International Federation for Information Processing (IFIP) Conference on Uncertainty Quantification

Charles Romine

Acting Associate Director for Laboratory Programs and Deputy Director, NIST

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

Topics

- **Introduction to NIST**
  - Mission and structure
  - NIST laboratories and research centers
- **Virtual Measurement Systems Program**
  - Metrology infrastructure for scientific computation
  - Uncertainty quantification

NIST

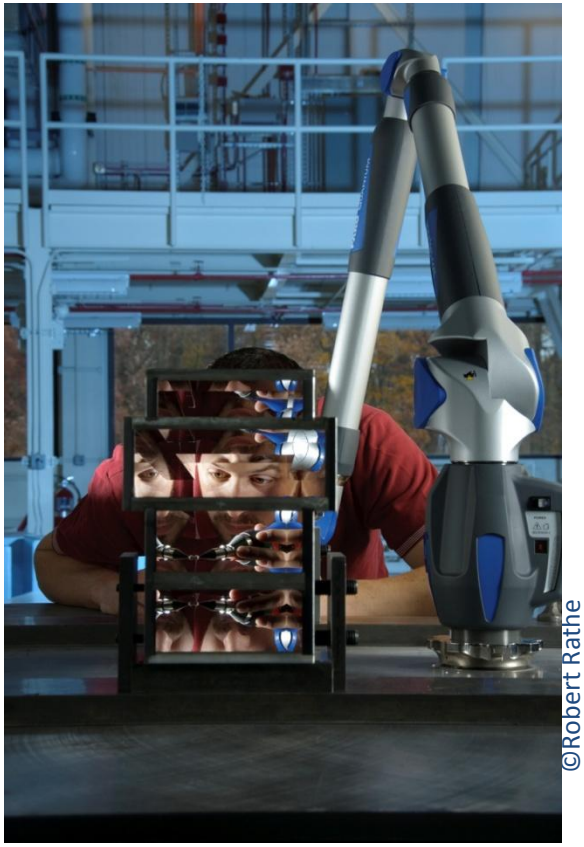
To promote U.S. innovation and industrial competitiveness by advancing

- measurement science,
- standards, and
- technology
- in ways that enhance economic security and improve our quality of life

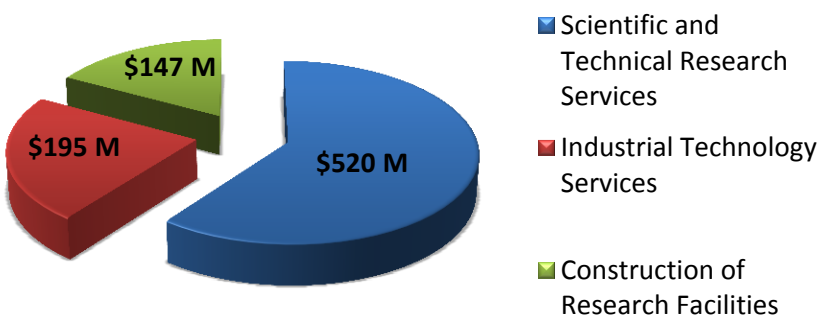
NIST: Basic Stats and Facts

•Major assets

- ~ 2800 federal employees
- ~ 2600 associates and facilities users/year
- ~ 1600 field staff in partner organizations (Manufacturing Extension Partnership)
- Two main locations, MD and CO
- Four collaborative Institutes (basic physics, biotech, quantum, marine)



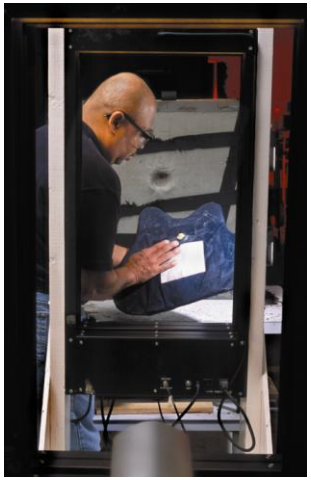
FY 2010 Appropriations $862 M



Measurement Science

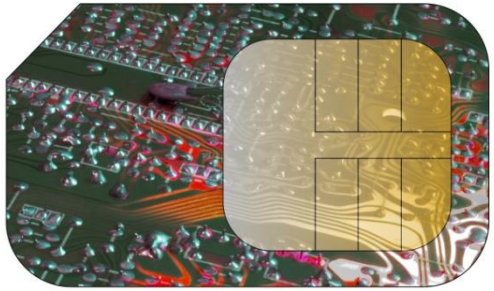
Physical Measurement Laboratory

- Fundamental units
- Applied measurements
- Calibrations
- Metric program
- State weights & measures programs



