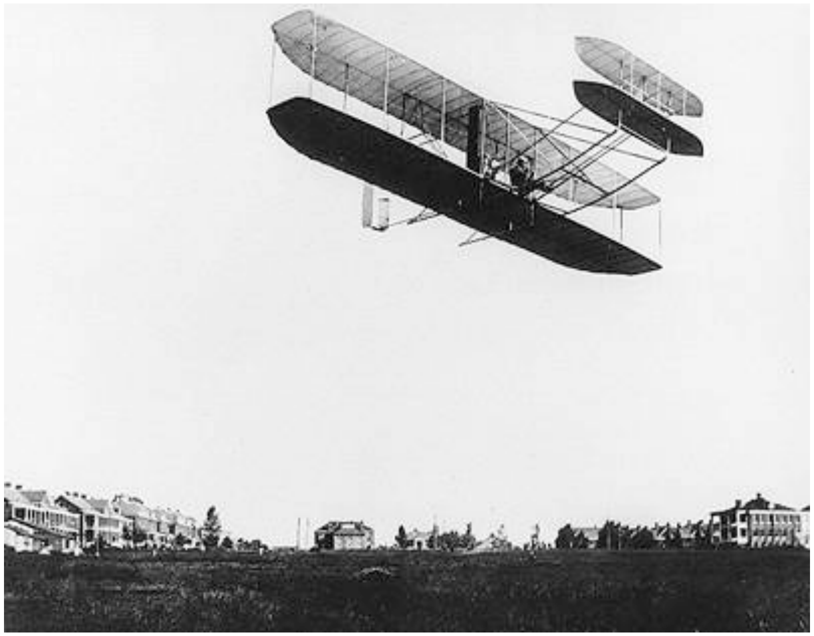
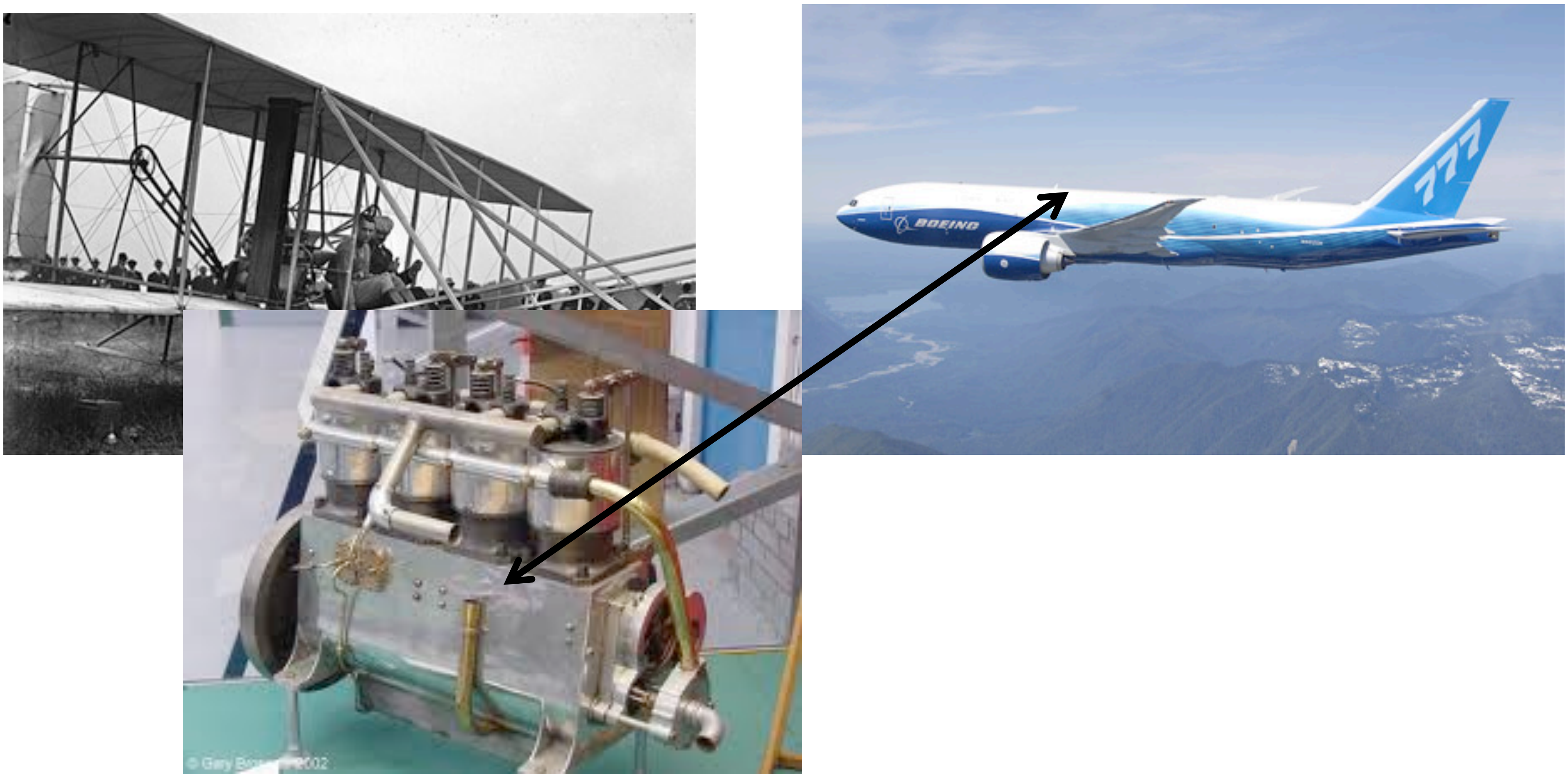
Computational Materials Science and the Materials Genome Initiative

