Advancing the Materials Genome Initiative

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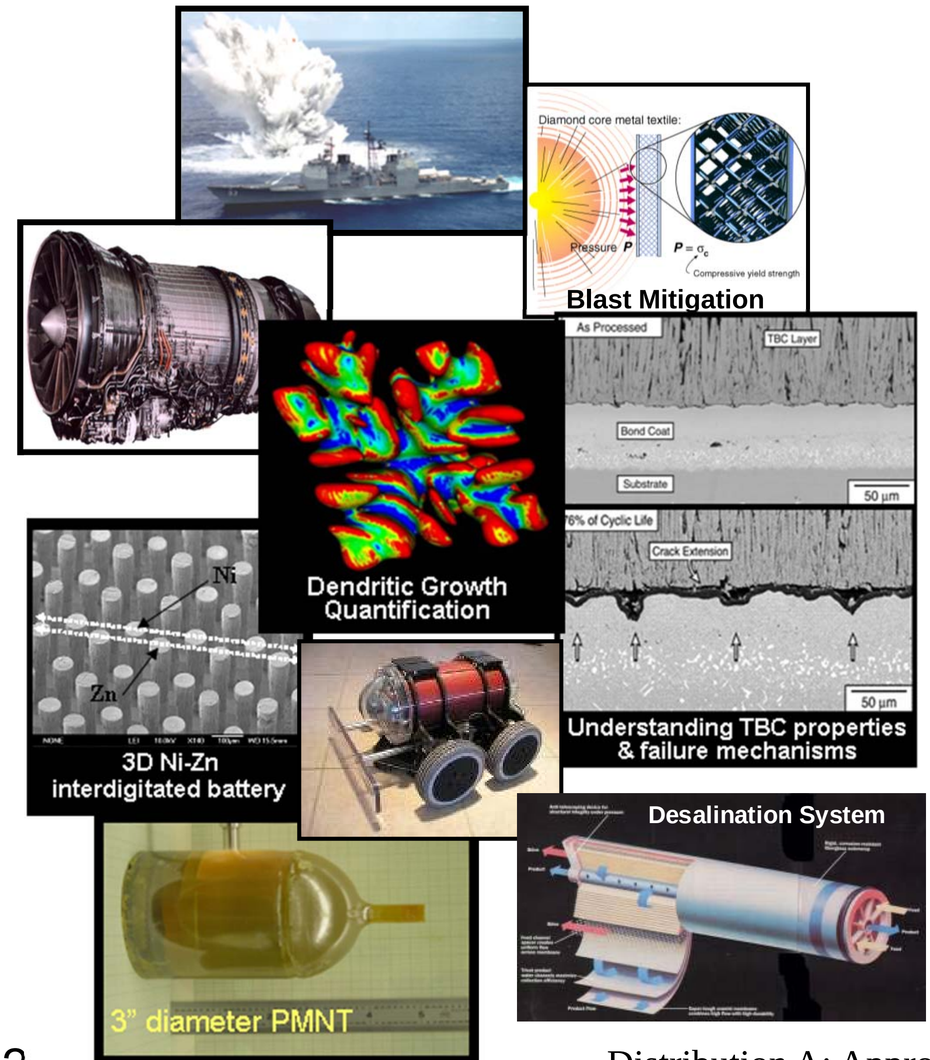
ONR
Revolutionary Research . . . Relevant Results

OFFICE OF NAVAL RESEARCH

Advanced Naval Materials

Integrated theoretical, computational and experimental programs to understand and develop the physics, chemistry, materials and processing that confidently meet critical naval needs



High Performance Functional Materials

- Power Generation & Energy Storage Materials
  - ✓ Electrochemical Materials
  - ✓ Polymeric and Organic Materials
- Piezoelectric Materials

High Performance Structural Materials

- Structural Metallic, Structural Cellular and Composite Materials
- High Temperature Turbine and Ultra-high Temperature Materials
- Welding and Joining
- Optical Ceramics

Environmental Quality

- Anti-fouling Release Coatings
- Solid and Liquid Waste Treatment

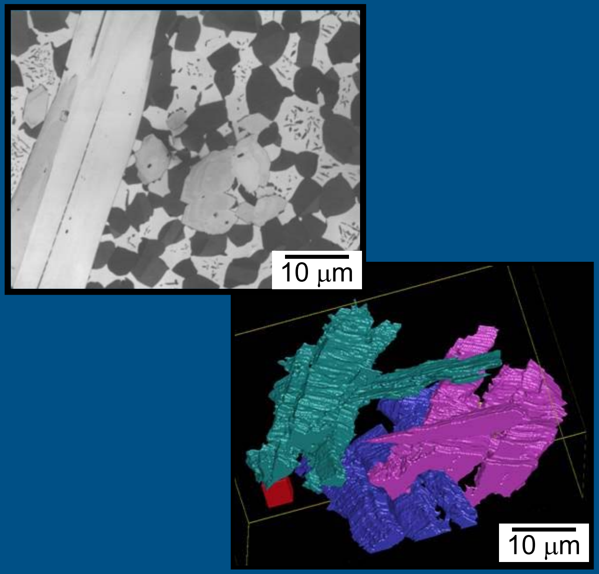
Optimization from Design thru System Life

- Computer Aided Materials Design
- Solid Mechanics and Fatigue
- Non-Destructive Evaluation and Prognostics
- Integrated Computational Materials Engineering

The Next Big Thing in Materials Isn't a New Class of Materials.

We are in the midst of a long drive to change the culture of material science from discovery to deployment

- Research becomes more rigorous and quantitative
- Processing models and experiments capture physical phenomena, uncertainty and stochastic behavior
- Design and manufacturing are linked to material processing to ensure performance and rapid qualification
- Life prediction/sustainment becomes more accurate, incorporating effects of specific processing and service histories

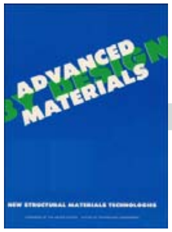


We are moving material science and engineering from the analog to the digital age

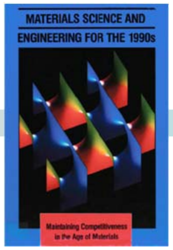
Historical Perspective

From Tresa M. Pollock
TMS 1st World Congress on Integrated Computational Materials Engineering
Seven Springs, PA
July 11, 2011

1988



COTA: *Advanced Materials by Design*



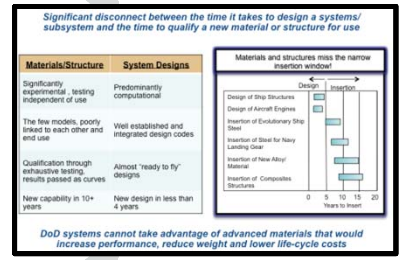
1989
0.8M
0.2GB

NRC: Materials Science & Engineering for the 1990s

DOE: Advanced Strategic Computing Initiative

1995
8M
1.1GB

Challenges for Materials Insertion



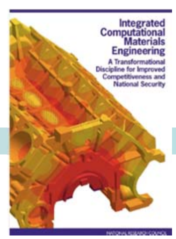
30M
10GB
1999
DARPA-AIM
Accelerated Insertion of Materials

