The Materials Genome Initiative, Data, Open Science, and NIST

James A Warren
Technical Program Director for Materials Genomics
Material Measurement Laboratory
National Institute of Standards and Technology
Executive Secretary, NSTC Subcommittee on MGI

Science advances one funeral at a time -Max Planck

The Perfect is the Enemy of the Good -Voltaire

NIST's Mission

To promote U.S. innovation and industrial competitiveness by advancing

measurement science,

standards, and

technology

in ways that enhance economic security and improve our quality of life

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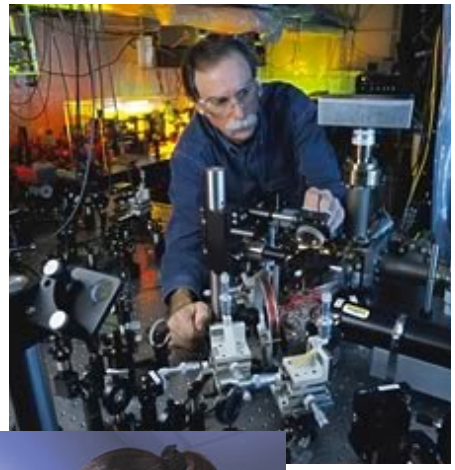
NIST at a Glance

Major Assets

- ~ 2800 employees ~(50/50 technical/admin)
- ~ 2600 associates and facilities users
- ~ 1600 field staff in partner organizations (Manufacturing Extension Partnership)



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Major Programs

- NIST Laboratories
- Baldrige Performance Excellence Program
- Hollings Manufacturing Extension Partnership

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NIST Products and Services


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Measurement Research

- ~ 2,200 publications per year

Standard Reference Data

- ~ 100 different types
- ~ 6,000 units sold per year
- ~ 226 million data downloads per year

Standard Reference Materials

- ~ 1,300 products available
- ~ 30,000 units sold per year

Calibration Tests

- ~ 18,000 tests per year

Laboratory Accreditation

- ~ 800 accreditations of testing and calibration laboratories

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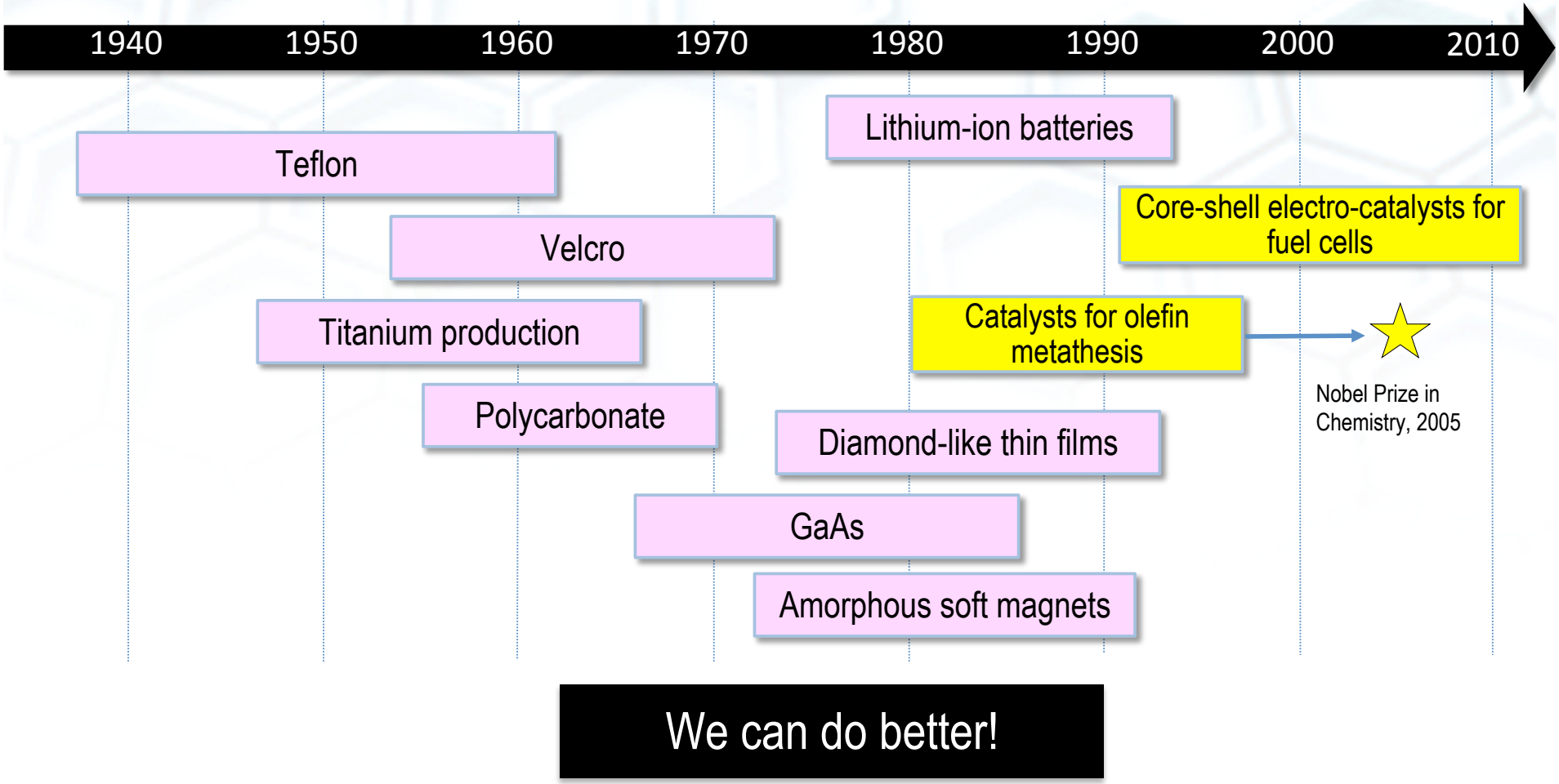
LAG FROM DISCOVERY TO APPLICATION OF NEW MATERIALS…



