Creating a Materials Innovation Infrastructure

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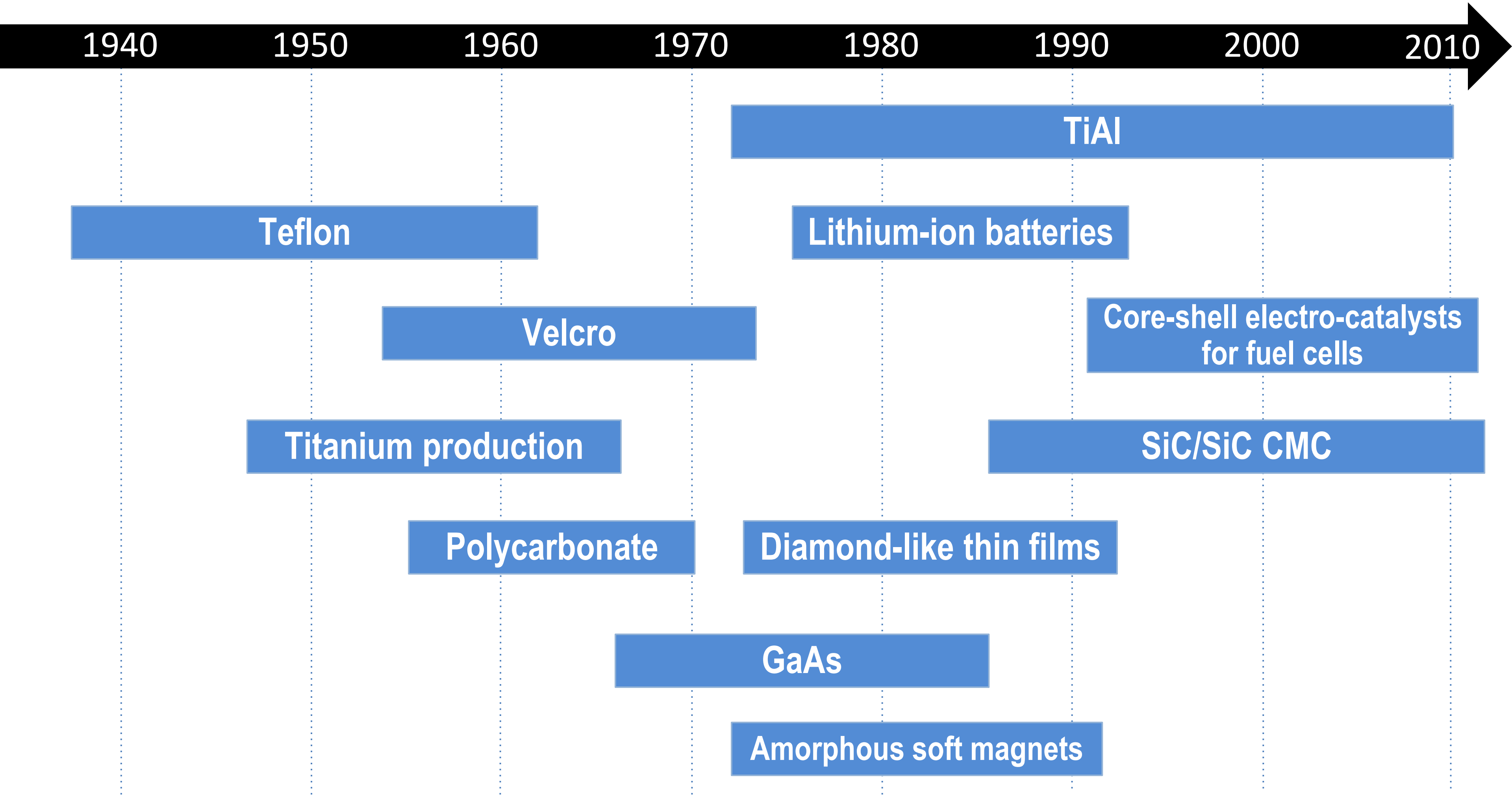
Integrity ★ Service ★ Excellence

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.

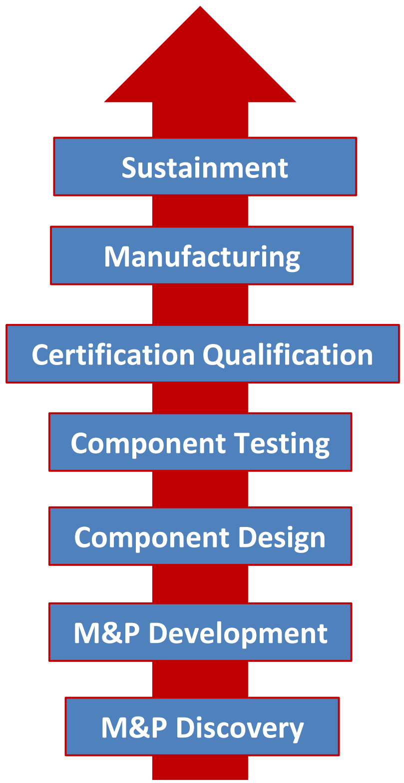
Integrated Computational Materials Science and Engineering (ICSME)*Materials Genome Initiative*

