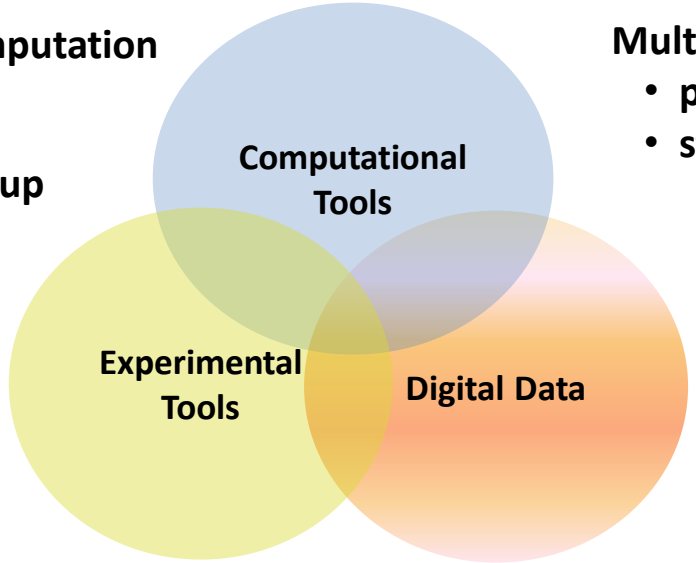
Materials discovery - first principles and atomistics

UQ and uncertainty management

High throughput computation

Multiscale Modeling
- process-structure
- structure-property

Process models for manufacturing and scale-up



Designer materials knowledge systems and representation

Verification and Validation - Experiment/Model coupling

Synthesis and processing, including high throughput

Databases, data sciences and material informatics

Sensors and in situ measurements; automation

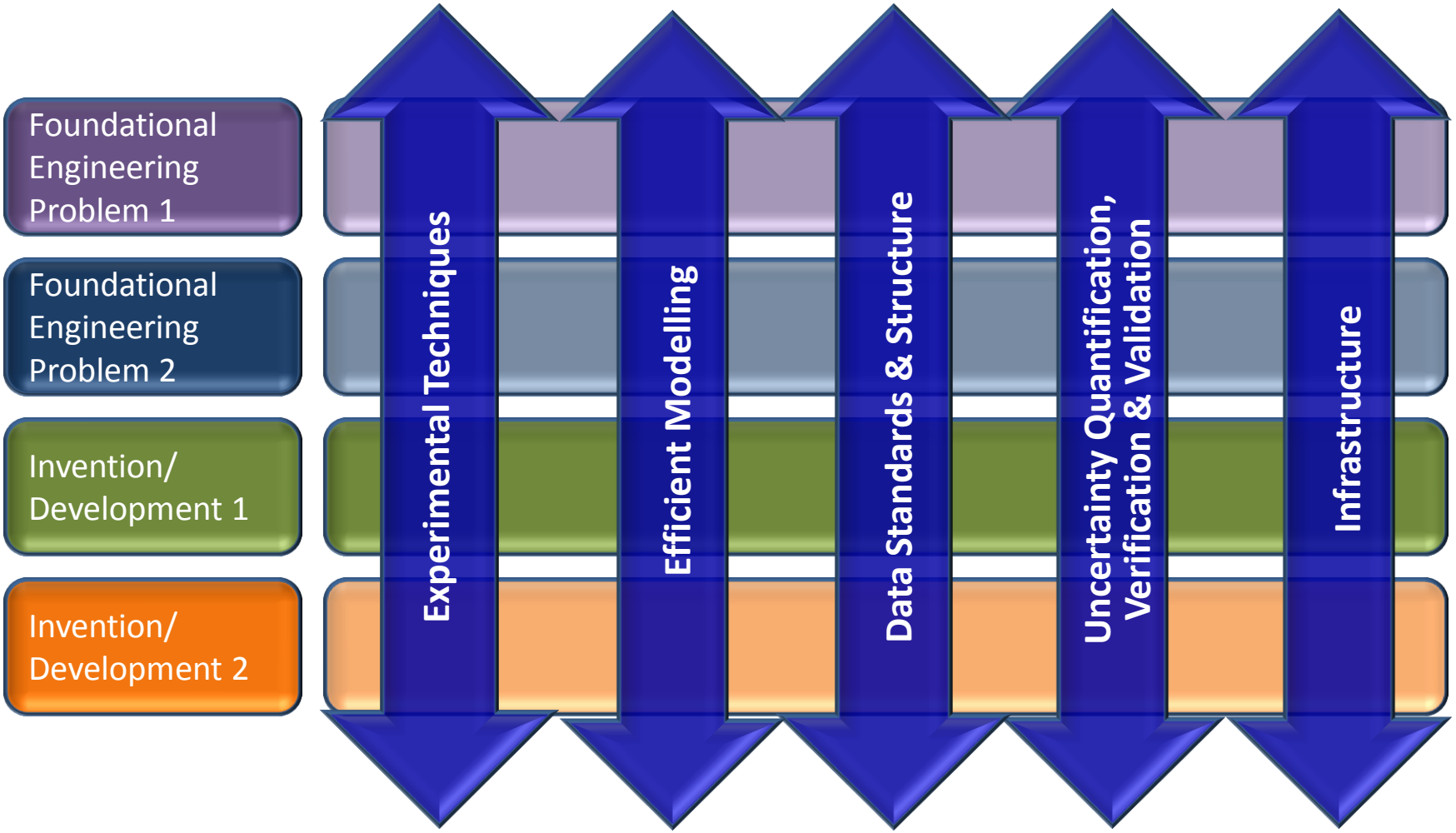
Materials characterization and microstructure representation

