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Computational Models in the Materials World
- We are nearly there….

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AIAA Conference
April 10, 2013
Boston, Mass.

Not Subject to the EAR per 15 CFR Part 734.3(b)(3)

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Report Documentation Page

Form Approved
OMB No. 0704-0188

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1. REPORT DATE **10 APR 2013**	2. REPORT TYPE	3. DATES COVERED **00-00-2013 to 00-00-2013**

4. TITLE AND SUBTITLE **Computational Models in the Materials World - We are nearly there...**	5a. CONTRACT NUMBER
	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S)	5d. PROJECT NUMBER
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **Pratt & Whitney,400 Main Street,East Hartford,CT,06118**	8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)
	11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution unlimited

13. SUPPLEMENTARY NOTES

14. ABSTRACT

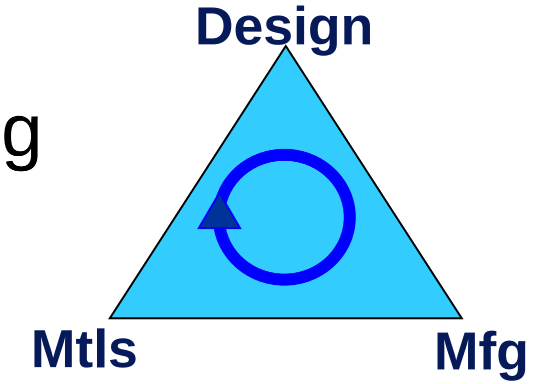
15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT **unclassified**	b. ABSTRACT **unclassified**	c. THIS PAGE **unclassified**	**Same as Report (SAR)**	**21**	

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std Z39-18

Engineering Materials Today

- Materials are critical for every engineered product
- Traditionally materials were developed by trial and error processes, separate from application requirements
- Materials are currently defined by static specifications based on empirical data
- Challenge and opportunity of Computational Materials Engineering is the linking of Materials, Manufacturing Processes and Component Designs



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Evolution of System Efficiency

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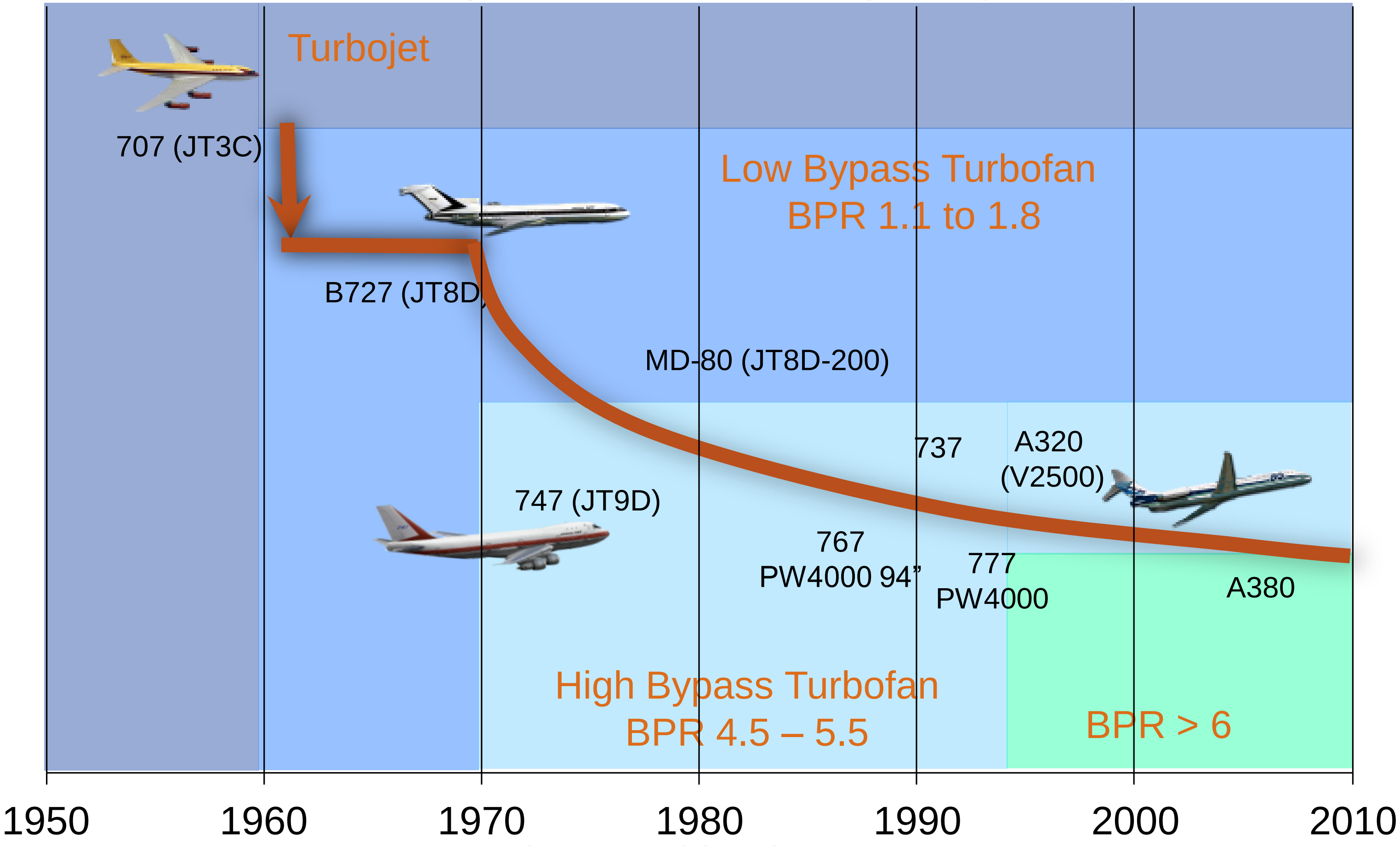
Thrust Specific Fuel Consumption (lb/hr/lb)