"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*

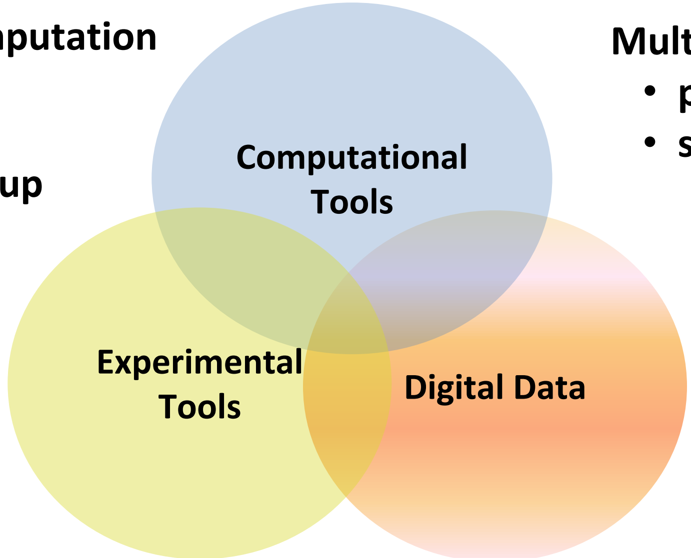
Materials discovery - first principles and atomistics

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

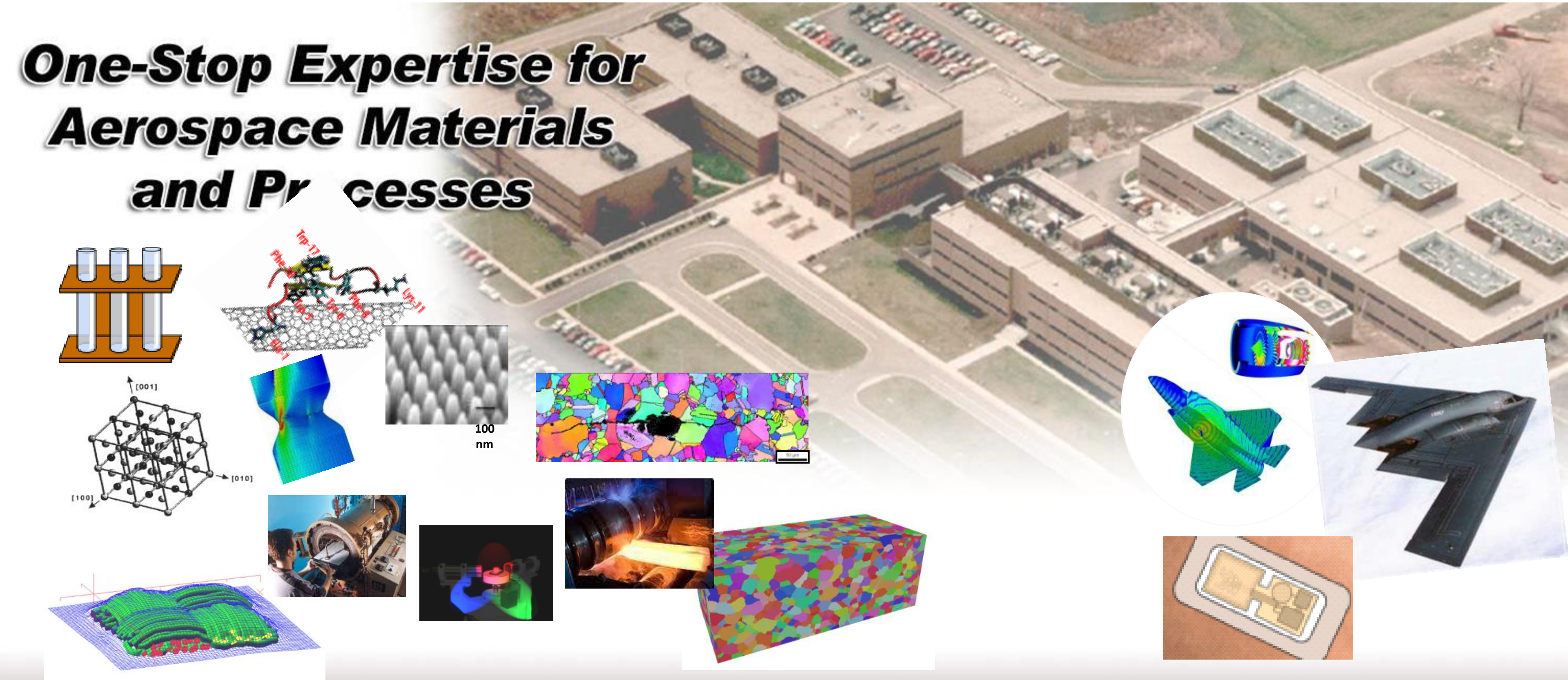
Materials characterization and microstructure representation

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

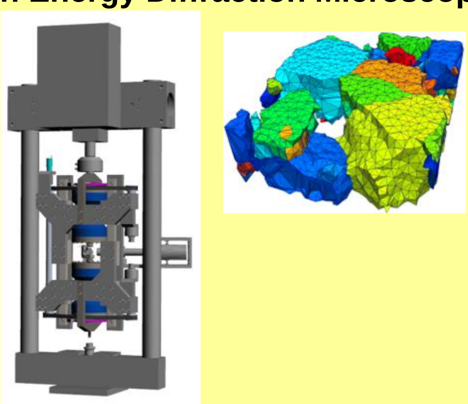
Structural / Propulsion / Weapons / Sensors / Survivability Applications

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

Materials and Manufacturing *Research Infrastructure*

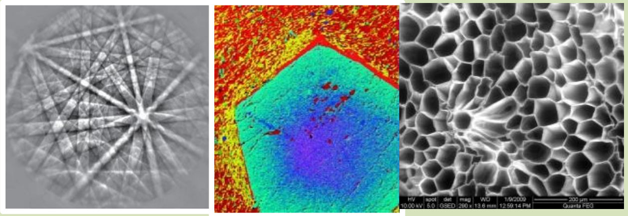
- 700+ scientists and engineers
- 108,000 sq ft lab space, 200 lab modules
- 750+ computers associated with research equipment
- 1000+ computers on desks: 2 separate networks
- 80+ scientific and engineering software packages
- Local computational clusters & remote HPC