Systems design and MDO
- Design exploration
- Detail design

Distributed collaborative networks

Expanded by D.L. McDowell, Georgia Tech, from OSTP MGI White Paper

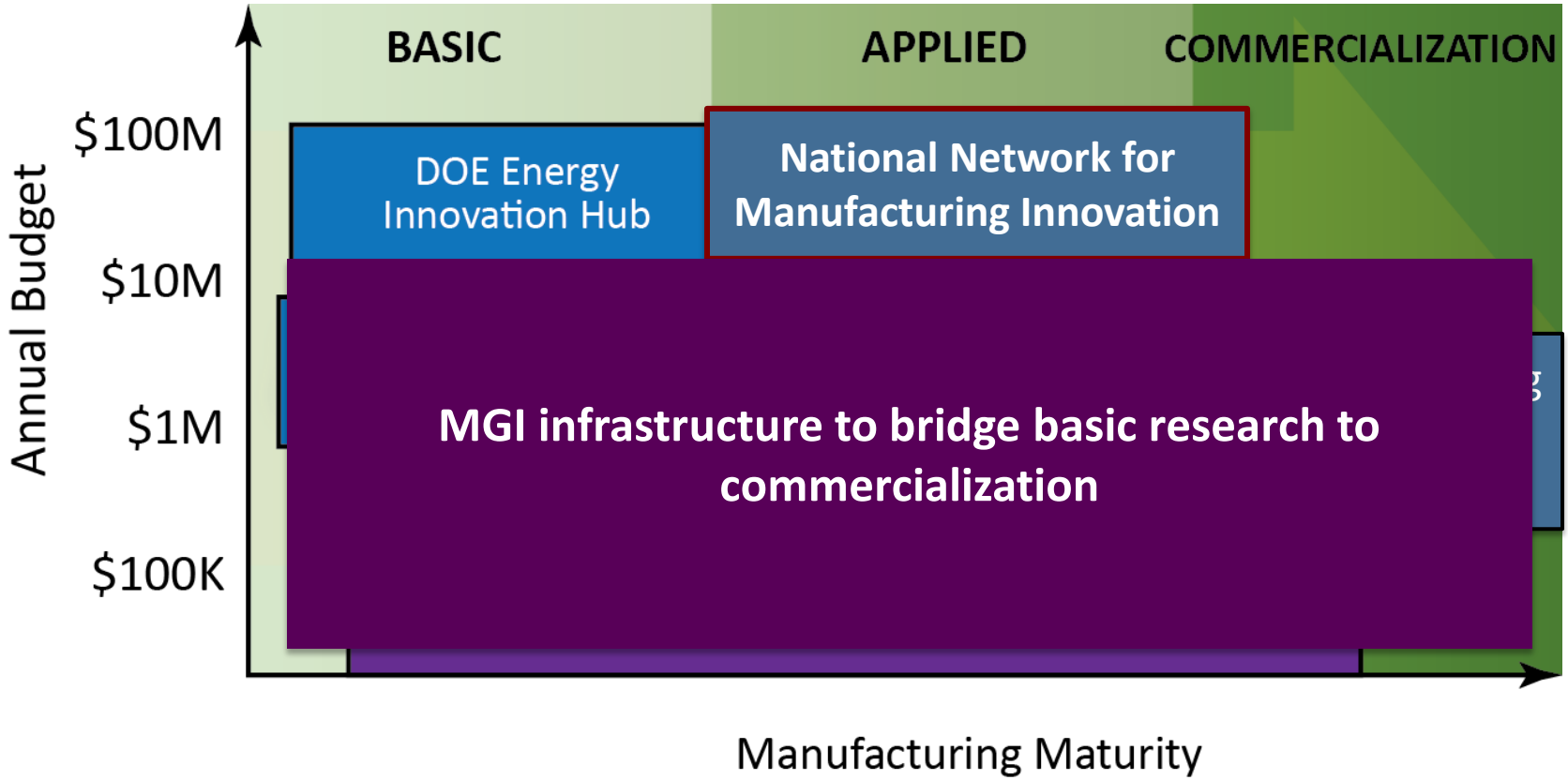
AFRL ICMSE Approach



Advanced Materials & Manufacturing Federal Funding

Basic science
Largely government funded

Commercialization
private sector owned/funded



MGI Funding ~ $125 million per year

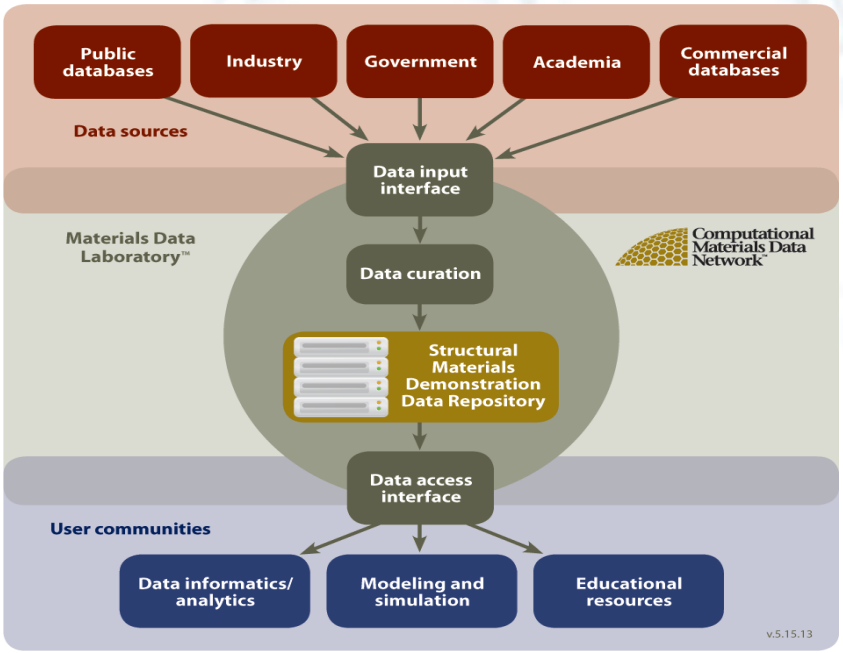
BUILDING THE DATA INFRASTRUCTURE
NIST EFFORTS IN DATA FOR MGI

Established Office of Data and Informatics

Goal: To Enable & Enhance Data Exchange

- building databases and possible federated databases and repositories
- developing tools for capture, mining, analytics
- developing standards for ontologies and metadata

ASM/NIST STRUCTURAL MATERIALS DATA DEMONSTRATION PROJECT



ASM
DOE/EERE
National Data Service…

Partnering is key to make materials data accessible on the scale that it happens in biology

NIST CENTER OF EXCELLENCE IN MGI

CHiMaD

THE CENTER FOR HIERARCHICAL MATERIALS DESIGN

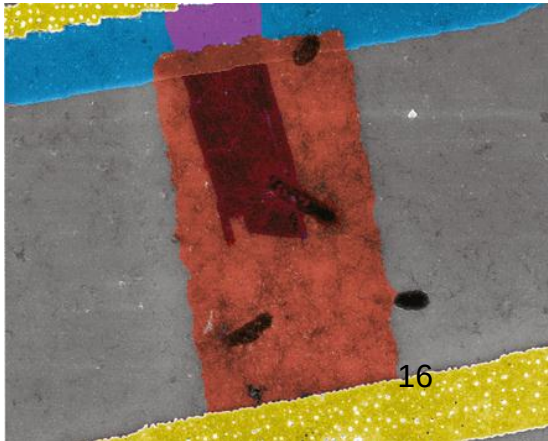
Peter Voorhees, Greg Olson, Northwestern University

Juan de Pablo, University of Chicago

$5M/y for 5y

- To foster hierarchical materials discovery, in accordance with the goals of MGI and NIST
- To serve, with NIST, as a national resource for verified codes and curated databases to enable proliferation of a materials-by-design strategy
- To foster the next generation of computational tools, databases and experimental techniques
- To provide opportunities to transition new breakthroughs in advanced materials to industry

Seed Project: Low D nanoelectronics
Goal: to understand and realize p-type and n-type doping in the low-dimensional limit



CNT-MoS_2 p-n heterojunction
(Hersam, Lauhon, PNAS, 2013)

Enabling Multi-Scale Management

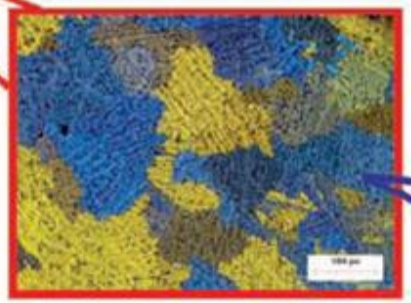
In construct of Objects with Attributes, higher-scale objects can have Attributes of lower-scale information

1 m

Element Object

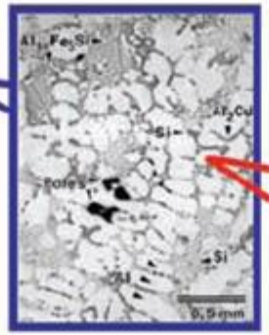
Feature Object

Ensemble Object(s)



1–10 mm
Macrostructure

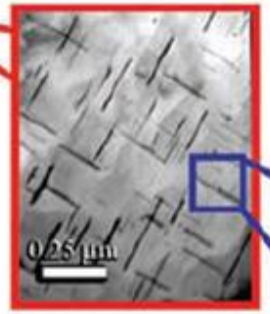
Ensemble Object(s)



10–500 µm
Microstructure

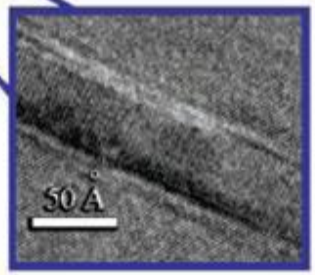
Element Object

Feature Object



1–100 nm
Nanostructure

Ensemble Object(s)



0.1–1 nm
Atomic Structure

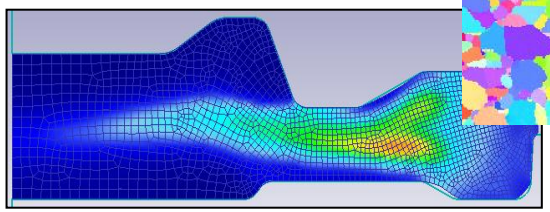
Ensemble Object(s)

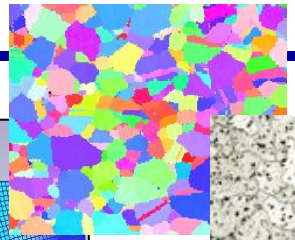
Multi-scale hierarchical management can occur with sufficient MSE guidance of links between scales and knowledge of digital representation

