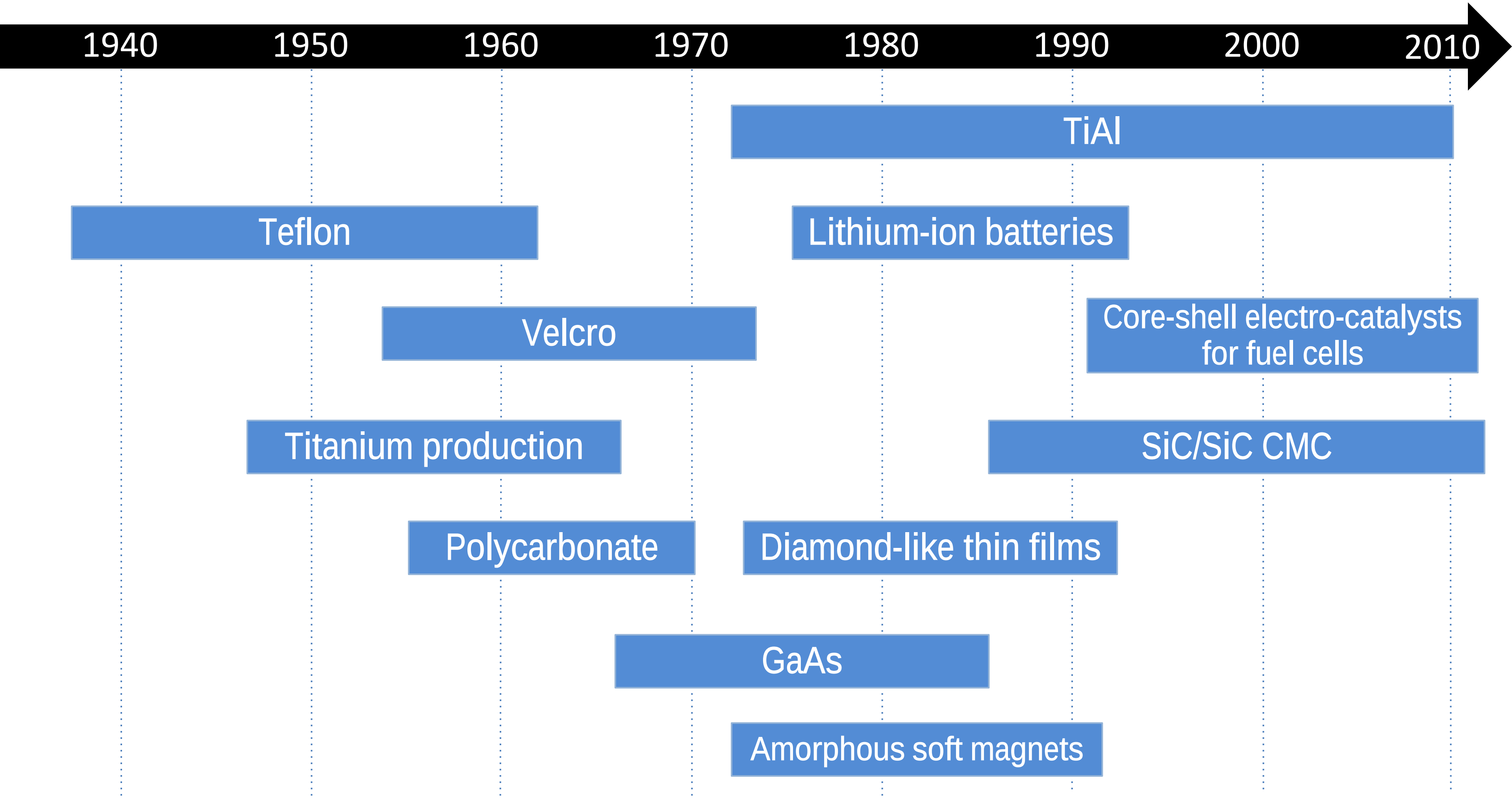
# Creating a Materials Innovation Infrastructure

**Charles Ward**
**Matthew Jacobsen**
**Materials & Manufacturing Directorate**

***Integrity ★ Service ★ Excellence***

# A long lag from discovery to application of new materials…




After Gerd Ceder (MIT); materials information from T. W. Eagar and M. King, Technology Review 98 (2), 42 (1995).
Catalysis information from R. Schrock et al. and R. Adzic et al.

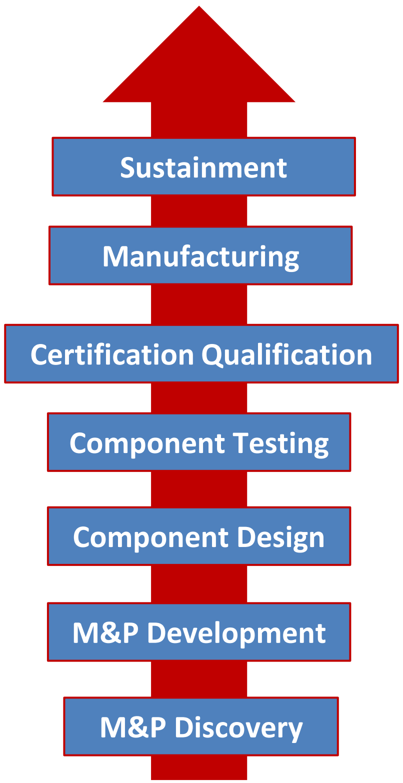
# Integrated Computational Materials Science and Engineering (ICSME)*Materials Genome Initiative*


***"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)**

- ICMSE is 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***

# Changing the Materials Life Cycle





**PAST**

Sequential
Qualitative
Empirical
*Ad Hoc*
Fragmented Data (in a drawer)
Disjoint Processes