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.

THE MATERIALS GENOME INITIATIVE: A NATIONAL PRIORITY

"To help businesses discover, develop, and deploy new materials twice as fast, we're launching what we call the Materials Genome Initiative.

The invention of silicon circuits and lithium ion batteries made computers and iPods and iPads possible, but it took years to get those technologies from the drawing board to the market place.

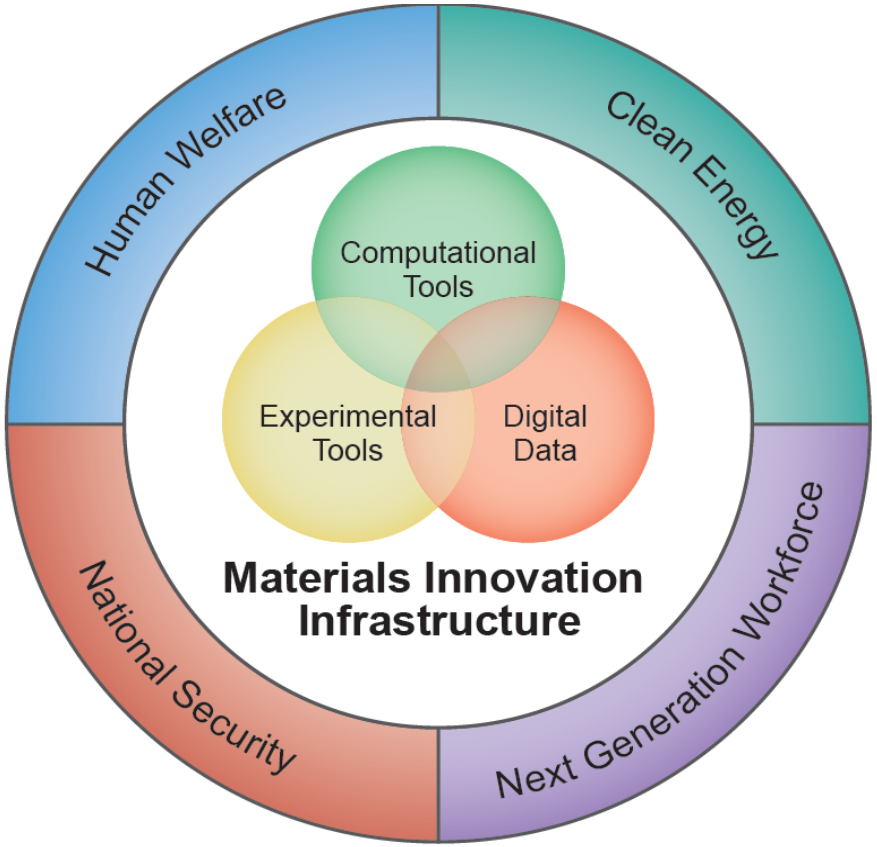
We can do it faster."