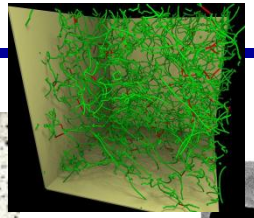
Computational management tools for structure hierarchy do not exist today

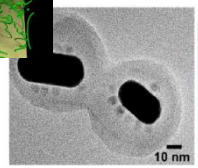
Abstract Hierarchical Scheme

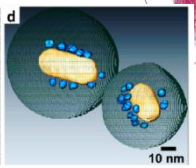
Image Courtesy of J. Miller











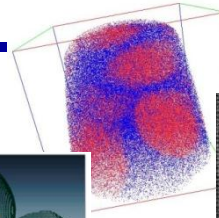
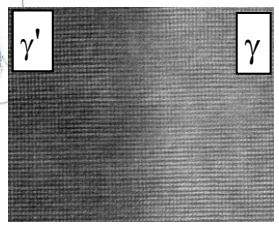
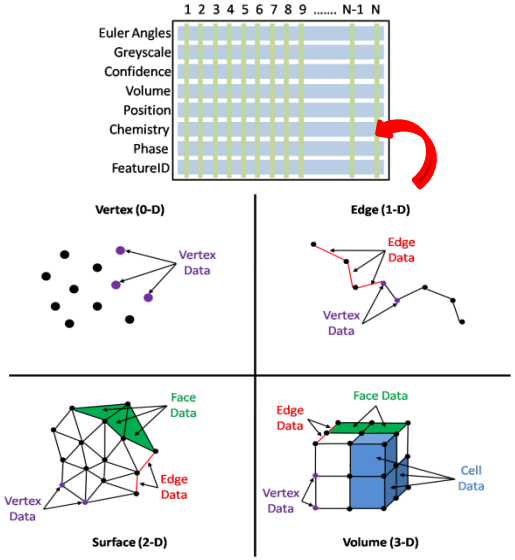


Image Courtesy of L. Drummy

Images Courtesy of J. Tiley

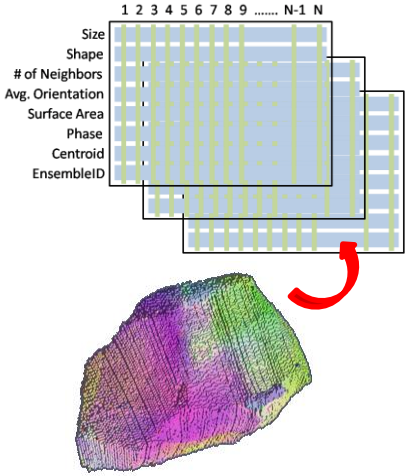


GEOMETRY, LABELING, STATISTICS



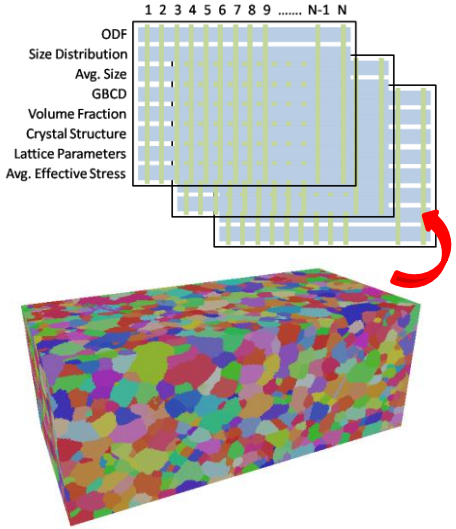
Element Object

100,000s – 1,000,000,000s of Objects



Feature Object

100s – 10,000s of Objects
(100s – 10,000s of Element Objects)



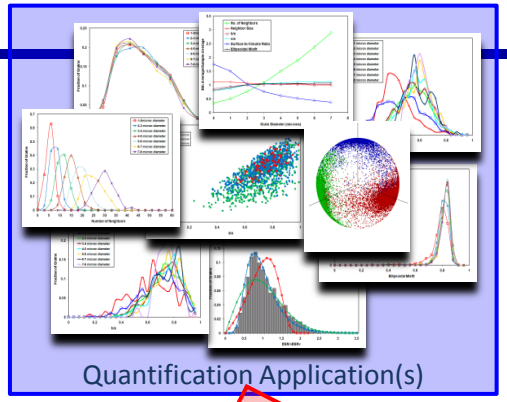
Ensemble Object

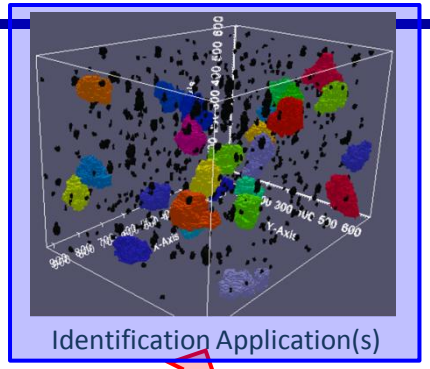
1s – 10s Objects
(100s – 10,000s of Feature Objects)

Object–Attribute construct generalizes storage of digital, spatial information

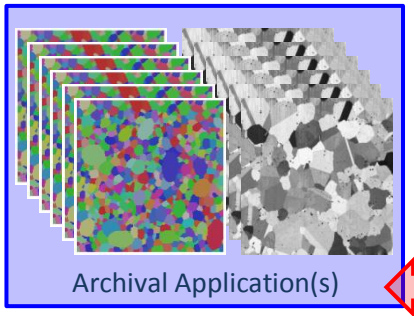
An App Suite for Materials

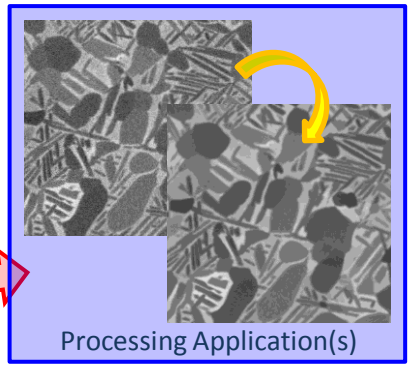
* Central box represents SIMPL as a broker/manager between applications


Quantification Application(s)


Identification Application(s)

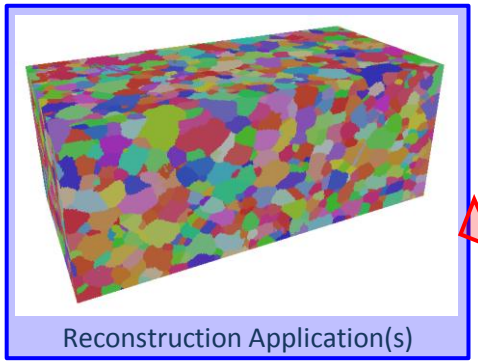
* Blue boxes represent a suite of applications for specific processes

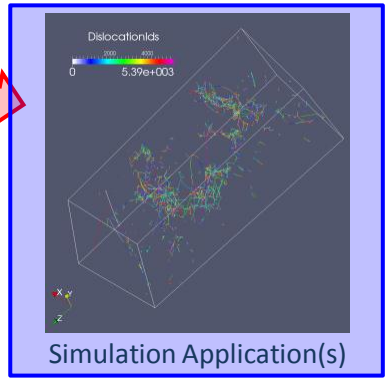

Archival Application(s)


Processing Application(s)

SIMPL

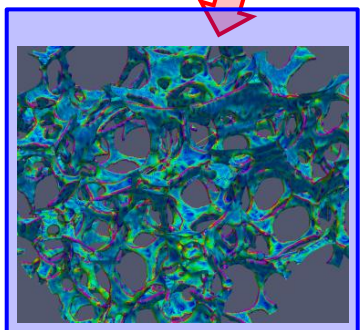
- Manages Current Object Versions
- Brokers Application Interaction
- Controls I/O
- Manages Digital History of Data

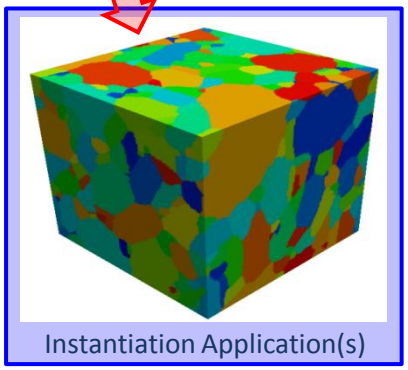

Reconstruction Application(s)