**FUTURE**

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

# Elements of the Materials Innovation Infrastructure *Materials Genome Initiative*

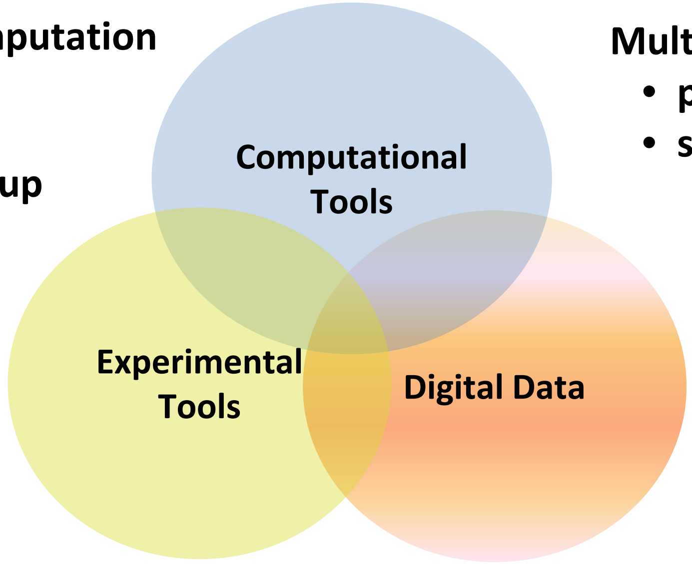
Materials discovery - first principles and atomistics

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

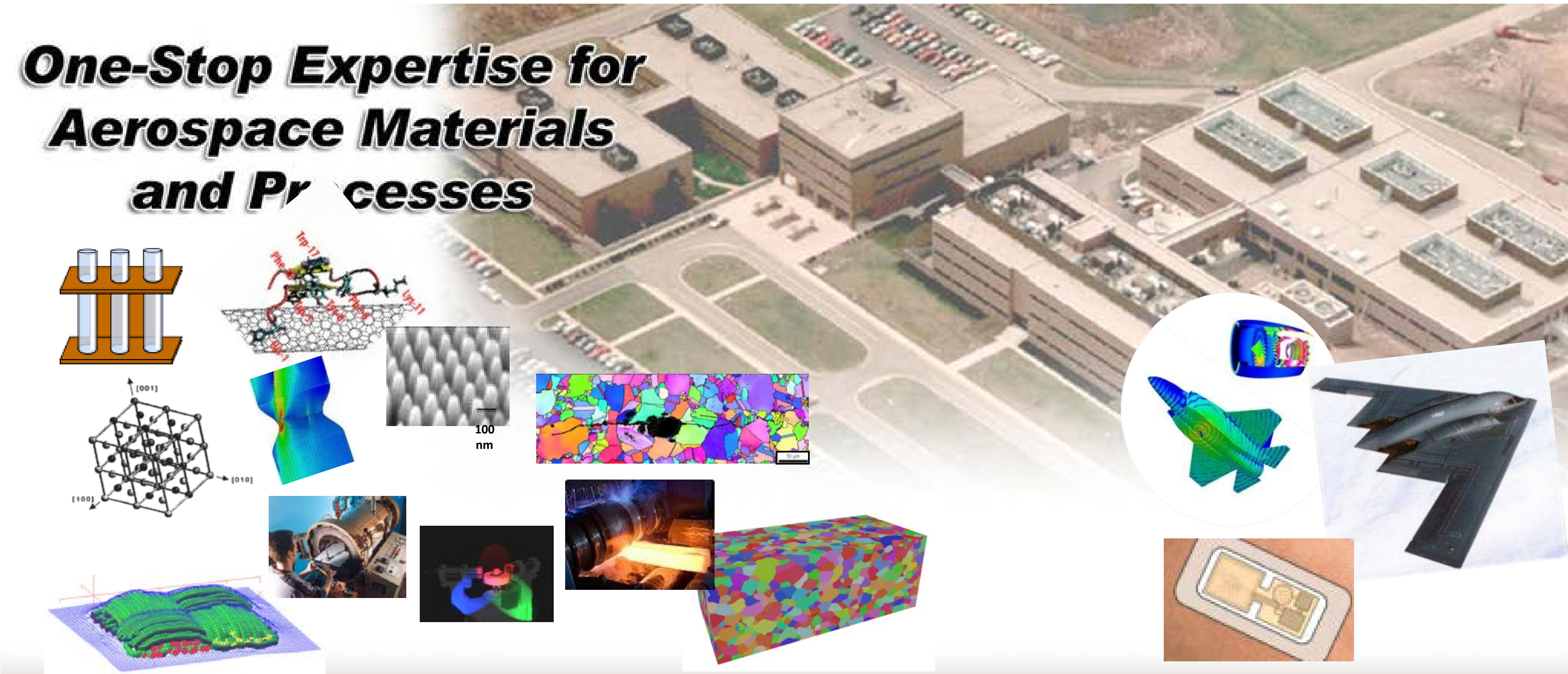
Materials characterization and microstructure representation

Systems design and MDO
- Design exploration
- Detail design

**Distributed collaborative networks**

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

# Air Force Research Laboratory
# Materials and Manufacturing Directorate




**A full spectrum materials & manufacturing organization:**

**Metals / Ceramics / Composites / NDE / Semiconductors / Polymers / Photonic Materials / Biomaterials**

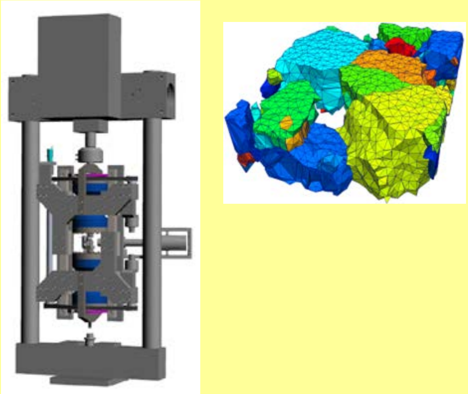
**Structural / Propulsion / Weapons / Sensors / Survivability Applications**