Material Measurement Laboratory

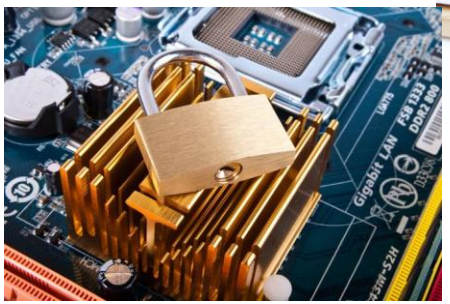
- Material composition & properties
- Validated methods & data
- Standard reference materials
- Laboratory accreditation



Technology

Information Technology Laboratory

- Cybersecurity
- Cloud computing
- Identity management
- Computer forensics
- Health IT
- Mathematical and Statistical Analysis



Engineering Laboratory

- Building technologies
- Fire research
- Smart Grid & energy technology
- Advanced manufacturing technology

Traceability

Property of a measurement result whereby the result can be related to a reference through a documented unbroken chain of calibrations, each contributing to the measurement uncertainty. (*International Vocabulary of Basic and General Terms in Metrology*, 2010)

Science: Precision leads to fundamental advance

Frequency precision of atomic clocks ⇒ Basis for GPS timing and synchronization solutions

Technology: Consistency provides stability

Quantitative standards in clinical chemistry ⇒ Improved diagnosis and long-time monitoring in health care

Commerce: Cross-comparability enables a fluid market

Measurement tools for energy ⇒ Marketplace for smart-grid technologies

Virtual Measurement Systems Program

Research and develop a metrology infrastructure in support of scientific computation and computer-assisted measurement.

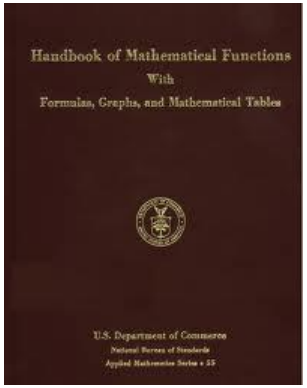
VMS research

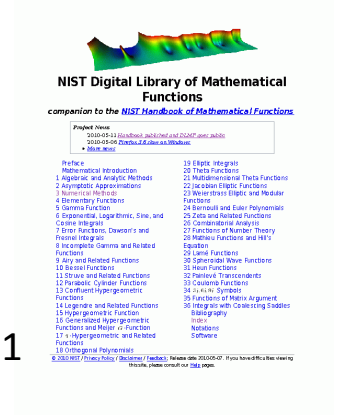
- Uncertainty quantification
- Benchmark problems
- Virtual measurement tools

Virtual Metrology at the Machine Level

<u>Special functions</u>

- Beloved Abramowitz and Stegun handbook
- Digital library of mathematical functions
- Numerical evaluation of special functions
  - Accuracy certificates on 100's of digits

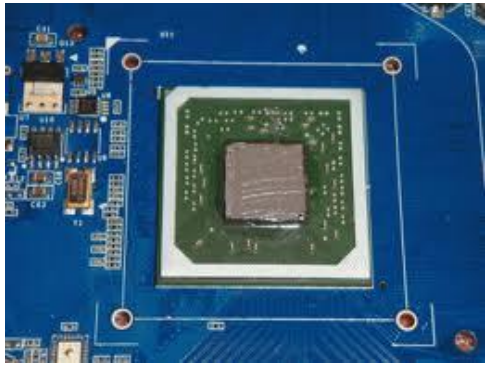




– – – 1.628904512232184058202113214339385978341713303560177196762158276066395108311917123297086800809 8096e+00 **± 2.88e-74**

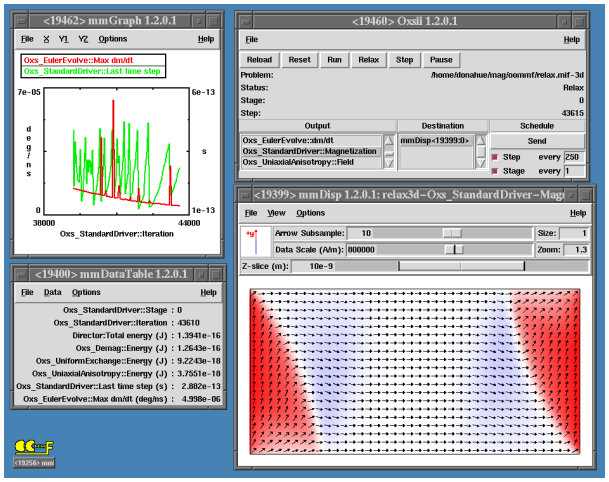
<u>General purpose graphics processing unit (GPGPU)</u>