2001
AFOSR-MEANS

ONR-D3D
100M
50GB

2004

NRC-ICME

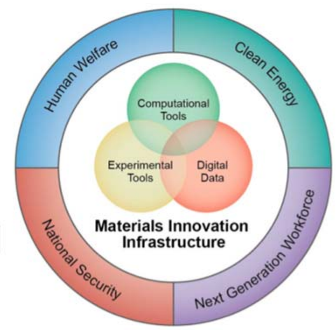


2008

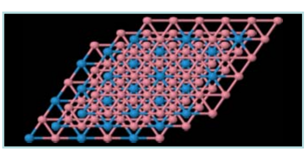
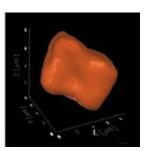
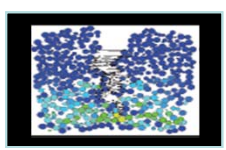
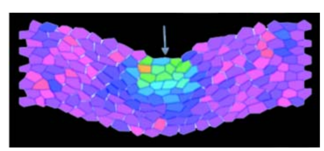
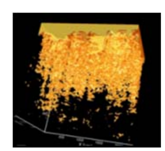
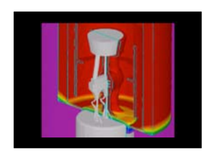
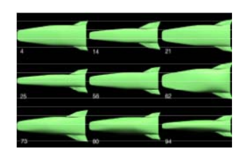
DOE-CMS&C

2,000M
1TB

2010



2011

Accelerated Insertion of Materials (AIM)

An efficient, robust, reliable and interactive process fully integrated into the available design tools and design community. Provides (generate) the right data at the right fidelity as it is needed.

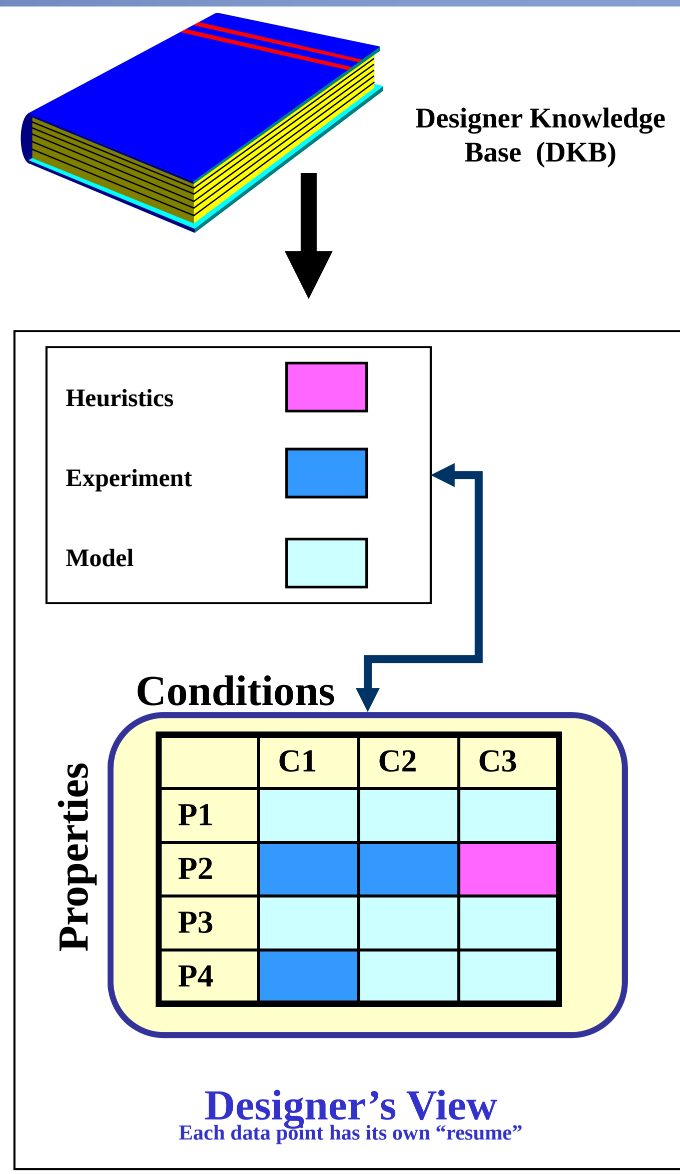
The right source (model, experiment, experience) to fill in the knowledgebase.

Confidence in the data and in the knowledge of errors and uncertainty.

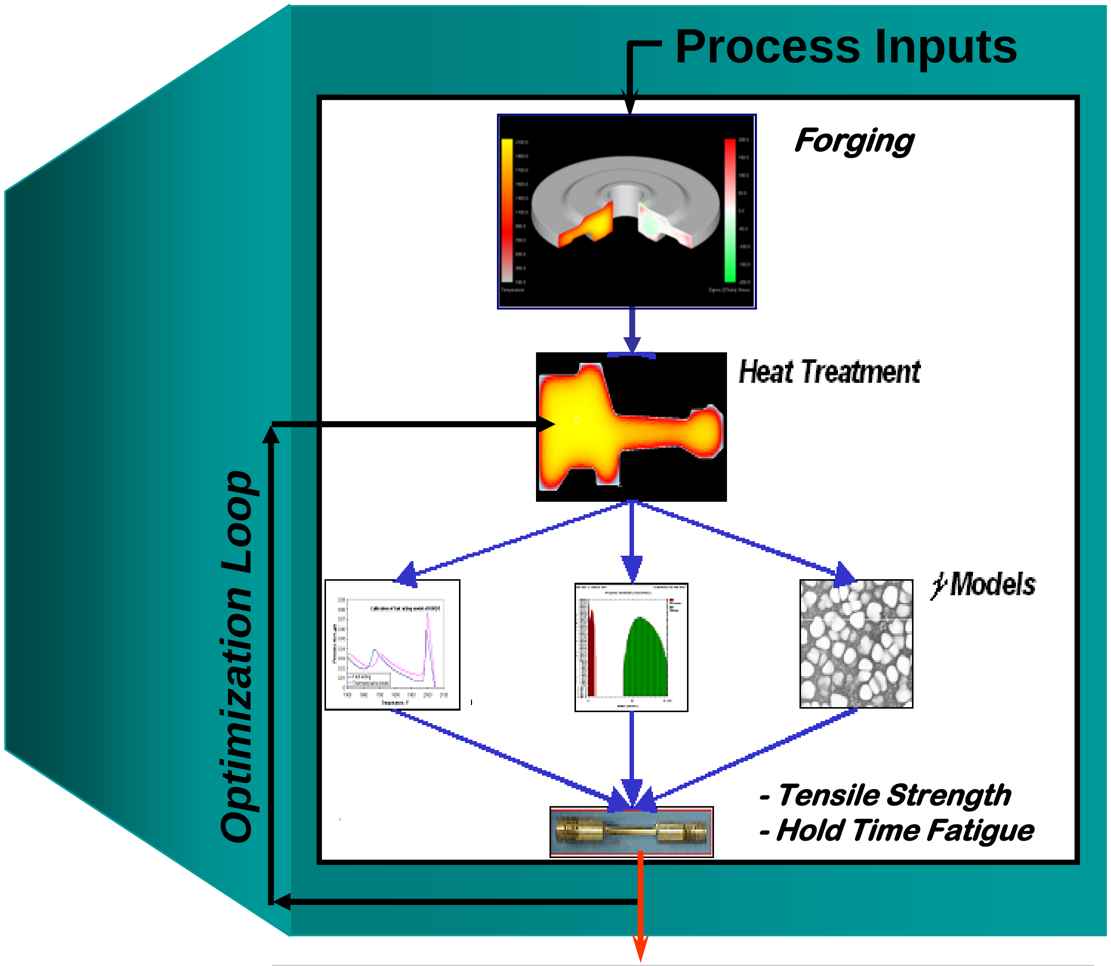
Models can (and will) evolve and are distributed