Peter W. Voorhees
Department of Materials Science and Engineering
Center for Hierarchical Materials Design
Northwestern University
Evanston, IL

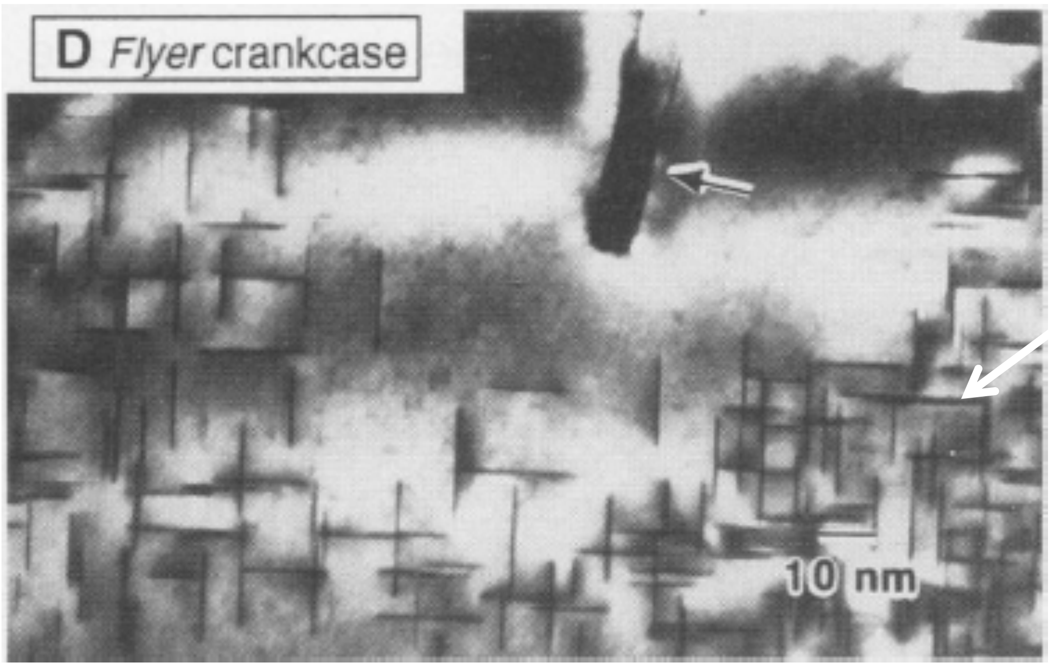
The Challenge:
What do these have in common?



The Materials For The Skin And Engine Block Are Both Al Alloys



Flyer Crankcase



Copper precipitates

Gayle and Goodway, Science 1994

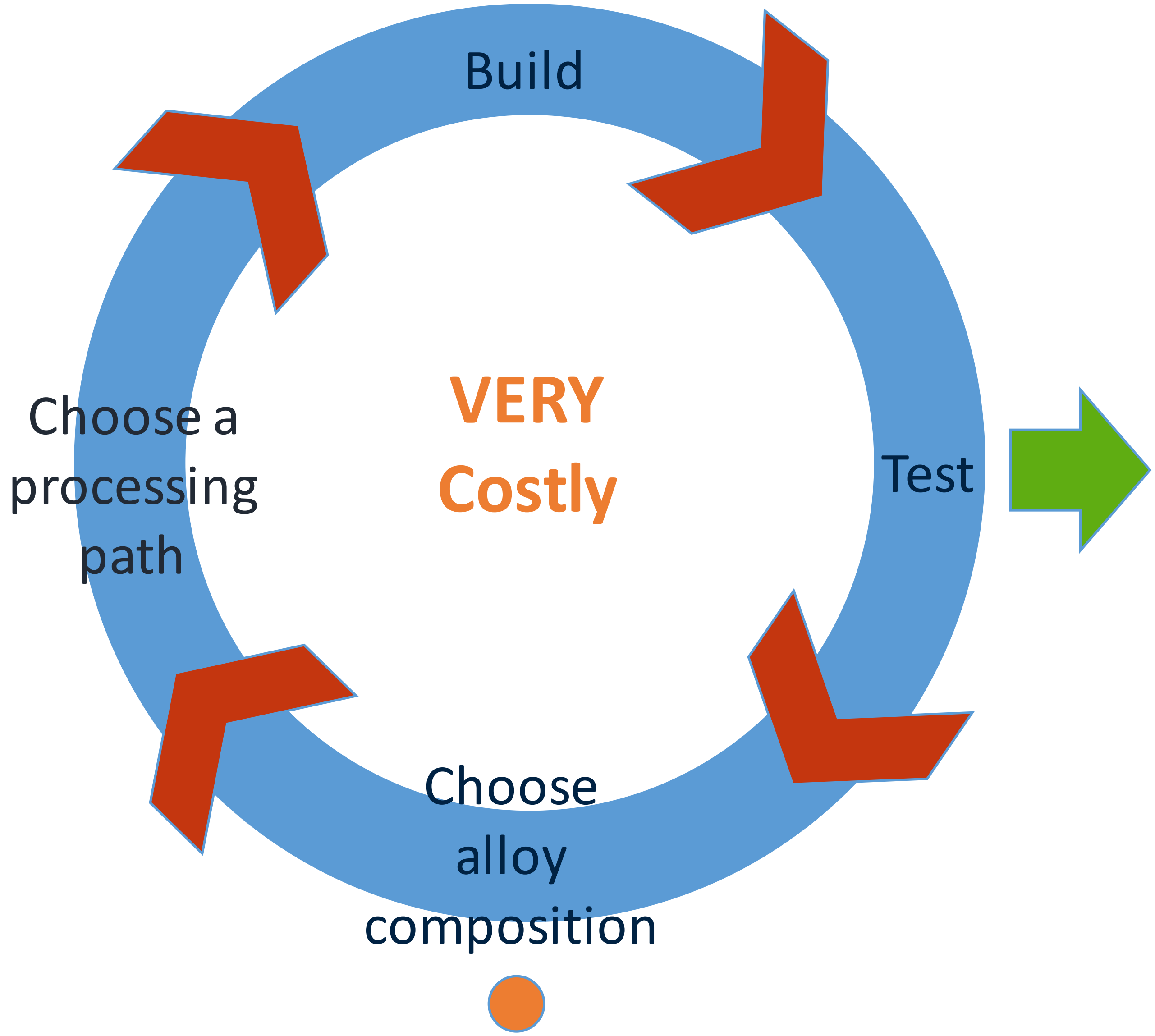
The Wright brothers created the first nanostructured material for aerospace applications