Engine Certification Date

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Propulsion History

Propulsion Innovations Enabled by Materials and Processing Technology


J58 Powered SR-71

DS blades, Cast &Wrought disks, 1st Gen Thermal Spray TBC coatings


JT9D powered Boeing 747

1st Gen SC blades, 1st Gen PM disk, 1st Gen EB-PVD TBC


F100 Powered F-15 / F-16

2nd Gen SC blades, Aluminide coatings, 2nd Gen PM/fracture tolerant disk


F119 Powered F-22

LFW Ti IBR, Dual Property Ni Disk, TBC blades, Burn resistant Ti, CatArc Metallic Coatings


F135 Powered F-35

Dual Property 3rd Gen PM disk, High modulus blade, 2nd Gen TBC coating


PW1133G Powered A320neo

4th Gen PM disk alloy, Hybrid metallic airfoils, 3rd Gen TBC

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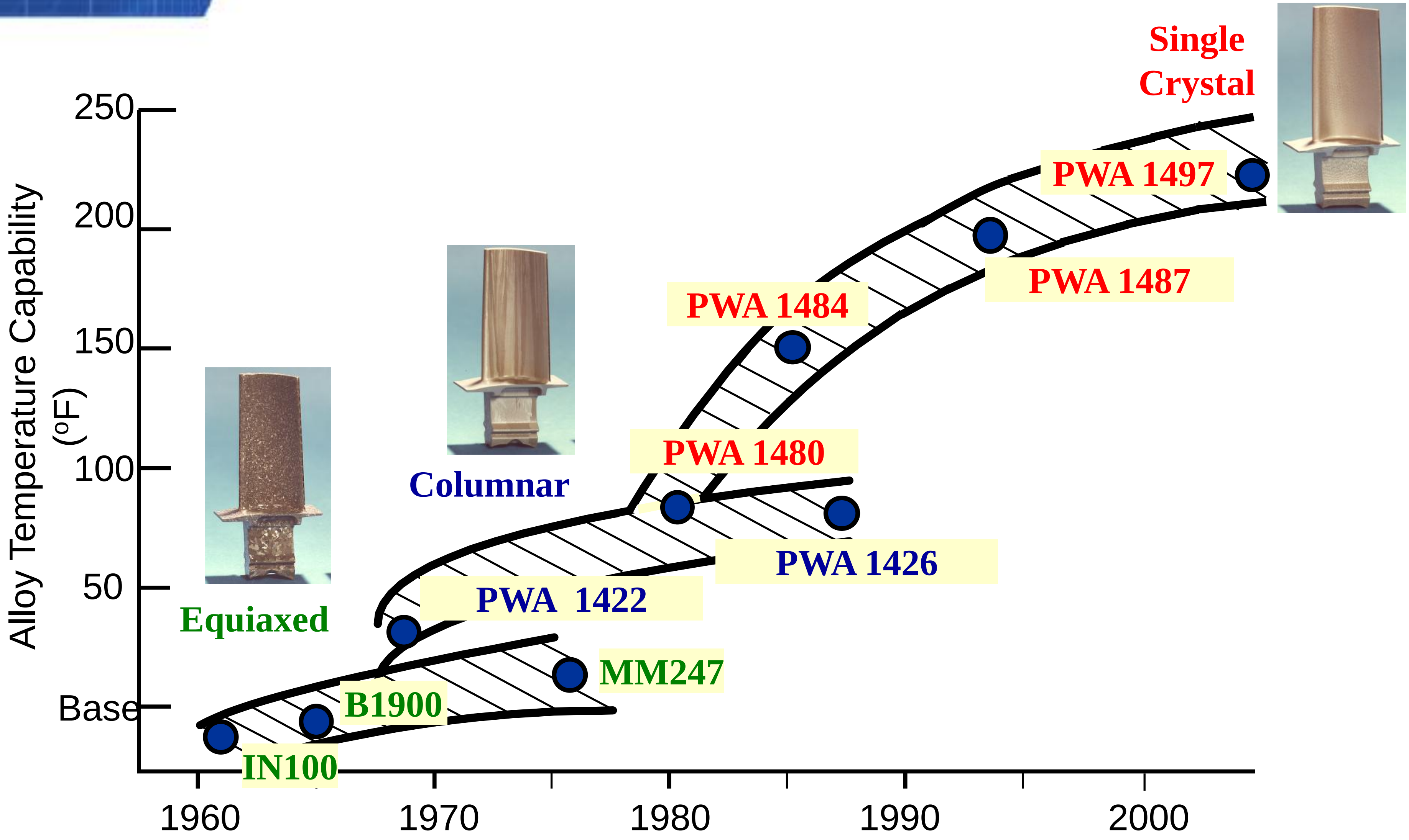
Ni Superalloy Turbine Airfoils: Significant Advances in Alloys and Casting Processes



