Applied and Computational Mathematics Division

Ronald F. Boisvert, Chief

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NASEM Board of Assessment

June 2024

Plan

Tuesday (here)

11:00 Division Overview
12:00 Lunch w/ Division Management
13:00 Technical Talks
14:30 Break
14:45 Technical Talks
16:45 Wrap up
17:00 Adjourn (rejoin others)

Wednesday (on NIST campus)

10:00 Technical Talks
11:00 Lab tour (quantum/viz)
12:00 Lunch w/ junior staff, postdocs
13:00 Technical Talks
14:30 Break
14:45 Lab tour (viz/quantum)
15:45 Wrap up
16:00 Adjourn (rejoin others)

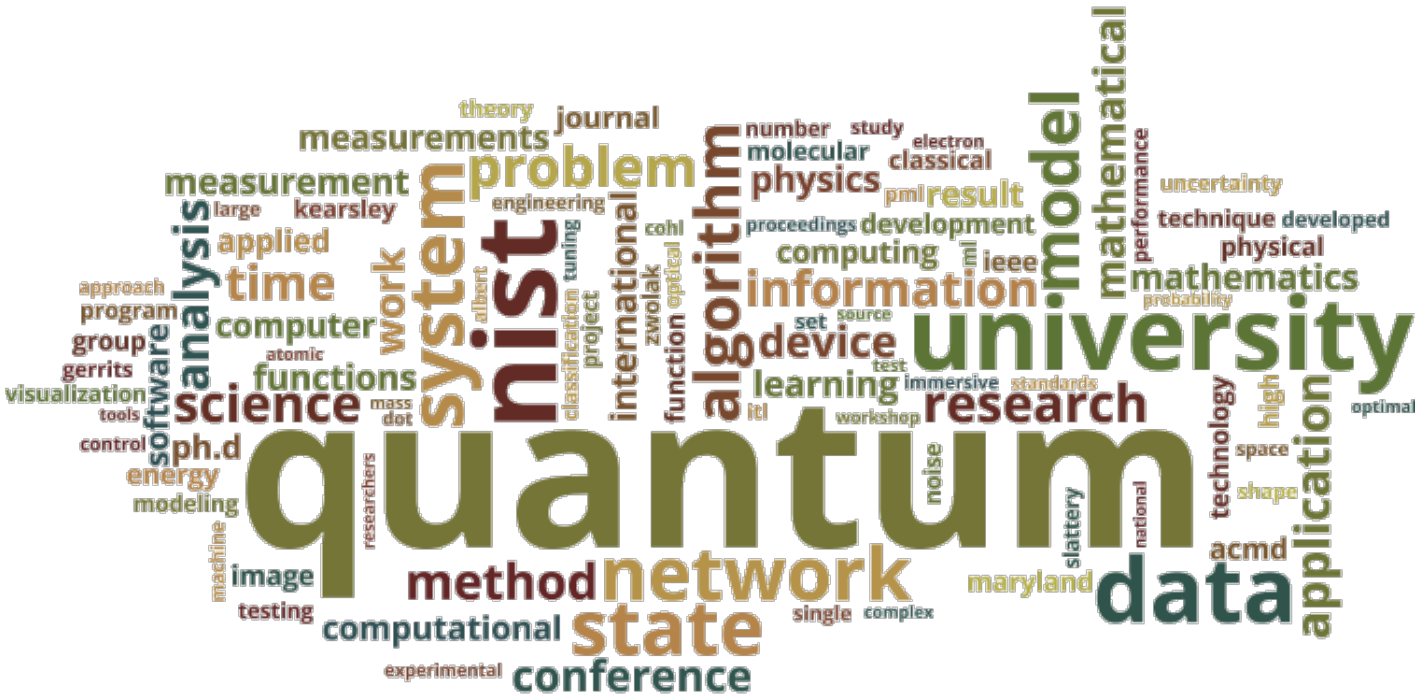
Background

ACMD Yearly Reports

1. *For FY 2023:*
   NISTIR 8518, April 2024
   https://doi.org/10.6028/NIST.IR.8518

2. *For FY 2022:*
   NISTIR 8466, May 2023
   https://doi.org/10.6028/NIST.IR.8466

3. *For FY 2021:*
   NISTIR 8423, April 2022
   https://doi.org/10.6028/NIST.IR.8423



https://www.nist.gov/itl/math

Main Messages

- Metrology is central to science, technology, industry
  - Leads to important, challenging mathematical/computational problems
  - Our work helps nurture trust in metrology and scientific computing
- NIST is a great place to be an applied mathematician / computational scientist
  - Wealth of fascinating problems in many application areas
  - Few barriers to collaboration
- We have good people, doing good science, and making a positive impact
  - Within NIST and beyond

Outline

- Context and Strategy
- Resources
- Technical Program
- Indicators
- Final Remarks

Context and Strategy

Context: External

Computational science is essential …

Computational science plays a crucial role in scientific discovery, the economy, and national security … we can look forward to

- more complex and accurate simulations
- the ability to simulate in real time and so to drive physical experiments
- the capacity to understand uncertainties and fully explore design spaces

But the landscape is changing dramatically …

- Science increasingly relies on large and complex data streams
- AI will create entirely new ways to do science

Context: External

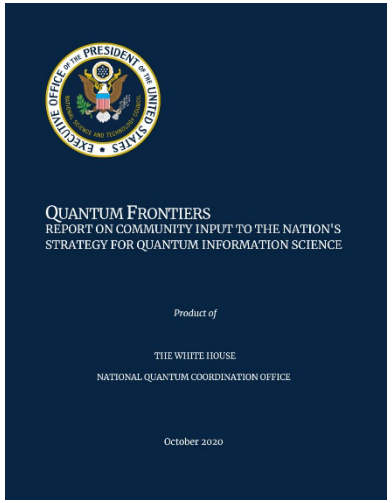
Computation itself is evolving …

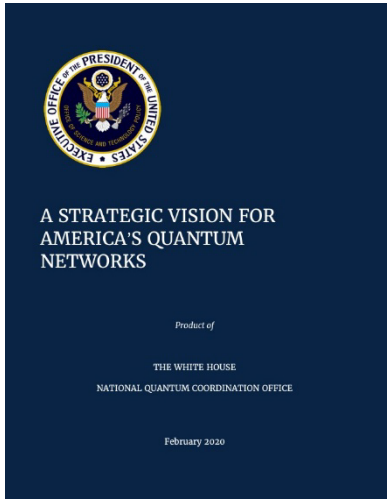
New technologies that harness unique quantum properties … are emerging. Major areas of inquiry :

- *discovering what is fundamentally possible, including practical quantum advantages and a deeper understanding of the classical-quantum trade space*
- *identifying potential applications for quantum resources*

As is networking …

- *Quantum networks will enable larger quantum computations*
- *Entangled sensor networks will enable precision metrology*
- *Quantum properties can also be utilized to secure communication*



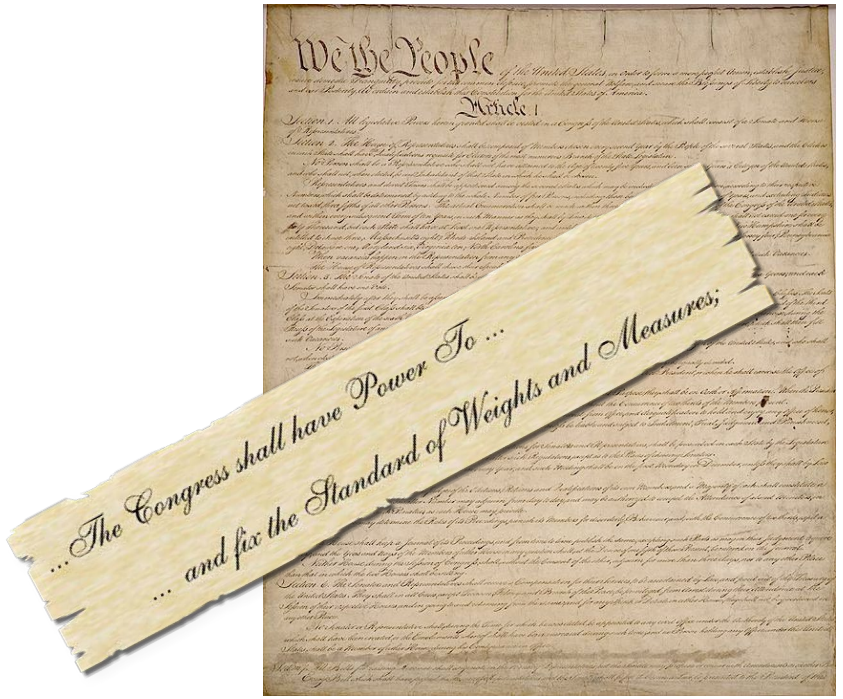


Context: NIST

Strengthen U.S. economy, improve the quality of life by working with industry to develop and apply technology, measurements, and standards

- US "National Metrology Institute"
  - Fundamental physical units, derived units
  - Evaluated data
  - Standard reference materials, calibrations
  - Measurement science R&D
  - National Standards Strategy
- Special Assignments
  - Building, fire investigations; forensic science
  - Federal information processing guidelines
- Collaboration with Other Federal Agencies