- **Establish a modular methodology**
- **Ensure configuration control**
- **Provide for appropriate remuneration of IP holders**

Materials become a true design variable (not a time consuming and expensive look up table)

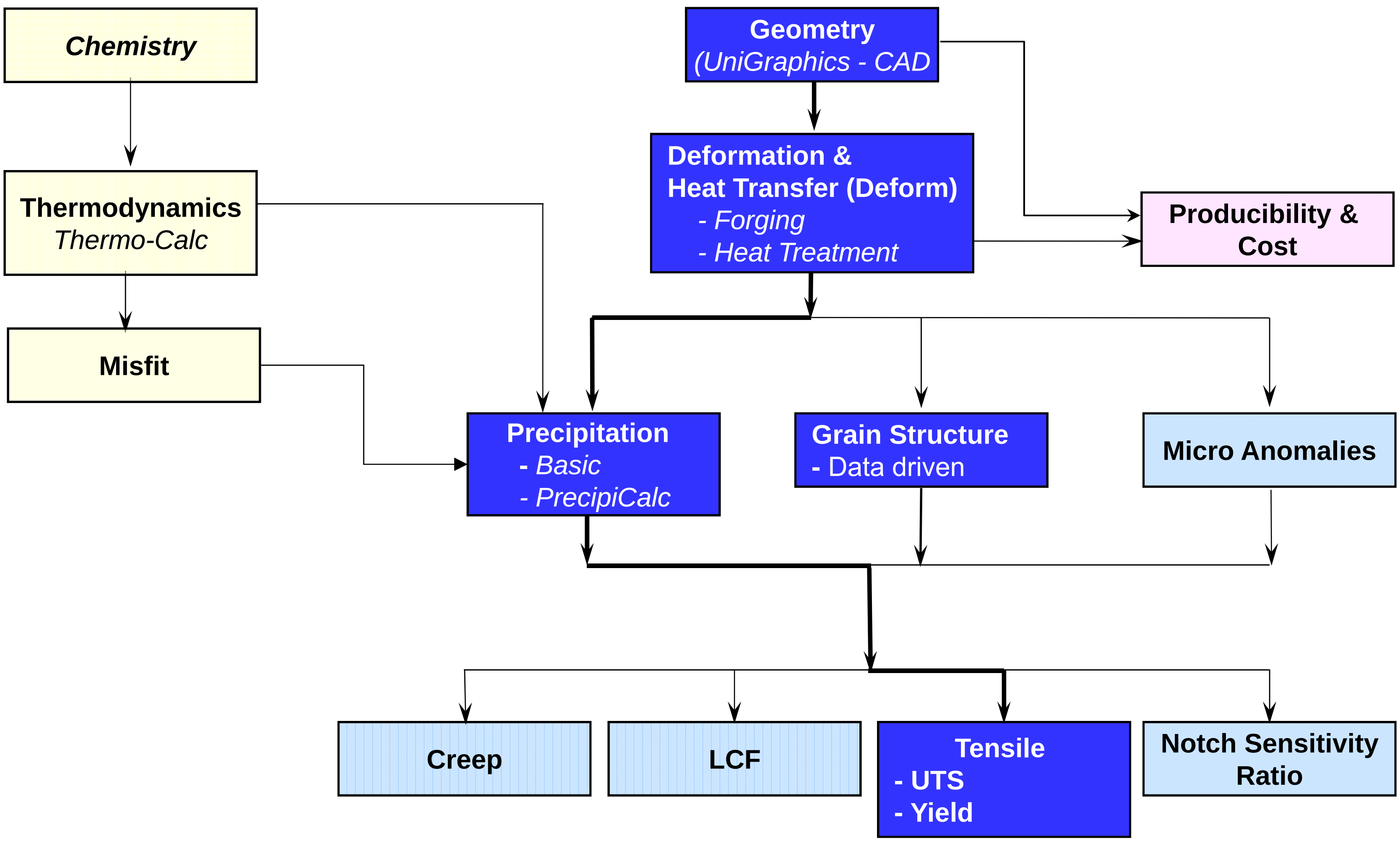


AIM Implementation



- *Strength* *@ Rim Increased* *5.7%*
- *Strength* *@ Bore Increased* *3.8%*
- *Crack Growth* *@ Rim Decreased* *25.9%*

Details of Materials Models Linkage



GE

Example: Elements of yield strength model

14%
Yield of Primary γ'

37%
Shearing of Secondary γ' (Pairs)

$$\sigma_{ys} = f_p\left\{\sigma(T)_{Ni3Al} + \sum_i \left(\frac{d\sigma}{dC_i}C_i\right)\right\} + M(1-f_p)0.43Gb\frac{\left(f_s / 1-f_p\right)^{1/2}}{d}\left(\frac{2.56d\Gamma_{APB}}{Gb^2}-1\right)^{1/2}$$

$$+ Mf_t\left\{\frac{\Gamma_{APB}}{b}\right\} + f_\gamma\left(\frac{T_o}{T}\right)\left\{\sum_i \frac{d\sigma}{dC_i^{1/2}}C_i^{1/2}\right\} + (1-f_p)k_y^\gamma d^{-1/2} + f_p k_y^{\gamma'} d^{-1/2}$$

Shearing of Tertiary γ' (Individual)
4%

γ Solid Soln Strengthening
8%

Hall-Petch γ Phase "Matrix"
25%

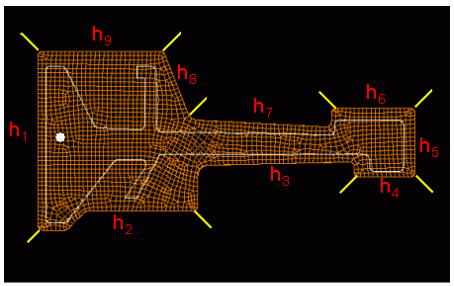
Hall-Petch Primary γ '
12%

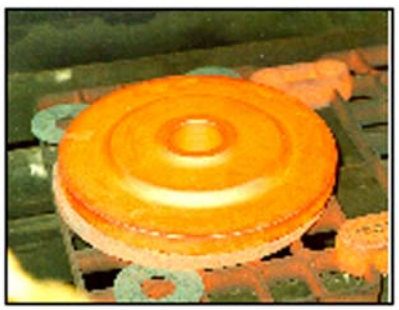
Web-Based Process Execution

Job Initiated at GE Lynn.

Objective: Estimate fracture load and location.