High Energy Diffraction Microscopy



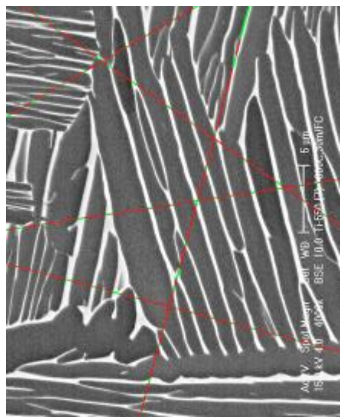
Sensor Survivability / Laser Hardened Materials Evaluation Laboratory

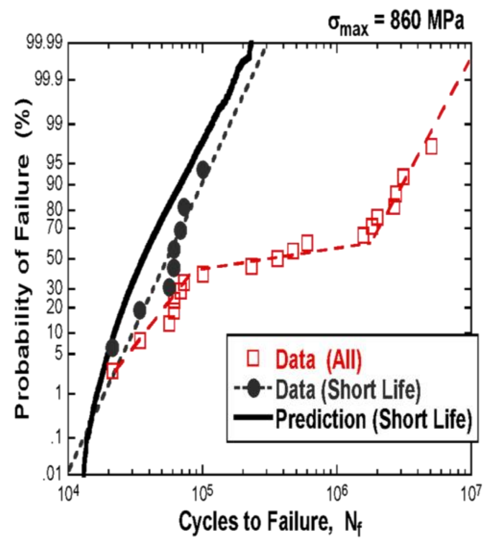
Materials Characterization Facility



And no supporting collaborative research environment

The Materials Science & Engineering Paradigm

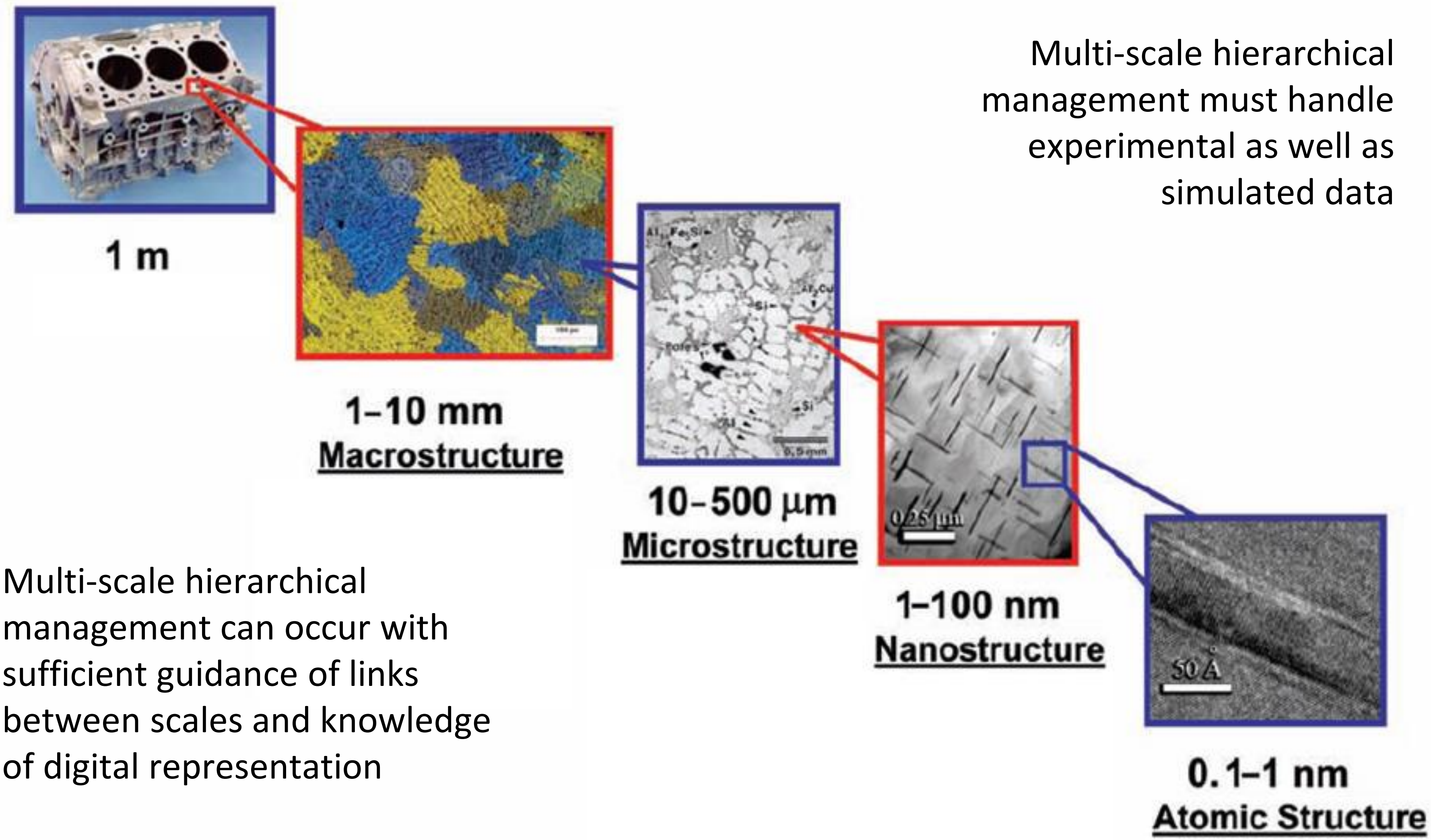




Processing → **Microstructure** → **Properties** → **Performance**

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

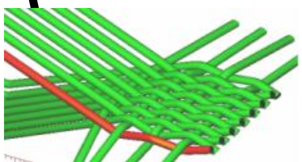
Computational management tools for structure hierarchy do not exist today

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

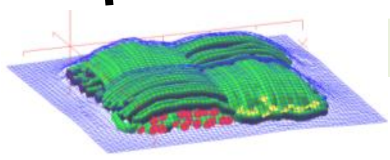
ICM2 aims to demonstrate . . .