Simulation Application(s)

* Images are example outputs from existing applications for specific processes


Meshing Application(s)


Instantiation Application(s)

* Red arrows represent the transfer of information to/from SIMPL to Application

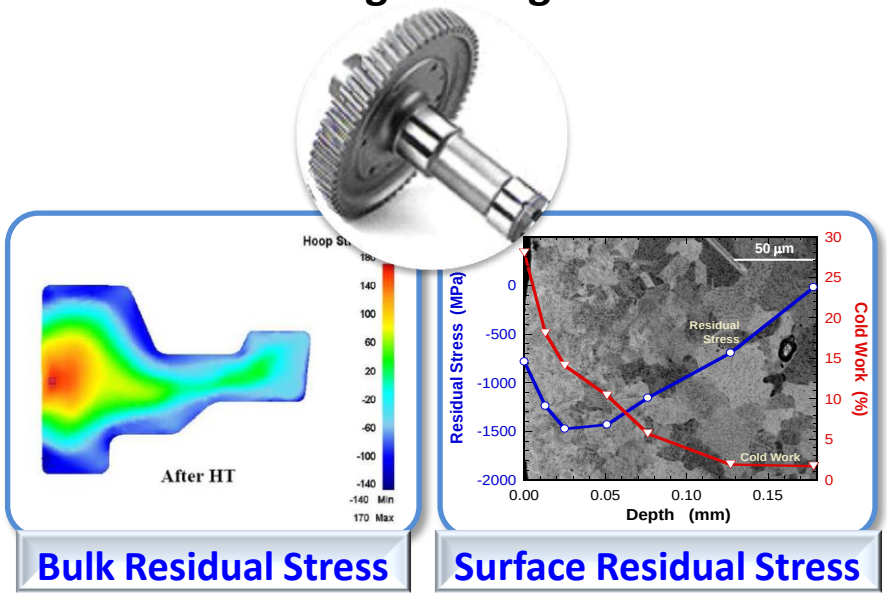
SIMPL is material independent; Apps may be material & data-type dependent

Foundational Engineering Problems
Objectives

- Develop & establish pervasive ICMSE technologies, methodologies, & protocols portable to other applications of interest
- Demonstrate a digital framework linking processing, property, structure relationships for material design to account for processibility, manufacturability, system performance and sustainability
- Demonstrate reduced cost & development time can be delivered using ICMSE on high return on investment components
- Identify infrastructure/technology gaps to be solved by the community
- Strengthen ICMSE competency & infrastructure within the supplier base

AFRL FEPs

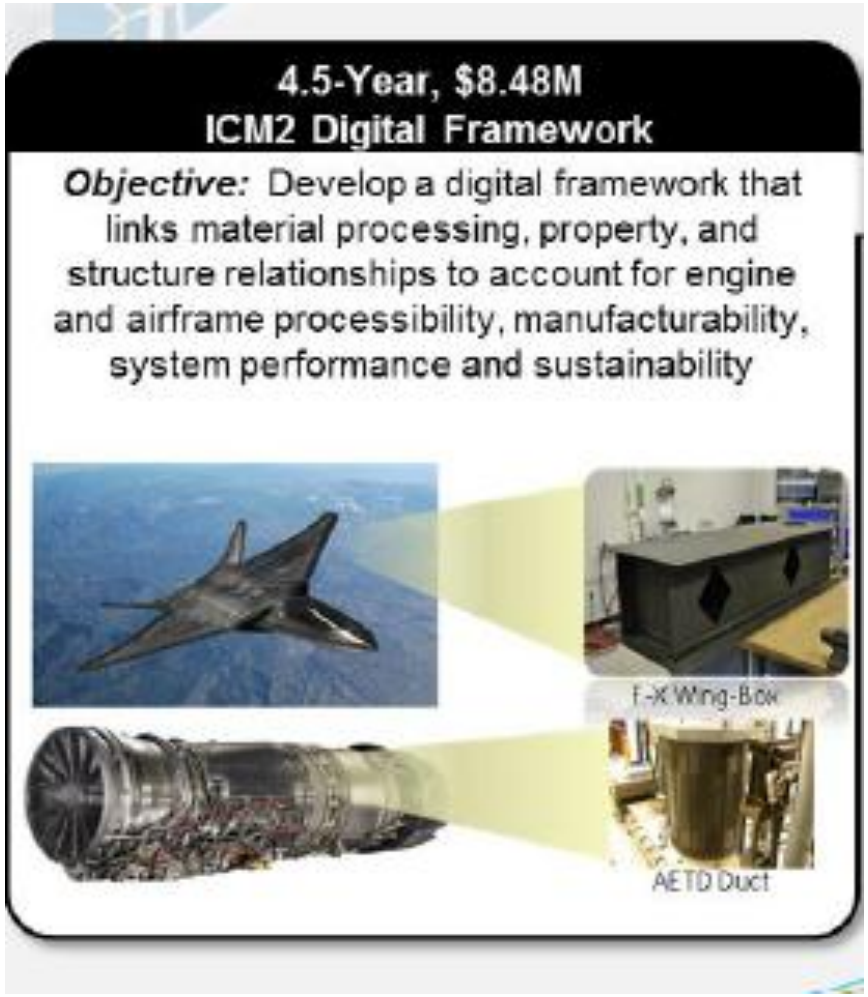
Residual Stress Engineering in Ni Structures



Bulk Residual Stress | **Surface Residual Stress**

- **Residual stress represents pervasive issue to metals industrial base**
- **Significant "tech pull" from OEM designers and materials suppliers**
- **Significant potential impact:**
  - Increased design efficiency
  - Reduced scrap at production and depot
  - Life extension of legacy components

Integrated Computational Methods for Composite Materials (ICM2)



DOE Vehicle Technologies – Foundational Engineering Problems

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

ICME Development of 3GAHSS

Apply ICME techniques to design steel chemistry, processing, and manufacturing for a body or chassis structure with 35% weight reduction at a cost of less than $3.18 per pound saved

- Connect experimental and modeling techniques across many length scales
- Identify steels exceeding 800MPa/1200MPa/30% and 1200MPa/1500MPa/25% (Tensile/Ultimate/Elongation)

DOE funding: $6M (1 award)

USAMP (PI), A/SP, EDAG, LSTC, U. Illinois, Brown U., Clemson U., Colorado Sch. Mines, Michigan State U., PNNL

Predictive Engineering Tools for Injection Molded Long Carbon Fiber Composites

Validate existing models for carbon fiber length and orientation in complex, 3D injection molded parts

- Integrate current state-of-the-art predictive tools and validate performance against experimental results

DOE funding: $1M/$740k (2 awards)

PNNL and partners, ORNL and partners

Advanced Alloy Development for Automotive and Heavy Duty Engines

Apply ICME to develop new Al (LD) and Fe (HD) alloys to enable higher peak cylinder pressures and improve efficiency

DOE funding: $3.3M/$3.5M/$3.5M/$3.5M (4 awards)