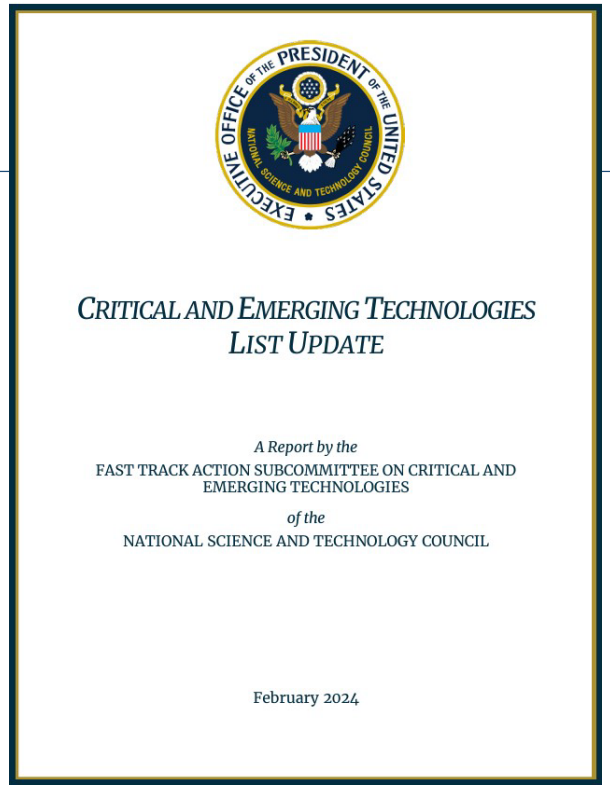
First "national lab"
Founded 1901



Context: NSTC → NIST

Critical and Emerging Technologies

- Advanced Computing
  advanced modeling and simulation, data processing and analysis
- Advanced Engineering Materials
  materials by design
- Artificial Intelligence
  machine learning, AI assurance and assessment
- Biotechnologies
  biometrology, computational biology, predictive modeling
- Semiconductors and microelectronics
  novel materials, specialized/tailored hardware
- Quantum Information
  quantum computing, quantum sensing, quantum communications
- Human-machine Interfaces
  virtual reality, augmented reality



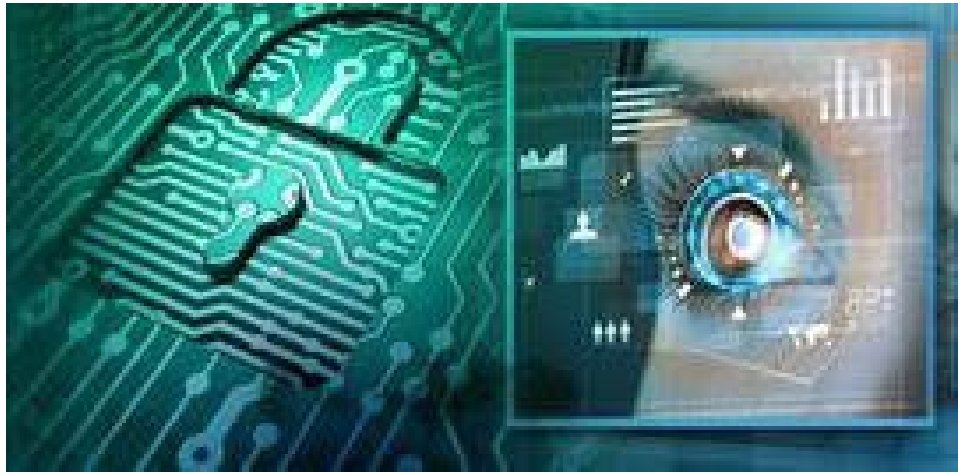
Related Interagency Initiatives

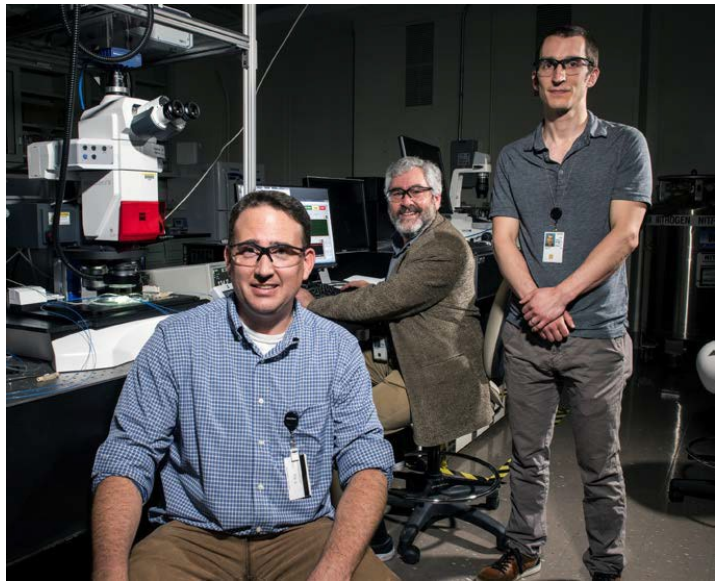
- Materials Genome (2011)
- National Quantum Initiative (2018)
- CHIPS & Science (2022)

Context: Information Technology Laboratory

Purpose: Cultivating Trust in IT and Metrology

Metrology for IT / IT for Metrology





Greg Cooksey (PML) with Tony Kearsley and Paul Patrone (ACMD)

* where IT includes applied math, statistics and CS

Context: Applied & Computational Math Division

Purpose: *Nurture Trust in Metrology and Scientific Computing*

- **Research**

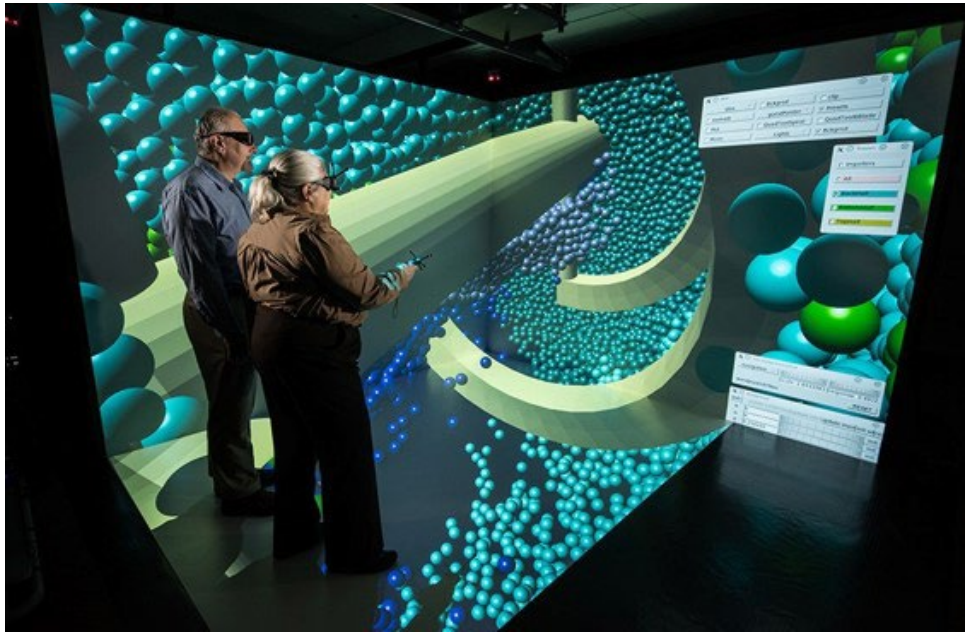
  Develop math, computational methods, tools, and facilities to enable world-class measurement science

- **Collaboration**

  Apply sophisticated math, computational expertise, tools to measurement and standards problems

- **Tech Transfer**

  Share results, reference data, tools, standards



Challenges

- NIST metrology must stay ahead of industry
  - Need for scientific and engineering reference data, standards accelerating
  - Industrial needs becoming more sophisticated as technology advances
- NIST targeted growth areas continually moving
  - Materials, biotechnology, quantum-based measurements, cybersecurity, AI, …
  - Often multidisciplinary
  - Becoming more data rich
- Every NIST project has math, computational components
  - We can’t be everywhere
- Operational issues
  - Flat budgets in core areas
  - Waves of retirement; difficult to compete for new hires in “hot” areas

Elements of Strategy

- Develop world-class research capability
  - establish environment that rewards innovation, initiative, excellence
- Hire most talented staff possible
  - educate to NIST role, then benefit from their creativity, insight; remove barriers; give leeway to innovate
  - use postdocs to bring fresh ideas; pathway to employment
- Don’t do everything, but span key technical domains
  - identify areas of high priority to NIST; nurture expertise over long period
- Identify key customers; develop their respect, trust
- Balance portfolio: large/small, long-term/short-term, basic/applied
  - build in time to explore
- Be efficient
  - develop tools that many can use; select activities with both internal and external impacts
- Leverage external expertise
  - maintain strong contacts with academia

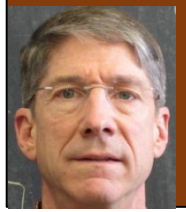
Resources

Resources: Organization

Based on April 15, 2024 org chart

Division Office
Ronald Boisvert
8 Staff
1 Postdoc

Mathematical Analysis and Modeling
Bradley Alpert
11 Staff
4 Postdoc
5 Faculty
9 Guests
2 Students