- 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

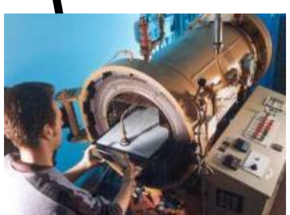


Virtual weaving



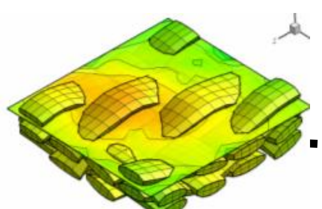
Virtual forming

Process modeling

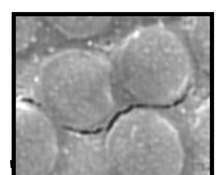


Residual stress/tool part interaction

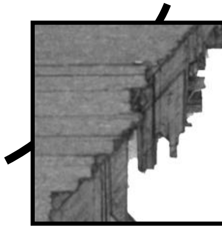
As-manufactured quality



Damage Modeling

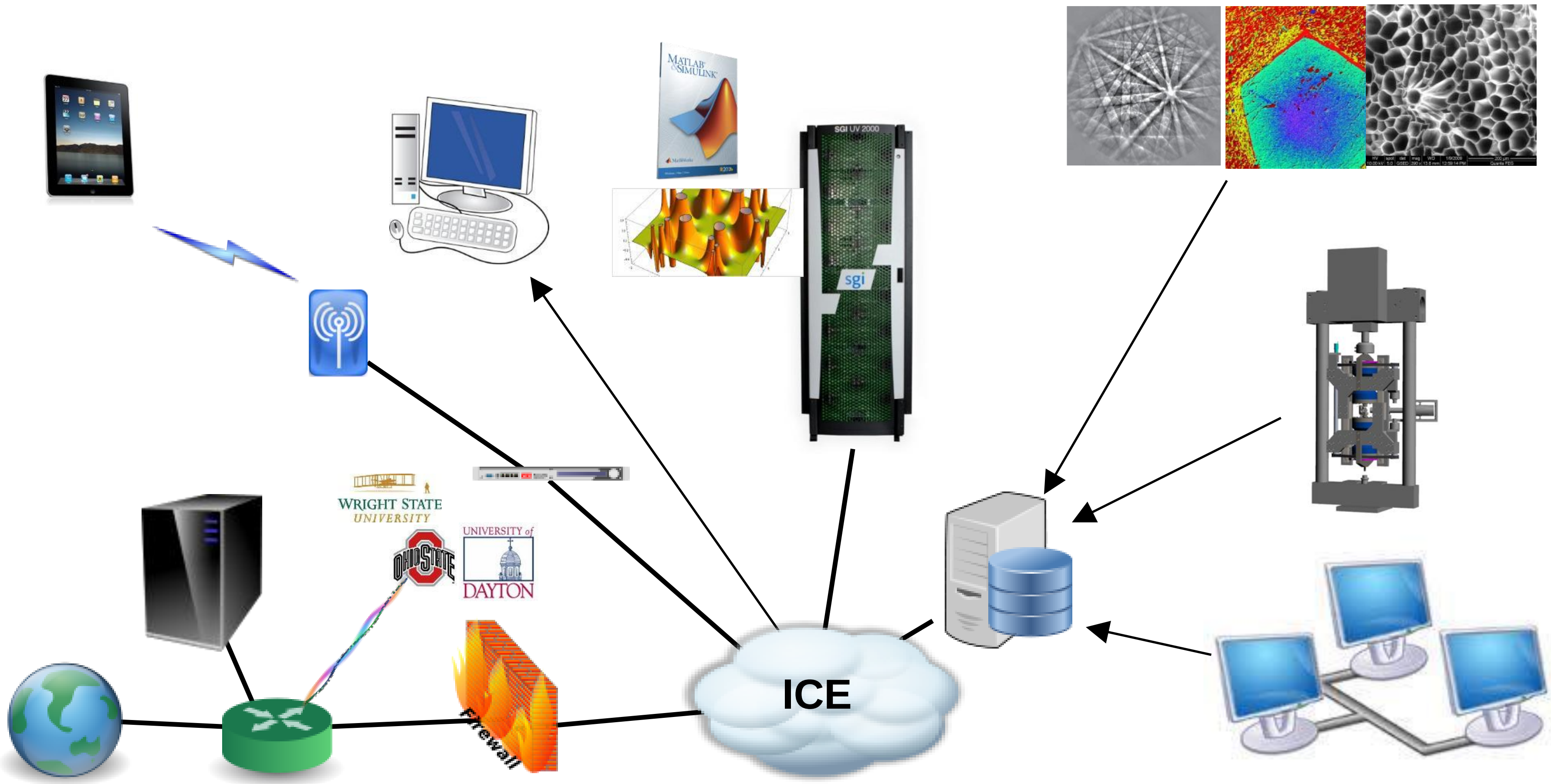


