Mathematical and Computational Science Research at NIST

Günay Doğan
Justyna P Zwolak
NIST Applied & Computational Mathematics Division

CMAI Industry Day, June 25, 2021

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

INFORMATION TECHNOLOGY LABORATORY

Outline

1. A Brief Tour of NIST
2. Applied & Computational Math Division
3. Examples of Our Work
4. Opportunities

NIST Origins

U. S. Constitution

"Uniformity in the currency, weights, and measures of the United States is an object of great importance, and will, I am persuaded, be duly attended to."

George Washington, State of the Union Address, 1790

Bureau of Standards established by Congress in 1901

Early Measurement Needs

1900

Eight different “authoritative” values for the gallon

1904

Out-of-town fire companies arriving at a Baltimore fire cannot couple their hoses to local hydrants. 1526 buildings destroyed.

1912

41,578 train derailments in the previous decade lead to NBS measurement and test program.

NIST Today

A Federal science and engineering lab within the US Department of Commerce

Promotes U.S. innovation and industrial competitiveness by advancing

measurement science, standards, and technology

Non-regulatory

©R. Rathe

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

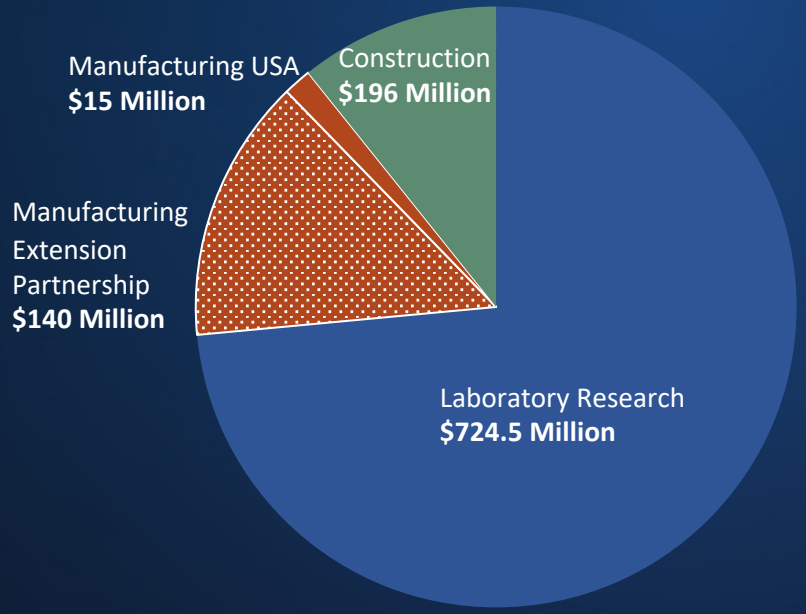
NIST At a Glance

3,400+
FEDERAL STAFF

3,500+
ASSOCIATES

2 CAMPUSES
GAITHERSBURG, MD
BOULDER, CO

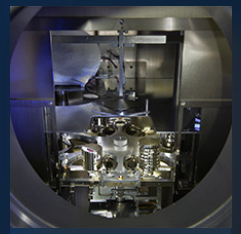
10
COLLABORATIVE INSTITUTES



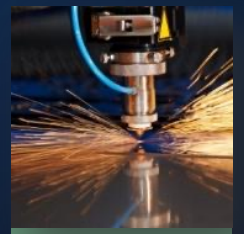
FY 2019 Appropriated Budget: $985.25M

6 Laboratory Programs


Material Measurement Laboratory


Physical Measurement Laboratory


NIST Center for Neutron Research


Engineering Laboratory


Information Technology Laboratory


Communications Technology Laboratory

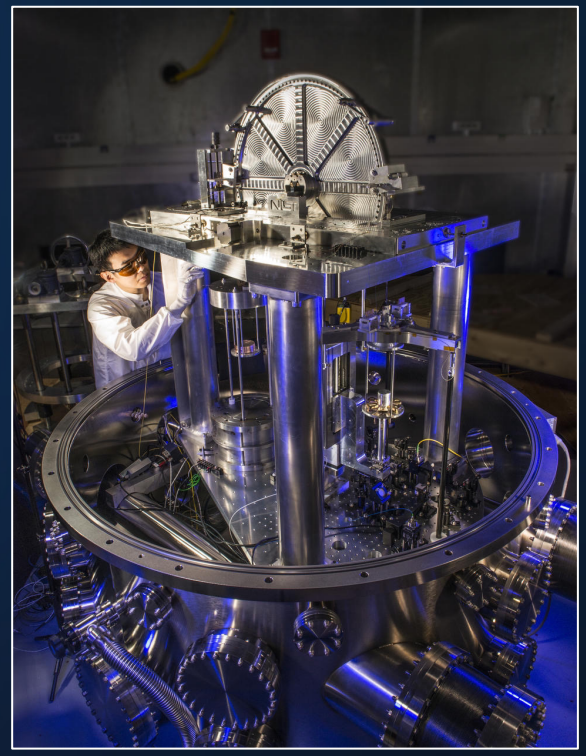
National Institute of Standards and Technology
U.S. Department of Commerce

NIST Labs: Your National Metrology Institute

Metrology: Science of Measurement

- Definition of units
- Realization in practice
- Characterization of uncertainty
- Traceability: linking measurements made in practice to reference standards

Fundamental → Applied → Legal



Scientific Foundations

2012 Nobel Prize
in Physics
Experimental
Quantum
Mechanics

2011 Nobel Prize
in Chemistry
Quasicrystals

Four NIST Nobel Prize winners in physics and one in chemistry

2005 Nobel Prize
in Physics
Frequency Combs

2001 Nobel Prize
in Physics
Bose-Einstein
Condensates

1997 Nobel Prize
in Physics
Laser Cooling