After 100+ Years of Alloy Development

"Al 319"

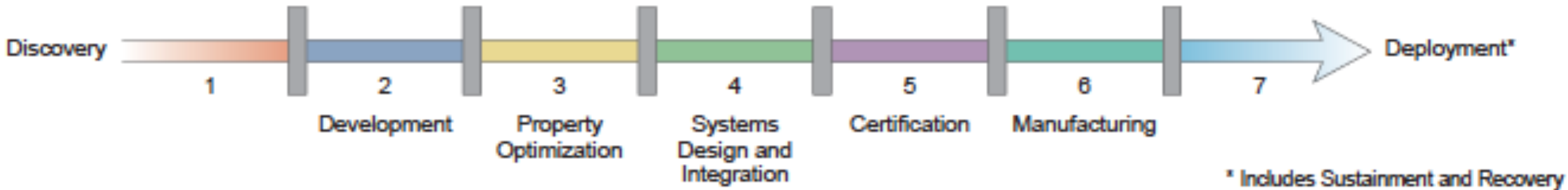
$Al_{88.08}Si_{7.43}Cu_{3.33}Mg_{0.22}Fe_{0.38}Mn_{0.24}Zn_{0.13}Ti_{0.12}Ni_{0.01}Cr_{0.03}Sr_{0.03}$

Traditional Approach



- Huge barrier to the introduction of new materials

Materials Development



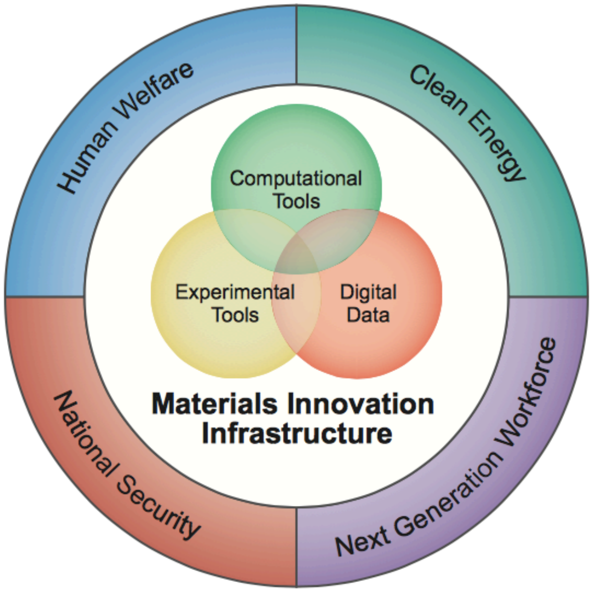
Solution:

Integrate computations, experimental tools, and digital data to speed up the design

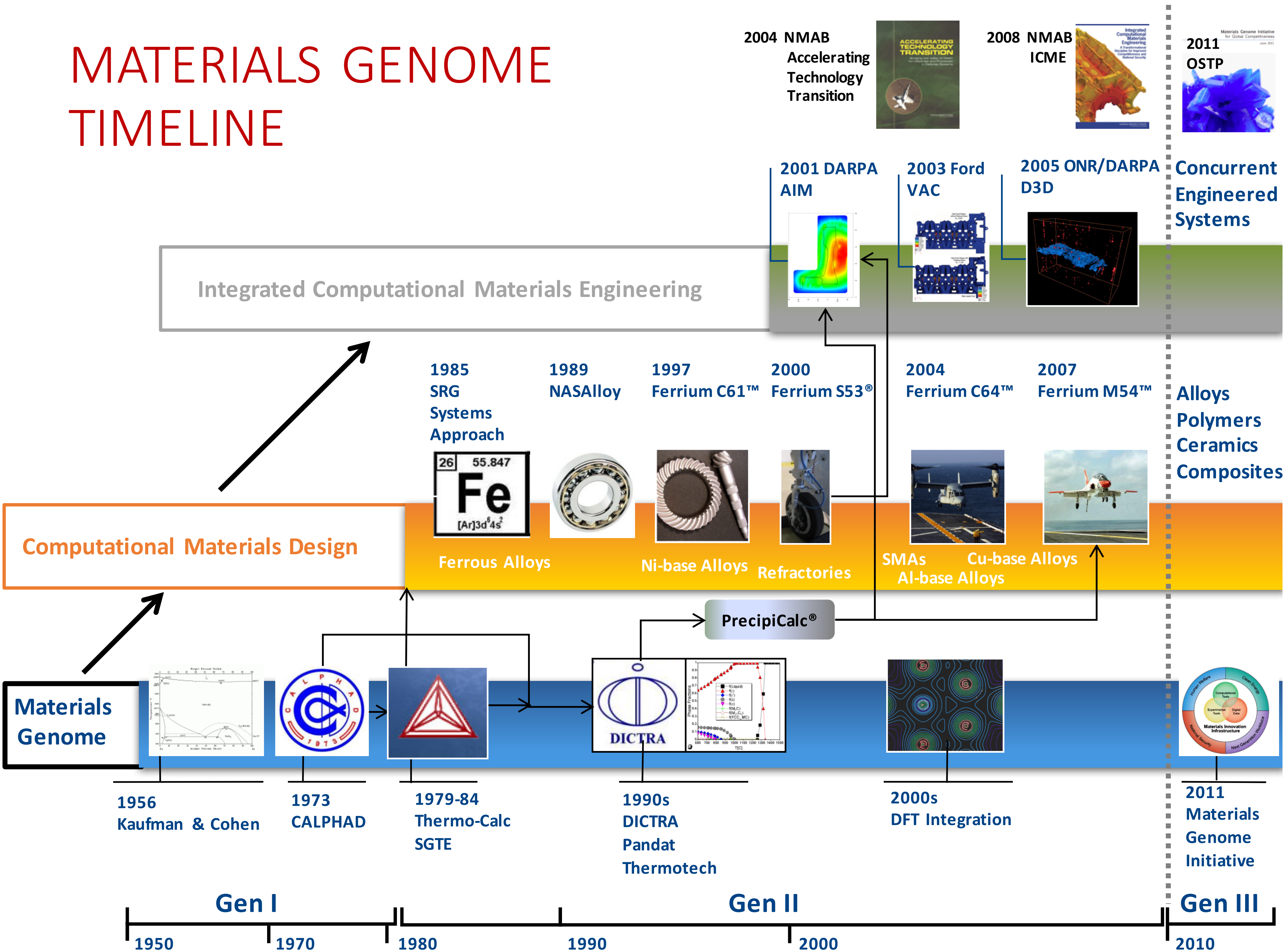
Materials Genome Initiative for Global Competitiveness – June 2011

