Scientific Computing and the The Materials Genome Initiative

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Outline

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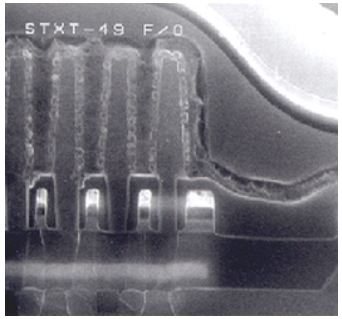
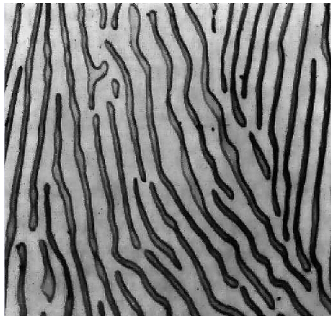
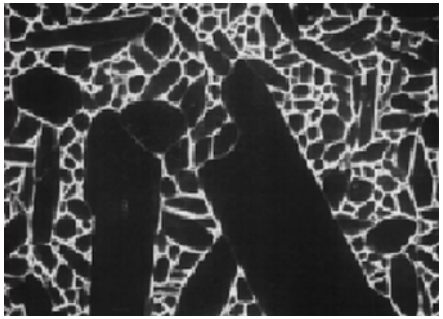
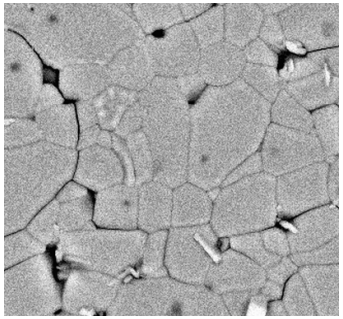
What's a Material?

A material is a particularly interesting or economically important arrangement of atoms, typically with several layers of structure.



Real materials typically embody a complex processing history, and remain far from equilibrium when in service.

What's Materials Science?

The study of the processing, structure, and properties of materials. Materials themselves are highly interactive, and so materials science is correspondingly interdisciplinary.

- Physics — solid mechanics and micromechanics, bulk properties
- Chemistry — reactions during processing, kinetics
- Modeling — approximate rules for behavior, interactions
  - Linear response is a common model

Outline

The Announcement

Announced in June of 2011 at Carnegie Mellon University:

"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."

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`http://www.whitehouse.gov/mgi`

The Objectives

Basic Goal: Reduce time-to-market for new materials by 50% or more.

- Develop a Materials Innovation Infrastructure
- Use advanced materials to reach goals in energy, security, and human welfare
- Educate the next generation materials workforce

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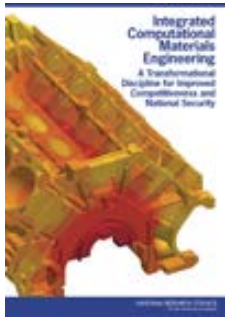
Precursors

QuesTek® INNOVATIONS LLC



The origin of the MGI reaches back in time...

- Academic research efforts
  - Steel Research Group / QuesTek (1990s)
- 2004 NRC report, uses “genome” terminology
- DARPA AIM
- ICME, successful aluminum alloy design
- Others...

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Multi-agency formulation

The MGI's origins also span many agencies...

NIST, DOE, NSF, DOD worked with OSTP to prepare the initial MGI white paper (2010-2011)

Precursor themes

These all had unifying themes:

- Bridge modeling length scales
  - Some institutions have these under one roof
- Use and/or build databases
- Solve the “inverse problem” — design a material!

Sound like anyone you know?

The issues addressed, and the breadth of scope, are familiar to the Python and SciPy communities.

SciPy is about the tools.

- SciPy co-hosted with DDANSE neutron-data effort, 2006
- Focus area on data science, 2011
- Focus area on HPC, 2012
- Focus area on machine learning, 2013
- Focus area on reproducible science, 2013

Government-wide response

MGI is administered by an NSTC Subcommittee whose members include NIST, DOE, DOD, NSF, NASA, NIH, USGS, and OMB.

This breadth reflects the breadth of the task, which calls for efforts in data science, workflow tools, parallel and high-performance computing, and high-throughput techniques of various kinds, as well as education.