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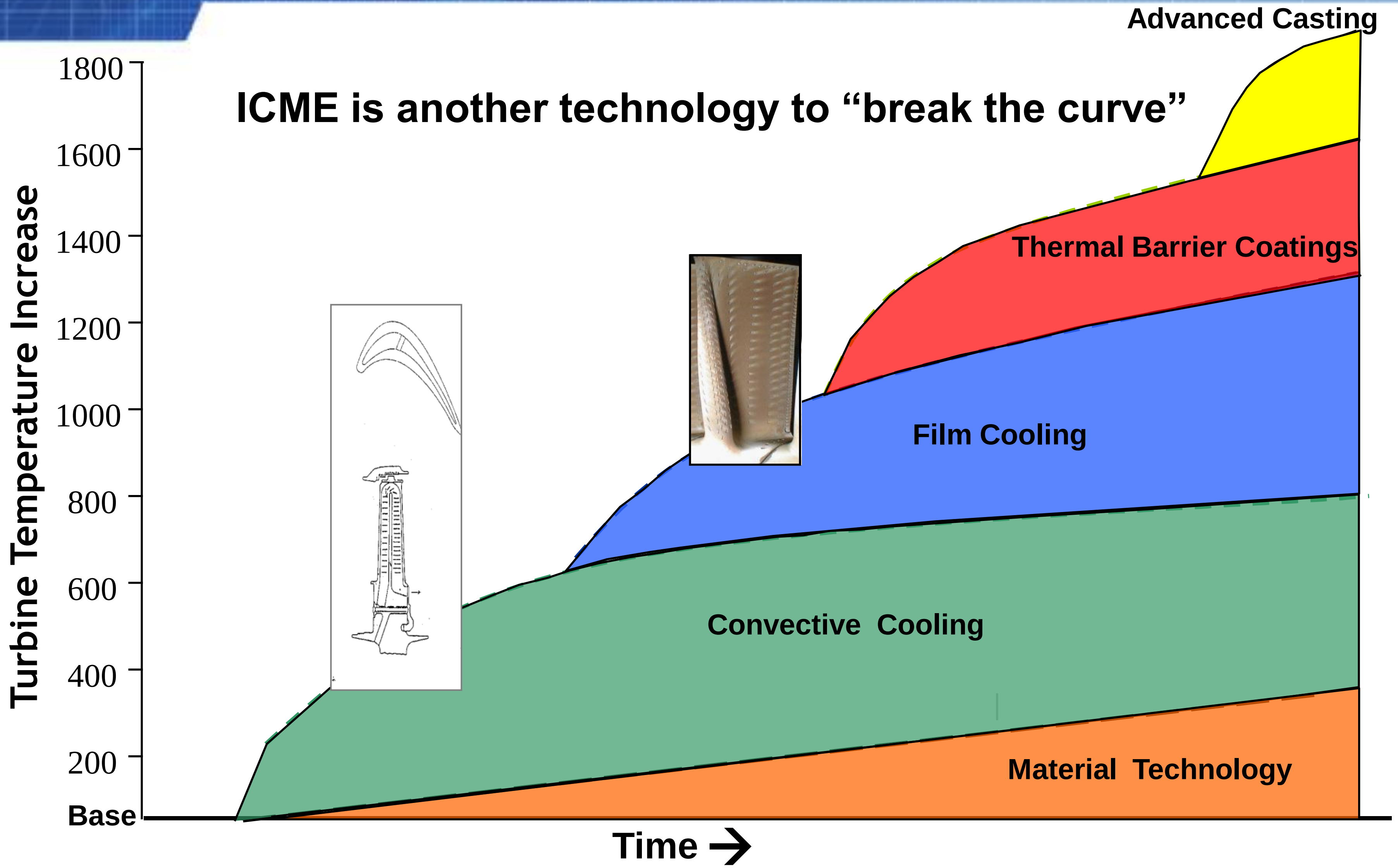
Key Technology Advances for Turbine Airfoil Materials



ICME is another technology to “break the curve”

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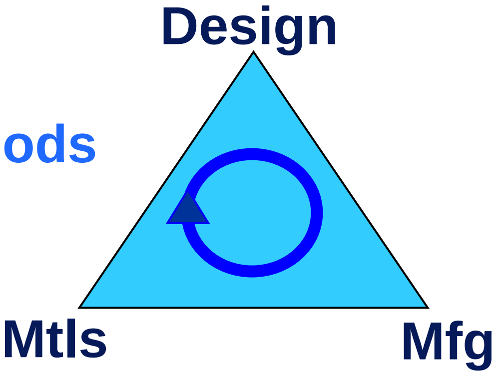
Materials & Product Engineering

Mechanical Properties = fn (chemistry and microstructure)

Microstructure = fn (chemistry and processing)

Processing = fn (component geometry)

Materials, Manufacturing Methods and Component Design are Strongly Coupled



ICME -Integrated Computational Materials Engineering

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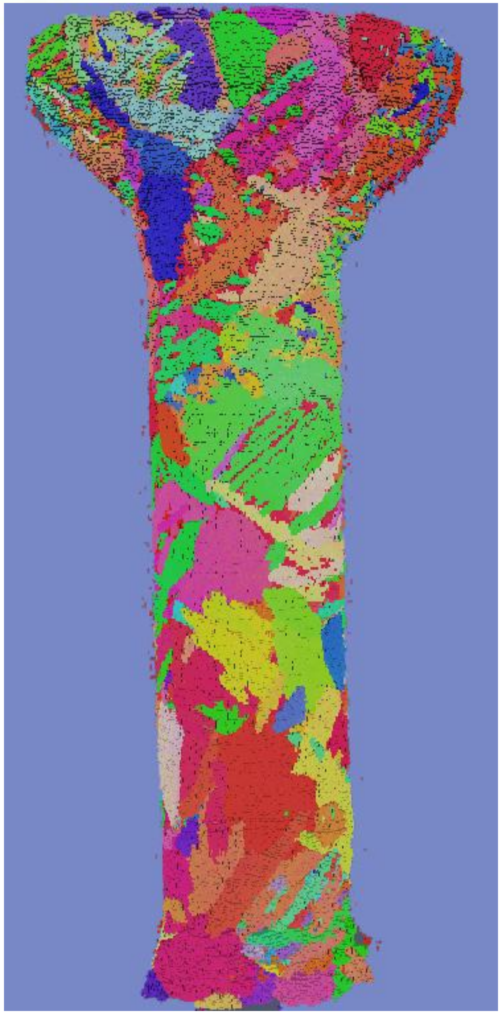
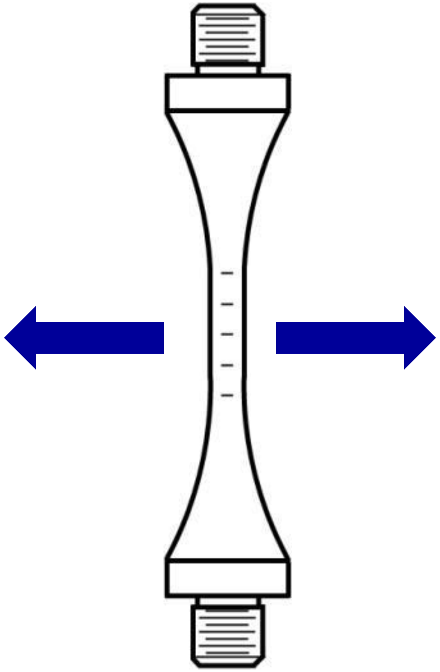
What a Tensile Test Looks Like…..