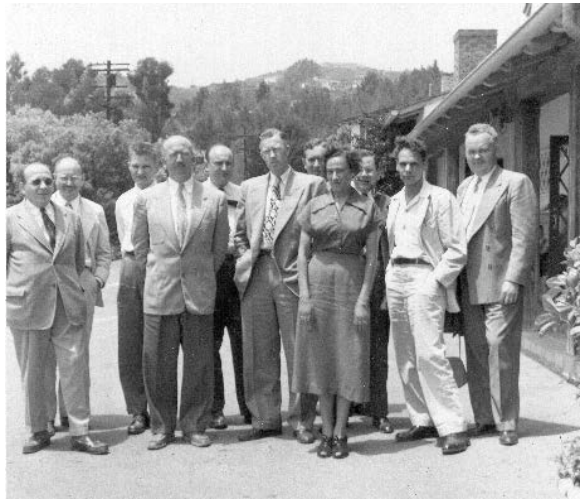


Mathematical Software
Bonita Saunders
10 Staff
3 Postdoc
1 Faculty
10 Guests
2 Students

Computing and Communication Theory
Ronald Boisvert
11 Staff
5 Postdoc
8 Guests
5 Students

High Performance Computing and Visualization
Judith Terrill
6 Staff
1 Faculty
2 Guests
4 Students

Resources: Personnel



NBS Institute for Numerical Analysis, 1950

NIST DLMF Project, 2011

- **62 Federal Employees**
  - 56 PhD, 3 administrative support
  - 52 FT / 10 PT (including 6 faculty appointees)
  - 48 Permanent / 14 Term appointees (incl. 6 NRC postdocs)
  - 46 Gburg / 9 Boulder / 7 remote
- **46 Associates**
  - 30 Guest researchers (some are postdocs)
  - 2 PREP Postdoc
  - 2 Contractors
  - 12 Students

As of April 2024

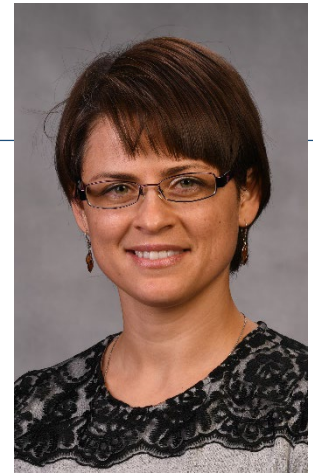
Federal Staff Distinctions

- AAAS Fellow: *Ronald Boisvert*
- ACM Fellow: *Ronald Boisvert*
- ASA Fellow: *Raghu Kacker*
- ASME Fellow: *Jeffrey Fong*
- APS Fellows: *Manny Knill, Barry Schneider*
- WAS Fellows: *Ronald Boisvert, Alfred Carasso, Michael Donahue, Raghu Kacker, Tony Kearsley, Paul Patrone, Bonita Saunders, Kamran Sayrafian, Justyna Zwolak*

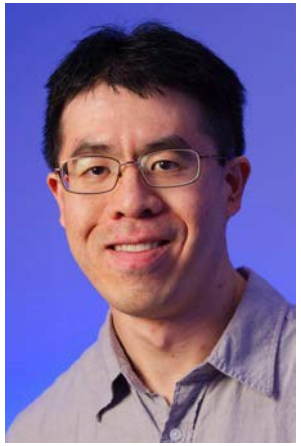
- - -

- NIST Fellows: *Manny Knill*
- QuICS Fellows: *Victor Albert, Yi-Kai Liu, Matthew Coudron*


Manny Knill


Justyna Zwolak


Barry Schneider


Yi-Kai Liu

Resources: Technical Expertise

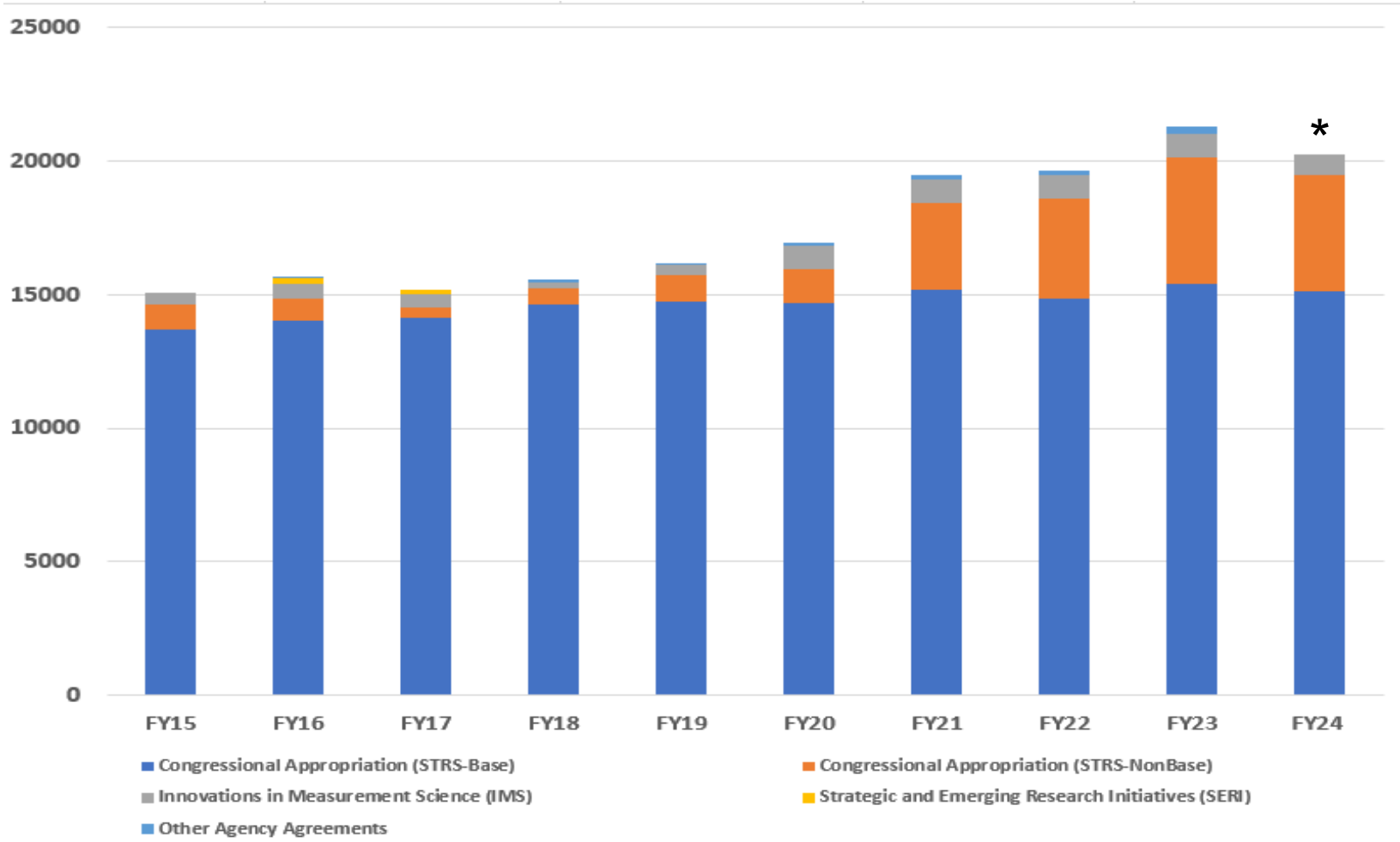
What we know includes …

- Signal processing
- Special functions
- Differential equations
- Nonlinear dynamics
- Inverse problems
- Optimization methods
- Monte Carlo methods
- Discrete mathematics
- Mathematical physics
- Mathematical modeling
- Computing theory
- Numerical analysis
- AI/machine learning
- Image processing
- Parallel algorithms
- Immersive scientific visualization
- Math software design
- Math knowledge management

Applications …

- Fluid, solid mechanics
- Electromagnetics
- AMO physics
- Quantum optics
- Quantum information
- Materials science
- Biometrology/Biomed
- Communication networks

Resources: Funding History



ACMD's total budget increased from **~$15 million** in FY 2015 to **~$20 million** in FY 2024.