Ford and partners, GM and partners, ORNL and partners, Caterpillar and partners

Courtesy Will Joost, DOE-EERE

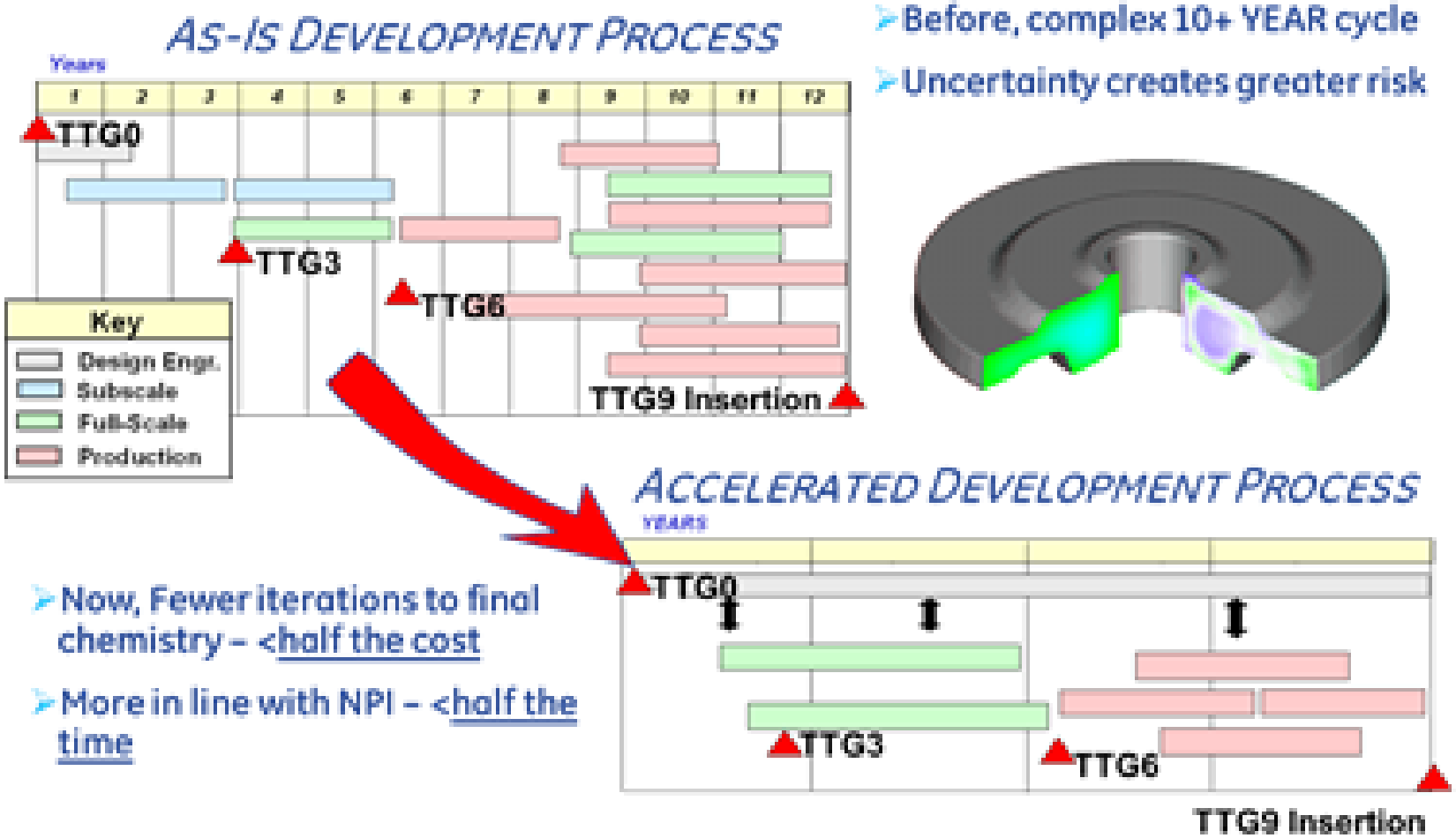
NNMI: starts with materials

Additive Manufacturing (DOD)	Power Electronics (DOE)	Digital Manufacturing (DOD)	Lightweight/ Modern Metals (DOD)
$50M fed, $60M matc Lead: Nat'l Center fo Defense Manufacturir and Machining Hub Location: Youngstown, OH Partners: >100	$70M fed, $70M match Lead: NC State Uni Hub Location: Research Triangle, N Partners: 17 industr 5 university, 3 othe	$70M fed, $24 match Lead: UI Lab Hub Location: Ch Partners: 41 ind 23 university/la other	$70M fed, $70M match Lead: EWI Hub Location: Detroit Partners: 34 industry, 9 university/labs, 17 other

Adv. Composites Manufacturing (DOE)	Integrated Photonics Manufacturing (DOD)	Solicitation TBA (DOD)	Solicitation TBA (DOE)
$70M fed Proposals und evaluation	$100M fed Proposals due December 19th		