To a Materials Engineer



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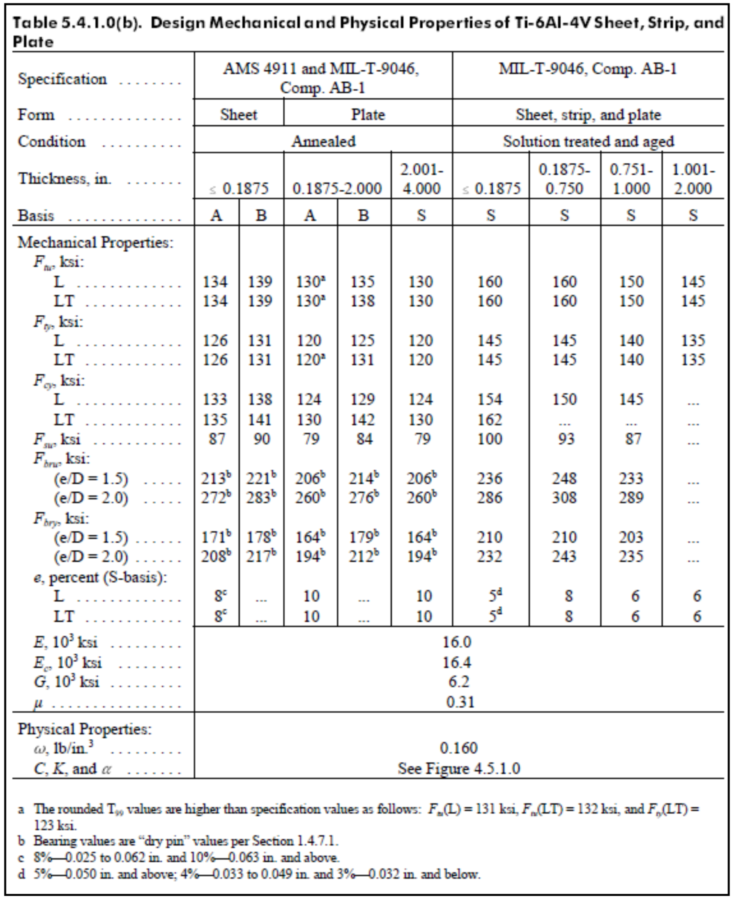

Table 5.4.1.0(b). Design Mechanical and Physical Properties of Ti-6Al-4V Sheet, Strip, and Plate

Specification	AMS 4911 and MIL-T-9046, Comp. AB-1					MIL-T-9046, Comp. AB-1			
Form	Sheet		Plate			Sheet, strip, and plate			
Condition	Annealed					Solution treated and aged			
Thickness, in.	≤ 0.1875		0.1875-2.000		2.001-4.000	≤ 0.1875	0.1875-0.750	0.751-1.000	1.001-2.000
Basis	A	B	A	B	S	S	S	S	S
Mechanical Properties:									
F_{tu}, ksi:									
L	134	139	130[a]	135	130	160	160	150	145
LT	134	139	130[a]	138	130	160	160	150	145
F_{ty}, ksi:									
L	126	131	120	125	120	145	145	140	135
LT	126	131	120[a]	131	120	145	145	140	135
F_{cy}, ksi:									
L	133	138	124	129	124	154	150	145	...
LT	135	141	130	142	130	162	...	...	...
F_{su}, ksi	87	90	79	84	79	100	93	87	...
F_{bru}, ksi:									
(e/D = 1.5)	213[b]	221[b]	206[b]	214[b]	206[b]	236	248	233	...
(e/D = 2.0)	272[b]	283[b]	260[b]	276[b]	260[b]	286	308	289	...
F_{bry}, ksi:									
(e/D = 1.5)	171[b]	178[b]	164[b]	179[b]	164[b]	210	210	203	...
(e/D = 2.0)	208[b]	217[b]	194[b]	212[b]	194[b]	232	243	235	...
e, percent (S-basis):									
L	8[c]	...	10	...	10	5[d]	8	6	6
LT	8[c]	...	10	...	10	5[d]	8	6	6
E, 10^3 ksi	16.0								
E_c, 10^3 ksi	16.4								
G, 10^3 ksi	6.2								
μ	0.31								
Physical Properties:									
ω, lb/in.^{3}	0.160								
C, K, and α	See Figure 4.5.1.0								

[a] The rounded T_{99} values are higher than specification values as follows: F_{tu}(L) = 131 ksi, F_{tu}(LT) = 132 ksi, and F_{ty}(LT) = 123 ksi.