Strength Prediction

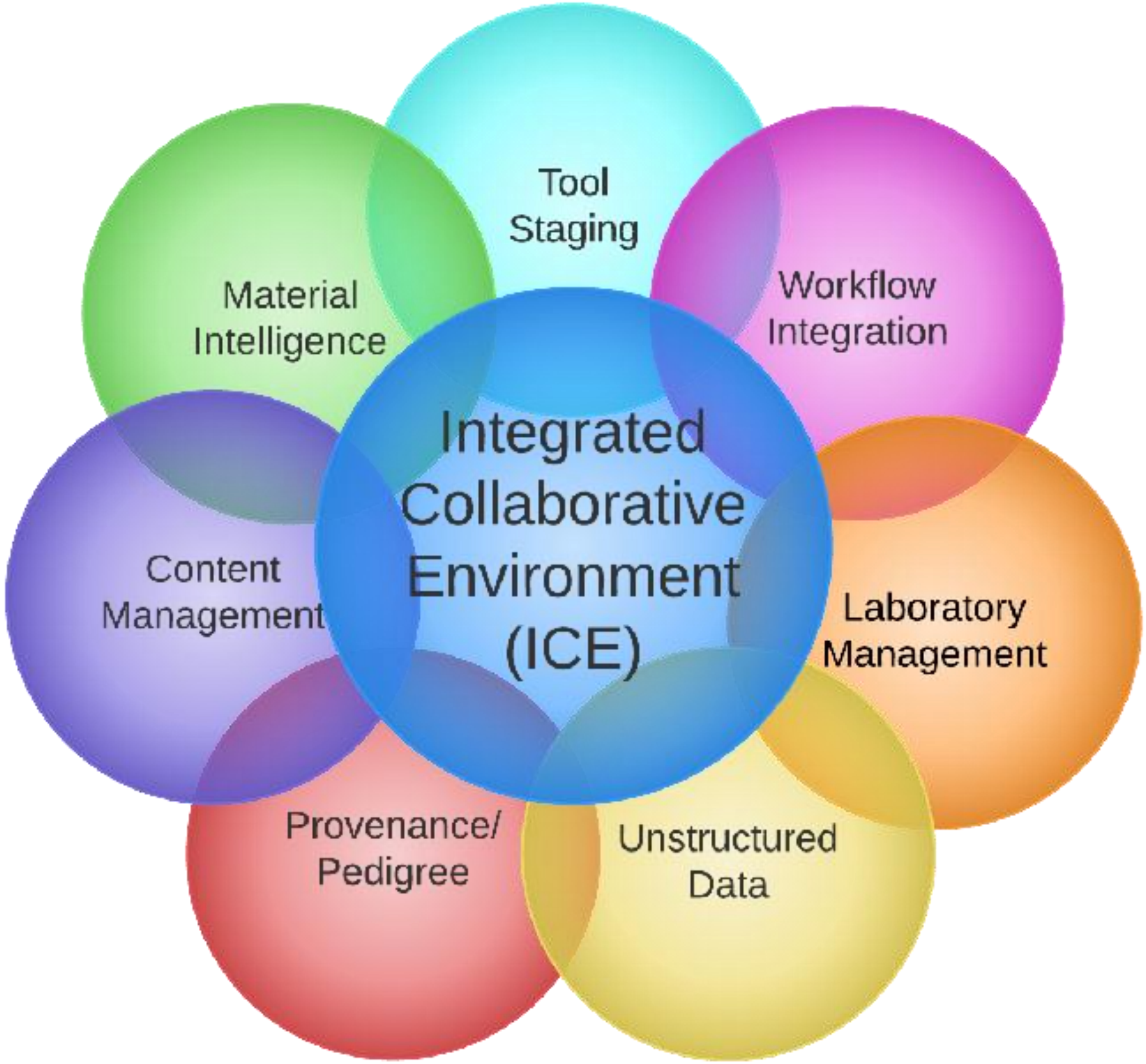


Integrated Collaborative Environment

+ Able to support ICMSE toolsets



ICE Context - Addressing ICMSE Needs

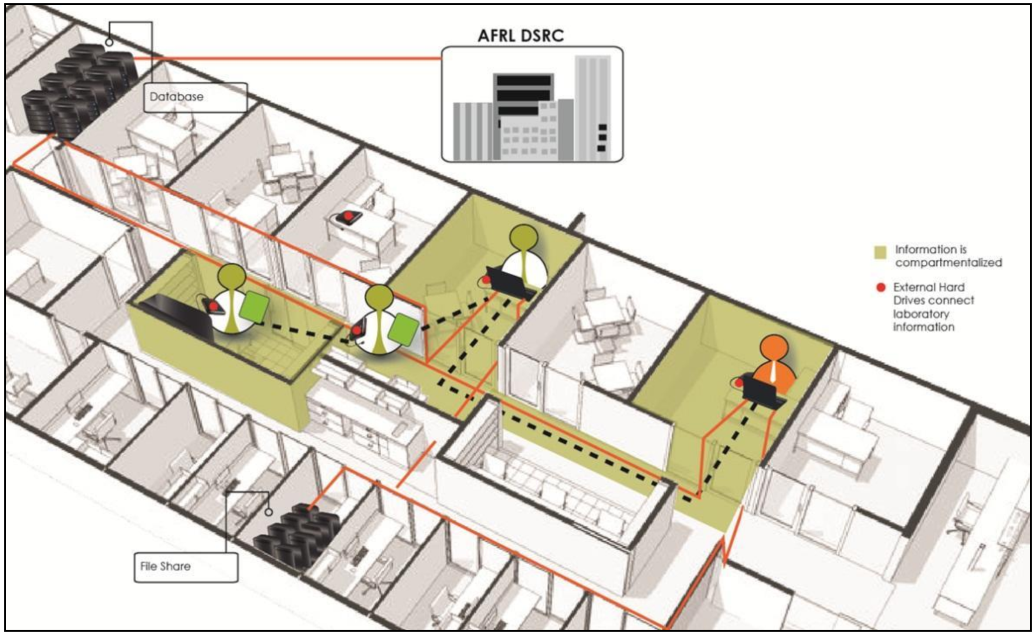


Problem Scope

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

- <u>Autonomously</u> 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.