Data-Driven Materials Development

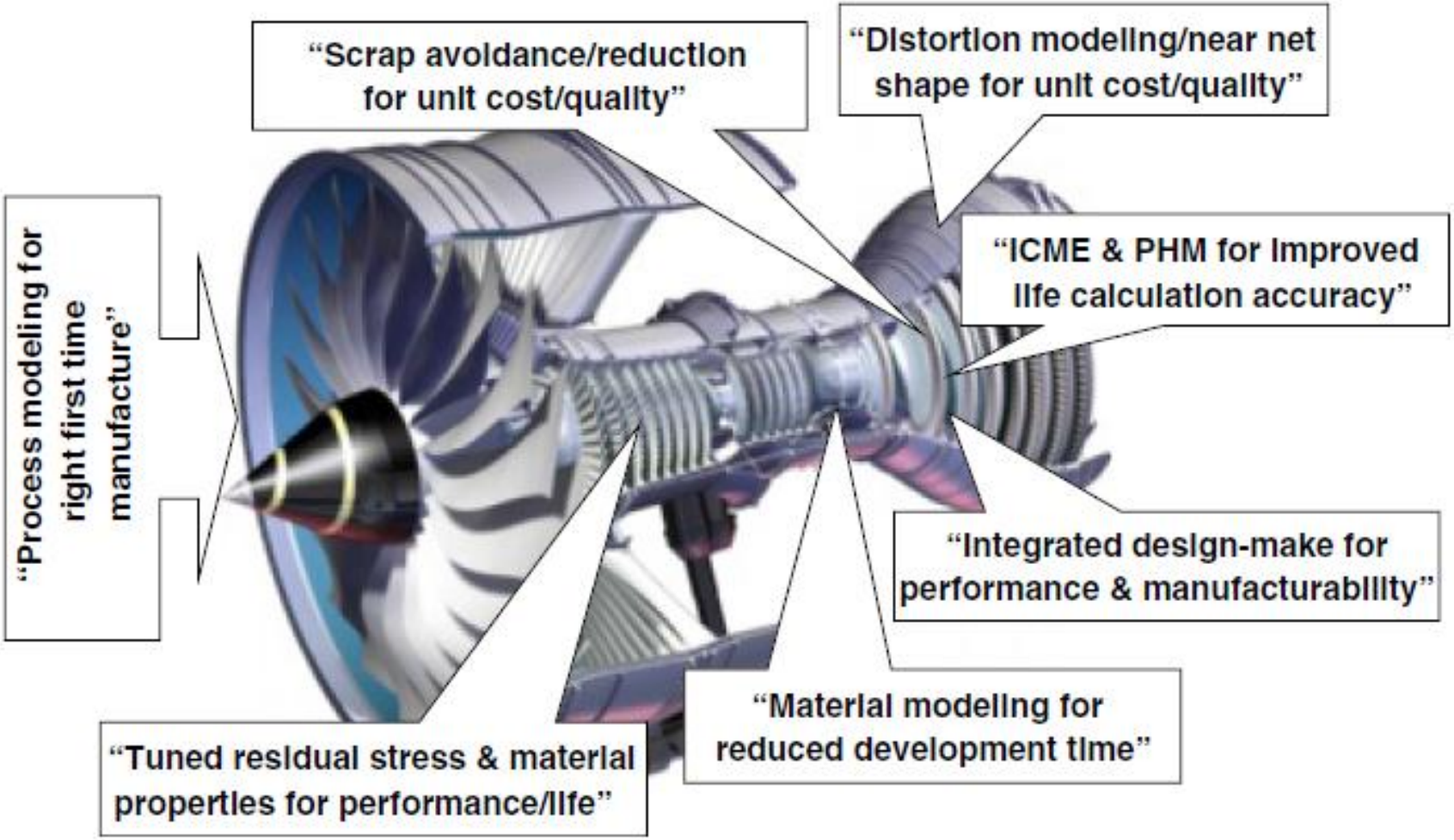
New Cast & Wrought Disk Alloy, R65



Source: *R. Schafrik, GE Aviation, RTO-MP-AVT-187, Oct 12*

ICMSE Case Study

Rolls Royce Plc



Bolcavage et al. Integrating Materials and Manufacturing Innovation 2014, 3:13

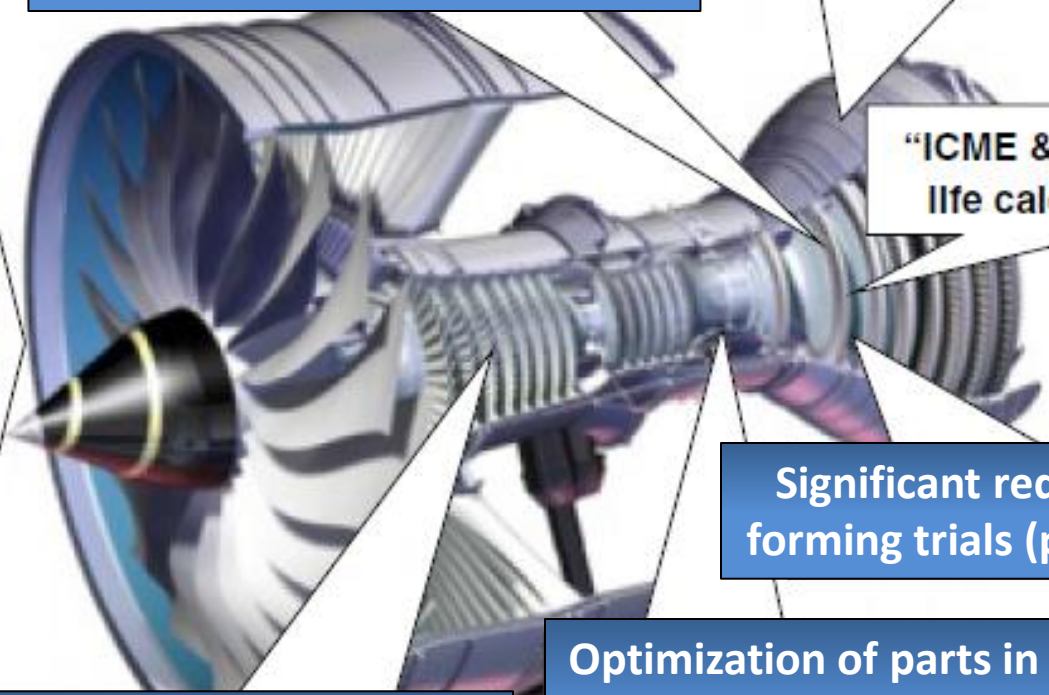
ICMSE Case Study

Rolls Royce Plc

Distortion prediction of forged parts resulting in less scrap, fewer concessions 99.98% Right First Time

Reduction in casting scrap
> > US$5M p.a.

Decreasing forging machining costs
50% cost reduction



"ICME & PHM for Improved life calculation accuracy"

Significant reduction (by 90%) of forming trials (powder HIP process)

Optimization of parts in furnaces to increase utilization; increasing stock-turn and lowering costs.

Increasing tensile strength
~ 5% on forged/formed parts

Bolcavage et al. Integrating Materials and Manufacturing Innovation 2014, 3:13

Verification & Validation in ICMSE

Cowles *et al. Integrating Materials and Manufacturing Innovation* 2012, **1**:2
http://www.immijournal.com/content/1/1/2

Integrating Materials and Manufacturing Innovation
a SpringerOpen Journal

RESEARCH Open Access

Verification and validation of ICME methods and models for aerospace applications

Bradford Cowles[1*], Dan Backman[2] and Rollie Dutton[3]

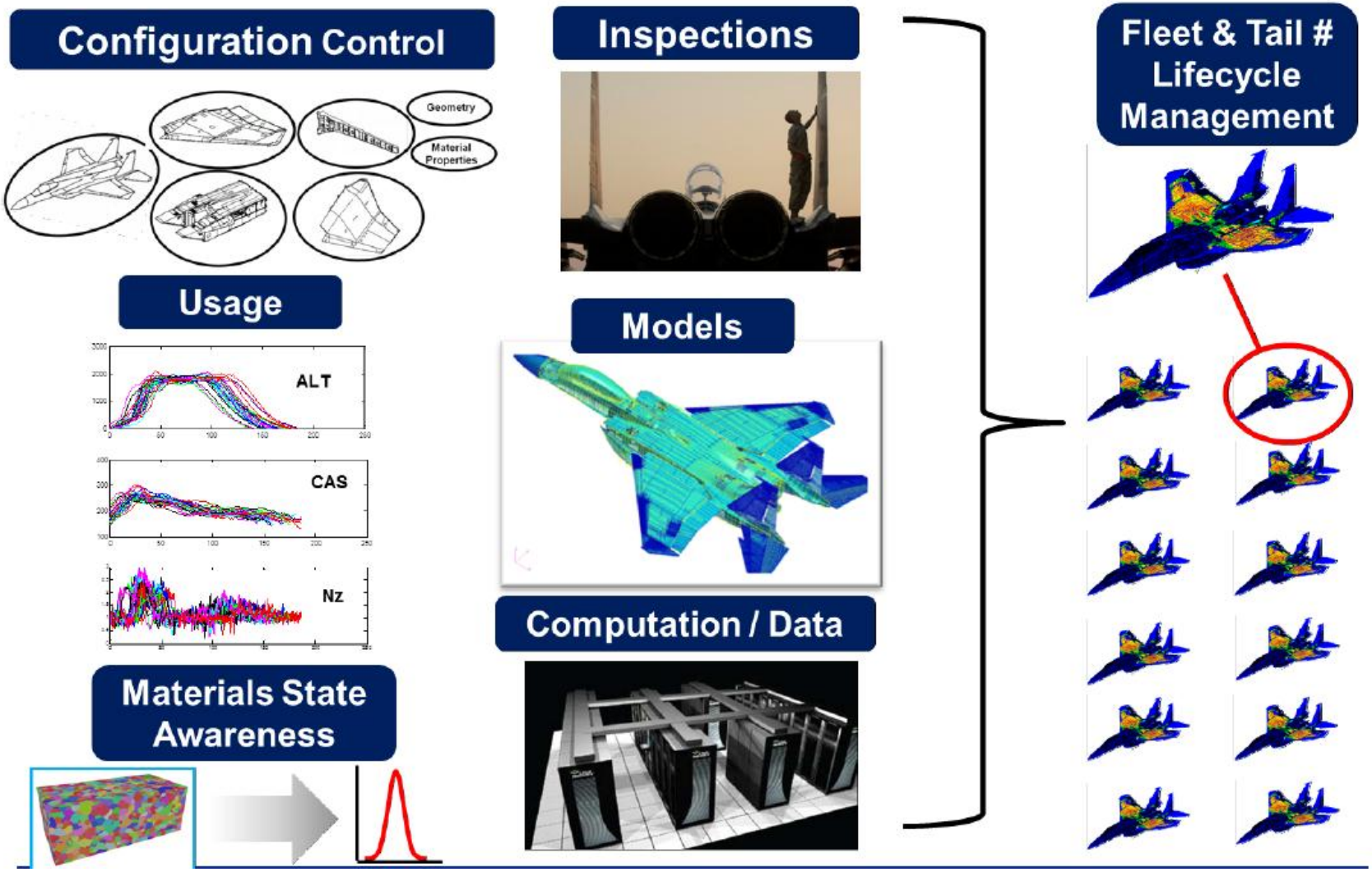
Abstract

Integrated Computational Mate
materials processing, microstruc
scales with an equally complex
who adapt these models rarely
uncertainty, and identify potent
of model applicability is limited
paper we provide a summary o
checklists, an ICME Tool Maturit
employed.