[b] Bearing values are "dry pin" values per Section 1.4.7.1.

[c] 8%—0.025 to 0.062 in. and 10%—0.063 in. and above.

[d] 5%—0.050 in. and above; 4%—0.033 to 0.049 in. and 3%—0.032 in. and below.

To a Mechanical Engineer

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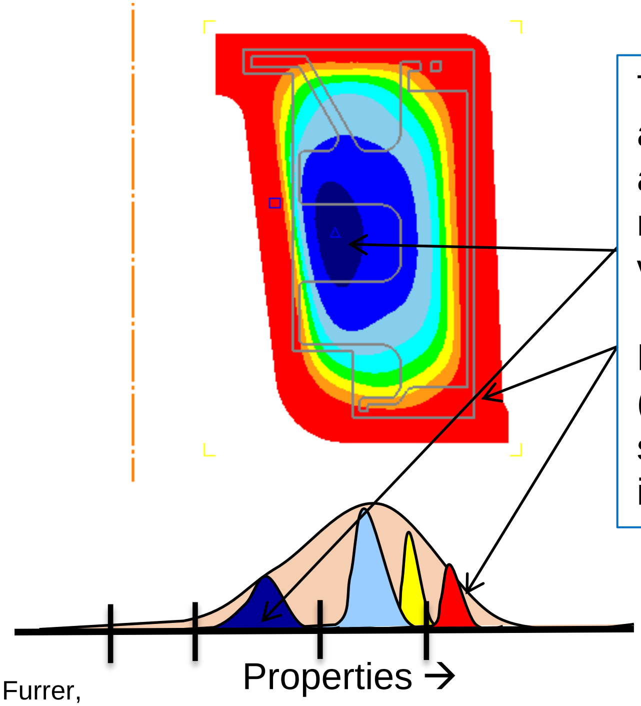
Materials Capability Definitions



True material capability and property distributions are controllable and reproducible; <u>not</u> "random variability".

Properties are a fn (chemistry, microstructure, stain, cooling rate, etc.); i.e. pedigree.

From D.Furrer,
OPTIMoM Conf., 2010

Materials properties are path dependent and are often "location-specific". Engineering specifications often treat entire material volume as single, homogeneous property capabilities.

Modeling and simulation can help enhance component property capability definitions

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Traditional Materials Definitions

- Design Curves – Empirical; Data Driven
- Specifications
- Prints Notes
- Fixed Process Requirements

Requires Defining Material Equivalency and Methods to Differentiate Material of One Control Pedigree from Another

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The Challenge: Need Models and Computational Infrastructure

Current materials definitions for design limit design flexibility and final component capabilities

There is a need for:

<u>Model-Based Materials Definitions</u>

Model-based material definitions enable location-specific prediction, analysis and optimization

Model-based materials definitions enable greater material, process and component definitions

Goal is prediction and control of capabilities

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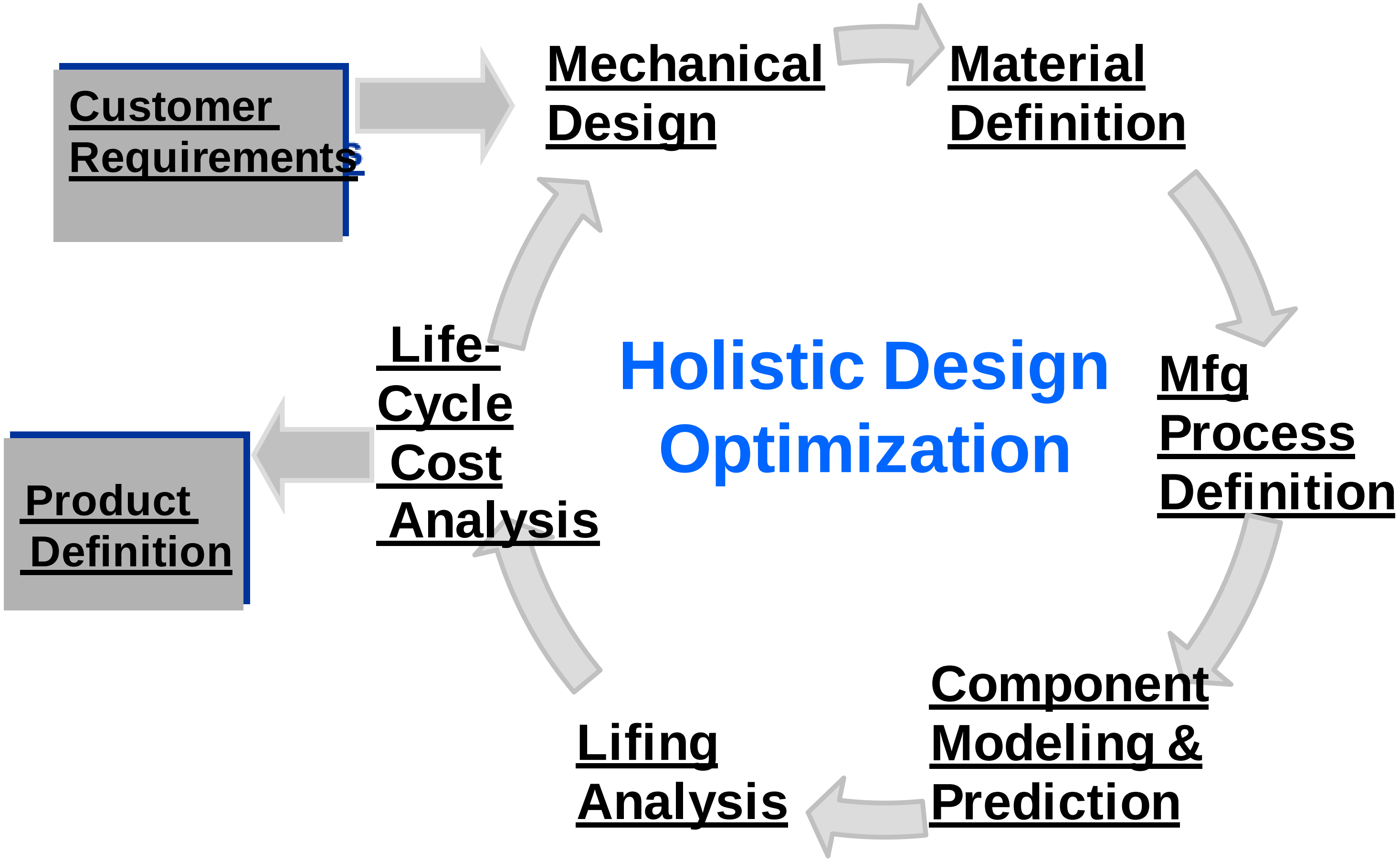
ICME Involved Linkage with Other Discipline Activities