* partial year only

Resources: FY 2024 Funding (unofficial)

Source	Percentage
Base STRS	71.0 %
STRS Budget Initiatives (non-base; tracked for 5 years)	8.2 %
ITL Building the Future	7.0 %
NIST Innovations in Measurement Science	3.5 %
Director's Office Funding for Postdocs (NRC, Fellows)	5.6 %
Misc (including other internal funding)	4.7 %
TOTAL	100.0 %

Resources: Computing

- Division Servers include
  - Ban - 3TB RAM 4-socket Xeon E7-8867v3 64 (real) cores (Win server 2022)
  - spiffy - 3TB RAM, 4-socket Xeon Platinum 8280, 112 (real) cores (Rocky Linux)
  - lanczos - 4TB RAM, 4-socket Xeon Platinum 8490H, 240 (real) cores (Ubuntu)

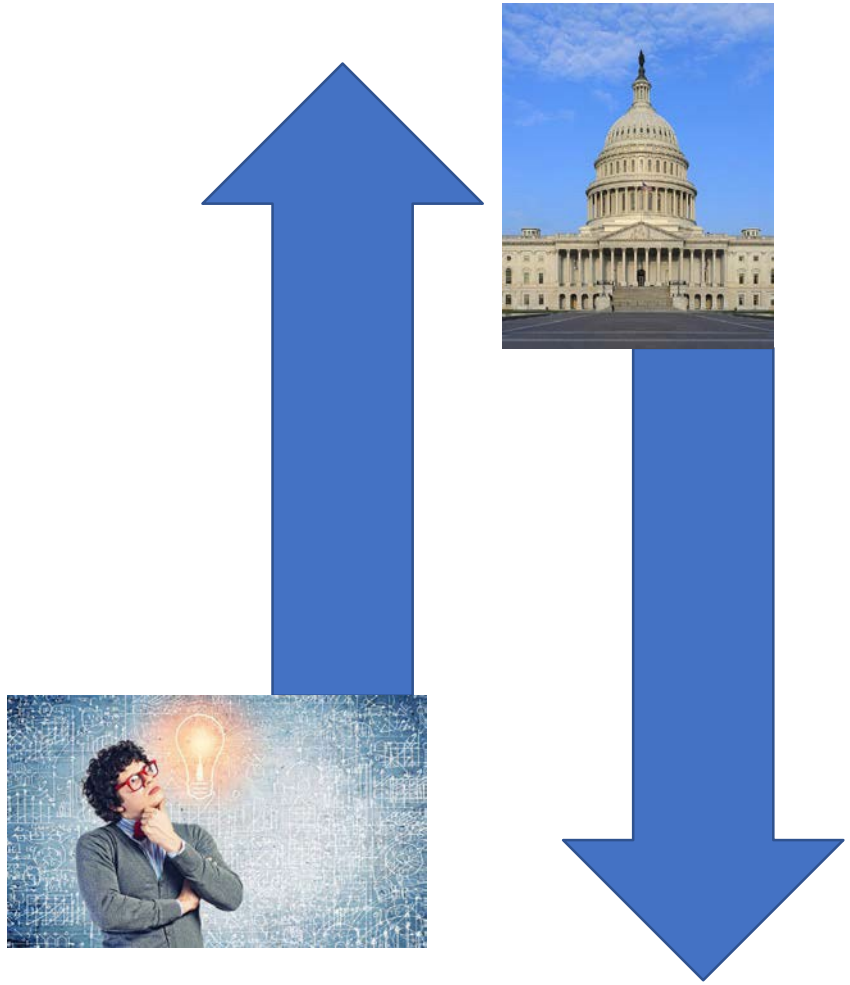
NBS SEAC, 1950

- Visualization Labs
  - 3-wall CAVE lab
  - head-mounted display lab
- NIST shared resources (maintained by NIST OISM, **in transition**)
  - Linux cluster ("Raritan"): 905 nodes, mix of Intel and AMD (21,648 cores); Infiniband; 200 TB Lustre parallel file system
  - Big data / ML cluster ("Enki"): 12 IBM Power9 nodes (Each: 2 20-core CPUs, 4 NVIDIA Tesla Volta GPUs); Infiniband
- Ad-hoc Access to External Resources
  - Via, e.g., NSF XSEDE, DOE INCITE

Technical Program

Project Selection

- Combination of top-down and bottom up
- Top Down
  - NIST Strategic Planning, Budget Initiatives
  - NIST Director Funding: SERI Program
- Bottom Up Proposals / Top Down Selection
  - NIST Innovations in Measurement Science Program
  - ITL Building the Future Program
- Bottom Up
  - Organic peer-to-peer collaborations
  - Personal “skunkworks”



Technical Program Areas

- Broad Areas
  - Mathematics of Metrology
  - High Performance Computing and Visualization
- Focus Areas
  - Mathematics of Biotechnology
  - Materials Modeling and Simulation
  - Quantum Information Science
  - Foundations of Measurement Science for Information Systems
  - Mathematical Knowledge Management

Mathematics of Metrology

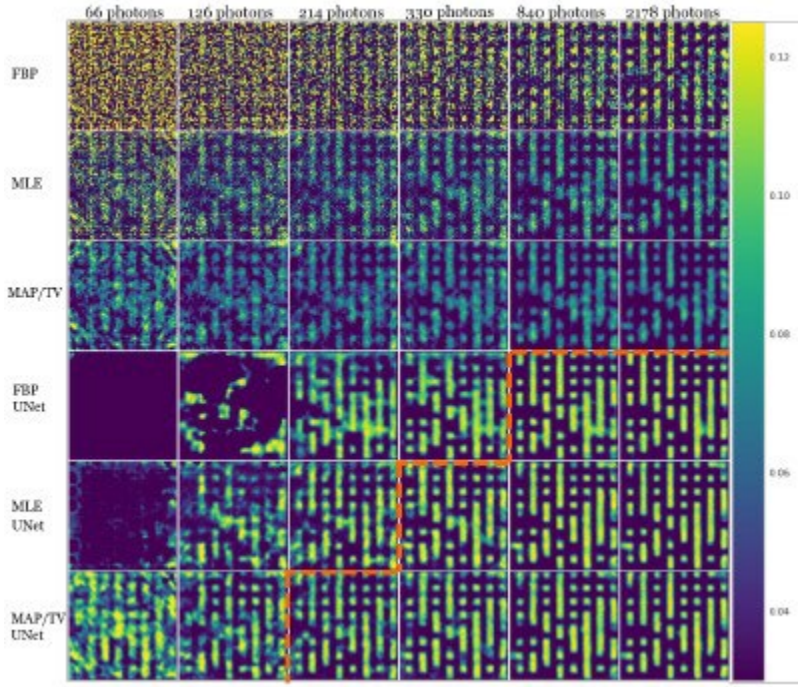
Develop mathematical methods and tools needed for NIST to continue as a world-class metrology institute and apply them to NIST problems.

Expertise

Modeling, PDEs
Signal processing
Image analysis
AI/machine learning
Numerical methods
Optimization

Applications

Atomic Physics
Electromagnetics
Chemistry
Forensics
Engineering



Comparison of tomographic reconstruction algorithms

Talks

Mass Spectral Data Analysis — Anthony Kearsley
Analysis of Separable Shape Ensembles — Zachary Grey

Mathematics of Metrology

Selected Recent Accomplishments

- Developed machine learning models to predict chemical reference data: Kovats retention indices, normal boiling points, infrared spectra. [FY21, p. 35. FY 22, p. 29. FY 23, p. 60]

  Barry Schneider, Anthony Kearsley, Chen Qu, Joel Bowman, Walid Keyrouz (ITL), Thomas Alison (MML), et al.

- Developed a physics-assisted generative adversarial network for X-ray tomographic reconstructions for low-photon nanoscale imaging for IARPA RAVEN project. [FY23, p. 49, FY22, p. 27]

  Bradley Alpert with colleagues in PML, Sandia National Laboratories, and MIT

- Led the development of the Atomic, Molecular, and Optical Science (AMOS) Gateway to make research software available to the community [FY22, p. 34. FY23, p. 53]

  Barry Schneider, with colleagues from CU Denver, Curtin U, IU, Drake U, Kennesaw State U, LBL, Ludwig-Maximilians U, Open U (UK), U Automata de Madrid, U Belfast

High Performance Computing, Visualization

Develop infrastructure and expertise necessary for high-performance computing and advanced visualization of scientific data and apply to NIST problems.

Expertise

Supercomputing
AI/Machine learning
Visual analysis
3D immersive visualization

Applications

Building materials
GHG analysis
Human body model
Standards

Development of 3D immersive visualization infrastructure to support **collaborations in a hybrid data analysis environment**

Develop 3D immersive environment into an **interactive measurement lab**.

Talks

CAVE Demo	Judith Terrill
Intelligent Tuning of Quantum Dot Devices	Justyna Zwolak

High Performance Computing and Visualization

Selected Accomplishments

- Developed a dense suspension simulation code which has applied from concrete to pharmaceuticals. Now studying the rheological properties of cementitious materials with suspended fibers, such as Ultra High-Performance Concrete. [FY23, p. 93. FY22, p. 66]

  William George, Nicos Martys (EL), Jeffrey Bullard (Texas A&M)

- Developed a transportable virtual reality (VR) system that approximates immersive VR for use at conferences and similar venues. Demonstrated at SC22, SC23. [FY22, p. 70]

  William Sherman, Simon Su

- Restructured ParaView classes to provide collaborative visualization functionality [FY23, p. 97]

  Simon Su, William Sherman, Judith Terrill

- Working closely with Kitware to extend ParaView for VR support, and the Khronos Group on immersive interfaces (OpenXR) and advance rendering (ANARI) standards.

  William Sherman, Sandy Ressler, Simon Su, Judith Terrill

- Extended use of explainable boosting machines to image data. [FY23, p. 30]

  Justyna Zwolak, Craig Greenberg (ITL), Rich Caruana (Microsoft), et al.