ICME Model Verification and Validation Checklist

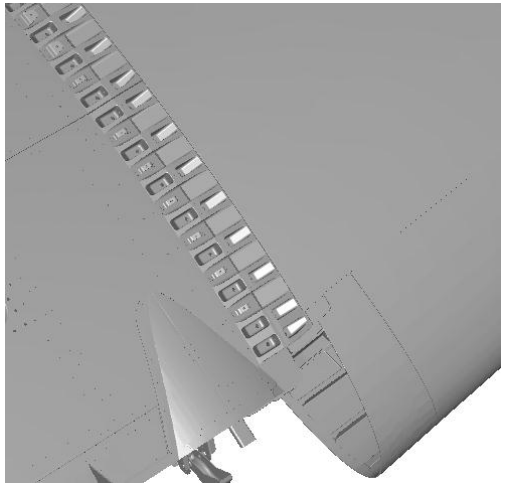
M1: ICME Model Development	• Established detailed modeling approach - Developed mathematical model and initial computational model - Conducted sensitivity studies to assess inputs, internal parameters & BC/ICs - Performed UQ to determine output uncertainty based on inputs uncertainty - Participate in system level uncertainty propagation analysis activities • Established detailed experimental approach to support model development - Established plan to measure internal parameters, inputs, and outputs - Conducted experiments to measure internal parameters, inputs, and outputs - Applied UQ to assess accuracy and variation for experimental results
M2: Experimental Support of Model Development and UQ	• Established experimental approach to support model development & UQ • Determined experimental methods and sources of uncertainty • Experiments conducted and UQ applied to determine uncertainty of results • Assess data and uncertainty in support of system level validation
M3: Model Verification	• Established model verification plan • Identified verification benchmark model and/or data • Checked and executed computational model to identify/fix coding problems • Compared model results against benchmark(s) • Identified and repaired computation model deficiencies
M4: Model Validation	• Established overall validation plan • Defined and executed experimental plan for validation - Analyzed results using UQ methods • Defined and executed modeling plan for validation - Analyzed results using UQ methods • Applied UQ methods to determine model accuracy & range of applicability • Completed activities and support to system level validation

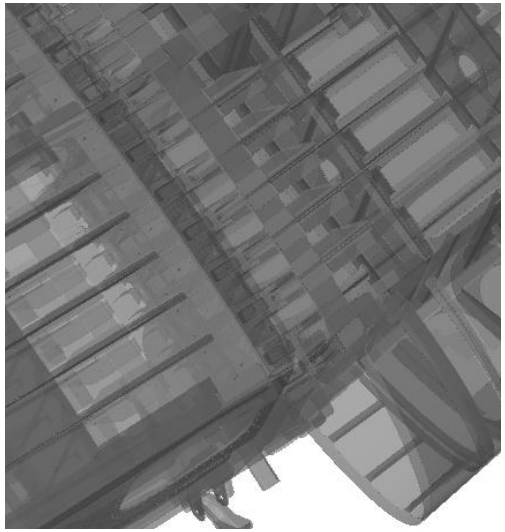
Digital Twin Aircraft



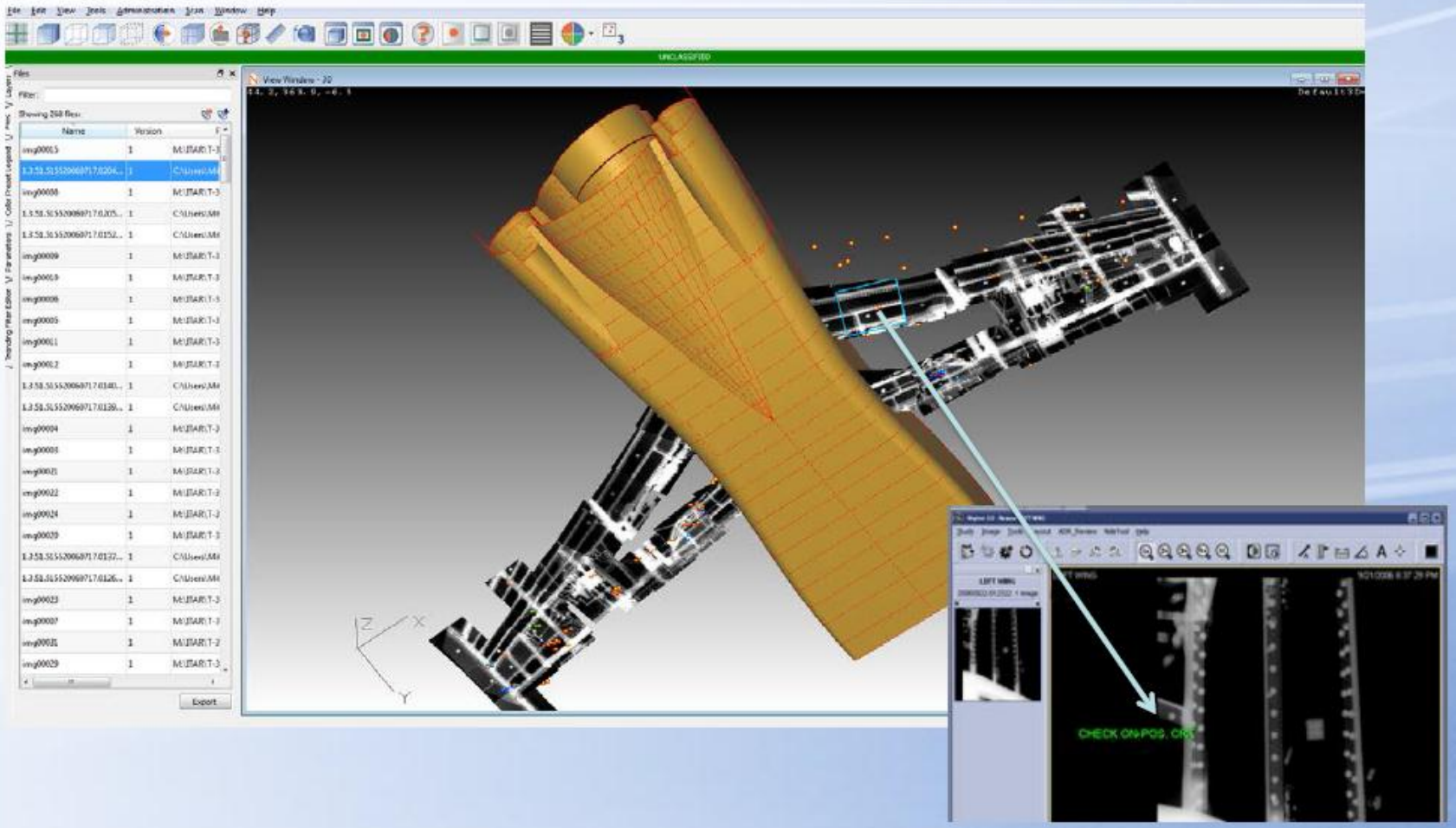
A-10 Current NLign Deployment

- **A-10 NLign current structure for ASIP support**
  - **Full 3D model with part tree**
    - **Basic 3D model functions**
  - **Serialized component tracking**
    - **Component hour tracking for major assemblies**
  - **Analysis support data**
    - **Analysis mapped visually onto 3D model**
      - **Clean metadata with AC (X,Y,Z)**
      - **Supporting documents ‘one-click’ away**
  - **Maintenance inspection data**
  - **Test and Teardown data**
    - **Each crack mapped onto 3D model**
      - **Supporting crack data ‘one-click’ away**
  - **All data verified for quality**





Link Back to NDI Data



Distribution A: Approved for public release; distribution unlimited USAF release number 88ABW-2013-4956, NAVAIR release number SPR-2013-961.