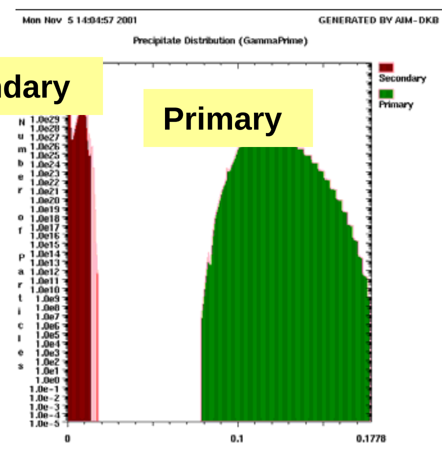
Disk CAD model (at GE Evendale)





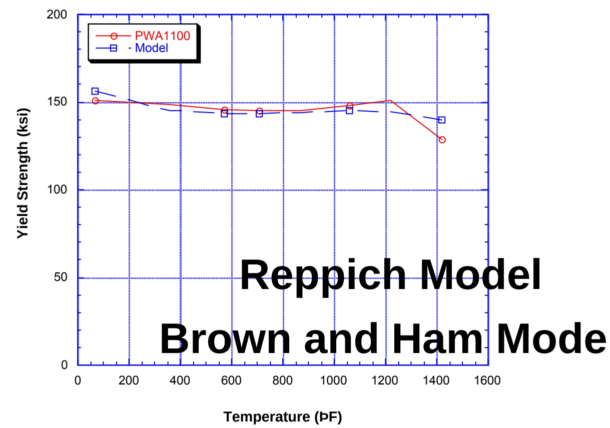
DEFORM - Heat Treatment
Model run at GE-CRD. Process variables (heat transfer conditions) from database at Laddish)

PRECIPICALC : γ' Model (Model Run at Questek)



Precipitate Size Distribution

Strength models
Models Run at U. of Michigan



Distribution A: Approved for Public Release

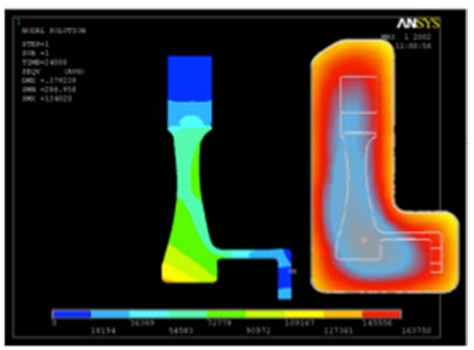
Full AIM Tool Demonstration at the Component Level

Case Study	Heat Treat	Forging	Part	Forge Wt	Part Wt	Burst Speed	Comments
1	Constant	Variable	Variable	-18%	-15%	+6%	Fixed Microstructure
2	Variable	Variable	Constant	-11%	n/a	+12%	Fixed Part Geometry
3	Variable	Variable	Variable	-21%	-19%	+19%	Full Opt. By AIM tool