Customer Requirements

Mechanical Design

Material Definition

Mfg Process Definition

Component Modeling & Prediction

Lifing Analysis

Life-Cycle Cost Analysis

Product Definition

Holistic Design Optimization

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Materials Technology Enablers

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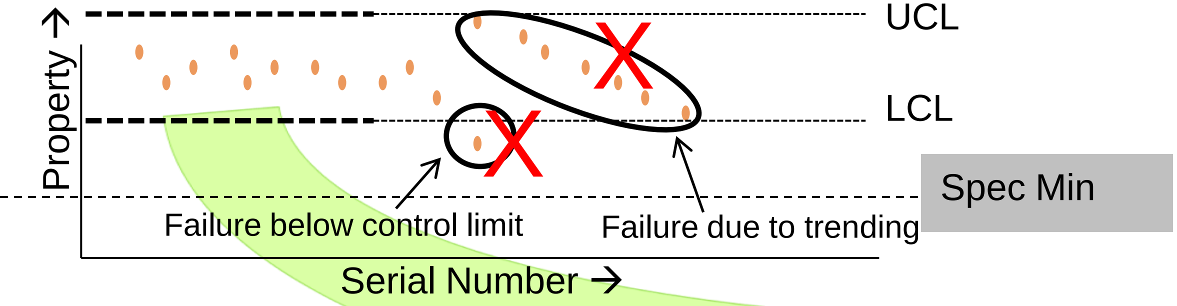
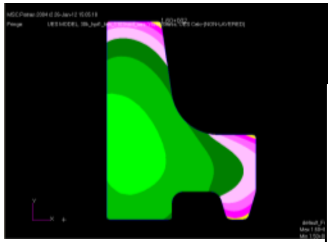
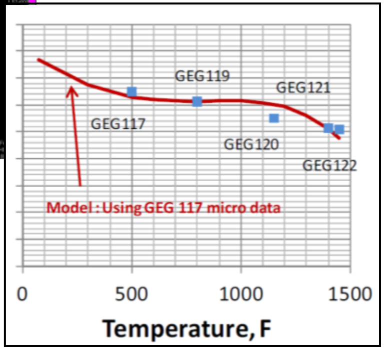
Computational Models and Advanced Data Management



Capture of developmental and production data to support model development

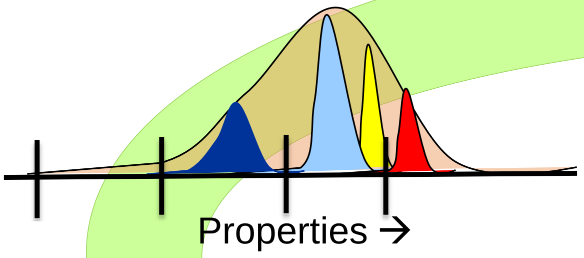


Predicted Material Properties

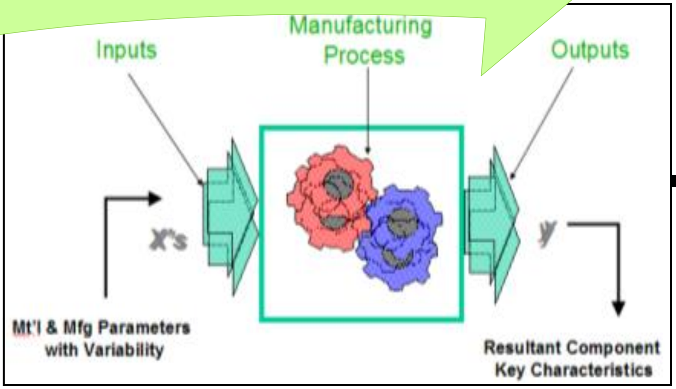


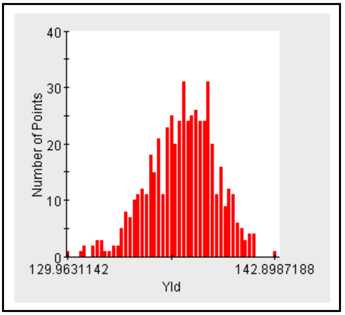
Goal is prediction and control of capabilities

Predicted Material and Component Properties



Traditional empirical property measurement and analysis migrating to materials models





Predicted Property Variability

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Material & Process Modeling Goals

- Develop Simulation Tools that Emulate Reality
- Develop Analytical Tools that Provide Insight in Material - Process - Property Relationships
- Implement Tools for Design and Manufacturing Benefits
  - Model-based Decisions
  - Tangible Improvements obtained based on Decisions

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Holistic Integration: Digital Thread