**Discover... Design... Manufacture... Transition... Support**

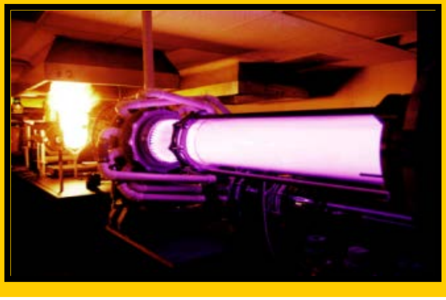
# Materials and Manufacturing *Research Infrastructure*

- **700+ scientists and engineers**
- **108,000 sq ft lab space, 200 lab modules**
- **750+ computers associated with research equipment**
- **1000+ computers on desks: 2 separate networks**
- **80+ scientific and engineering software packages**
- **Local computational clusters & remote HPC**

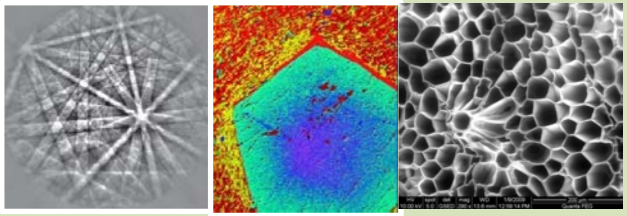
**High Energy Diffraction Microscopy**



**Sensor Survivability / Laser Hardened Materials Evaluation Laboratory**

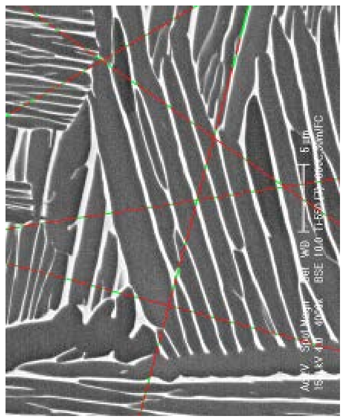


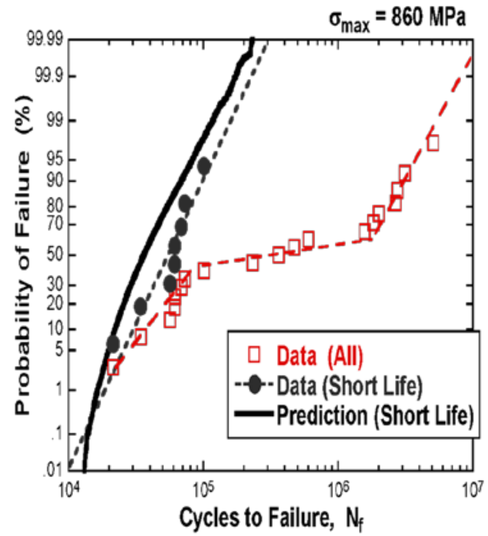
**Materials Characterization Facility**



***And no supporting collaborative research environment***

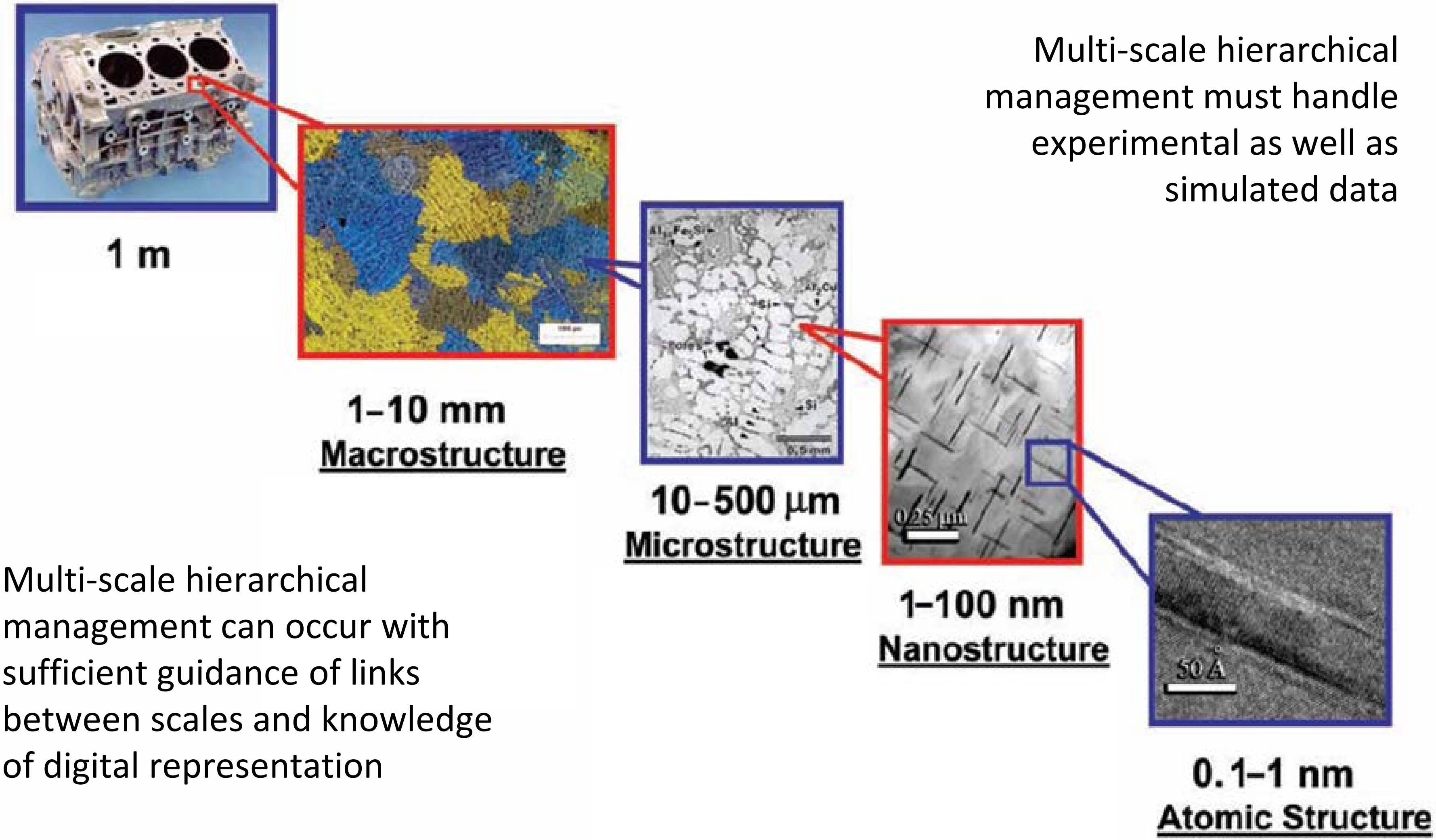
# The Materials Science & Engineering Paradigm