-President Obama (6/11)

There are two groups of people that don't like the name Materials Genome Initiative

THE MATERIALS GENOME INITIATIVE

to decrease time-to-market by 50% while <$$



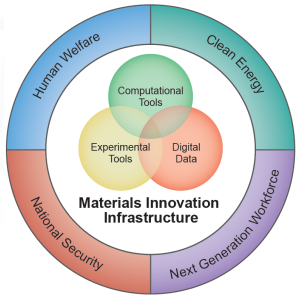
Develop a Materials Innovation Infrastructure

Achieve National goals in energy, security, and human welfare with advanced materials

Equip the next generation materials workforce

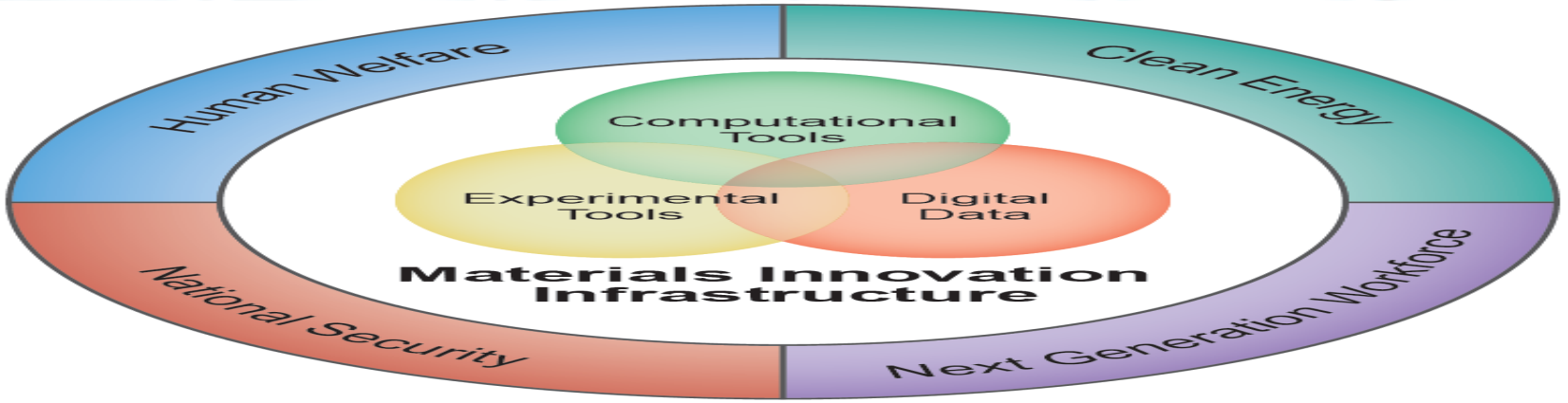
Materials Genome Initiative for Global Competitiveness