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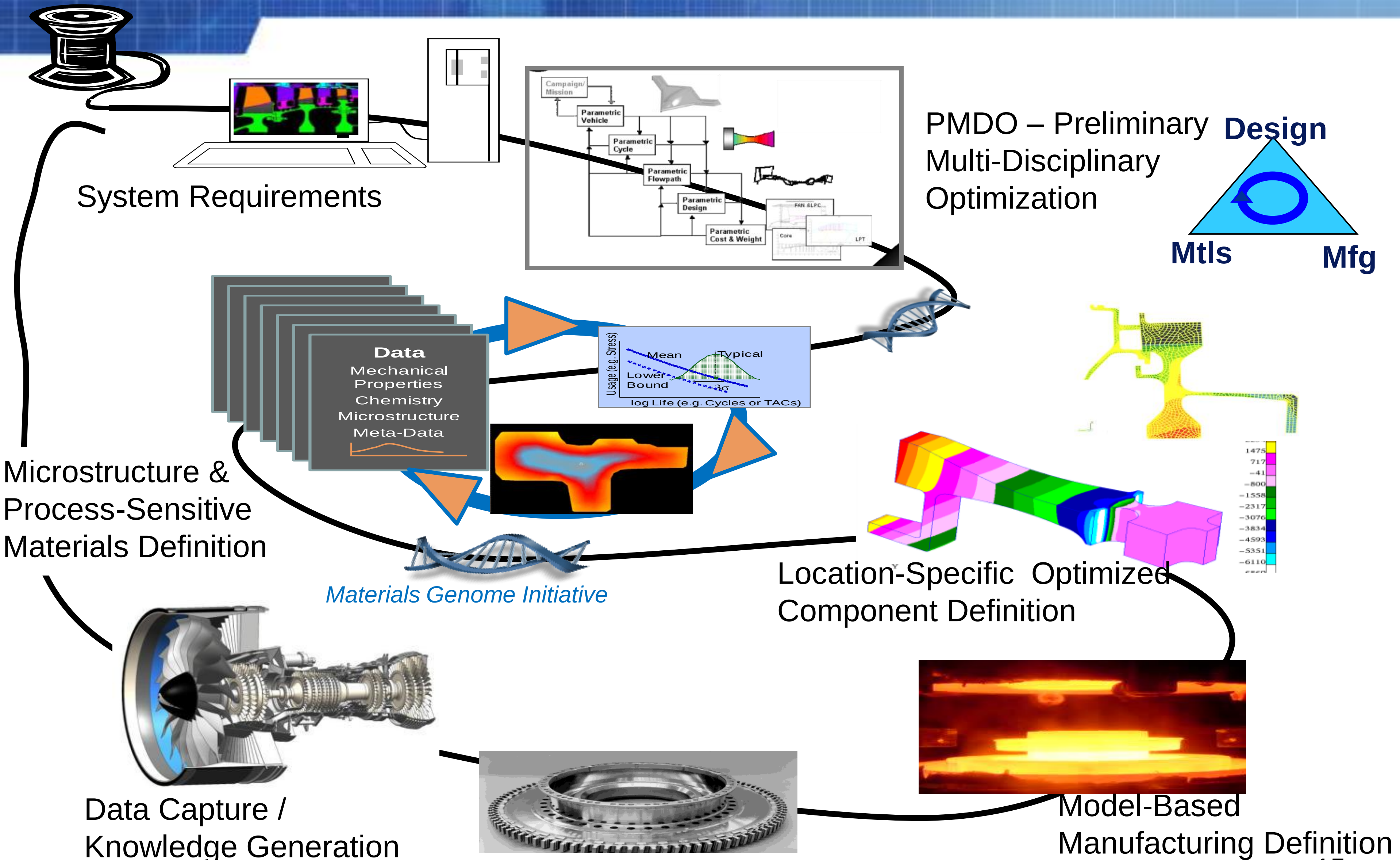
Example of Integrated Computational Materials & Mfg Engineering



System Requirements

PMDO – Preliminary Multi-Disciplinary Optimization

Microstructure & Process-Sensitive Materials Definition

Materials Genome Initiative

Location-Specific Optimized Component Definition

Data Capture / Knowledge Generation

Model-Based Manufacturing Definition

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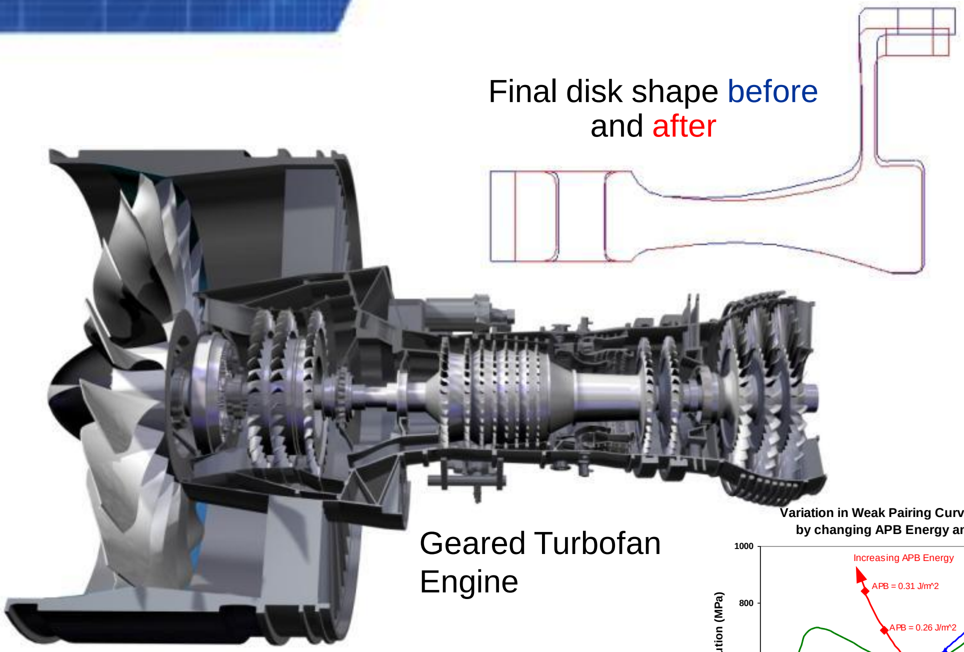
Example of ICME Application