Fundamental databases and tools enabling reduction of the 10-20 year materials creation and deployment cycle by 50% or more

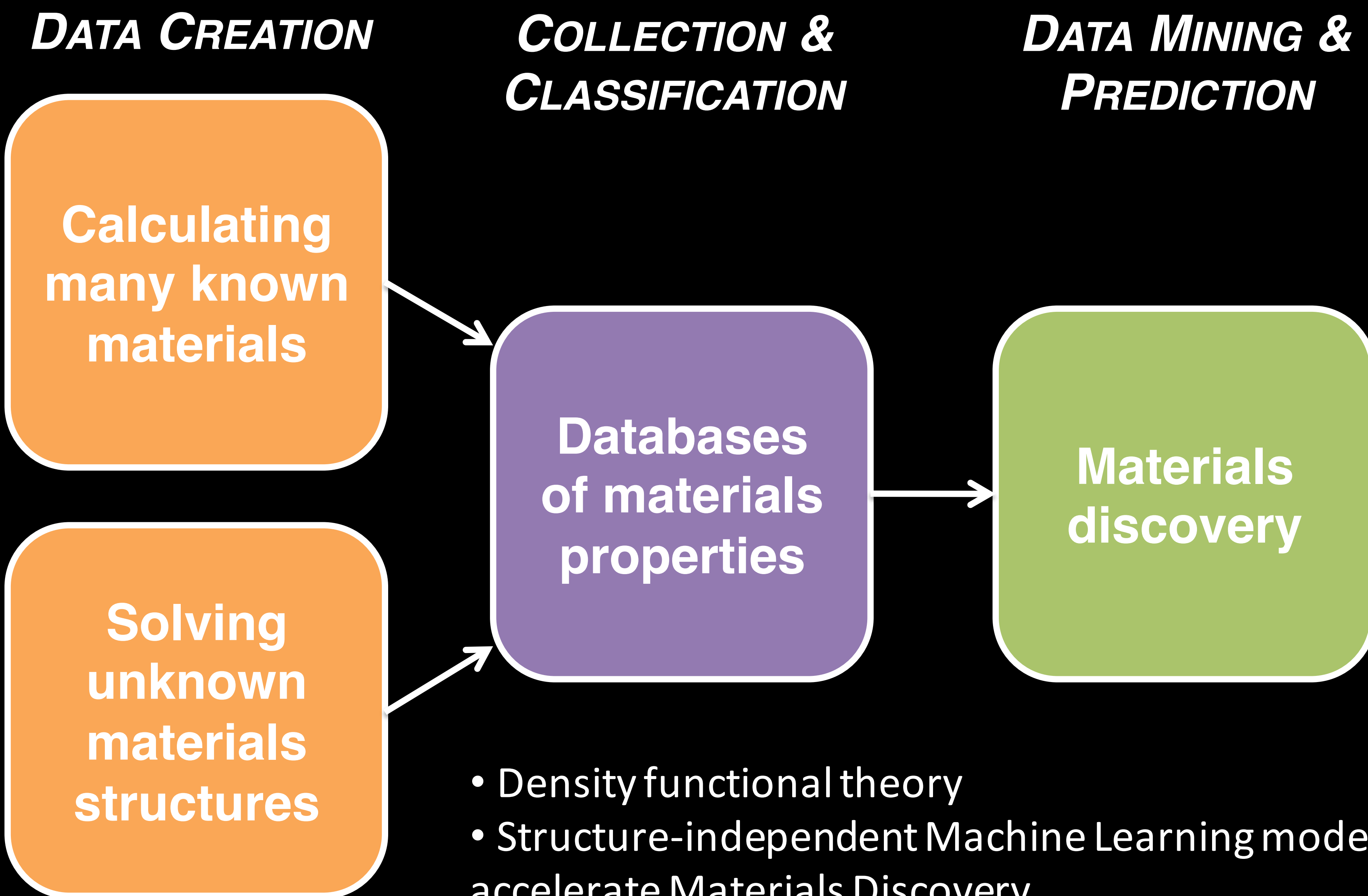
- Developing a Materials Innovation Infrastructure
  - Integrated experimental, computational, and data informatics tools
  - Span entire materials continuum
  - Open-access/Open-source
- Achieving National Goals with Advanced Materials
  - Develop the *infrastructure* to design new materials
- Equipping Next Generation Materials Workforce
- Engaging all stakeholders
  - Government, academia, and industry



www.whitehouse.gov/sites/default/files/microsites/ostp/materials_genome_initiative-final.pdf