**Processing** → **Microstructure** → **Properties** → **Performance**

# Enabling Multi-Scale Management




Multi-scale hierarchical management must handle experimental as well as simulated data

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

***Computational management tools for structure hierarchy do not exist today***

# Integrated Computational Methods for Composite Materials (ICM2) *Foundational Engineering Problem*

**ICM2 aims to demonstrate . . .**

- Application and integration of material and process models into the product design cycle
- How integrated models can be used within a digital framework to reduce risk and testing requirements as a program moves to full scale testing

GE Aviation

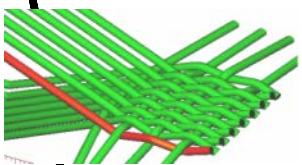
LOCKHEED MARTIN

AUTODESK.

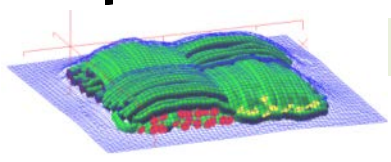
CONVERGENT

MICHIGAN

UDRI



Virtual weaving

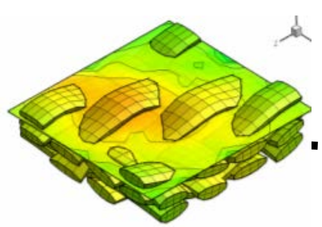


Virtual forming

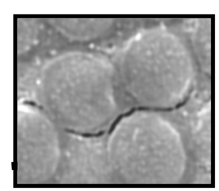