Cost Benefit | System Benefits

Superalloy disk burst test validates the methodology

Rim initiated fracture

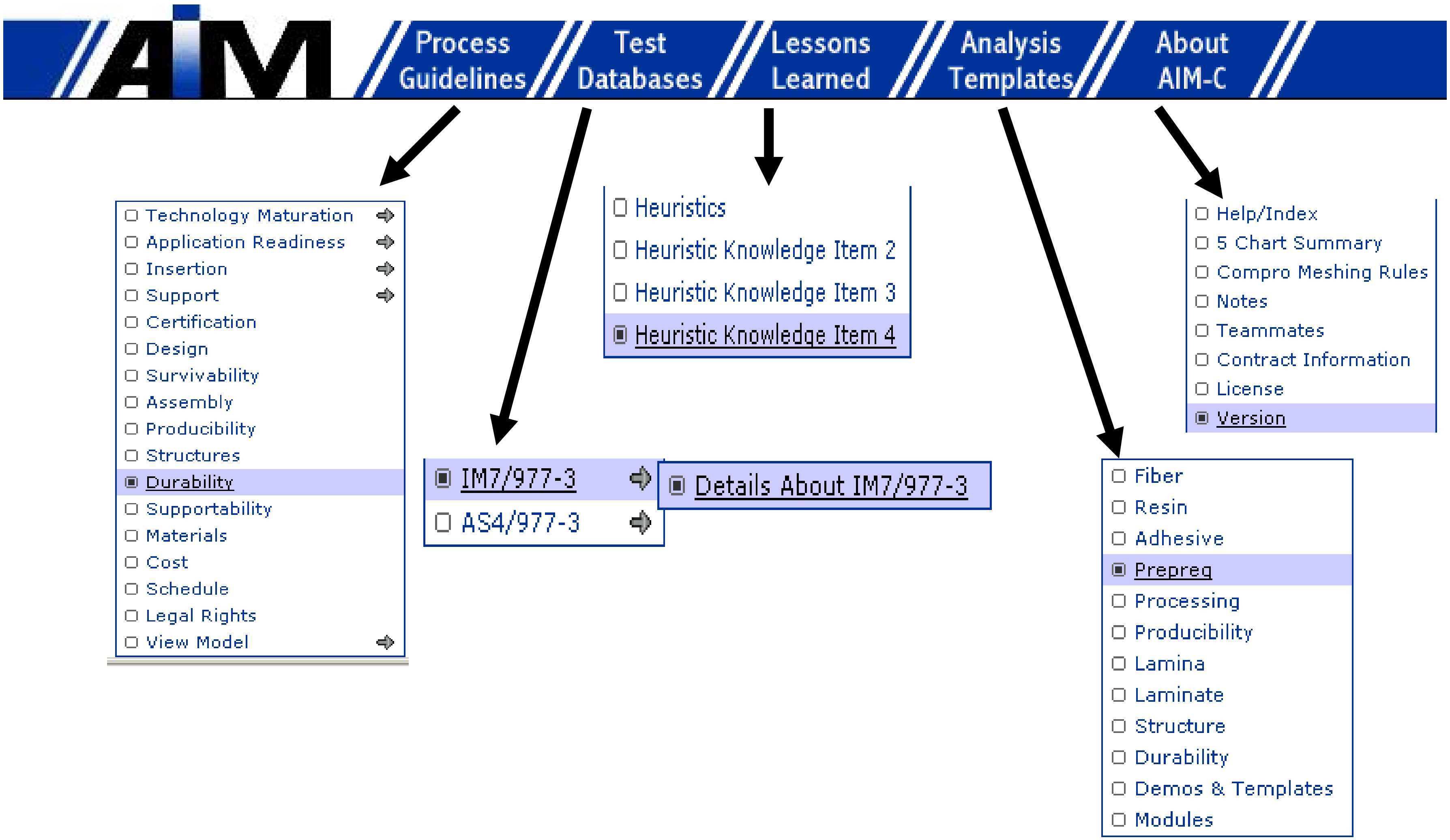


Bore initiated fracture

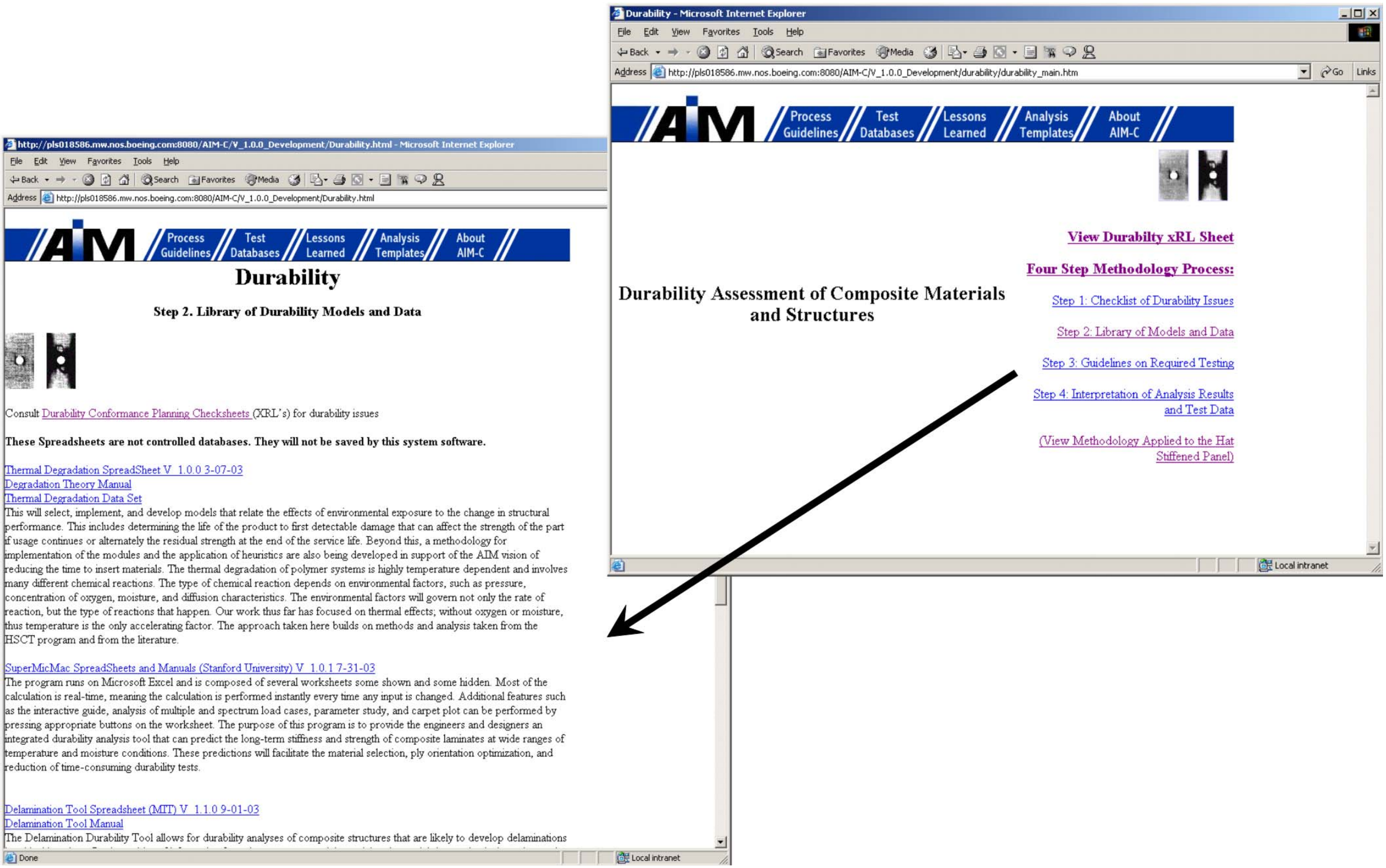
Integrated tool & models reduced development and test cycle by greater than 50%

- demonstrated improved design capability (5% in speed)
- identified and tested process outside of experience base
- eliminated subscale experimentation
- mapped & integrated material property spatial variation into structural performance
- provided insight into material impact (failure location)
- readily integrated and responded to evolving model capability