MATERIALS GENOME TIMELINE
2004 NMAB Accelerating Technology Transition
2008 NMAB ICME
2011 OSTP
2001 DARPA AIM
2003 Ford VAC
2005 ONR/DARPA D3D
Concurrent Engineered Systems
Integrated Computational Materials Engineering
1985 SRG Systems Approach
1989 NASAlloy
1997 Ferrium C61™
2000 Ferrium S53®
2004 Ferrium C64™
2007 Ferrium M54™
Alloys
Polymers
Ceramics
Composites
Computational Materials Design
26
55.847
Fe
[Ar]3d6 4s2
Ferrous Alloys
Ni-base Alloys
Refractories
SMAs
Cu-base Alloys
Al-base Alloys
PrecipiCalc®
Materials Genome
DICTRA
1956 Kaufman & Cohen
1973 CALPHAD
1979-84 Thermo-Calc SGTE
1990s DICTRA Pandat Thermotech
2000s DFT Integration
2011 Materials Genome Initiative
Gen I
Gen II
Gen III
1950
1970
1980
1990
2000
2010

How to discover new compounds?



- Density functional theory
- Structure-independent Machine Learning model to accelerate Materials Discovery

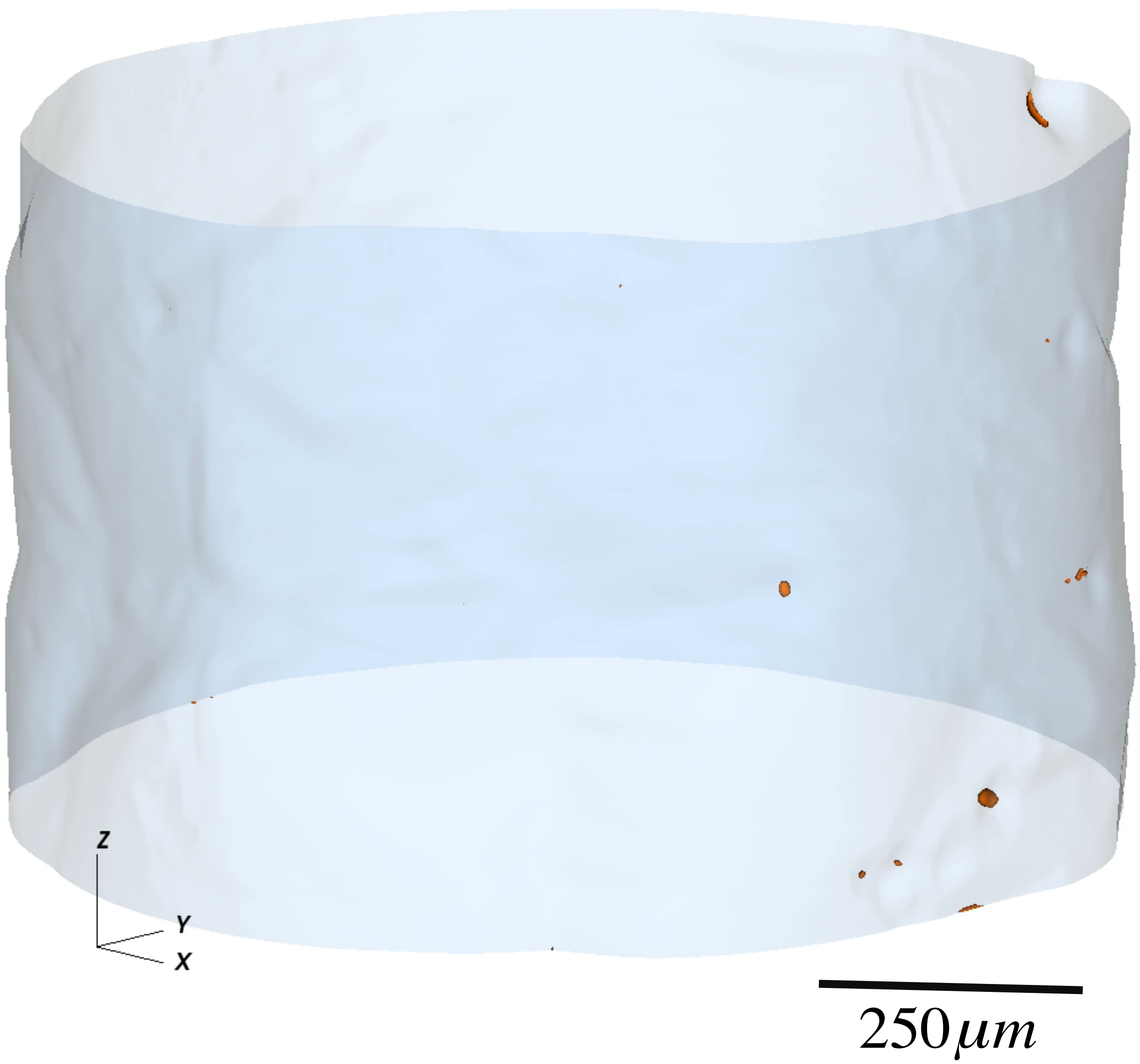
(C. Wolverton, Northwestern University)