DESIGNING MATERIALS TODAY



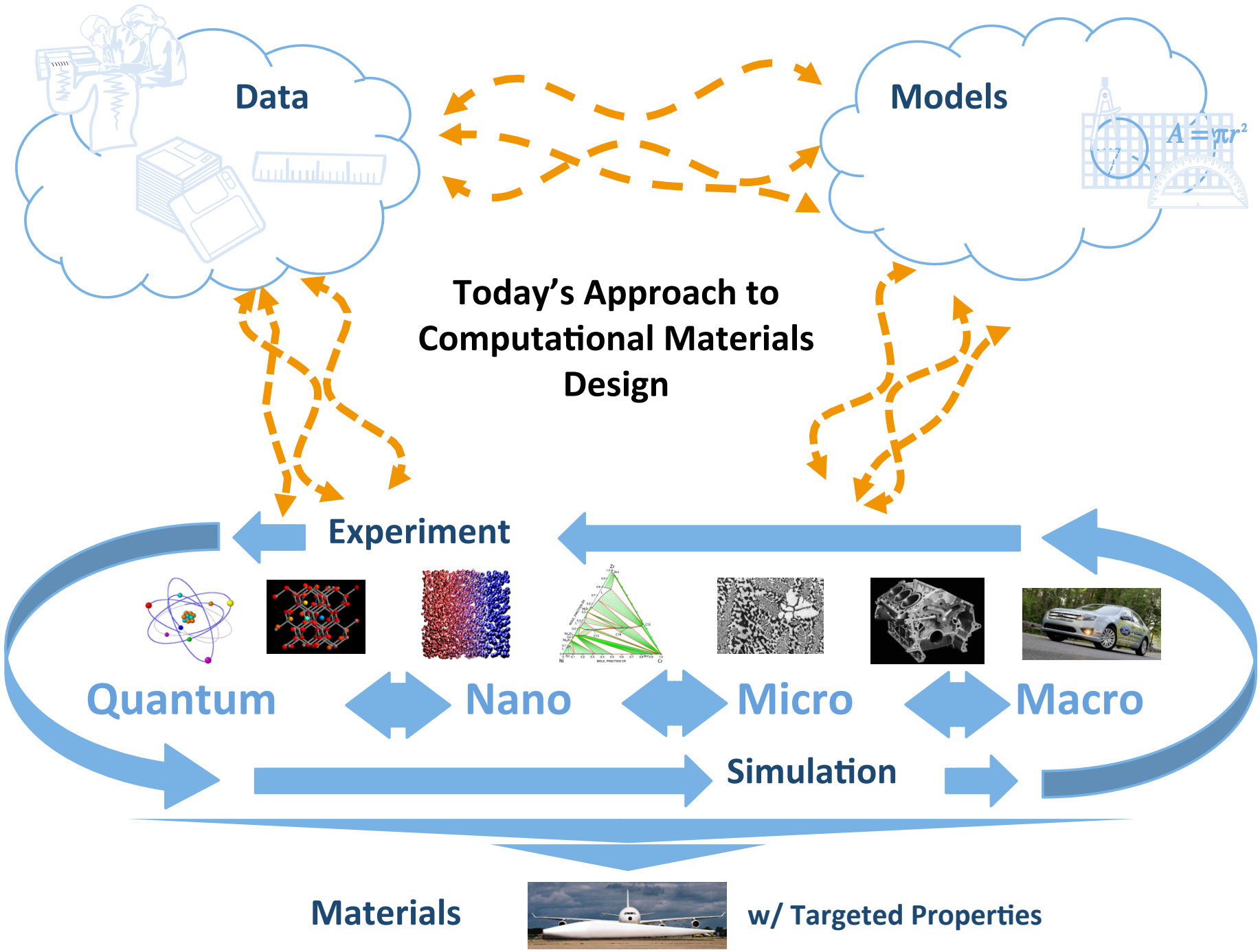
Discovery → Development → Property Optimization → Systems Design and Integration → Certification → Manufacturing → Deployment

DESIGNING NEW MATERIALS IN THE FUTURE



Discovery | Development | Property Optimization | Systems Design and Integration | Certification | Manufacturing | Deployment

Formulating the NIST Role in MGI


Data
Models
$A = \pi r^2$
Today's Approach to Computational Materials Design
Experiment
Quantum
Nano
Micro
Macro
Simulation
Materials
w/ Targeted Properties

SCOPE: Goals of Initiative at NIST

To foster widespread adoption of the MGI Paradigm both across and within the multitude of materials development ecosystems

Goal 1: NIST establishes *essential materials data and model exchange protocols*

Goal 2: NIST establishes the *means to ensure the quality* of materials data and models

Goal 3: NIST establishes *new methods, metrologies and capabilities* necessary for accelerated materials development.