Drop Down Menus

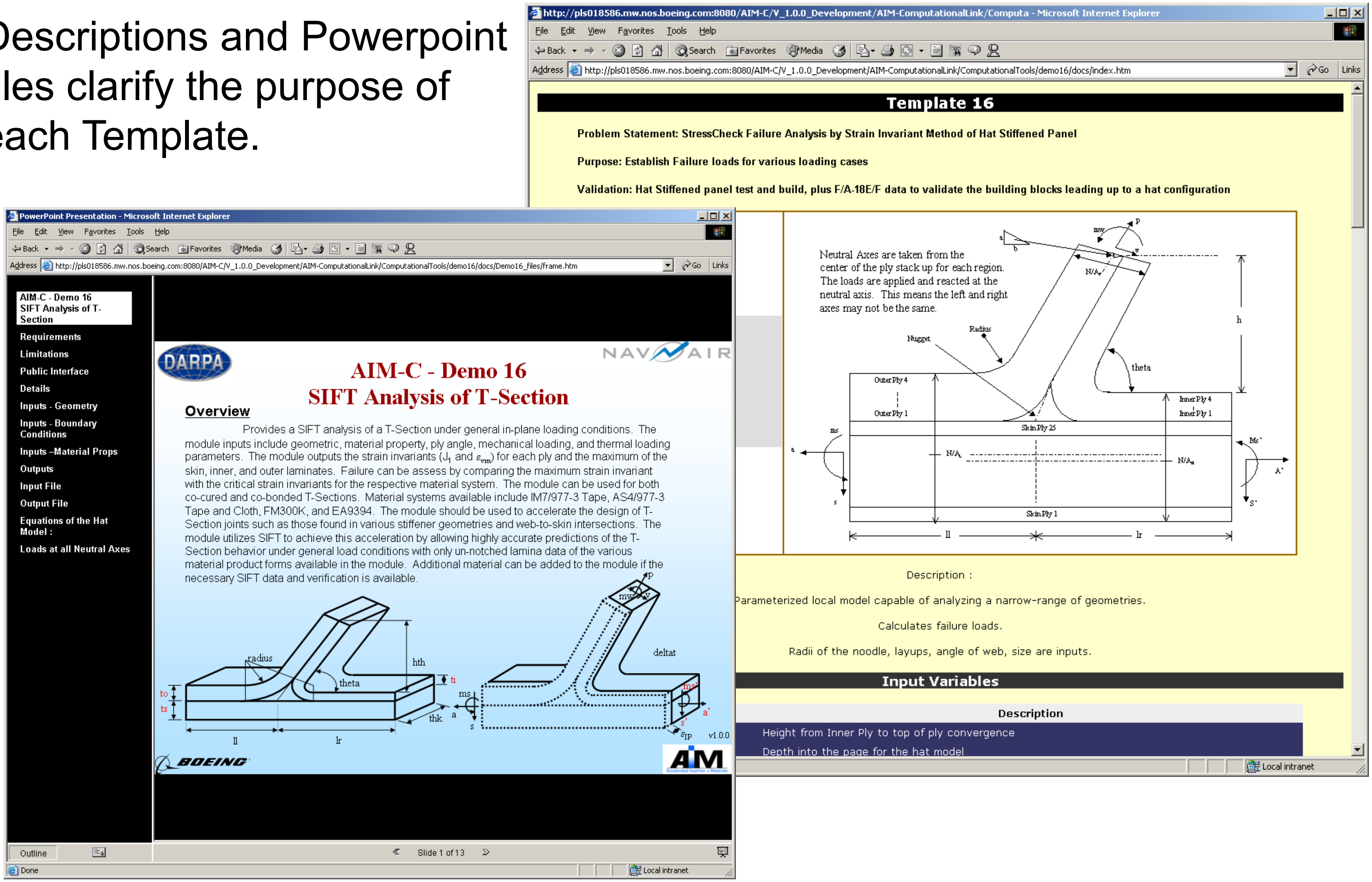


Tools, e.g. Durability

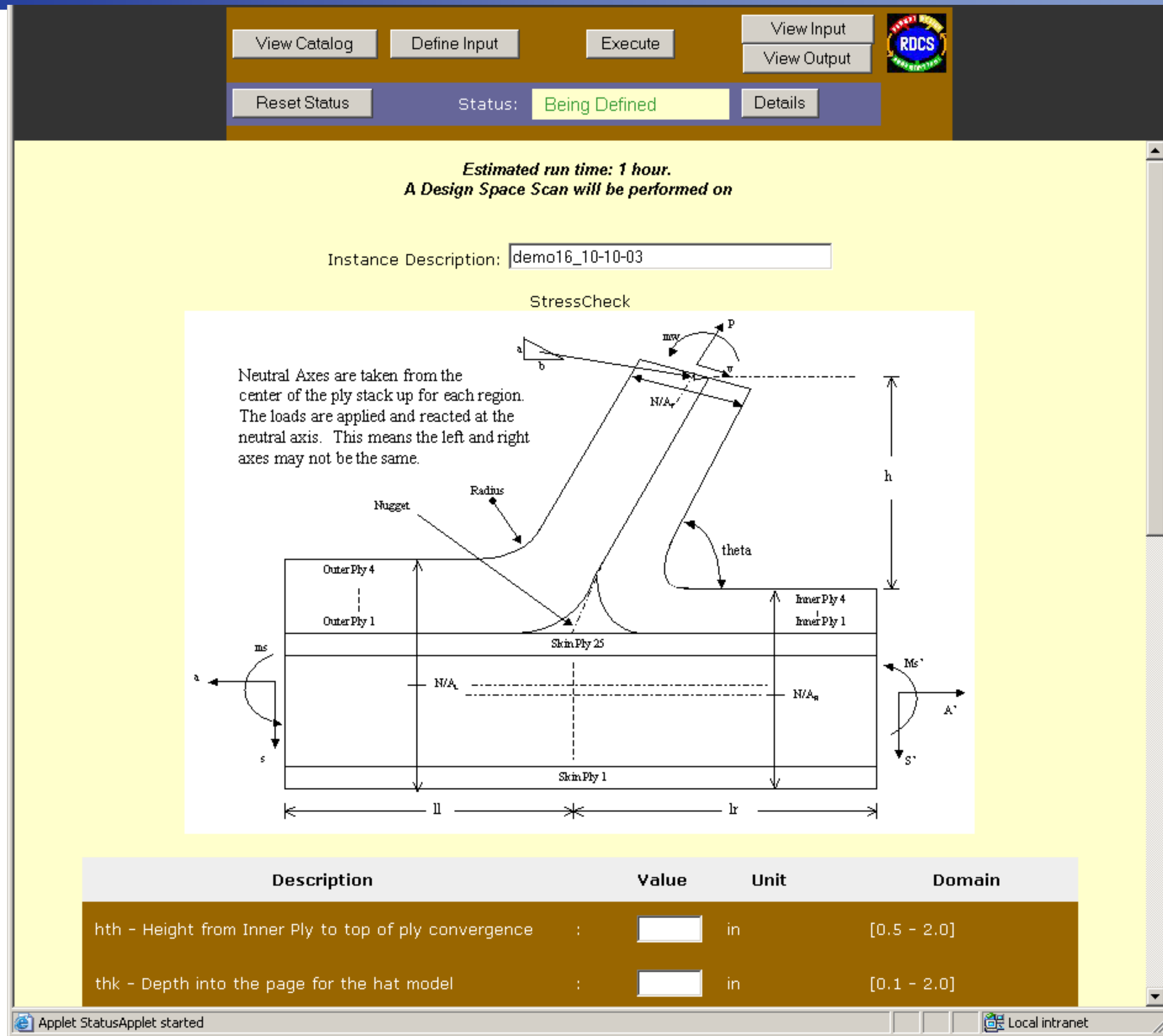


Template

Descriptions and Powerpoint files clarify the purpose of each Template.



Input Screens for the Templates



Impact of AIM on a Specific System

F/A-18 component

Using AIM Methods and Tools

- 46% Savings in Labor
- 53% Savings in Time
- Lower Risk

	AIM-Developed	Baseline
Stress at Crack Initiation (tension)	50.9 ksi	13.4 ksi
Stress at Failure (tension)	78.0 ksi	34.2 ksi

AIM part is better quality, slightly lighter, and simpler to manufacture than baseline.