Databases via High Throughput DFT Calculations

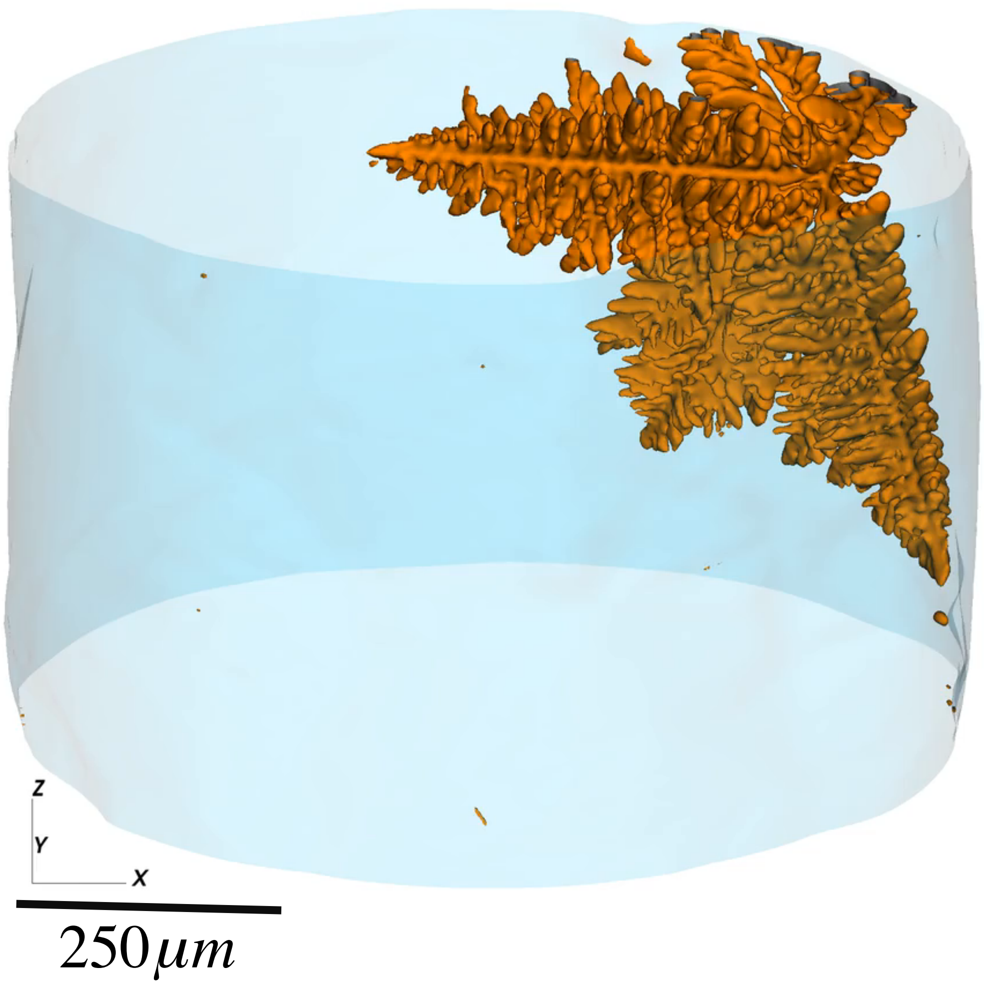
- DFT Databases: Materials Project (LBL), Open Quantum Mechanical Database (NU), and AFLOW (Duke), …
- For example, OQMD (OQMD.org, C. Wolverton) has thermodynamic and structural properties of 285,000 compounds “synthesized” on the computer
- This data can be mined to screen compounds for: Li-ion battery coatings, precipitates in Mg and Al alloys, high-efficiency thermoelectrics
- Accuracy? Metadata?

The looming Big Data Problem and the Challenge of Computing the Evolution of Interfaces in 3D

- 4D tomography of dendritic solidification



The Big Data Problem and Computing the Evolution of Interfaces in 3D

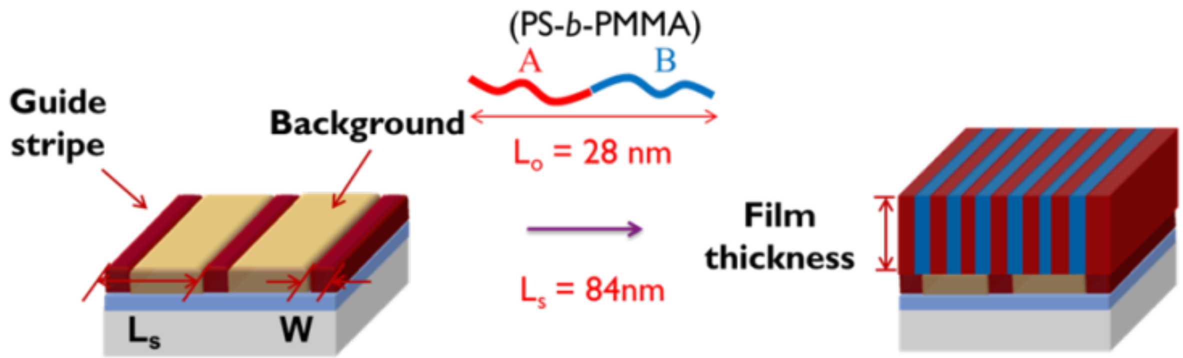


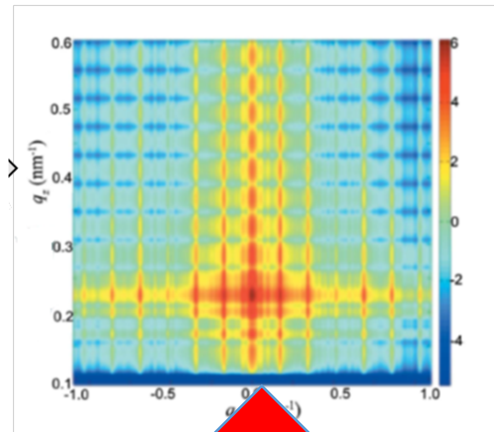
- Secondary arm spacing sets the fatigue life of the alloy
- It is not possible to compute the evolution the evolution of such a dendrite
- Typical data sets are 1-2 TB