*Enable & Enhance **Exchange***

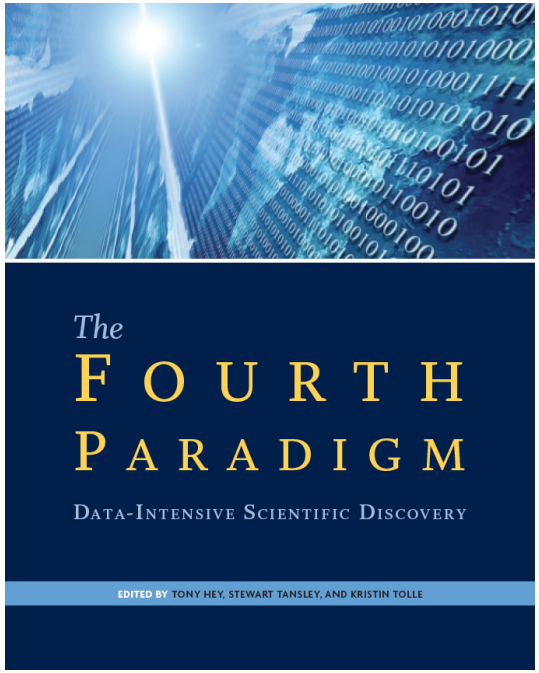
- Develop and deploy repositories
- Develop and disseminate materials informatics infrastructure
  - Enable data discovery through tools and standards
  - Capture data from scientific workflows and archival sources
  - Engage with stakeholders to determine needs and disseminate best practices
- Integrate across length and time scale
- Build and Test infrastructure through Pilots