Mathematics of Biotechnology

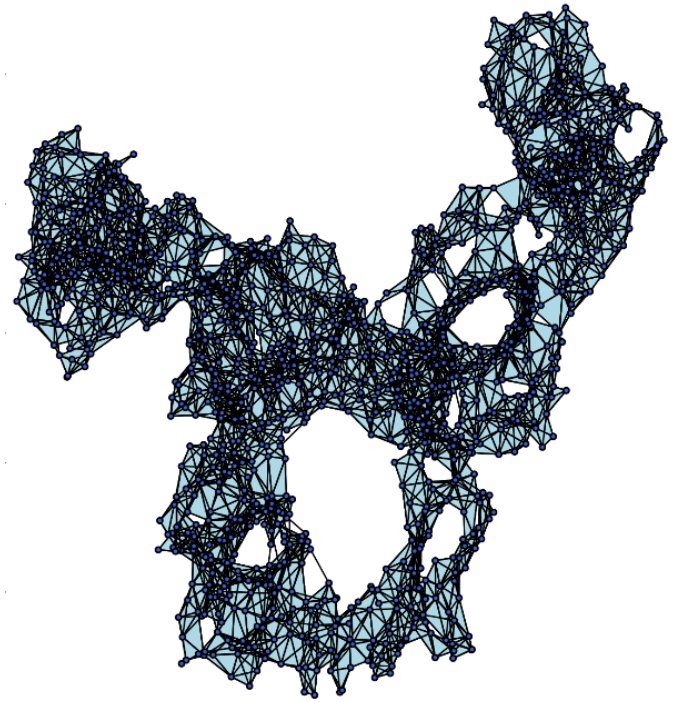
Characterize and measure biological technologies for healthcare and manufacturing.

Expertise

Math Modeling
Data analysis
AI/machine learning
Uncertainty quantification
Classification theory

Applications

Microfuidics/cytometry
qPCR
Diagnostics
Cryobiology
Low-field MRI
BioFETs



NISTmAb represented as a simplical complex

Talks

Analysis of Diagnostics — Paul Patrone
Modeling of Biological Field-Effect Transistors — Ryan Evans
Wearable System to Monitor Pulmonary Edema — Kamran Sayrafian

Mathematics of Biotechnology

Selected Accomplishments

- Developed and analyzed concept for a wearable device to detect pulmonary edema (fluid buildup in the lungs) A patent is pending. [FY21, p. 15]

  Kamran Sayrafian and Katjana Ladic with colleagues at Bogazici University (Turkey)

- Biological field effect transistors (Bio-FETs) have potential for rapid, accurate, low-cost, and portable measurements. We have developed the first dynamic model for Bio-FET experiments that accounts for physically relevant transport effects. [FY23, p. 85]

  Ryan Evans and Anthony Kearsley with Seulki Cho and Arvind Balijepalli (PML)

- Developed an innovative flow-cytometer enabling time-dependent measurements of cell behavior. With cell classification accuracy of 99.5 % and tracking errors of fewer than 1 in 10,000 at a throughput of 1 million cells per hour it is a revolutionary improvement over existing techniques. A company (Lumos Nanolabs) was created to commercialize. [FY23, p. 71]

  Paul Patrone and Anthony Kearsley with Greg Cooksey and Matt DiSalvo (PML)

Materials Modeling

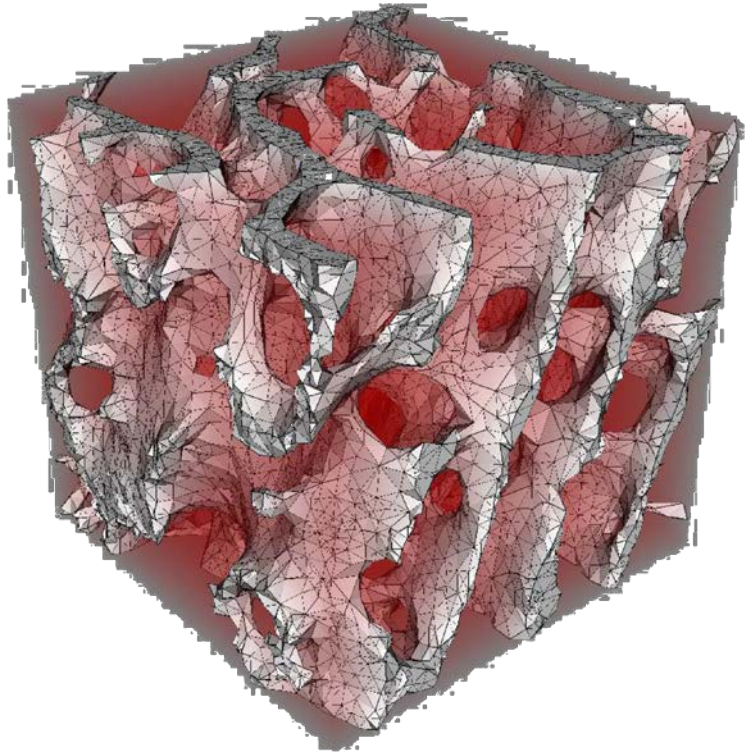
Promote more efficient creation of advanced materials through modeling and simulation.

Expertise

Modeling
Numerical analysis
Uncertainty quantification
Software development

Applications

Micromagnetics
Microstructures
Engineering Reliability



Talks

OOMMF - Public Domain Micromagnetics

Michael Donahue

Materials Modeling

Selected Accomplishments

- With more than 3,600 citations[1] touting its use, ACMD's Object-Oriented Micromagnetic Modeling Framework (OOMMF) has become a valuable tool in for research community. It has also been critical to in the NIST Innovation in Measurement Science project Thermal MagIC, developing nano-sized ultra-sensitive thermometers based on magnetics. [FY23, p. 90]

  Michael Donahue and Donald Porter

- Electron backscatter diffraction (EBSD) is a SEM used to probe material grain structure and orientations at the microscale. Such scans may be noisy, resulting in errors and missing data. ACMD has developed postprocessing techniques that greatly improves the quality of such imagery. [FY23, p. 25]

  Gunay Dogan with colleagues at Clarkson University

[1] https://math.nist.gov/oommf/oommf_cites.html

Quantum Information Science

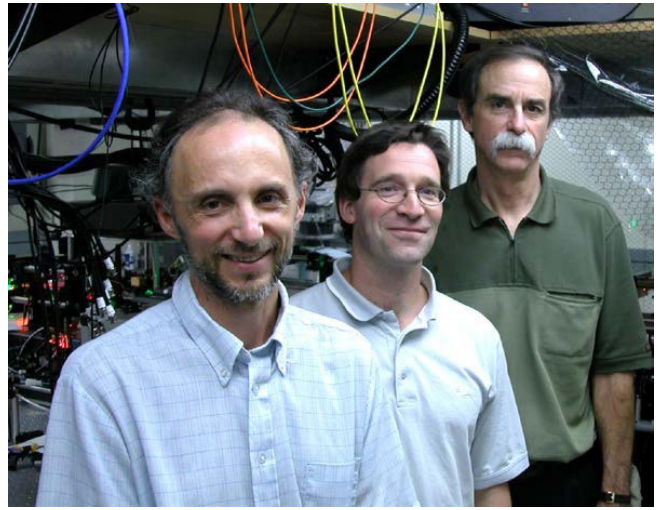
Understand potential of QI to revolutionize information science. Develop, apply techniques and tools for the reliable assessment of quantum-based systems.

Expertise

CS Theory
Math physics
Quantum optics
Tomography
Experimentation

Applications

Computing
Networking
Algorithms
Cryptography
Randomness



Manny Knill (ACMD) with Didi Leibfried and Dave Wineland (PML)

Talks

QuICS, Quantum Algorithms, and Post-Quantum Cryptography	Yi-Kai Liu
Quantum Algorithms and the Power of Forgetting	Matthew Coudron
Characterizing Performance of Quantum Bits	Scott Glancy
Quantum Communications Lab Tour	Oliver Slattery

Quantum Information Science

Selected Accomplishments

- *Physics World*'s top breakthrough of 2021 was the demonstration of the entangling of two macroscopic drumheads[1] "thereby advancing our understanding of the divide between quantum and classical systems." [FY21, p. 99]

  Ezad Shojaee, Alex Kwiatkowski, Shawn Geller, Scott Glancy, and Manny Knill, with colleagues in NIST PML

- Error correction is a critical technology for scalable quantum computation, and many such schemes have been proposed. ACMD has developed the Error Correction Zoo[2], an online taxonomy of more than 750 classical and quantum codes [FY23, p. 120]

  Victor Albert, with colleagues at Freie Universitat Berlin, Amherst College, and Caltech

- Developed a dictionary that defines terms and metrics relevant to the characterization of single-photon detectors and sources. It is now being propagated to formal standards organizations. [FY23, p. 129]

  Thomas Gerrits, Paulina Kuo, and Oliver Slattery with Joshua Bienfang, Alan Migdall, and Sergey Polyakov of PML

[1] https://www.science.org/doi/10.1126/science.abf2998
[2] https://errorcorrectionzoo.org

NIST / University of Maryland

Joint Center for Quantum Information and Computer Science

Established in 2014

Goal: Foundational research in quantum CS and information theory

How does quantum mechanics inform the theory of computing and communication?

What insight does computer science shed on quantum computing?

What are the consequences of quantum information theory for fundamental physics?

How can theoretical advances be applied?