- Feasibility of full design integration demonstrated
  - ➢ Over 600 design loop runs with coupled part geometry and material capability driving design evolution
  - ➢ Realistic case studies



Final disk shape before and after

Geared Turbofan Engine

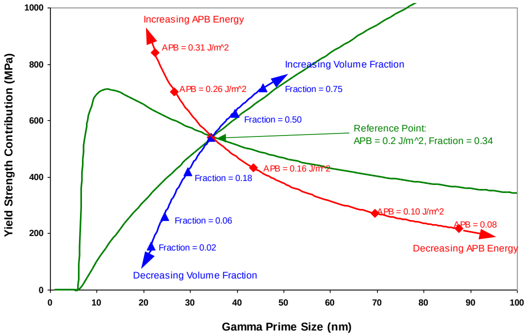
Yield of Primary γ'

Shearing of Secondary γ' (Pairs)

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

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

Shearing of Tertiary γ' γ Solid Soln Strengthening Hall-Petch γ Phase Hall-Petch Primary γ '



Variation in Weak Pairing Curve - Strong Pairing Curve Intersection by changing APB Energy and Volume Fraction Independently

Cost Benefit

System Benefits

>50% Reduction in Design Cycle Time

Case Study	Heat Treat	Forging	Part	Forge Wt	Part Wt	Burst Speed	Comments
1	Constant	Variable	Variable	-18%	-15%	+6%	Current State of the Art
2	Variable	Variable	Constant	-11%	n/a	+12%	Final Part shape constrained
3	Variable	Variable	Variable	-21%	-19%	+19%	Full impact of tool

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Disciplines Touched by ICMSE

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Integration of Computational Materials Science and Engineering is Complicated

- Materials
- Manufacturing
- Design
- Structures
- Quality
- Supply-Chain

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Challenges to Effective ICME Deployment

- Accurate computational models
- Efficient simulation software tools
- Data and databases for model application
- Industry standard methods and protocols
- Computational methods for design linkages
- Well trained interdisciplinary workforce

Unique engineering skill sets are required to support each challenge

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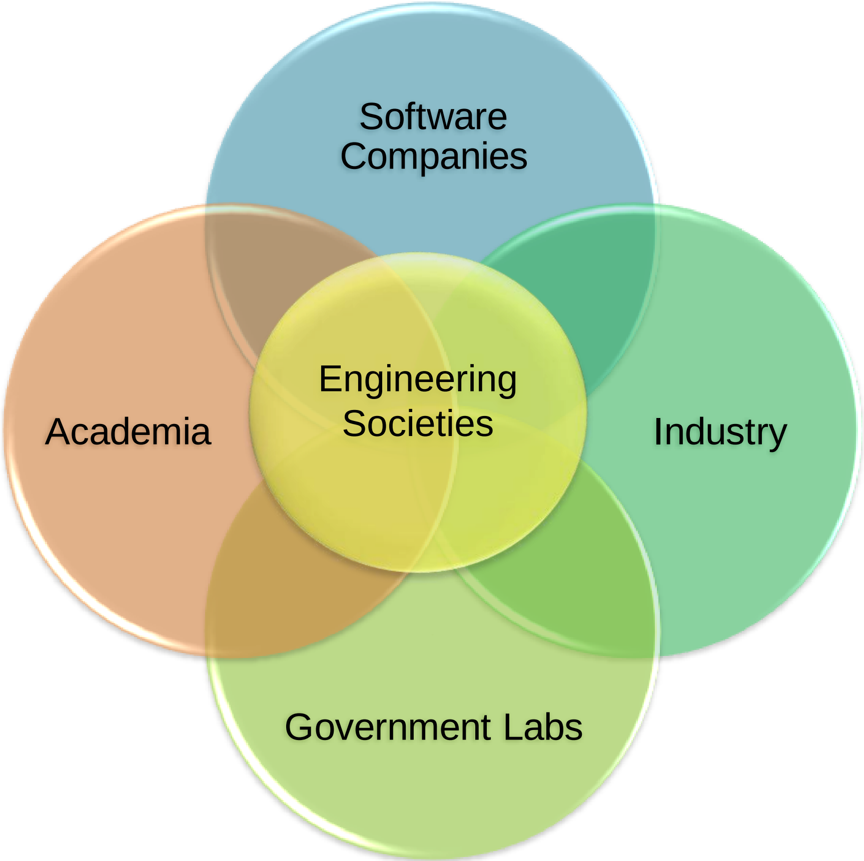
Computational Supply-Chain

A series of well-established, capable and viable organizations that provide necessary portions of the ICME Value Chain

- Fundamental Model Development
- Model Integration into Software Packages
- Maintenance of Software Tools
- Database Generation
- Application Engineering
- Customer Approval and Certification
- Education and Training



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Conclusions

- ICME: Potential for dramatic changes to development time, cost, and product capabilities
- Computational materials engineering enables virtual manufacture and component testing for optimization and risk mitigation
- Application of ICME has several challenges: trained practitioners; tools and methods; and computational infrastructure

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Any Questions?