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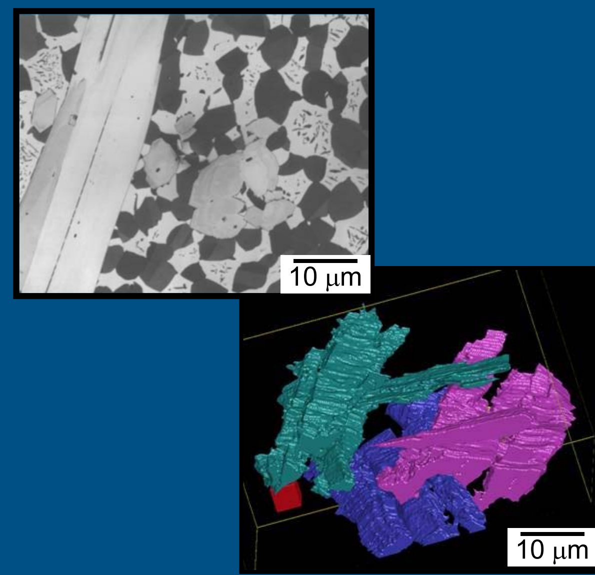
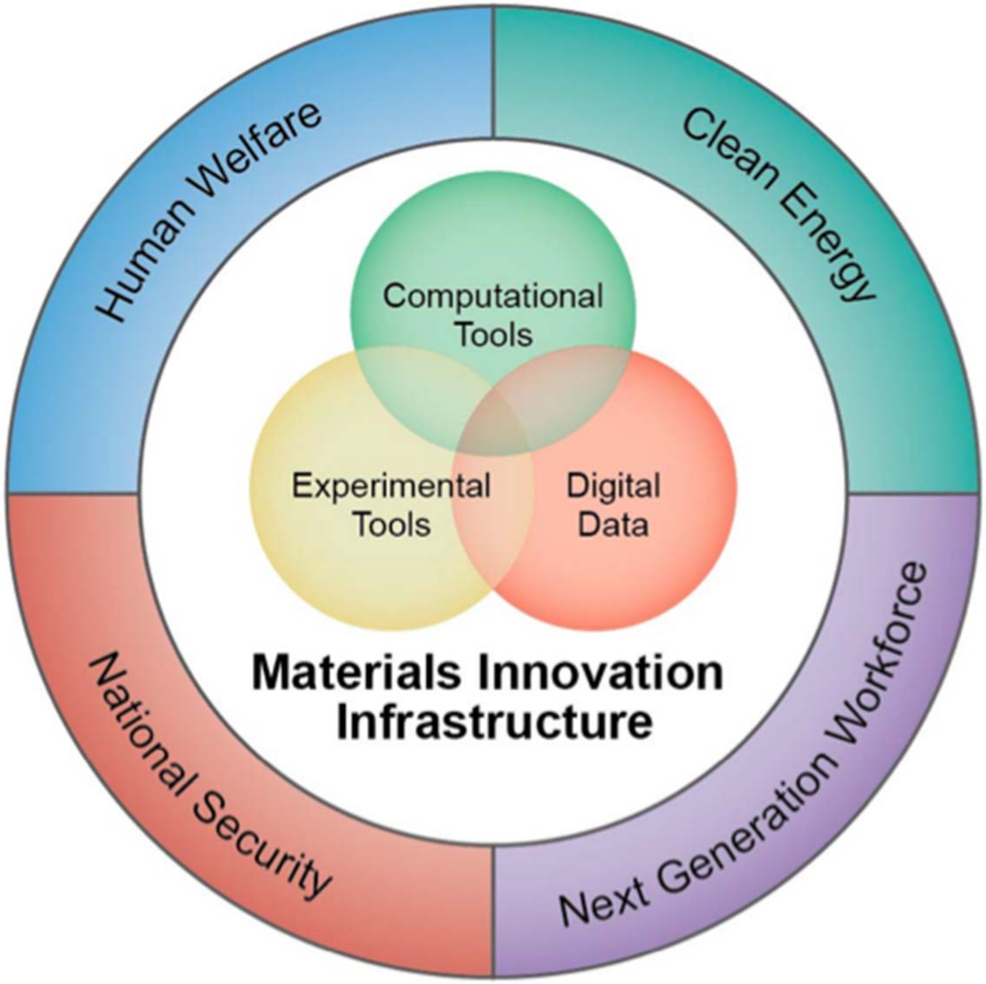
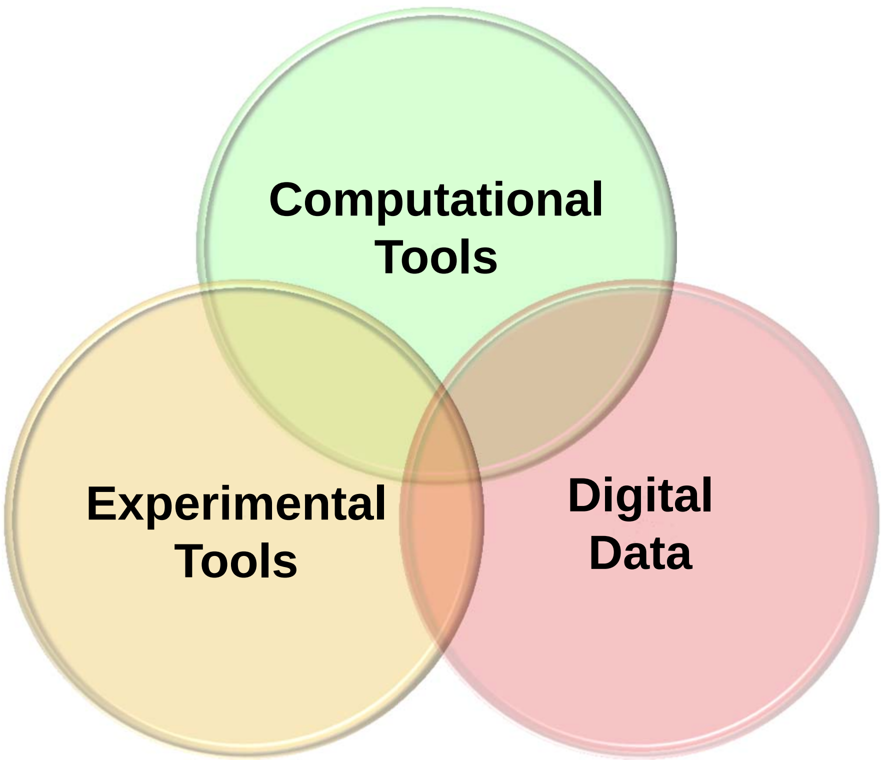


We are moving material science and engineering from the analog to the digital age



http://www.whitehouse.gov/blog/2011/06/24/materials-genome-initiative-renaissance-american-manufacturing

Materials Innovation Infrastructure



Computational Tools

- Develop validated models to predict performance of materials under a diverse set of conditions
- Guide and minimize traditional experimental testing matrices
- Ensure software is modular and simple to use

Digital Data

- Establish new databases, standards, assessment methods, quality assurances, and preservation systems for material properties, software, and experimental results.
- Effective retrieval and analysis of materials data in this new paradigm
- Approaches for data sharing and protection of IP

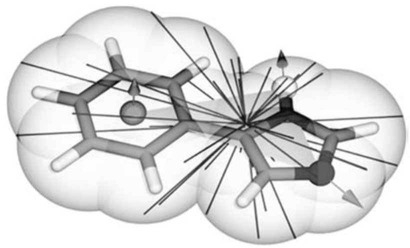
Experimental Tools

- Accelerated methods for automation, interpretation, and visualization, including visualization of structure in 3-dimensions
- New approaches that link materials science experiments in a way that efficiently fills in empirical data and models where computations fall short
- Seamless exchange of experimental data with models, input to provide material-specific parameters, and output to validate model predictions.

COMPUTER-AIDED MATERIALS DESIGN (CAMD)

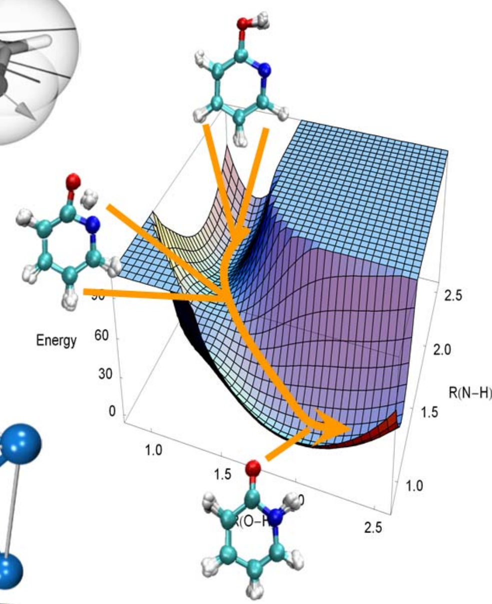
Revolutionary Research . . . Relevant Results

Developing Fundamental Understanding and the Tools for Discovery



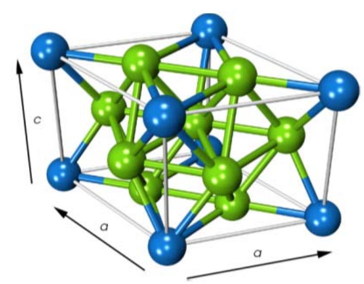
De Nuevo Calculations and Exploration

- Design strategies for new material creation
- Expand DoD materials portfolio



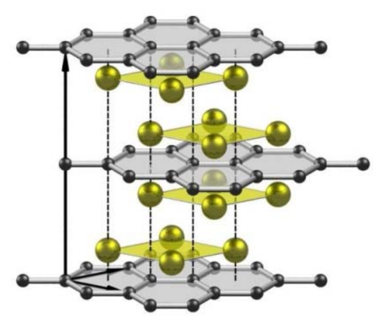
Introduce New Approaches / Develop New Tools