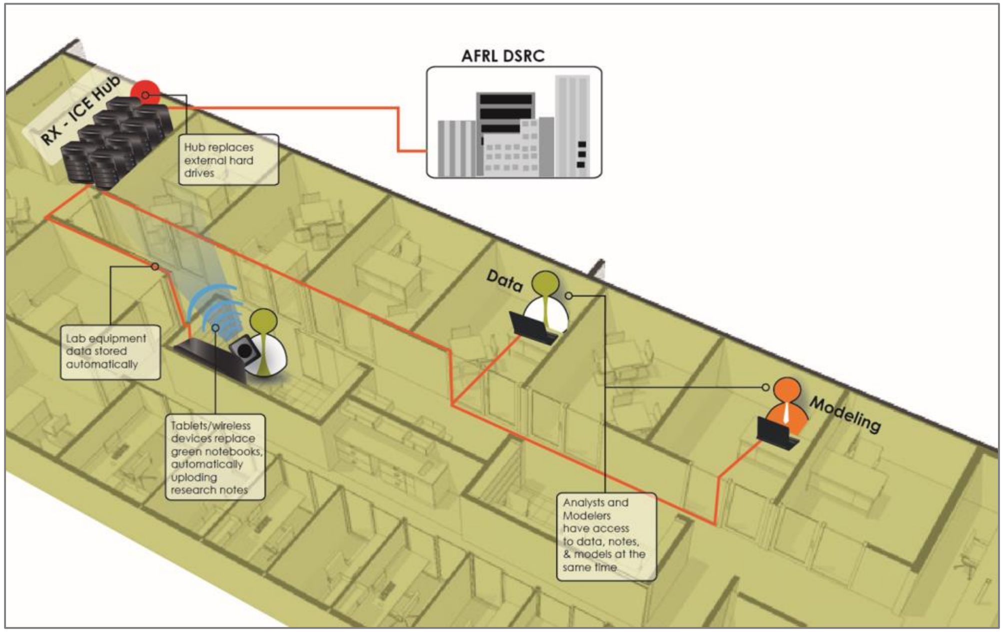
- ICE is/will be a federated, centralized, enterprise data management system.

- 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

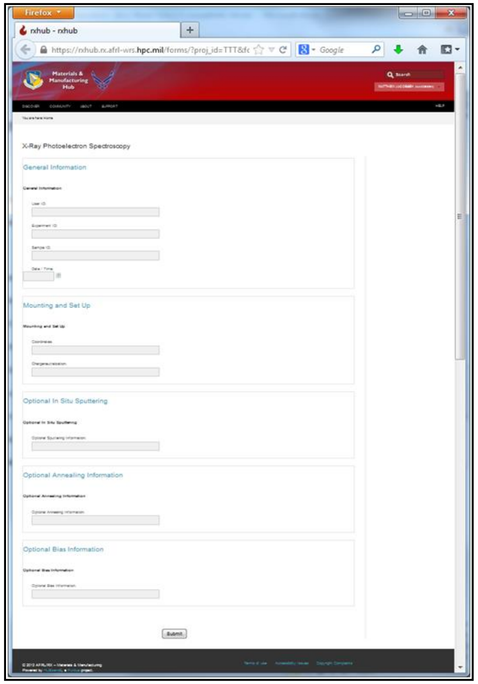
- The coordination and management of research activities
- The collection of research data (structured and unstructured)