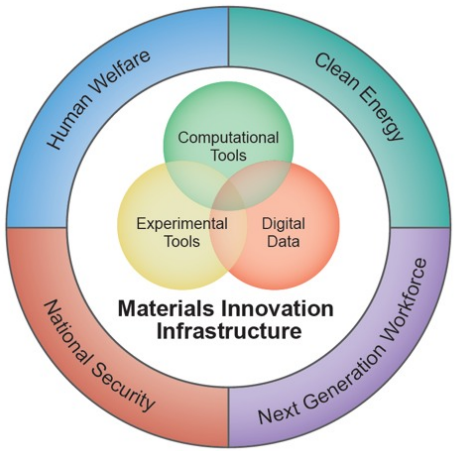
Outline

NIST in the World

Mission: To promote US innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve our quality of life.

Vision: NIST will be the world's leader in creating critical measurement solutions and promoting equitable standards. Our efforts stimulate innovation, foster industrial competitiveness, and improve the quality of life.

NIST Tasks



Work with the materials community to develop:

- Computational tools, validated databases, data assessment tools, and standards
- Reference models and simulations
- Information exchange mechanisms based on community consensus
- A Center of Excellence

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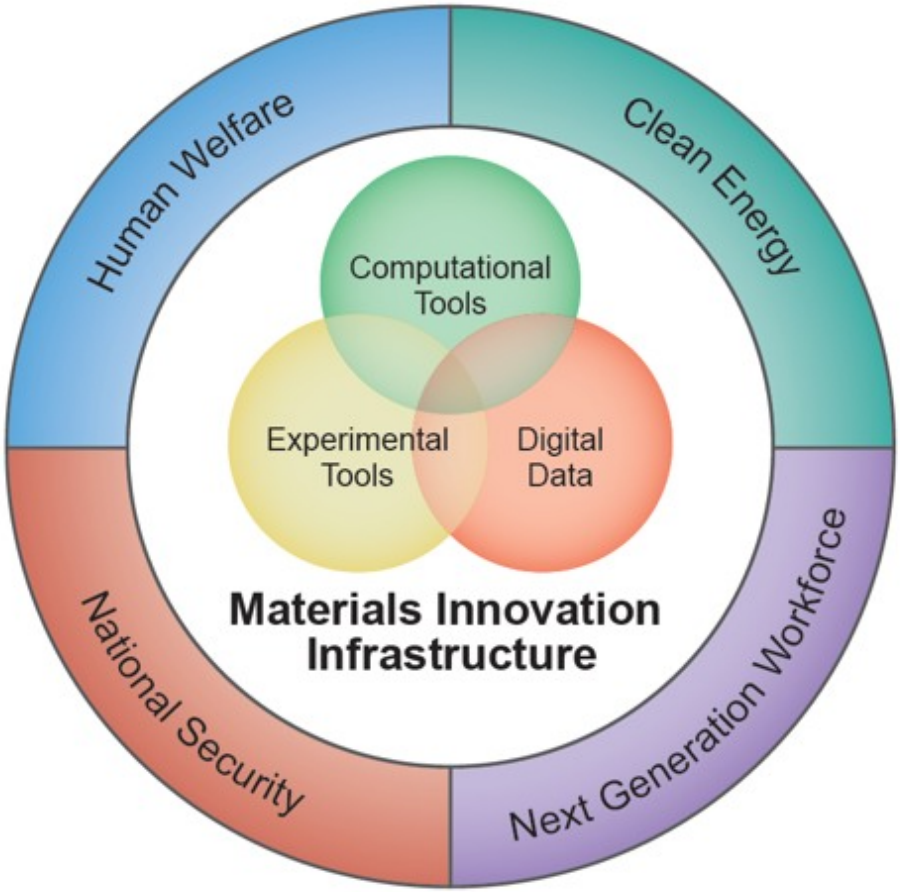
Materials Innovation Infrastructure



The Government Environment

The NIST response is also framed by related activities coming from the White House

- The “Holdren Memo” — February 22, 2013, commits Federal science agencies to increase public access to the results of research funded by the Federal Government
  `http://www.whitehouse.gov/sites/default/files/microsites/ostp/ostp_public_access_memo_2013.pdf`
- The May 9, 2013 Executive Order — describes an Open Data Policy making machine-readable, web-accessible form the default for public data
  `http://www.data.gov`

The Government Environment

Sidebar: Government Starts to Get It

The current White House has a CTO, Todd Park, who has a background in small business and entrepreneurship.