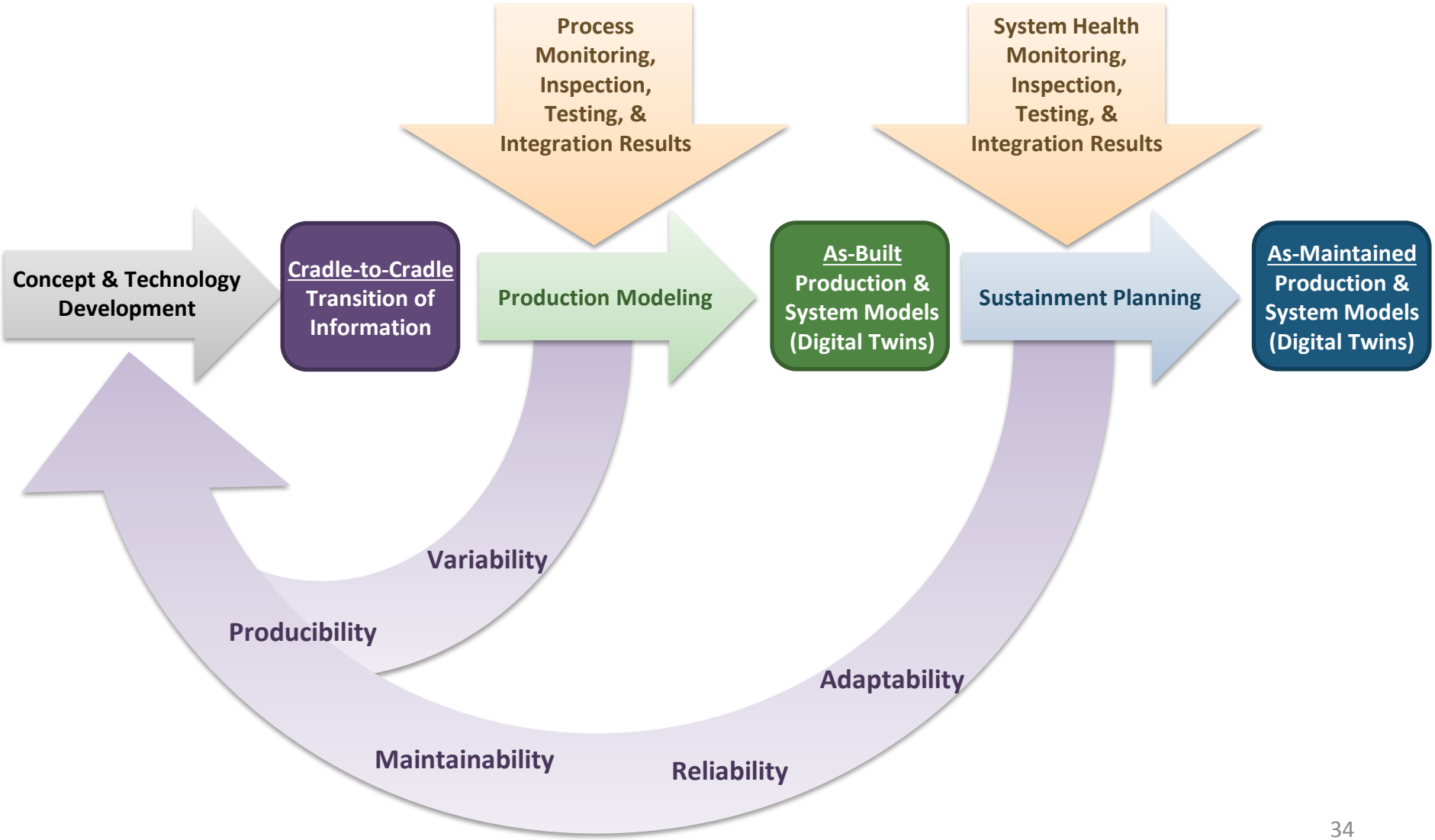
Summary

- Tremendous community-wide challenges and opportunities that require augmented approaches to materials science & engineering to integrate with structural design
- Requires coupling between experiment, computation and data and a seamless link to structural design
- “New” technology gaps defined by integration, VVUQ, high throughput experimentation and computation, data management, reuse and integration, and infrastructure
- MGI & ICMSE will be a long-term commitment to change the way in which we approach materials science and engineering
- Materials, manufacturing, structural design & sustainment all migrating toward the same end point—digitally enabled, integrated engineering

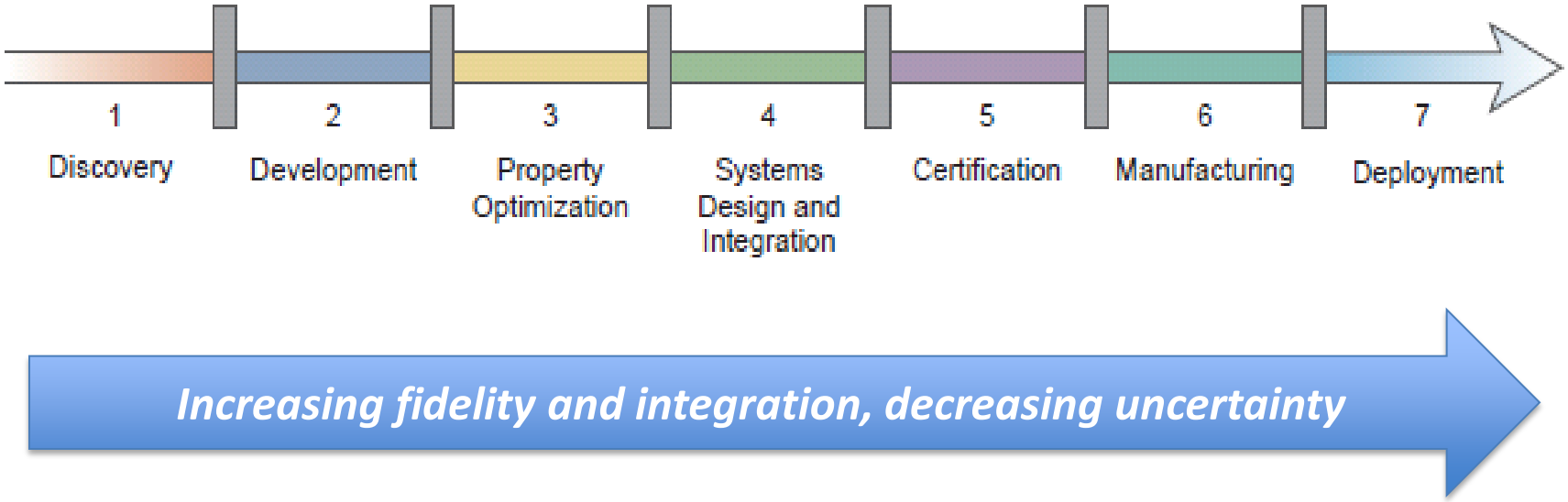
Key Technical Challenges

- **Improved physical understanding and models to relate processing, structure, property and performance of materials**
- **Integration across vast time and length scales, *and with other engineering disciplines***
- ***Application of verification, validation and uncertainty quantification methodologies***
- ***Novel and high throughput experimental techniques***
- ***Acceptance of digital materials data as a valuable research & engineering asset, and standard means of information flow***
- ***A materials information infrastructure to support research and engineering including informatics techniques***

Digital Thread Concept



Progress Toward the Vision

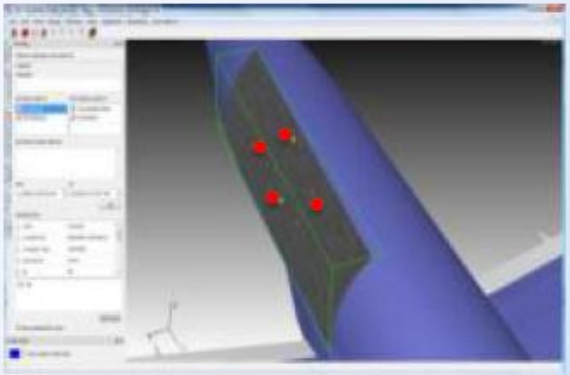


Success depends on your perspective

Software Overview

Collect-Organize-Archive-**Analyze**

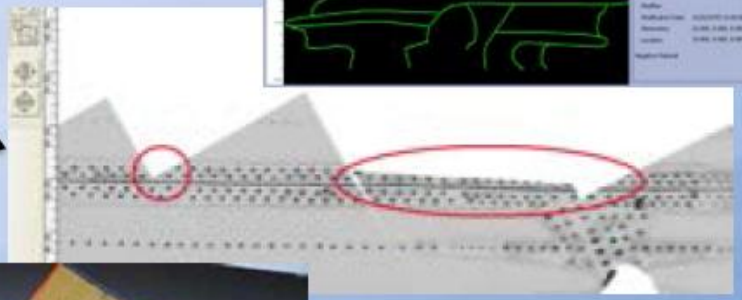
Map ultrasound C-Scan to 3-D model with trending (colored dots) to find problem areas



Map digital radiography to 2-D model with trending and show trending results (colored dots) to identify problem areas

Analyze

- Reporting
- Visualization
- Trending
- Coverage checking
- Analysis integration



Integrated reporting Tools
- Scatter plots
- Histograms
- Bar charts
- Line charts
- Excel Export

Map eddy current C-scan to model to check for inspection coverage

Repair design tool shows multiple layers of data

Distribution A: Approved for public release; USAF 88ABW-2013-4956, NAVAIR SPR-2013-961.