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

Project Objectives

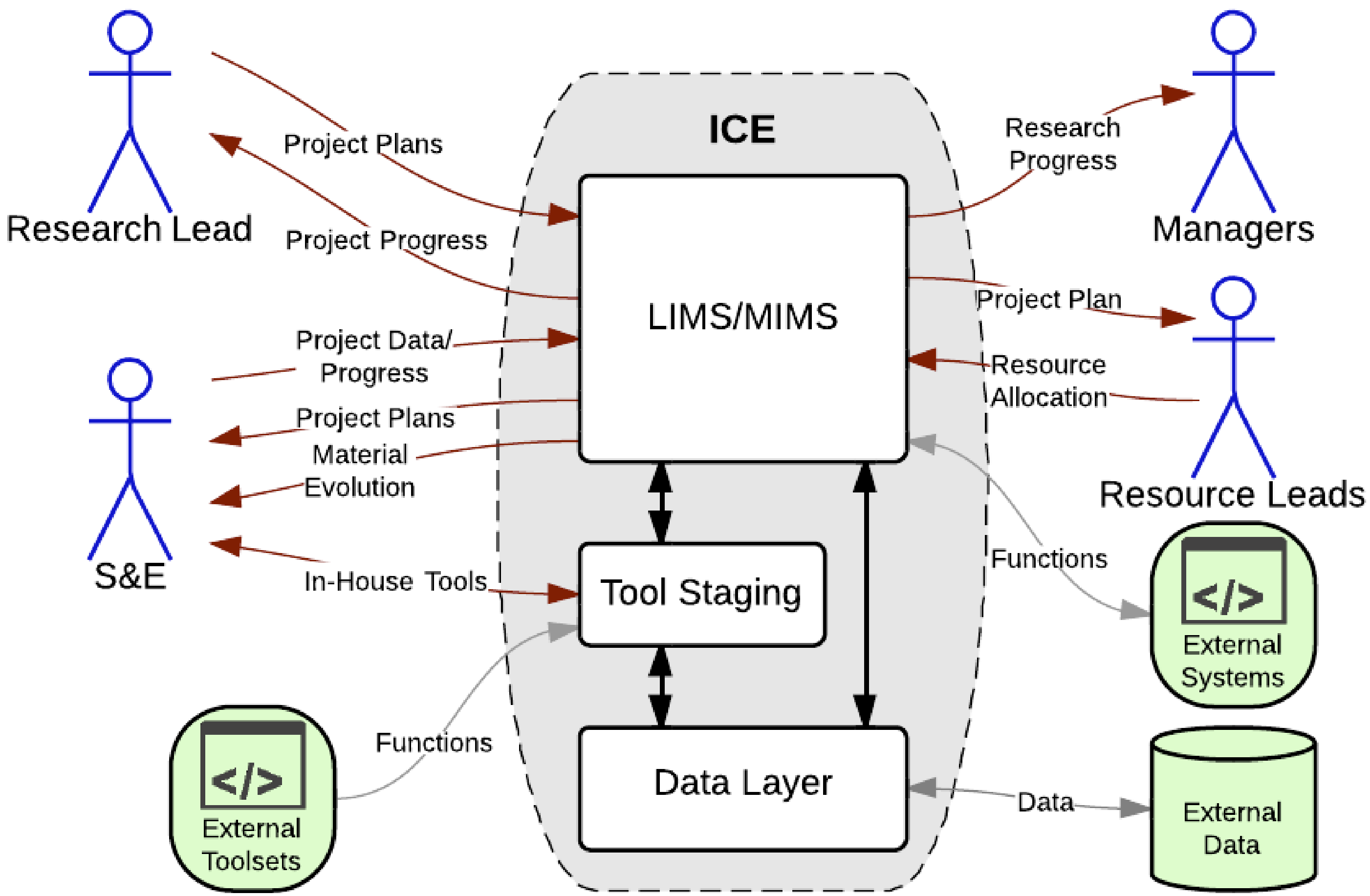
- Convert 90% of existing paper methods of to digital formats.



- 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.