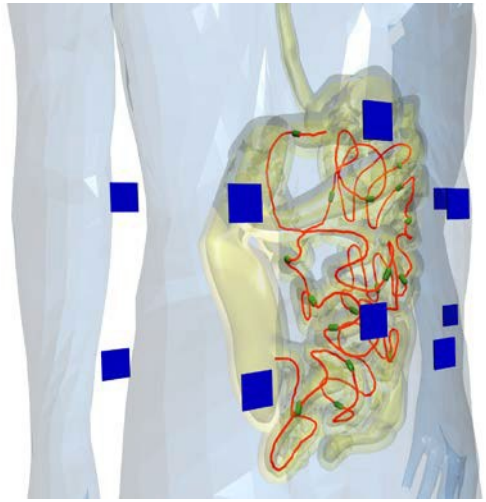
- 13 Fellows (8 NIST, 5 UMd); 20 postdocs; 67 students
- In 2023: 70 research papers; 88 seminars; 2 major events
  - 13th International Conference on Quantum Cryptography (QCrypt), August 2023
  - 14th International Conference on Post Quantum Cryptography (PQCrypto), August 2023

ITL PML LPS UMIACS

Department of Computer Science

Metrology for Information Systems

Develop mathematical foundations to create, apply measurement science to enable trust in complex information systems

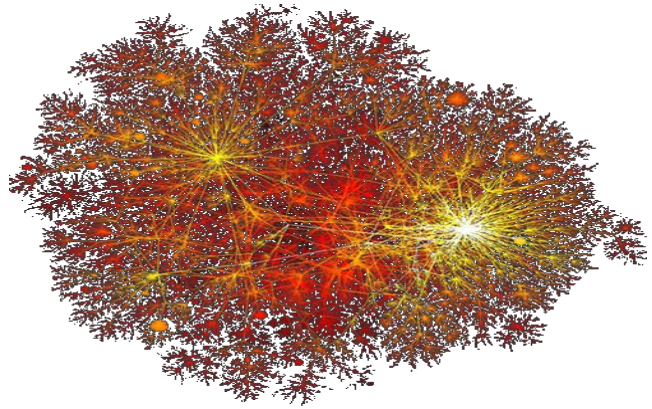


Expertise

Math modeling
Discrete event simulation
Combinatorics
AI/machine learning
Graph theory
Electromagnetics

Applications

Network characterization
Software testing
Internet of Things for Health
Neuromorphic computing



Talk

Neuromorphic AI Andrew Dienstfrey

Metrology for Information Systems

Selected Accomplishments

- The paper, "ACTS: A Combinatorial Test Generation Tool," presented at the 2013 IEEE International Conference on Software Testing, Verification and Validation was recognized at the 2023 conference as the Most Influential Paper Award (MIP) of the Decade in the category of MIP Practical. [FY23, p. 146]

  Raghu Kacker with Rick Kuhn (ITL/CSD), and colleagues of the University of Texas at Arlington

- Studied the effect of using more refined exposure thresholds in automated exposure notification systems on virus propagation, providing the basis for a variety of optimizations. [FY23, p. 78]

  Brian Cloteaux, Vladimir Marbukh, Kamran Sayrafian

- Completed a major comparative survey of algorithms for the k-median problem for real-world graphs, which requires identifying a subset of k vertices that minimize the total distance to all other vertices in a graph. [FY23, p. 140]

  Roldan Pozo

Mathematical Knowledge Management

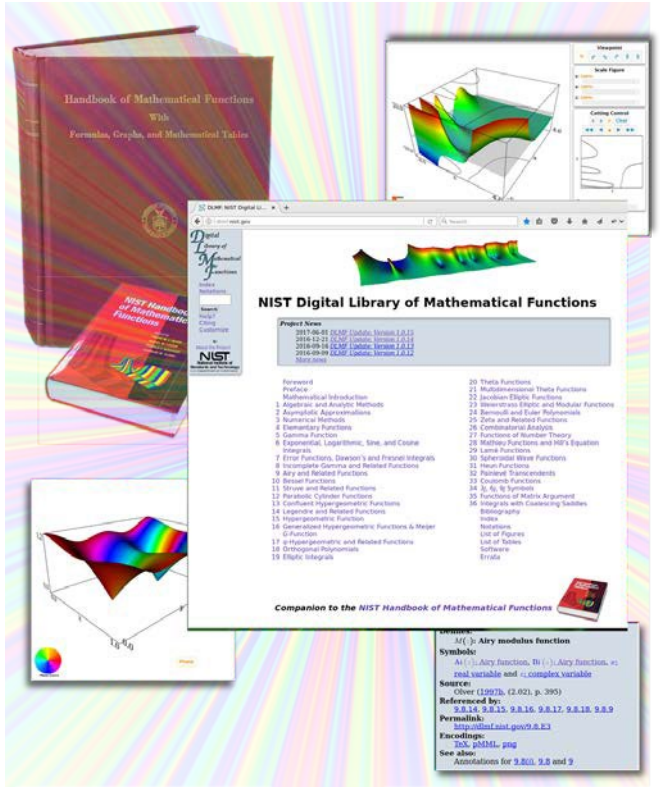
Enable unambiguous representation, exchange, and use of mathematical data. Serve as a trusted source of reference data for special functions.

Expertise

Representation
Semantics
Search
Visualization
Special functions

Applications

Digital Library of Mathematical Functions (DLMF)
Function Tables on Demand
LaTeXML



Talk

NIST's DLMF and Math Knowledge Management

Bonita Saunders

Mathematical Knowledge Management

Selected Accomplishments

- The arXiv preprint repository is now using ACMD's LaTeXML tool to create HTML/MathML versions of submitted TeX/LaTeX manuscripts in order to promote *accessibility*.

  Bruce Miller

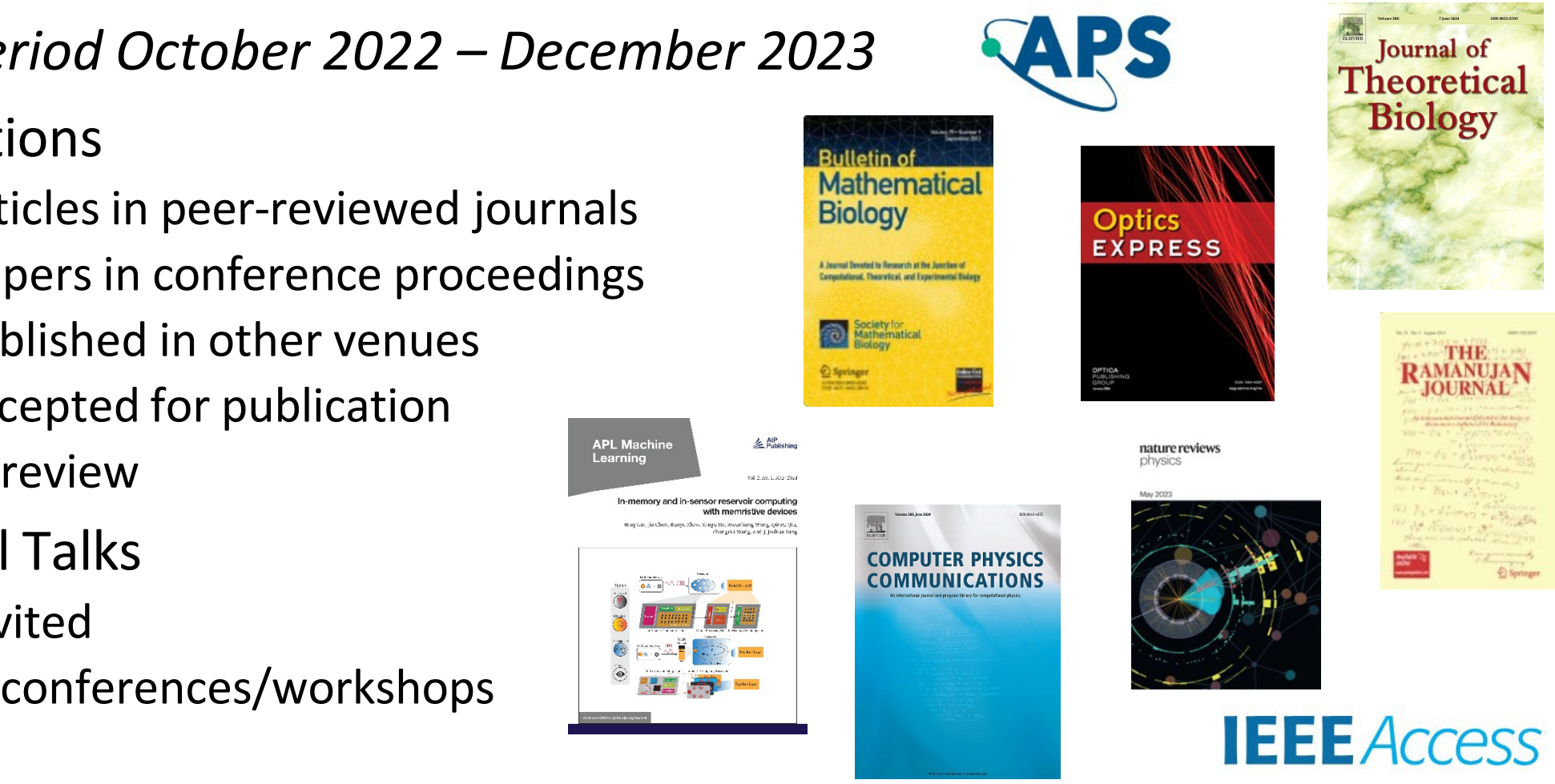
- Originally released in 2010, Digital Library of Mathematical Functions (DLMF) usage remains high. 5.1 M pages downloaded by 351,000 unique visitors during calendar year 2023. >9,550 citations since 2010. A major revision to the chapter on orthogonal polynomials was recently released, and a new chapter on Orthogonal Polynomials of Several Variables is nearing completion. [FY23, pg. 152]

