Welcome!

Jim Warren, National Institute of Standards and Technology
Executive Secretary, Interagency Working Group on the Materials Genome Initiative

Outline

- Whither MGI?
- What we need to do
- Current thoughts on where we are headed

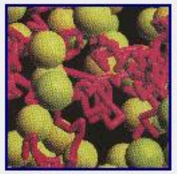
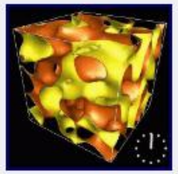
1996

NIST

Center for Theoretical and Computational Materials Science

ctcms

A center of expertise in computational materials research that develops tools and techniques, and fosters collaborations.


MISSION PROJECTS SEARCH

PEOPLE

ARCHIVES

REGISTER

1724 visitors since 1-18-96.

THE NIST CENTER FOR THEORETICAL AND COMPUTATIONAL MATERIALS SCIENCE

The Center's mission is to:

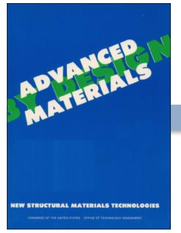
- investigate important problems in materials theory and modeling with novel computational approaches;
- create opportunities for collaboration where CTCMS can make a positive difference by virtue of its structure, focus, and people;
- develop powerful new tools for materials theory and modeling and accelerate their integration into industrial research.

The CTCMS story...

Historical Perspective

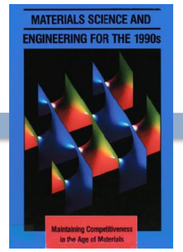
The Pursuit of Computation-guided Experimentation in Materials Research

1988



COTA: *Advanced Materials by Design*

1989



NRC: Materials Science & Engineering for the 1990s

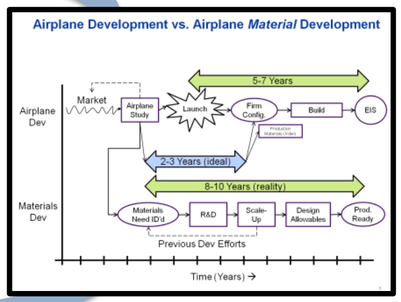
1995

DOE: Advanced Strategic Computing Initiative

1997

ONR: Computational Materials Engineering Grand Challenge Program

The Problem



1999

DARPA-AIM

Accelerated Insertion of Materials

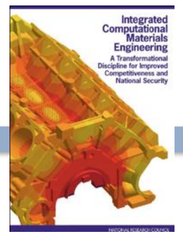
2001

AFOSR-MEANS

ONR-D3D

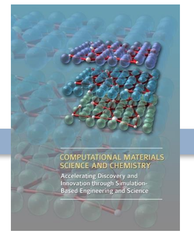
2004

NRC-ICME

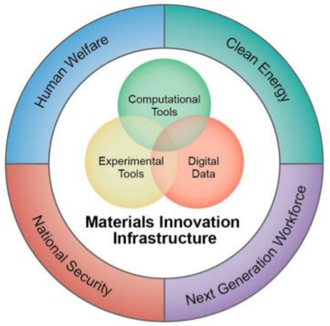


2008

DOE-CMS&C



2010



2011

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Adapted from T. Pollock, July 2011

Key Objectives

- Continue pushing for the development of state-of-the-art data and models that enable predictions of materials properties
  - Note that this includes all of the materials innovation infrastructure
- Leverage knowledge and capacity across the government and with key stakeholders worldwide
- Enable the US to achieve its objectives where advanced materials play a critical role

None of this works without data

And MATERIALS DATA IS EXPENSIVE

How do we get more?

THE GRAND VISION

- The MGI developed many new materials but insertion into manufacturing remains very challenging (bridging across many TRLs)
- Self driving labs not only can rapidly deliver targeted materials but also can generate the vast quantities of data required to create AI-based “surrogate models” of materials processes and properties that can substitute for traditional physics/chemistry models which are often very slow (but are still the benchmark for all modeling)
- These surrogate models can be used as “materials digital twins” which can operate at the speed of manufacturing, inserting materials knowledge into the manufacturing paradigm.
- This would accelerate materials R&D towards realizing engineering impact

AI REMAINS AT THE HEART OF THIS VISION!

Have a fantastic workshop!