- Develop heuristic-based modeling methodologies, akin to what is done in the pharmaceutical industry for “drug design,” to create new materials from new “lead” materials
- Develop design principles from the atomistic level through processing of bulk material (physics-based, multi-scale modeling methods)
- Develop data mining methods capable of exploring well established chemical databases for alternative materials



D&I Investments to Advance Materials Science and Application

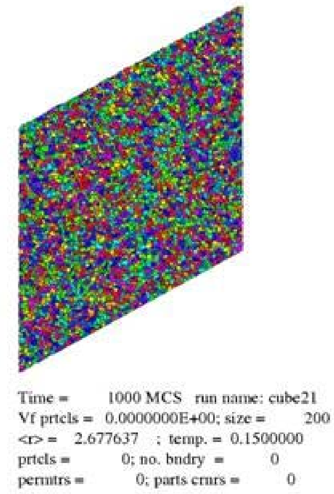
- Theoretical tools are being developed to explore potential energy surfaces so that dynamical processes of molecules can be predicted.
- A new Hf/Sc alloy predicted by high-throughput quantum theory; now a candidate for synthesis and testing.
- A CAMD superconducting material; higher Tc materials are now being considered.



Integration of Advanced Analysis with Materials Research

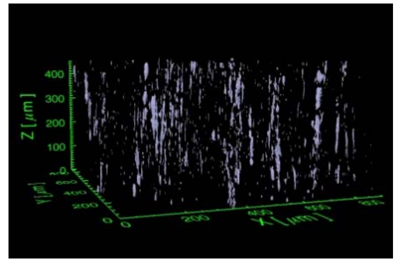
Objective: Materials design toolset

- Define a coherent framework for prediction & optimization of material properties
- Explore new approaches for modeling
- Computational efficiencies: less data but more information
- New approaches to performing calculations
- Exploit tight collaboration of experiment, characterization, modeling, and computation
- Rapid identification of new physical phenomena



Approach: Draw advanced analysis into each stage

- Explore reduced-order descriptions of microstructure
- Capture stochastic micromechanics of microstructure evolution
- Constitutive modeling that includes inherent randomness and emergent behavior
- Process modeling
- Investigate mappings of microstructure evolution models into reduced-order random-field descriptions
- Performance optimization



3D reconstruction of $LaSO_4$ inclusions in C-61 steel, created from 240 serial sections.

ICME/MGI for Structural Materials

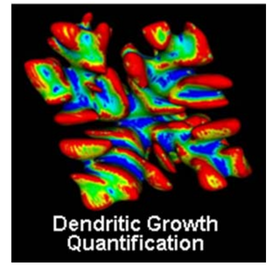
Building Tools to Integrate Theory, Computation & Experiment to Accelerate Materials Discovery through Implementation

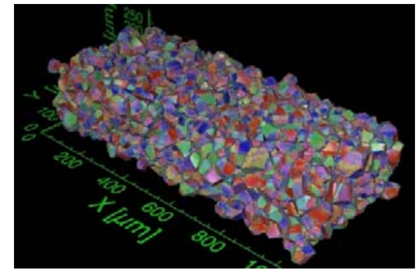
Basic Research enabling ICME

- Advance multi-scale and multi-physics experimental capabilities that move material science from the analog to the digital age
- Emphasize model-guided experimentation at the nano-, meso- and macro- scales to discover, understand and articulate interactions
- Anticipate the random nature of microstructure, and non-linear effects of processing variations that lead to localized variations in materials performance
- Link basic research to reliable, cost-effective processing-manufacturing design for accelerated qualification and service life management

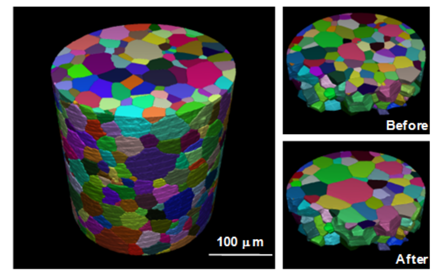
Lightweight Structural Materials Research

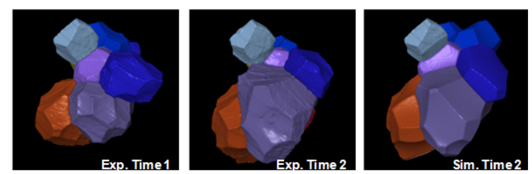
- Demonstrate utility of approach and establish “best practice” to reduce certification costs by 75%
- Develop thermodynamic, kinetic, deformation, and microstructure models and data sets
- Integrate applications with iSight
- Calculate microstructures, validate system
- Develop similar 7XA models for Flexible Infrastructure

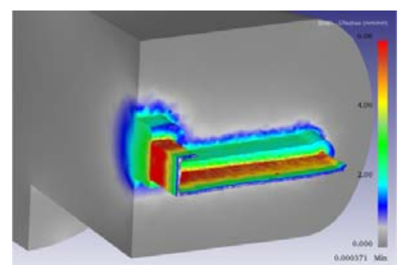




3-D experimental data of Ti-β-21S







Simulation of extrusion of AA6082 for an LCS-2 sidewall panel

ICME/MGI Efforts in Electrochemistry

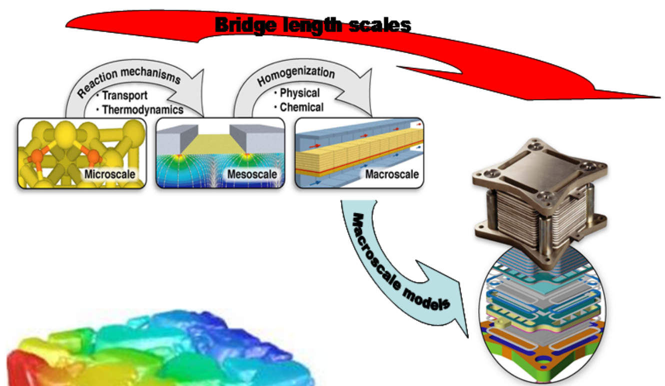
Quantifying Surface/Interface Reactions for Advanced Battery and Fuel Cell Design

Objective: New high-performance electrochemical energy storage and power conversion systems

- Develop effective design tools and integrate validated physical models into robust CFD codes
- Collaborate with designers to develop and improve high-performance power systems
- Incorporate physical knowledge into real-time process control

Approach: Focus on science, tools, and systems

- Develop new approaches for modeling charge-transfer incorporating fundamental physics, chemistry, and electrochemistry
- Develop fully resolved models to represent effective properties of composite electrodes
- Develop model-predictive process-control algorithms for tubular SOFC stacks
- Develop model-predictive process-control algorithms for rechargeable battery design
- Initially develop and validate for solid oxide fuel cell (SOFC)
  - Apply to design a class of all-ceramic microchannel heat-exchangers and fuel-processing reactors
- Extend SOFC modeling tools to Li-ion batteries



Simulated transport in a reconstructed Li-ion cathode

All ceramic microchannel heat exchanger and reactor