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

Best part of working here …

… the challenging science found along the way

- ❑ Semiconductor electronics
- ❑ Electromagnetic technology
- ❑ Atomic and optical physics
- ❑ Radiation physics
- ❑ Quantum science/engineering
- ❑ Manufacturing engineering
- ❑ Biotechnology
- ❑ Analytical chemistry
- ❑ Nanotechnology
- ❑ Material science
- ❑ Structural engineering
- ❑ Fire science
- ❑ Environment/climate
- ❑ Public safety
- ❑ Forensics
- ❑ Healthcare technology
- ❑ Information technology
- ❑ Cybersecurity
- ❑ Statistics
- ❑ Mathematic

NIST Applied & Computational Mathematics Division

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

Organizational Context

Information Technology Lab

- Advanced Networking
- Computer Security
- Applied Security
- Information Access
- Software and Systems
- Statistical Engineering
- Applied & Computational Math

ACMD Purpose:

Nurturing trust in metrology and scientific computing.

How?

Ensure that the best mathematical and computational methods are applied.

How we work

- Collaborative Research
  - Within NIST: interdisciplinary
  - Bring expertise, facilities / high local payoff
  - With academia: access specialized expertise
- Underlying R&D
  - Research in math, stat, CS anticipating needs
  - Develop tools, facilities to make us, customers more efficient
- Technology Transfer
  - Community-based measurement, standards
  - Online information services
  - Wide distribution of tools

Staff Expertise

Mathematics

- *Real & complex analysis*
- *Differential equations*
- *Nonlinear dynamics*
- *Linear algebra*
- *Optimization*
- *Game theory*
- *Group theory*
- *Numerical analysis*
- *Computational geometry*
- *Combinatorics*
- *Graph theory*
- *Approximation theory*
- *Signal processing*
- *Statistics*

Computer Science

- *Algorithms*
- *Complexity theory*
- *Software carpentry*
- *Software testing*
- *Machine learning*
- *Image processing*
- *Computer graphics*
- *Parallel algorithms*
- *Computational science*

Applications

- *Mathematical physics*
- *Network Science*
- *Computational chemistry*
- *Computational materials science*

Examples of Our Work

Computational Tools for Image and Shape Analysis

by Günay Doğan

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

Machine Learning Tools to Enhance and Control Quantum Experiments

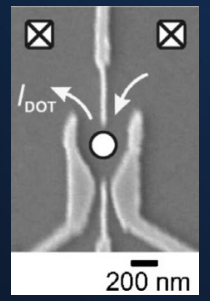
by Justyna P Zwolak

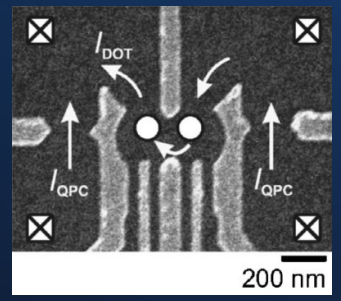
National Institute of Standards and Technology
U.S. Department of Commerce