Indicators

Output: Papers and Talks

During period October 2022 – December 2023

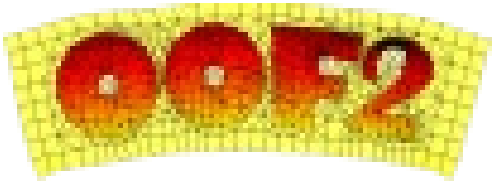
- Publications
  - 61 articles in peer-reviewed journals
  - 39 papers in conference proceedings
  - 6 published in other venues
  - 17 accepted for publication
  - 40 in review
- External Talks
  - 79 invited
  - 74 in conferences/workshops



Output: Software

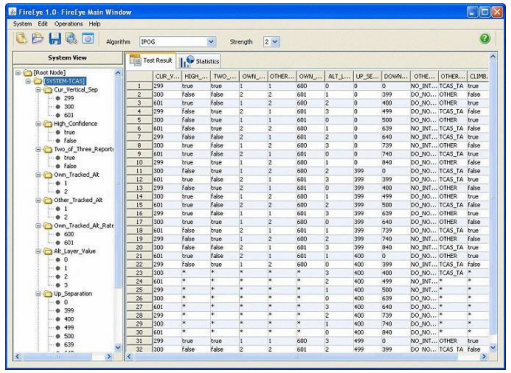
- OOMMF (micromagnetic modeling)
  5,200 downloads from 3,300 clients in FY23. Overall: >3650 citations (including 25 dissertations, 45 US patent applications) >30 YouTube tutorials; also on nanoHub

- OOF (modeling material microstructures)
  Available on nanoHub, exercised 4,300 times in FY23 (69,000 times since 2007)



- ACTS (combinatorial testing)
  Downloaded by 4,775 distinct users since 2014.

- Other software currently under development/distribution includes …
  - ✓ LaTeXML (TeX/LaTeX to HTML/MathML converter)
  - ✓ Scikit-shape (Python package for shape and image analysis)
  - ✓ G2Aero (Python package for separable shape tensors)
  - ✓ Software for Joint Quantum State Tomography

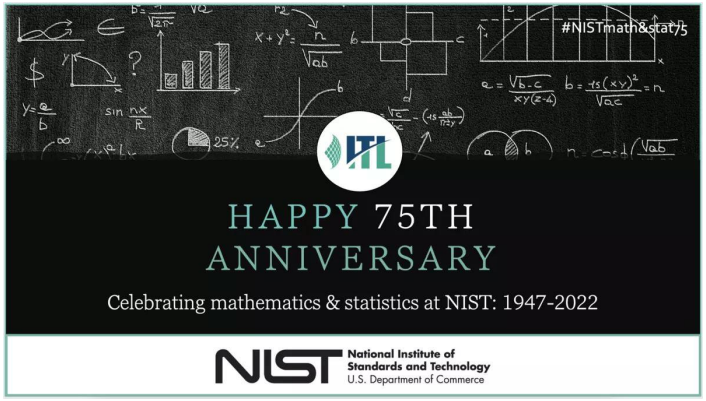


Output: Data

- Division Web Server (math.nist.gov)
  In calendar 2023: 2.2M pages downloaded (9.5 pages/visit) by 238K visitors

- Digital Library of Mathematical Functions (dlmf.nist.gov, properties of special functions)
  5.1 M pages downloaded by 351,000 unique visitors during calendar year 2023. >9,550 citations since 2010.

- Other ACMD data being distributed includes …
  - ✓ Dark solitons in BECs dataset (supports machine learning)
  - ✓ QFlow (quantum dot data for machine learning)



Digital Library of Mathematical Functions

Celebrating Our People

- Department of Commerce Ron Brown Award
  - Anthony Kearsley and Paul Patrone (2023, for the invention of serial cytometry)
- Department of Commerce Gold Medal
  - Anthony Kearsley and Paul Patrone (2023, for the invention of serial cytometry)
  - Scott Glancy and Manny Knill (2022, for quantum entanglement of two macroscopic mechanical resonators)
- Department of Commerce Silver Medal
  - Thomas Gerrits (2021, for first demonstration of an array of superconducting nanowire single-photon detectors with more than one thousand pixels)
  - Ryan Evans and Tony Kearsley (2021, for advancing the state-of-the-art in methods for determining the higher order protein structure of biotherapeutics)
- Department of Commerce Bronze Medal
  - Thomas Gerrits (2023, for precision measurement techniques for molecular absorption of photon pairs)
- Washington Academy of Sci: Excellence in Research in Applied Math
  - Justyna Zwolak (2023), Paul Patrone (2022), Michael Donahue (2021)

Patents Awarded

1. G. Cooksey, **A. Kearsley**, and **P. Patrone**. Optical Flow Meter for Determining a Flow Rate of a Liquid. Patent US 11035707, June 15, 2021.

2. J. Ullom, G. O'Neil, L. Avila, K. Silverman, D. Swetz, R. Jimenez, W. Doriese, G. Hilton, C. Reintsema, D. Schmidt, **B. Alpert**, J. Uhlig, Y. Joe, W. Fullagar, V. Sundstrom, I. Maasilta, and J. Fowler. X-Ray Spectrometer. Patent US 10,914,694 B2, Feb. 9, 2021.

Patent Applications in Process

1. S. Buckley, A. McCaughan, **A. Dienstfrey**, S. Nam. System and Method for Parameter Multiplexed Gradient Descent. Provisional Patent Application, NIST Docket 22-051US1, July 19, 2023.
2. A. Balijepalli, J. Majikes, A. Kanwal, P. Vallone, K. Kiesler, E. Romsos, and **A. Kearsley**. US Department of Commerce, assignee. Agile Nucleic Acid Sensor and Measuring a Biomarker. Patent Application US 17/845,682. October 13, 2022.
3. **K. Sayrafian**. Lung Fluid Monitor and Monitoring Fluid Level in a Lung. Patent Application Serial Number PCT/US22/48217, October 28, 2022.
4. G. Cooksey, **A. Kearsley**, and **P. Patrone**. Multiplexed Amplitude Modulation Photometer and Performing Multiplexed Amplitude Modulation Photometry. Provisional Patent Application 20210055201.
5. G. Cooksey, **A. Kearsley**, and **P. Patrone**. Serial Flow Cytometer. Provisional Patent Application 20210302300.
6. **A. Kearsley**, **P. Patrone**, E. Romsos, and P. Vallone. System and Method for Data Analysis in Quantitative PCR Measurements. Provisional Patent Application 20210395807.

External Community Engagement

- Memberships include …
  - B. Saunders: SIAM Board of Trustees
  - O. Slattery: Co-Chair. OSTP Working Group on Quantum Networks
  - R. Boisvert, NSTC Subcommittee on Future Advanced Computing Ecosystem
  - S. Ressler: W3C Advisory Committee
  - B. Miller: W3C Math Interest Group
  - D. Porter: TCL Core Team
  - R. Boisvert, A. Dienstfrey: IFIP WG 2.5 (Numerical Software)
  - K. Sayrafian: IEEE802.15 Task Group 6ma (Body Area Networking)
  - W. Sherman, S. Su: Khronos OpenXR Working Group

Editorial, Conferences and Workshops

Staff members …

- Hold 11 journal editorial positions, including
  - Barry Schneider, Associate Editor-in-Chief, IEEE's *Computing in Science and Engineering.*

- 30 positions on conference committees, including
  - Y.-K. Liu. General Chair. 14th International Conference on Post-Quantum Cryptography. College Park, MD, August 16-18, 2023.
  - K. Sayrafian. Lead Organizer and Co-Chair: 5th International IoT-Health Workshop. IEEE International Conference on Communications. Rome, Italy, June 1, 2023.
  - O. Slattery. Co-Chair. QCRYPT 2023, College Park, MD. August 14 -18, 2023.
  - J. Zwolak. Co-organizer. Workshop on Advances in Automation of Quantum Dot Devices Control, Rockville, MD, July 19-20, 2023.

Tech Transfer: Testimonials

Regarding the DLMF …

- "I recently stumbled upon your resource [sic] and I have to say that I am very impressed by the scope and depth of the content. I have used Abramowitz and Stegun for a while now and having 3D visualizations and relations all in one place and so easily accessible is a very nice thing." – Prof. Nicholas Mecholsky, Catholic University of America

Regarding work on automation of quantum dot experiments …

- "I am also writing to express my appreciation for the in-depth collaboration Justyna [Zwolak] has built with us, on the auto-tuning, calibration and operation of these gate-controlled qubits. Her ideas around physics-informed algorithms for quantum hardware and condensed matter measurements and characterization are also of great value to the community and to experimentalists" -- Prof. Anasua Chatterjee, Delft U. of Tech.

Tech Transfer: Testimonials

Regarding OOF …

- "In studying microstructures and their impact on material properties, OOF2 (Object-Oriented Finite Element Analysis) stands out as specialized software … By simulating the relationship between microstructure and mechanical properties, OOF2 facilitates investigations into the influence of diverse microstructural features on material behavior. " – Prof. Albert Linda, Indian Inst. Of Tech.