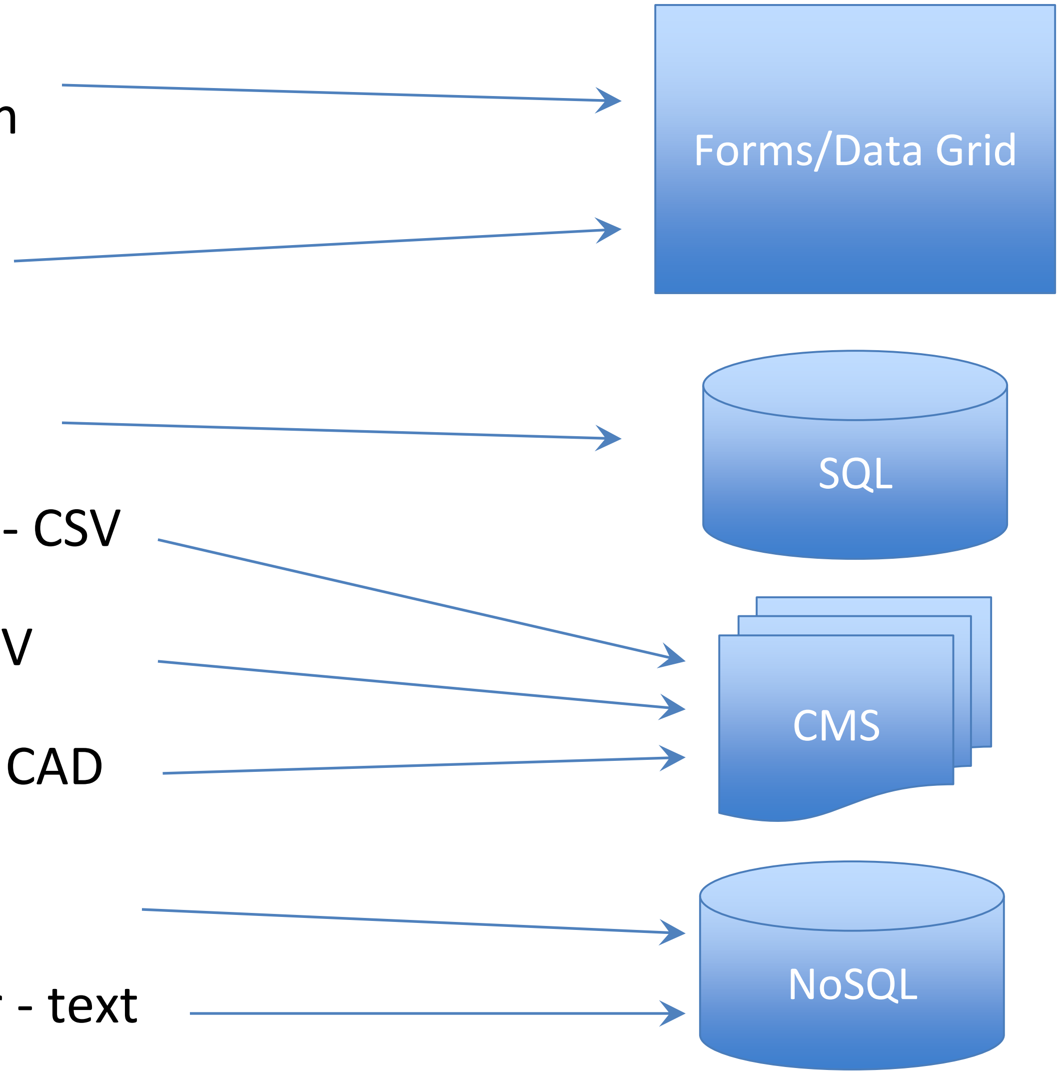
System Context

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



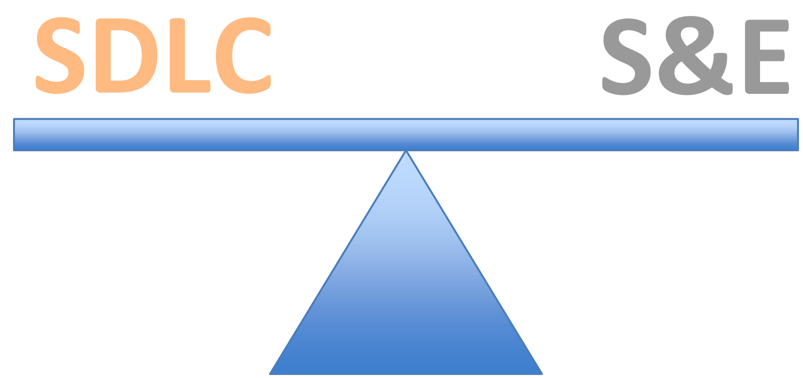
Example Process Elements

- 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

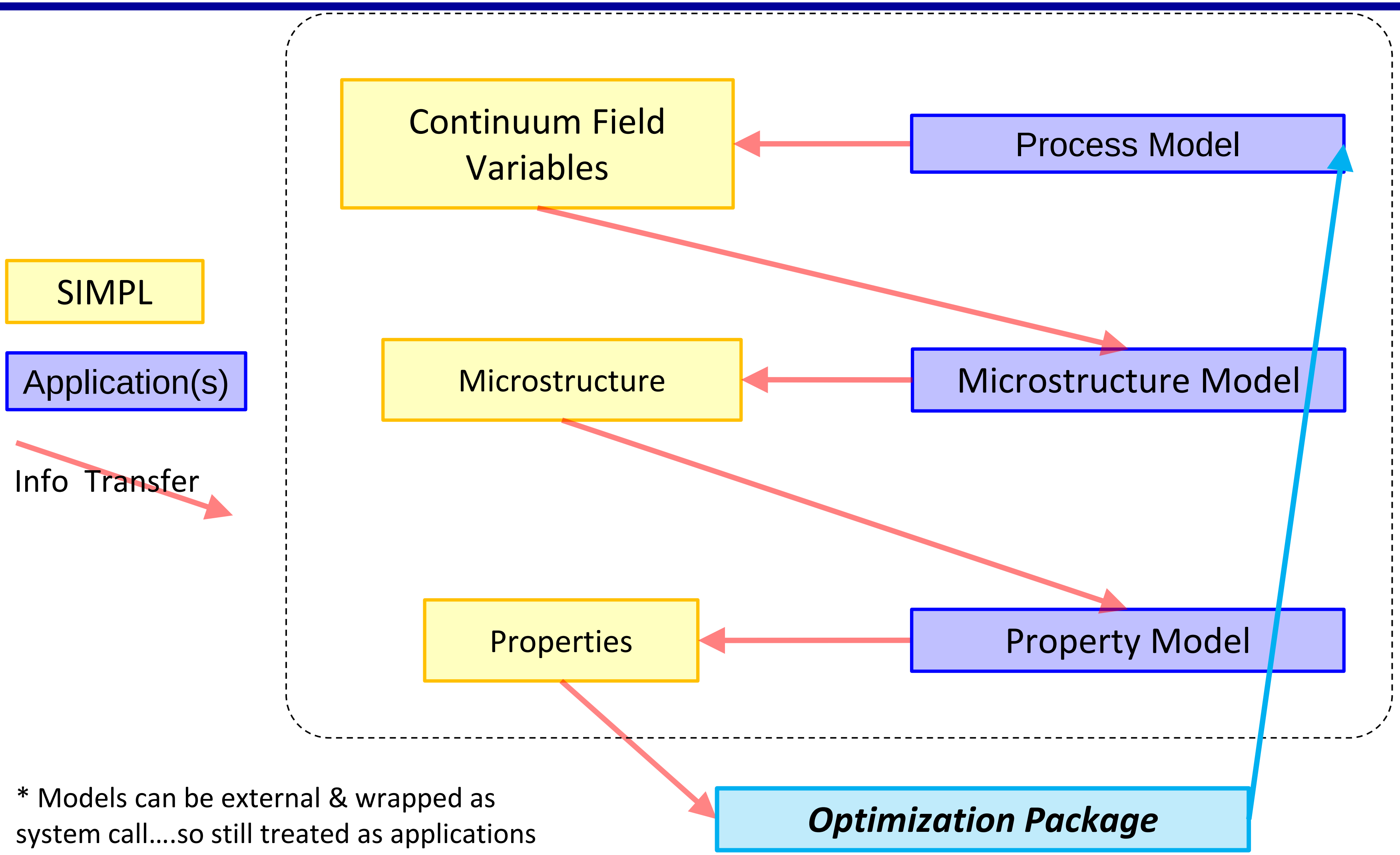
- Experiment and computation must work together more synergistically: requires a collaborative research environment

- 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

AIR FORCE RESEARCH LABORATORY

Enabling Management of Process Design



* Models can be external & wrapped as system call….so still treated as applications (Ex. Los Alamos FFT code)

SIMPL arbitrates model interactions & modularizes process