Process modeling

Residual stress/tool part interaction

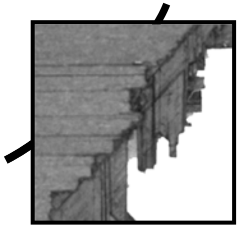
As-manufactured quality



Damage Modeling

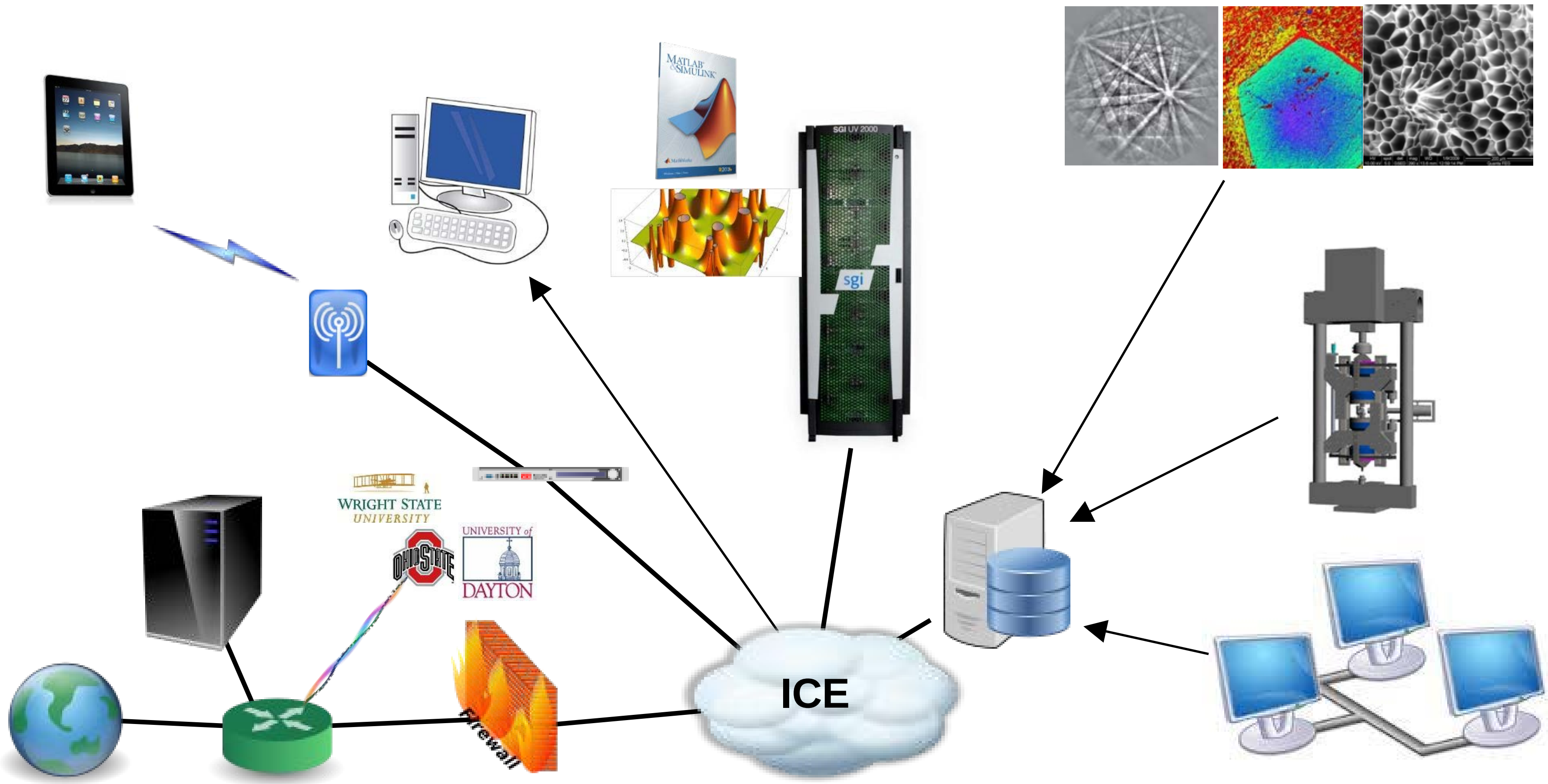


Strength Prediction

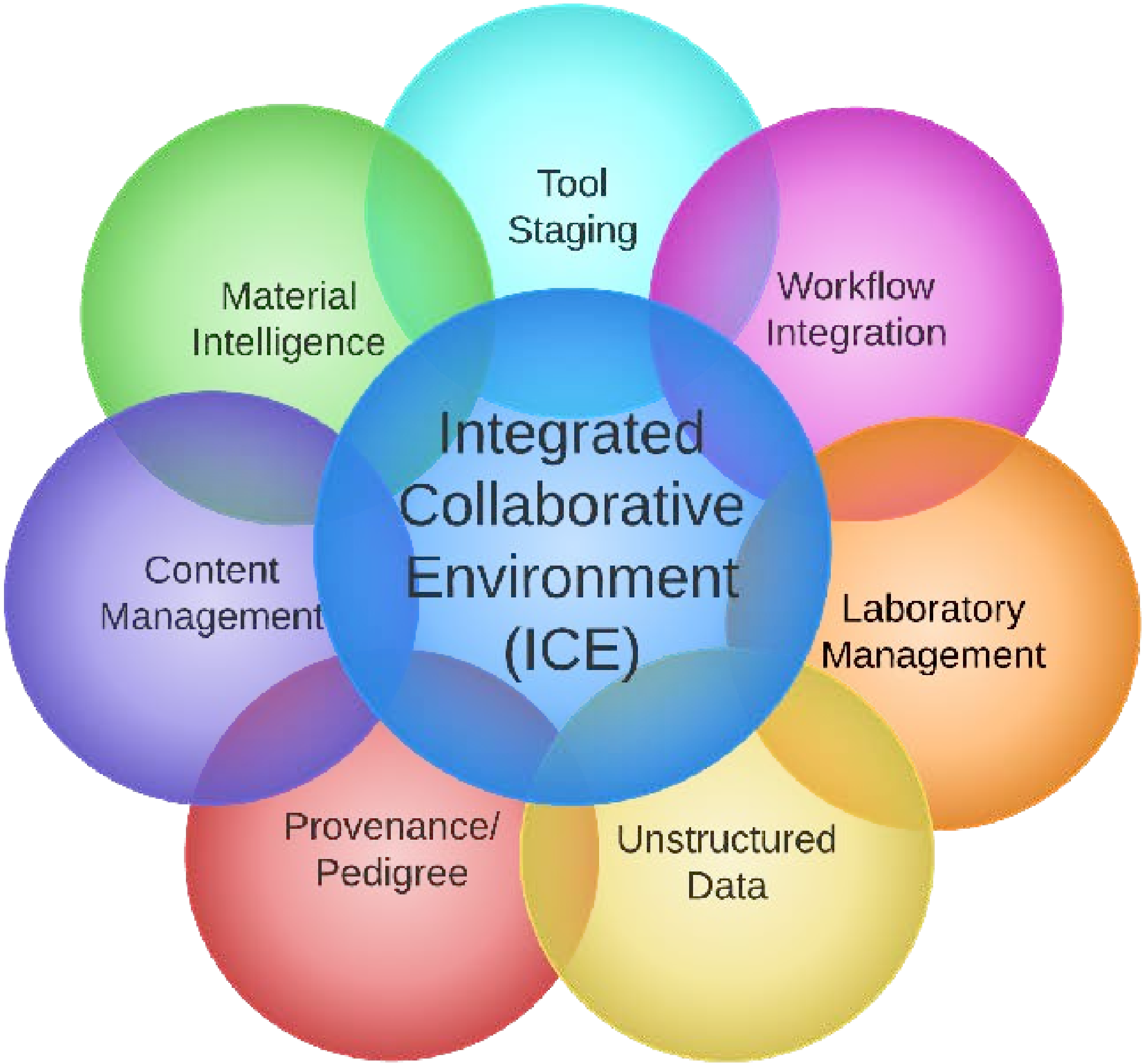


# Integrated Collaborative Environment

+ Able to support ICMSE toolsets



# ICE Context - Addressing ICMSE Needs

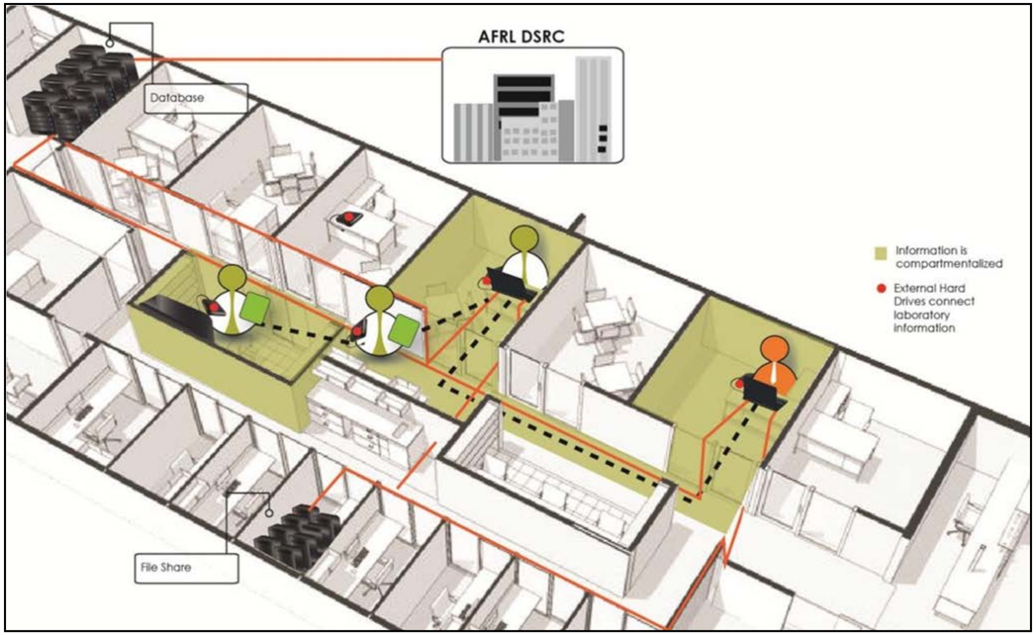


# Problem Scope

Gaps in all research deliverable attributes result in increased cost and lead time for warfighter capabilities

Symptoms:

- Data loss/inaccuracies
- Duplication of effort
- Increased process lead times
- Wasted manpower




- Non-regulated, disorganized and outdated methods and systems

# Problem Scope - Drivers

- Autonomously defined laboratory management solutions


- Reliance on legacy/insufficient tools and communication channels (the usual suspects)
- Disconnected solution development results in a lack of interoperability