J.W. Gibbs et al, Sci. Reports, 2015

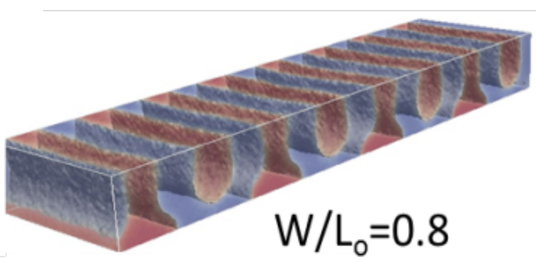
Directed Self Assembly: Nano Lithography

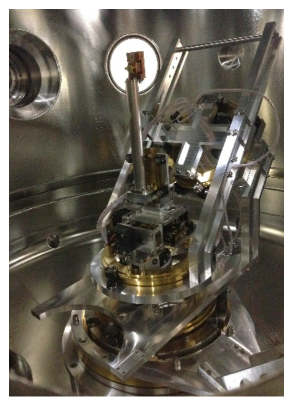
Paul Nealey and Juan De Pablo, University of Chicago



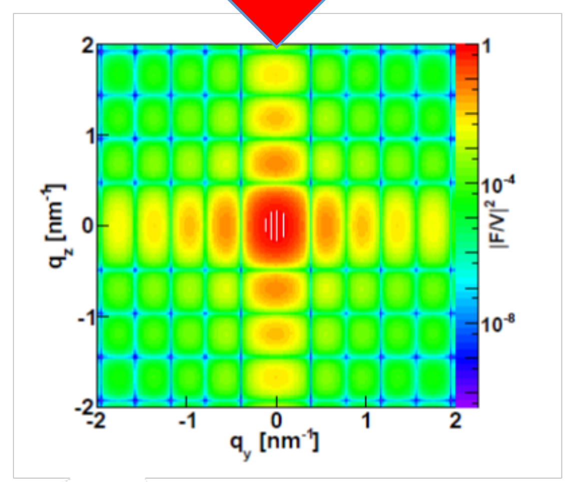


HiPG XS (LBNL)