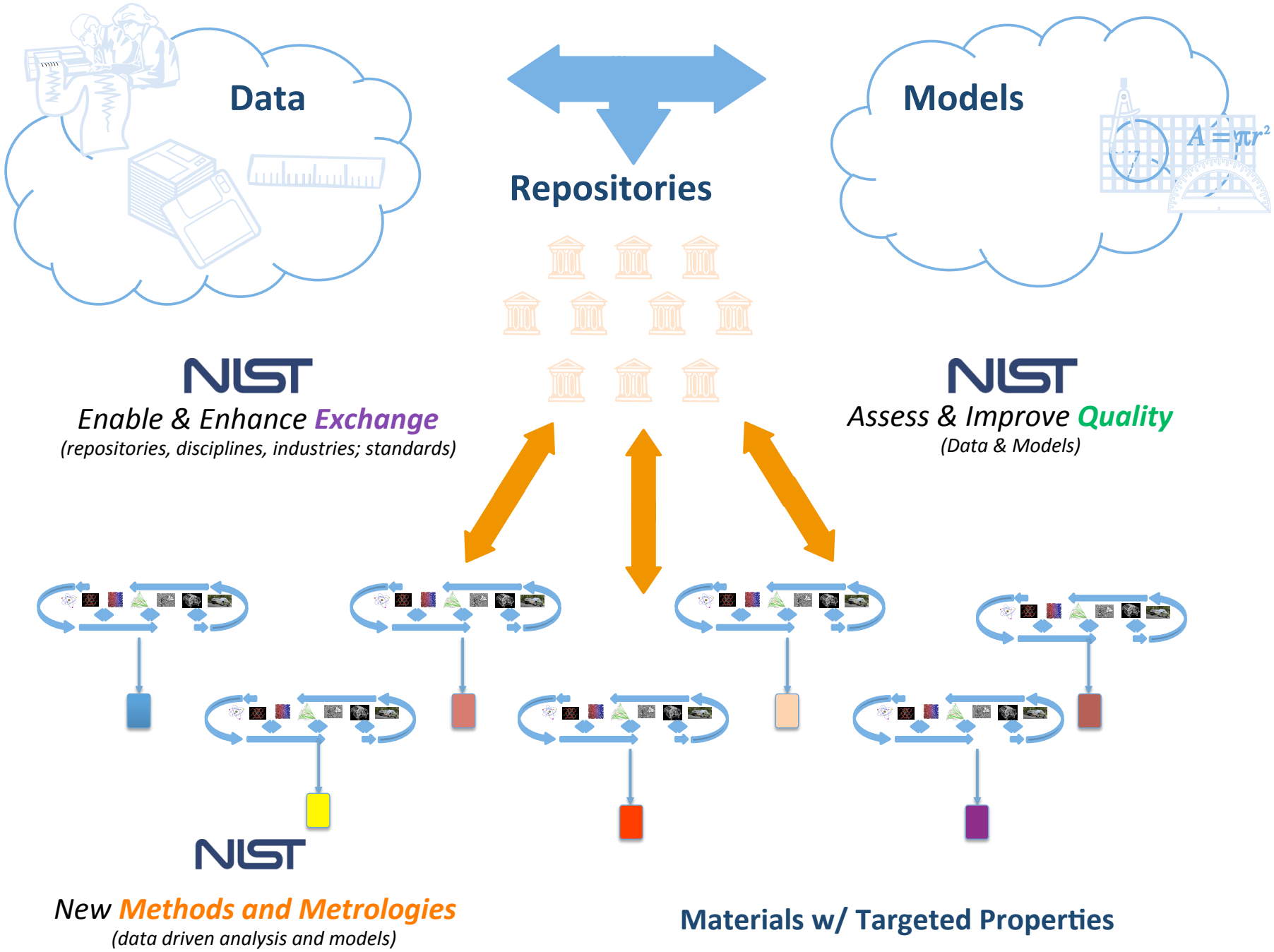
*Assess & Improve **Quality***

- Validate Experiments and Models
- Verify Model accuracy
- Quantify Uncertainty
- Quantify Sensitivity
- Define Next Generation of Experiments and Models

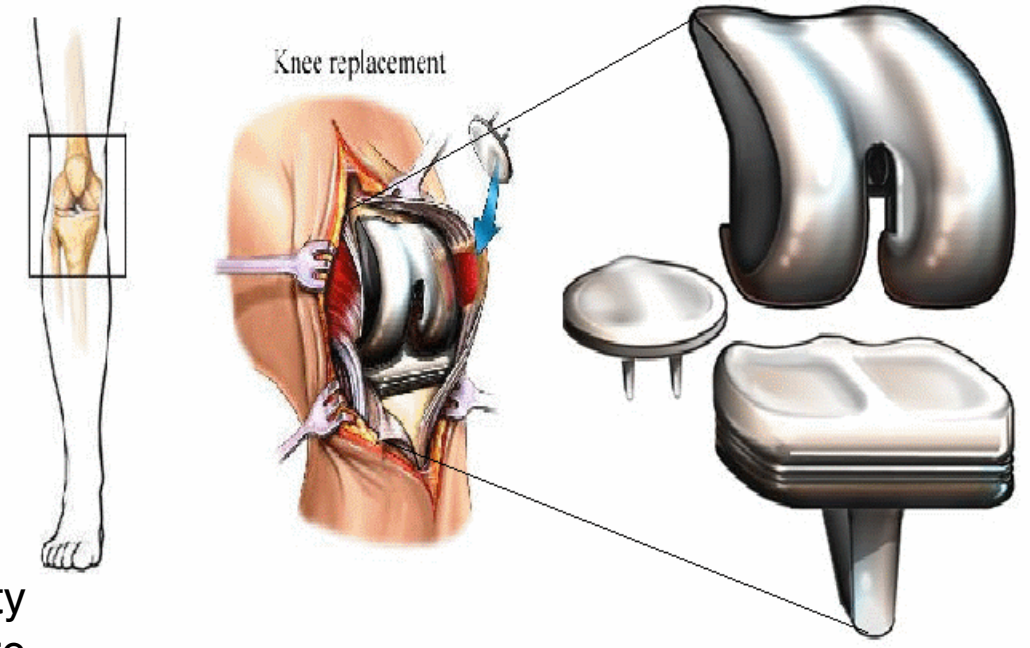
New ***Methods and Metrologies***

- Develop Data Driven Materials Science
- Integrate with Modeling Expertise
- Enable Crowdsourced/Open Science
- Achieve targets in Materials by Design/ICME




Data
Repositories
Models
$A = \pi r^2$
NIST
Enable & Enhance Exchange
(repositories, disciplines, industries; standards)
NIST
Assess & Improve Quality
(Data & Models)
NIST
New Methods and Metrologies
(data driven analysis and models)
Materials w/ Targeted Properties

Use Case Example



Required Data

- Crystallographic data (X-Ray info)
- Strength
- Stiffness
- Fatigue
- Wear Resistance, Toughness, Ductility
- Statistical metrics of the microstructure
- Microstructure images (from electron or optical microscopes)
- Cost
- It must comply with many other FDA regulations
- It must be amenable to manufacturing techniques needed to shape and finish the component (additive processes?)
- It must be made of bio-compatible material (Metrics of bio-compatibility include corrosion properties as well as allergic reactions)
- It must undergo a large number of deformations without significant degradation in properties (probably it needs to last at least 20 years under normal use for FDA approval). The larger this number can be made without degrading other properties, the better,

Search Requirements

Searches over multiple repositories **for data** on known materials that meet all of the above constraints, **simultaneously**