- Lack of cross-functional expertise between software development and engineering

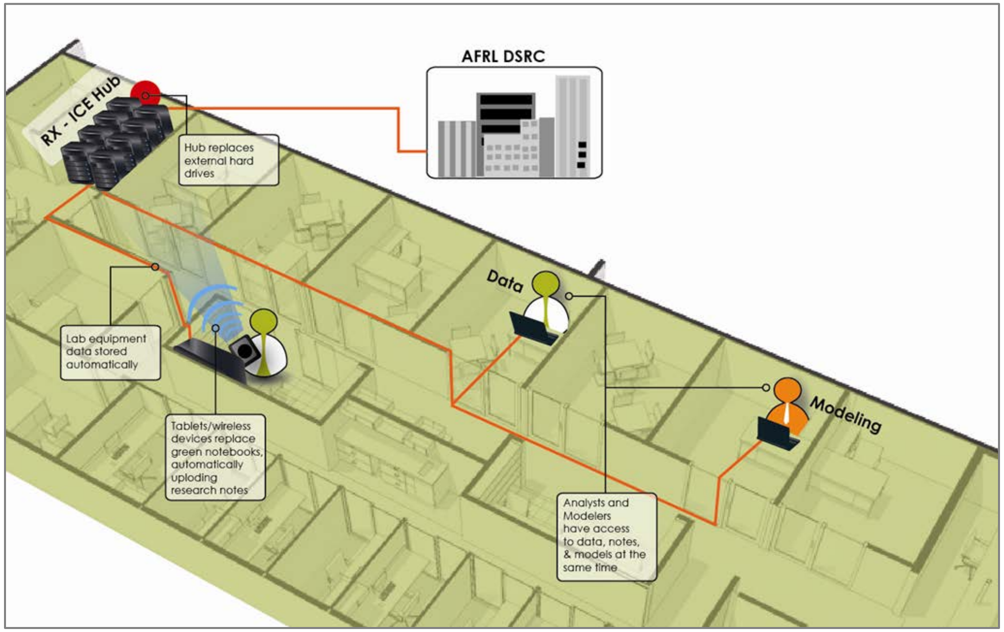
# Solution:
# Integrated Collaborative Environment (ICE)

- ICE must serve as the backbone of major ICMSE initiatives.
- ICE is/will be a federated, centralized, enterprise data management system.


- ICE will serve the S&E community, which includes management, modelers, experimenters, and support staff, with a reliable lab and data management solution.
- ICE will be developed in a partnership between the S&E community and in-house software development resources.

# ICE-Enabled Capabilities

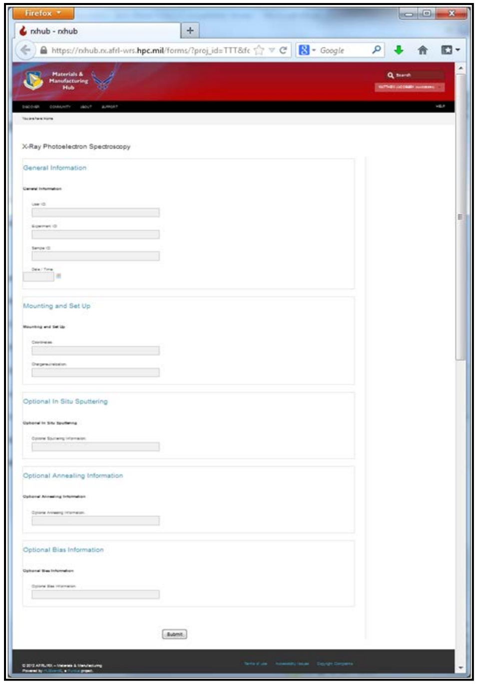
- The coordination and management of research activities
- The collection of research data (structured and unstructured)




- Complete traceability of material evolution
- Autonomous data sources to continue to exist in many cases
- Growth of the RX ICMSE culture

# Project Objectives

- Convert 90% of existing paper methods of to digital formats.