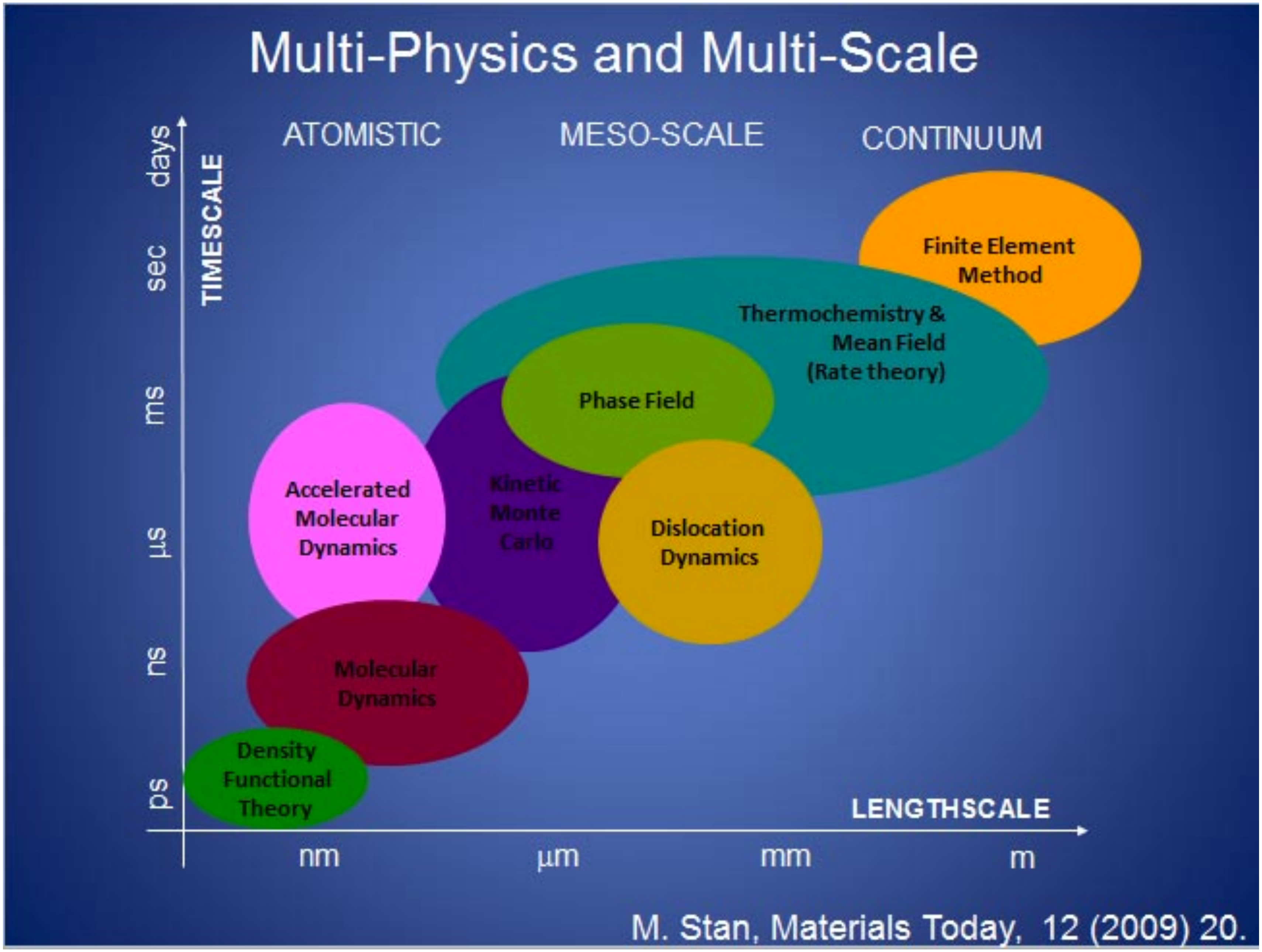




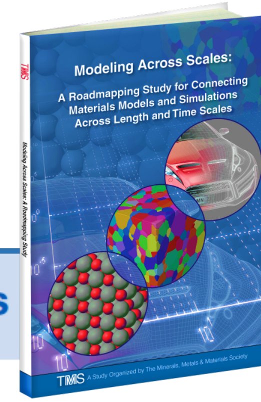
Diffractometer

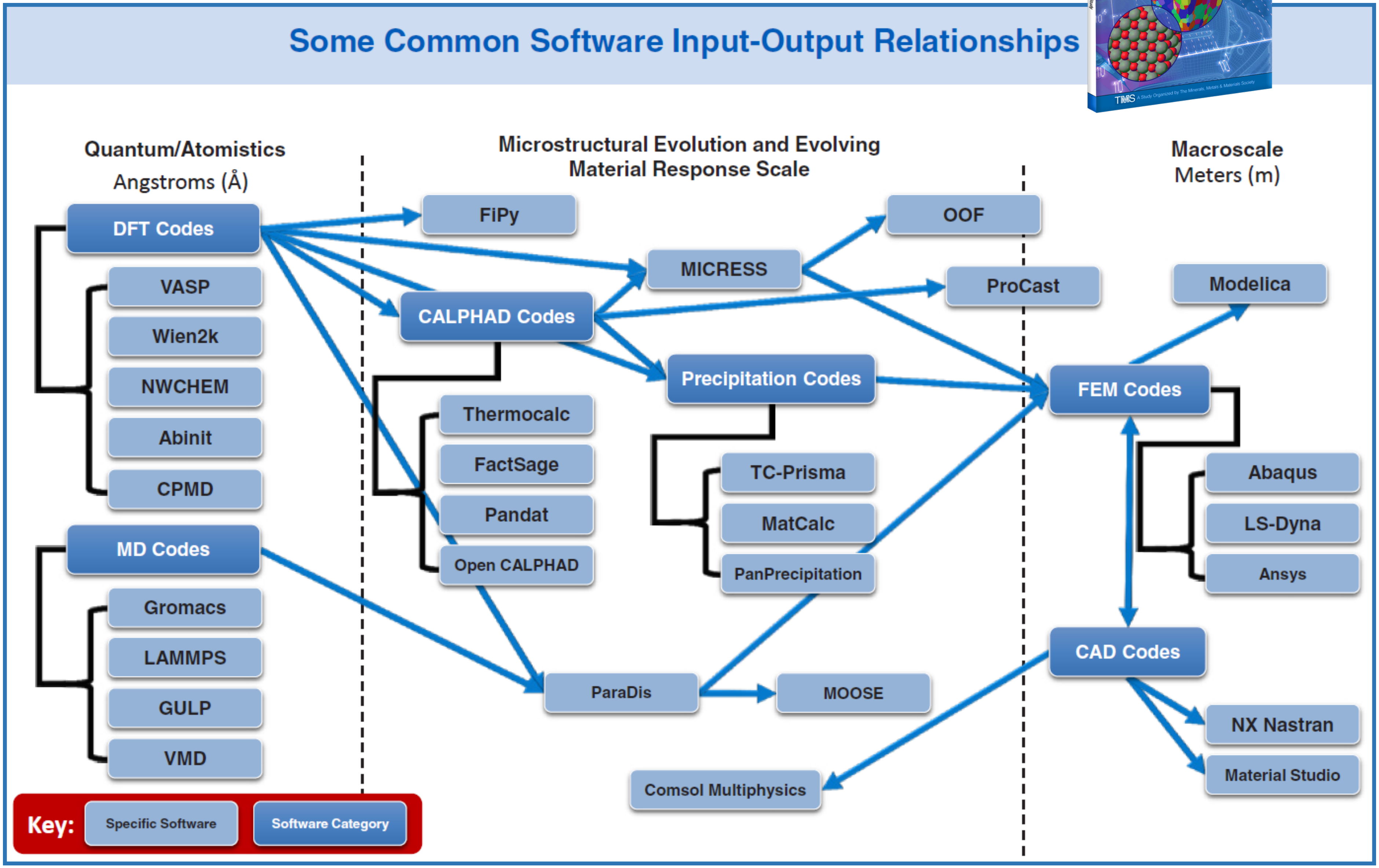


The challenge of modeling hierarchical materials structure



Current State of the Art





TMS Materials Models and Simulations Across Length and Time Scales Study

Selected recommendations:

- Develop initiatives that address uncertainty quantification and propagation (UQ/UP) across multiple models describing a range of material length and time scales
- Develop strong coupling methods that allow bidirectional communication between deformation and microstructural evolution models
- Develop focused research efforts addressing interfacial properties and nucleation effects, with particular emphasis on systematic studies that couple theory, experiments, and simulations across length and time scales
- Devise methods and protocols for taking into account rare events and extreme value statistical distributions