Searches on ***models*** that allow for parametric variation of processing and composition variables, to design new materials with improved properties

Data Sharing is Important Beyond MGI & NIST

OSTP "Public Access" Memo
Feb 22, 2013

EXECUTIVE OFFICE OF THE PRESIDENT
OFFICE OF SCIENCE AND TECHNOLOGY POLICY
WASHINGTON, D.C. 20502

February 22, 2013

MEMORANDUM FOR THE HEADS OF EXECUTIVE DEPARTMENTS AND AGENCIES

FROM: John P. Holdren
Director

SUBJECT: Increasing Access to the Results of Federally Funded Scientific Research

1. Policy Principles

The Administration is committed to ensuring that, to
constraints possible and consistent with law and the
federally funded scientific research are made availat
the scientific community. Such results include peer-

Scientific research supported by the Federal Govern
drive our economy. The results of that research becc
for progress in areas such as health, energy, the envi

Access to digital data sets resulting from federally fi
resources and efforts on understanding and exploitir
data underpins the forecasting industry, and making
spawned many biotechnology innovations. In additi
publications and scientific data in digital formats wi
services related to curation, preservation, analysis, a
publications and data for re-use through preservatio
the impact and accountability of the Federal researcl
scientific breakthroughs and innovation, promote en
growth and job creation.

Executive Order
May 9, 2013

For Immediate Release

May 09, 2013

Executive Order -- Making Open and Machine Readable the New Default for Government Information

EXECUTIVE ORDER

MAKING OPEN AND MACHINE READABLE THE NEW DEFAULT
FOR GOVERNMENT INFORMATION

By the authority vested in me as President by the Constitution and the laws of the United States of America, it is hereby ordered as follows:

Section 1. General Principles. Openness in government strengthens our democracy, promotes the delivery of efficient and effective services to the public, and contributes to economic growth. As one vital benefit of open government, making information resources easy to find, accessible, and usable can fuel entrepreneurship, innovation, and scientific discovery that improves Americans' lives and contributes significantly to job creation.

Decades ago, the U.S. Government made both weather data and the Global Positioning System freely available. Since that time, American entrepreneurs and innovators have utilized these resources to create navigation systems, weather newscasts and warning systems, location-based applications, precision farming tools, and much more, improving Americans' lives in countless ways and leading to economic growth and job creation. In recent years, thousands of Government data resources across fields such as health and medicine, education, energy, public safety, global development, and finance have been posted in machine-readable form for free public use on Data.gov. Entrepreneurs and innovators have continued to develop a vast range of useful new products and businesses using these public information resources, creating good jobs in the process.

OMB "Open Data" Memo
May 9, 2013

EXECUTIVE OFFICE OF THE PRESIDENT
OFFICE OF MANAGEMENT AND BUDGET
WASHINGTON, D.C. 20503

THE DIRECTOR

May 9, 2013

M-13-13

MEMORANDUM FOR THE HEADS OF EXECUTIVE DEPARTMENTS AND AGENCIES

FROM: Sylvia M. Burwell

Officer

ficer

ice of Information and Regulatory Affairs

ging Information as an Asset

ource and a strategic asset to the Federal Government, its
at the Federal Government is taking full advantage of its
and agencies (hereafter referred to as "agencies") must
s life cycle to promote openness and interoperability, and
Managing government information as an asset will increase
e services, support mission needs, safeguard personal
luable government information.

ible, discoverable, and usable by the public can help fuel



Office of Data and Informatics

Material Measurement Laboratory

Robert J. Hanisch, ODI Director

NIST
National Institute of
Standards and Technology
U.S. Department of Commerce

MATERIAL
MEASUREMENT
LABORATORY

About ODI

- Overall goal: establish the technical infrastructure and foster a culture of first-class data management for MML, eventually for all of NIST
- Near term initiatives
  - Update Standard Reference Data collection
    - Web-based user interfaces
    - Application Programming Interfaces (APIs)
  - Implement OMB/OSTP open access data policy
    - Laboratory-wide Data Management Plans
    - NIST-wide Enterprise Data Inventory, data.gov
  - Build solution inventory for data management systems
    - Storage
    - Metadata
    - Electronic Lab Notebooks
- Informatics / data analytics consulting
- ODI works closely with Materials Genome Initiative