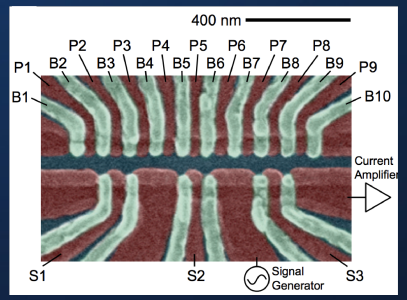
Automation of Quantum Dots Experiments

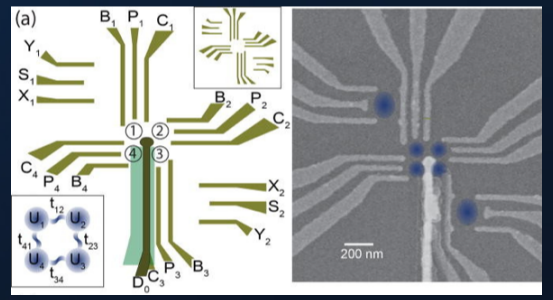
Quantum dots are semiconductor nanostructures that confines the motion of conduction band electrons, valence band holes, or excitons.

Spin states of coupled single-electron quantum dots were first proposed as a platform for realization of quantum bits by Loss and DiVincenzo back in 1998.







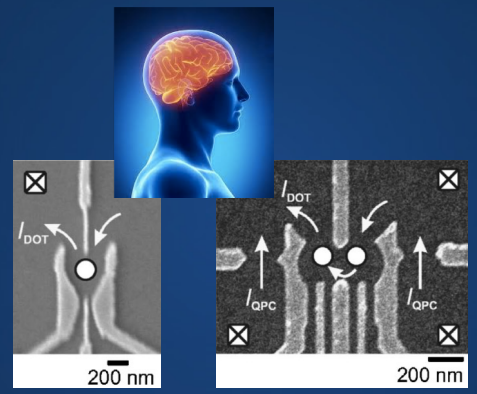


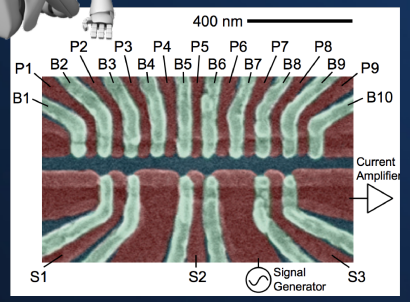
National Institute of Standards and Technology
U.S. Department of Commerce

R. Hanson, L. P. Kouwenhoven, J. R. Petta, S. Tarucha, and L. M. K. Vandersypen, Rev. Mod. Phys. **79**, 1217 (2007)
D. M. Zajac, T. M. Hazard, X. Mi, E. Nielsen, and J. R. Petta Phys. Rev. Applied 6, 054013 (2016)
U. Mukhopadhyay, J. P. Dehollain, et al. Appl. Phys. Lett. 112, 183505 (2018)

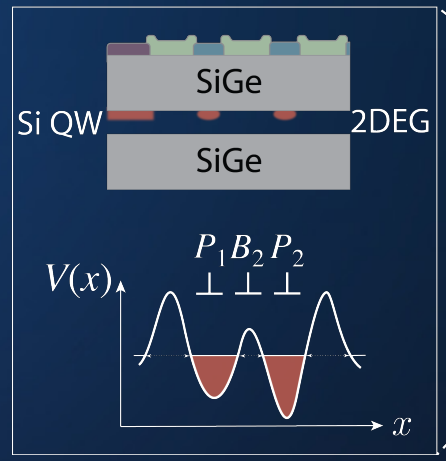
Automation of Quantum Dots Experiments

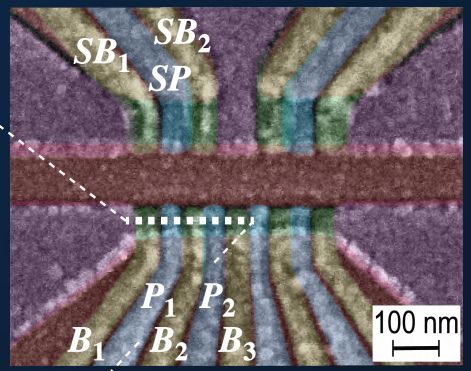
Traditional approach: heuristic and intuition





Can we use machines?