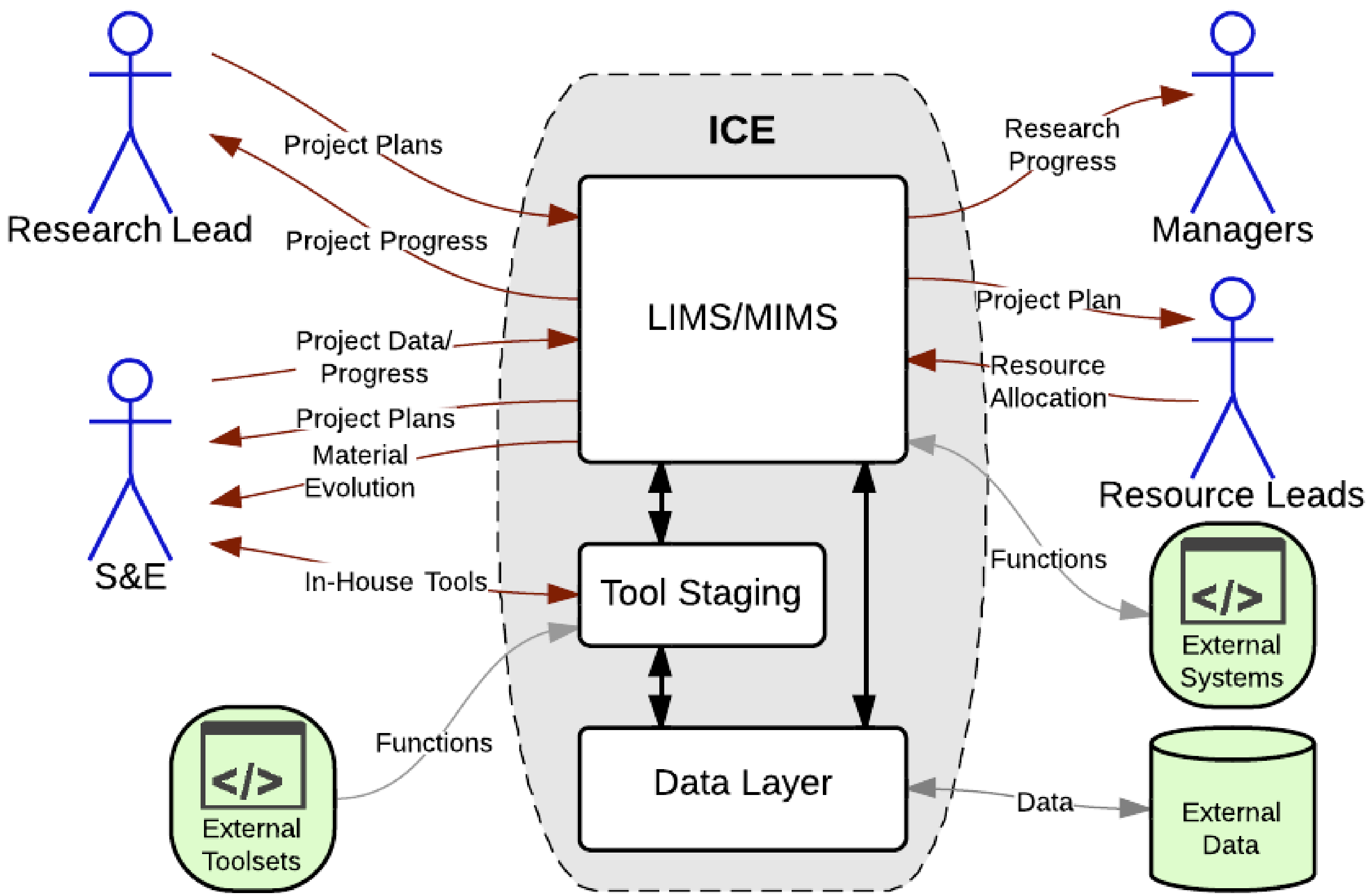

- Achieve 100% connectivity and data sharing between the all existing research data networks and data repositories (file servers, etc).

- Connect 90% of non-networked experimental equipment to at least one of the existing research data networks.

- Reduce the data management workload on the S&E from 40% FTE to 10% FTE.