- Some Federal agencies are workshopping “innovation strategies”
  - How to efficiently leverage existing data and resources
- Importance and utility of open data is understood at very high levels
- White House hackathon (March, 2013) is perhaps part of this trend

NIST Institutional Response

NIST is setting up data repositories in support of pilot efforts

- DSpace general data repository for MGI data
- Advanced Composites Pilot
- Cobalt-based Superalloy Pilot
- Structural Alloys Pilot
- Workflow tools
- Uncertainty analysis

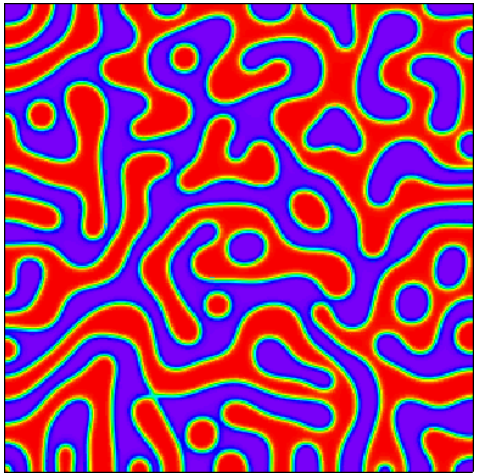
Significant presence of computer scientists working on data mining, machine learning, and discoverability

MGI SciPy and Python at NIST

- The FiPy PDE solver
- IPython as a workflow tool
- The OOF finite-element software

FiPy

FiPy is a finite-volume-based PDE solver, written in Python, and using the SciPy libraries, which can model microstructural evolution at the finest continuum length scales.



- Phase field evolution
- Phase transformations
  - Polycrystalline
  - Dendritic (solidification)
  - Electrochemical
- Electrodepostion

FiPy at SciPy

Look for Dan Wheeler's talk at this conference about using Sumatra to manage scientific workflow, featuring FiPy.

9:50 am Thursday, room 106.

`http://www.ctcms.nist.gov/fipy`

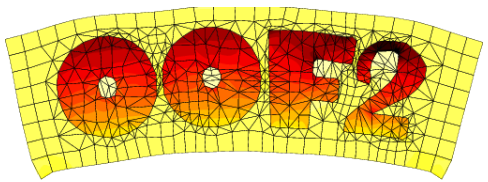
IPython and workflow

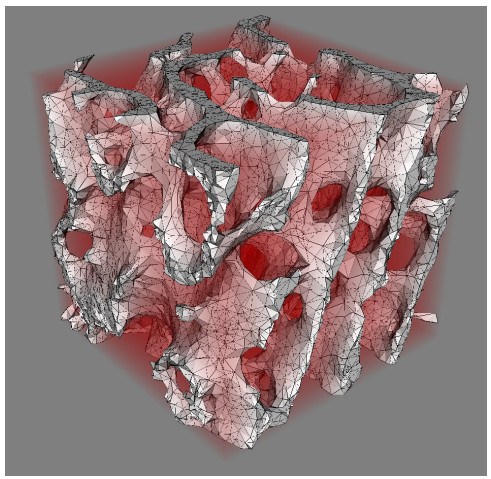
Zachary Trautt is using IPython to anchor a workflow development effort designed to scale up investigator productivity to match the size and complexity of the MGI task.

- Large increase in productivity compared to scripting
- Self-describing data, re-usable workflows
- Automated dispatch of compute tasks for good scaling

Also speaking at this conference,
12:00 noon Thursday, room 106.

OOF





"Object-Oriented Finite Elements", a Python and C++ (but not SciPy) tool for building microstructure-based meshes, and easily handling custom constitutive rules.

Well adapted to the larger continuum length scales. MGI role is as the platform for crystal-plastic modeling of sheet metal materials.

Outline

The Value of SciPy and Python

Obviously:

- Python provides high-level glue code for highly sophisticated materials modeling efforts
- SciPy provides numerical tools with good flexibility and scalability

The Python and SciPy Community

Less obviously:

- Python and SciPy are the core of a software ecosystem selected for power and flexibility
- The Python and SciPy community is made up of tool-builders

  This is a pretty good model for an innovation infrastructure.

So now what?

Through the MGI, the government is starting to formally recognize and articulate requirements that Python SciPy tools are well-prepared to meet.

Keep an eye out for CFPs and RFPs from Federal agencies where you can contribute.

Look for emerging MGI communities, and join them!

`http://www.whitehouse.gov/mgi`
`http://www.mgidata.org`
`http://materialsinnovation.tms.org`

Coming soon: `http://www.nist.gov/MGI`