- IEEE 754 – Standard for Floating-Point Arithmetic
- Port *paranoia* to perform compliance testing and analysis



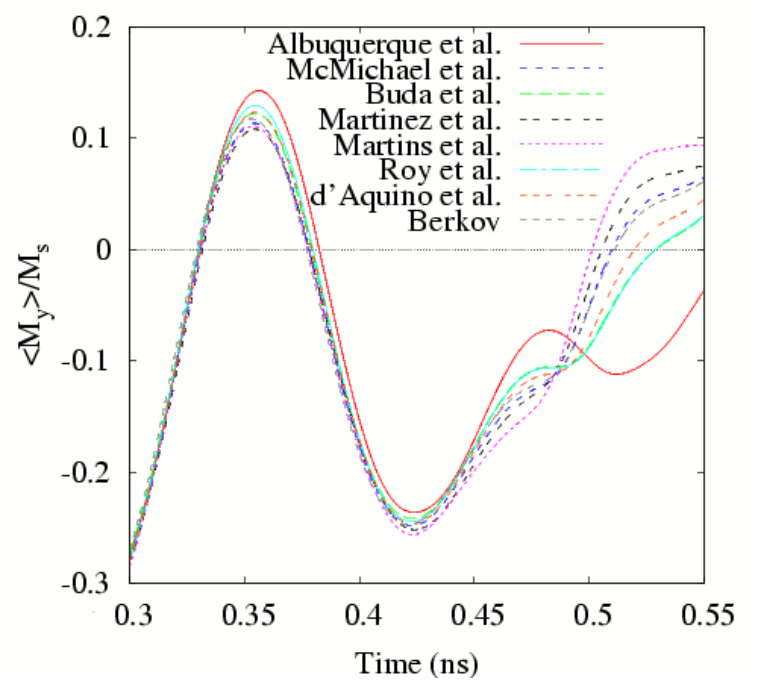
Virtual Metrology at Nanoscale

Micromagnetics – Object oriented micromagnetics framework (OOMMF)



Numerical tool OOMMF

- Open source development
- Landau-Lifshitz-Gilbert Reference solver
- Over 1000 citations in refereed journals



Micromagnetic physics benchmark problems

- Defined in consultation with stakeholders
- Simulations are compared

Virtual Metrology and Decision Making

Fire Measurement at NIST

Deep history of physical measurement

- Structural analysis and building codes
- NIST called upon for post-9/11 analysis

Recent growth of virtual measurements

- Two NIST fire models subjected to rigorous V&V as part of NUREG-1824 series
- Certified models will assist NRC in risk analysis for nuclear power plant safety

Summary

Present status of Uncertainty Quantification at NIST

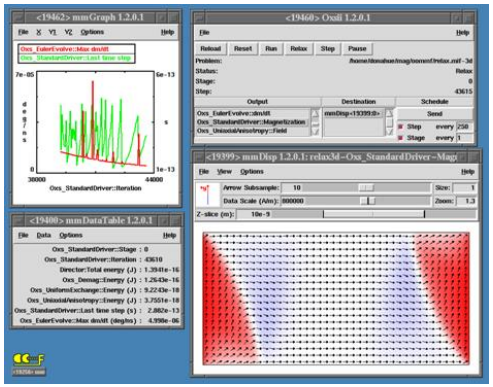
- Uncertainty analysis is a foundational topic for NIST. UQ for scientific computation represents the natural evolution of this topic.
- NIST charter covers a broad range of scales and application areas.
- Our core strength in precision physical measurement is an asset.

Next steps

- Continued outreach within NIST as well as to external stakeholders.
- New presidential initiative, “Materials Genome,” could provide essential resources to spur application of UQ technology to computational material science.
- Continued research on analysis and applicability of UQ.


NIST Digital Library of Mathematical Functions
companion to the NIST Handbook of Mathematical Functions

Thank You




Test 3
3.6.1999