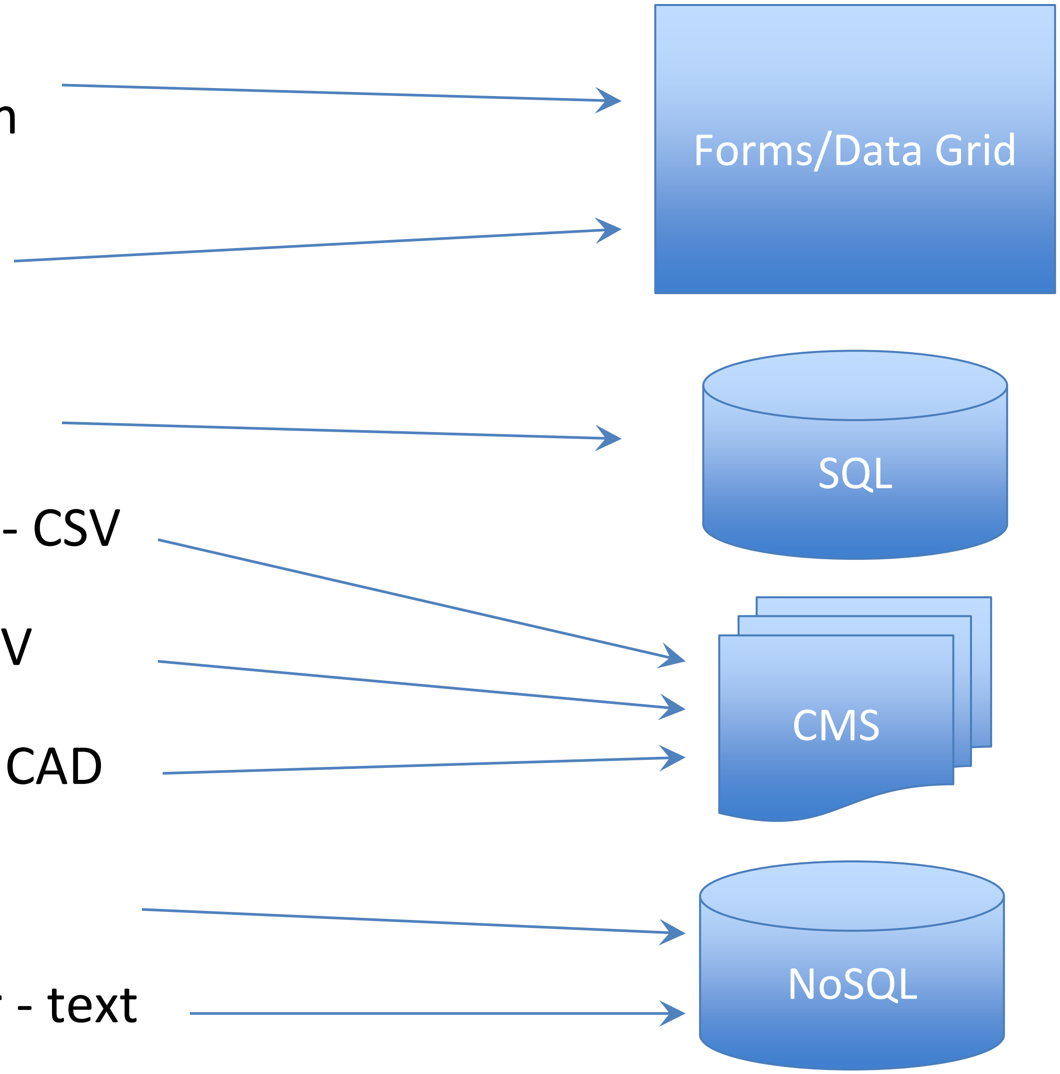
# System Context

The context diagram illustrates high-level actor behaviors in the proposed system.



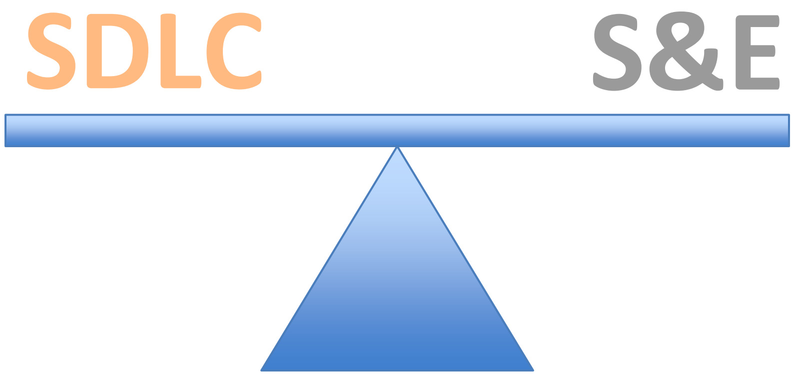
# Example Process Elements

- Process Monitor –
  Excel Dashboard/Plan
- Test Monitor –
  Excel Dashboard
- Process Metadata
- Mold Configurations - CSV
- Process run data - CSV
- Casting model files – CAD
- Process Sheets - text
- Notes from Operator - text



# Challenges

- Preserve the autonomy of the research process
- Enhance existing processes with data-centric behaviors
- Provide easy to use community tools to organic teams of S&Es




- In short, **balancing** the **conflicting needs** of insuring long term viability by utilizing software design best practices, with immediacy of user needs for simple, flexible, autonomous and secure information management.

# The Hub in AFRL *Initial Impressions*

- Excellent representation of the organization with groups
- A wide array of options for project teams (files, wikis, tasks, etc)
- Joomla!/Hub framework appeared to reduce re-work for routine customization tasks
- Workspaces/Rappture provided unprecedented capability

# The Hub in AFRL *Strengths*

- Tool staging requirements can be met with workspaces and Rappture
- Groups/Projects can be used to represent the vast majority of the RX organization
- File management capabilities are superb

# The Hub in AFRL*Considerations*

- Dynamic data collection for pedigree development and workflow management would add value for a research organization like RX

- De-coupled ‘proper’ Hub and database groups presents challenges for naturally linking projects and associated meta-data

- Organizations with in-house development capability will benefit from close communications with other Hub developers, including lessons learned (workflow development, template based views, etc)

# Opportunities*Outstanding needs*

- Customizable, light-weight tool staging (de-coupled workspaces/Rappture model)
- Data linkage between tool staging and ICE (ensuring provenance)

# Summary

- A viable Materials Innovation Infrastructure—both globally and locally--is essential to providing predictive and quantitative tools in materials science and engineering
- Experiment and computation must work together more synergistically: requires a collaborative research environment
- The breadth of materials classes, their complexity and their applications and need for integration with other engineering disciplines provides a complex challenge
- Any component of a Materials Innovation Infrastructure must be flexible, adaptable and extensible