Regarding collaboration with NREL …

- "This collaboration led to breakthrough inverse design and uncertainty quantification capabilities for wind turbine blades using separable shape tensors and invertible neural networks ... NIST's mathematical expertise in this project contributed to a significant dimension reduction and ultimately a 100x computational speedup over prior methods. " – Dr. Ryan King, National Renewable Energy Lab

Tech Transfer: Student Training

FY 2023: ACMD supported 40 student interns

19 graduate students, 17 undergraduates, and 4 high school students

- "Thank you so much for all your support last summer. I didn't get into MIT, but I got into Carnegie Mellon. I'm planning on studying Electrical and Computer Engineering there." -- High school student Angela Shen writing to mentor Oliver Slattery

Final Remarks

Federal Staffing

Retirements* (2021-present)

- Roldan Pozo (Computer Scientist)
- Timothy Burns (Mathematician)
- Geoffrey McFadden (NIST Fellow)
- Steven Satterfield (Computer Scientist)
- Marjorie McClain (Mathematician)
- James Sims (Physicist)

Needs (currently unfunded)

- 1+ AI/data analysis for biotechnology/forensics applications
- 1 Mathematical knowledge mgmt
- 1 Linux system administration
- 1 Research software engineer

Recruitment

- **Permanent Federal Hires** (2021-present)
  - 3 physicists (quantum)
  - 2 computer scientists (visualization)
  - 2 mathematician (data analysis/AI, soft materials/PDES)
  - 2 administrative assistants
- **Term Appointees** (2021-present)
  - 7 NRC Postdocs (special functions, classification, mathematical physics, topological data analysis, bio)
  - 1 NRC postdoc (quantum) in process

** 18 FTP Federal staff members (41%) are eligible to retire today*

Recommendation of FY 2018 Panel

"RECOMMENDATION: The ACMD should evaluate its organizational and recruiting practices in order to better meet the challenges it faces. Ideas that should be considered include the use of contractors to broaden the pool of potential participants in the ACMD mission; the use of sabbatical opportunities for career staff to broaden the range of skills in response to new areas for ACMD; and development of a more effective pipeline for graduate students into ACMD through, for example, a broad-based university affiliates program."

Response

We have greatly increased our pool of participants. During the period October 2022 – December 2023 we :

- Hosted 7 NIST/NRC postdoctoral associates
- Engaged with 12 postdoctoral or senior researchers through the PREP program, contracts, or grants
- Supported 2 technicians via contracts
- Supported 13 graduate research assistants through the PREP, the NIST foreign guest researcher program, and the NSF Math Science Internship program
- Supported the part time work of 8 faculty members
- Formally engaged with many others as unpaid guest researchers
- Informally engaged with many additional collaborators worldwide

Of the 105 names on the March 2024 Division org chart, only 45 are "regular" Federal employees. In contrast, in June 2018 there were 87 names on our roster, 43 of whom were regular Feds.

Recommendation of FY 2018 Panel

"RECOMMENDATION: The ACMD should engage in a formal strategic planning exercise with the following goals:

- *Identify current core competencies and match them to NIST needs;*
- *Identify gaps and new opportunities—mapping what its strategic goals are to resources (budget and staff)—in emerging areas such as artificial intelligence and machine learning; and*
- *Engage the next generation of ACMD leaders in developing this plan, so that what emerges can be enthusiastically executed by them. (Chapter 6)."*

Response

An *Applied and Computational Mathematics Division Capability Plan* was developed in 2019 which has the requested features.

Table of Contents

1. Introduction: the Division and Its Operations
   - Customers
   - Approach
   - Relation to Internal Customers
   - Relation to External Customers
   - Project Selection
2. Capabilities Needed for the Future
   - 2.1 Math and Comp Foundations of Adv Metrology
   - 2.2 Future Computing Technologies
   - 2.3 Mathematical Knowledge Management
3. Meta Issues
   - 3.1 Coping with a Wave of Retirements
   - 3.2 Ensuring Diversity in the Workforce
   - 3.3 Developing Competencies in New Areas
   - 3.4 Developing the NIST Customer Base
   - 3.5 Physical Location of NIST Staff
4. Staffing Trends and Needs

Response

Technical Areas Identified for Growth

- Quantum based measurements
- Bioscience
- Measurement science for information technology
- Data, machine learning and AI
- Dynamic metrology
- Imaging systems as metrological devices
- Multiscale material modeling
- Metrology for modeling and simulation
- Quantum information theory
- Quantum architectures, benchmarking and testing
- Quantum communication systems and components
- Neuromorphic computing
- Mathematical knowledge management

While there has been activity in all of these areas, those in red have seen the biggest increases

Recommendation of FY 2018 Panel

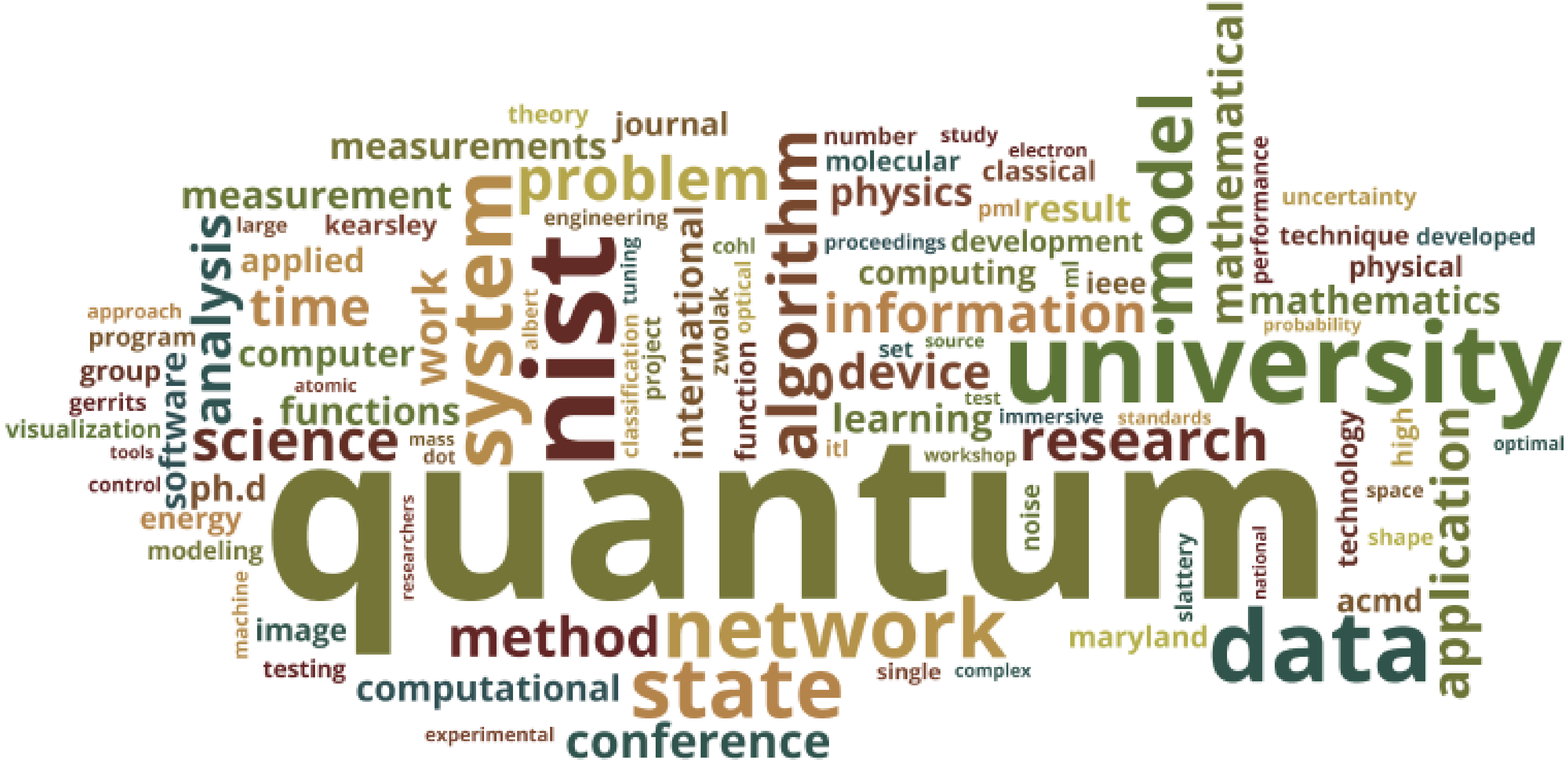
RECOMMENDATION: The ACMD should evaluate simulation software development practices in light of the disruptive changes in high-performance computing technology.

Response

Individual staff members have continued to engage in self-study to increase knowledge, skills, and abilities in this area. Machine learning techniques and workflows is one example. Research software engineering is an area in which we would like to grow, and we have had some recent contract support in this area, but budgetary and recruiting considerations make expansion a challenge.

Final Thoughts

- Vibrant program with broad impact
  - Have embraced/excelled in emergent areas (e.g., quantum, bio)
- No better place to be an applied mathematician
  - Problems exciting, important
  - Staff talented, motivated, (generally) happy
- Staffing continues to be a challenge given needs of collaborators and impending retirements


quantum
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