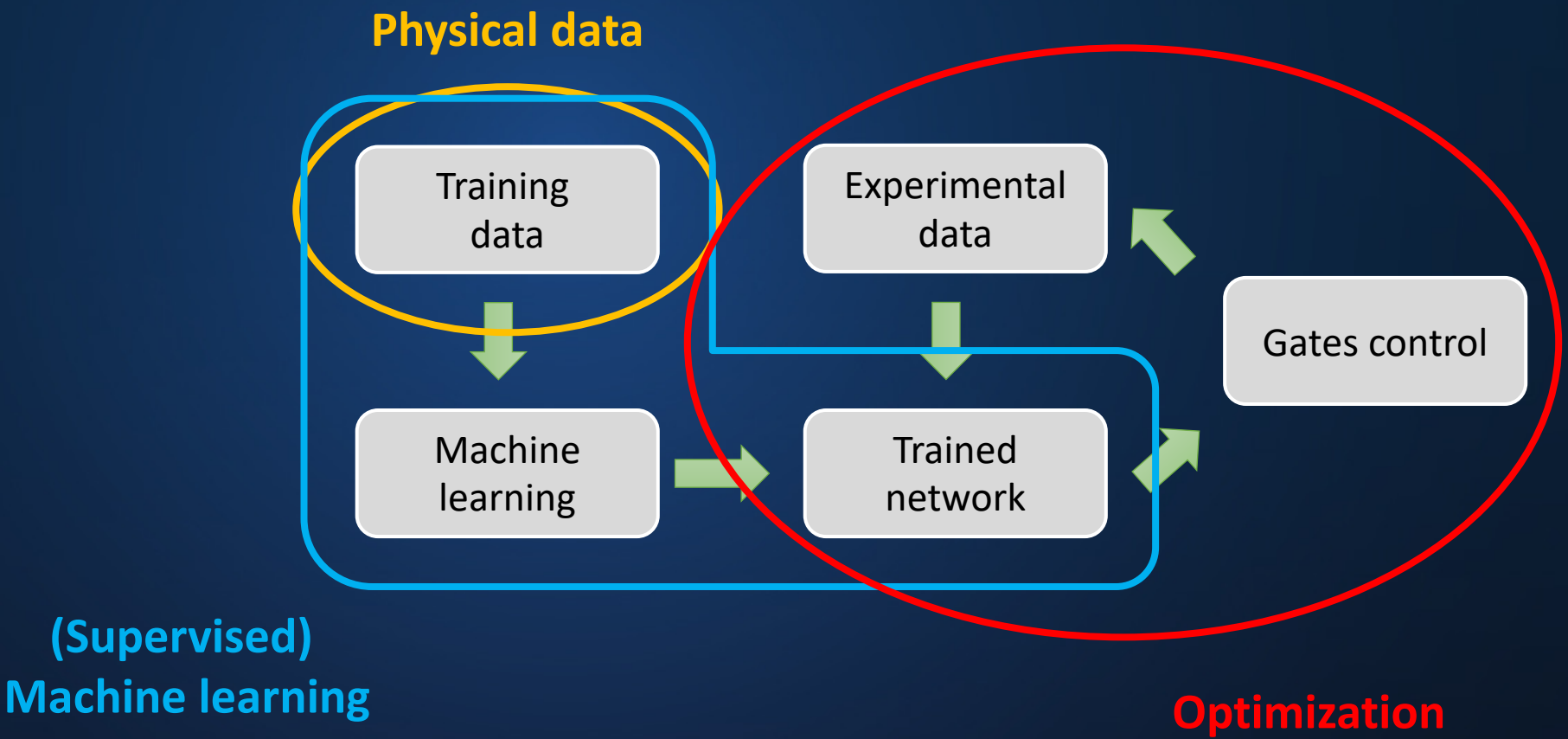




National Institute of Standards and Technology
U.S. Department of Commerce

R. Hanson, L. P. Kouwenhoven, J. R. Petta, S. Tarucha, and L. M. K. Vandersypen, Rev. Mod. Phys. **79**, 1217 (2007)
D. M. Zajac, T. M. Hazard, X. Mi, E. Nielsen, and J. R. Petta Phys. Rev. Applied 6, 054013 (2016)

Automation of Quantum Dots Experiments



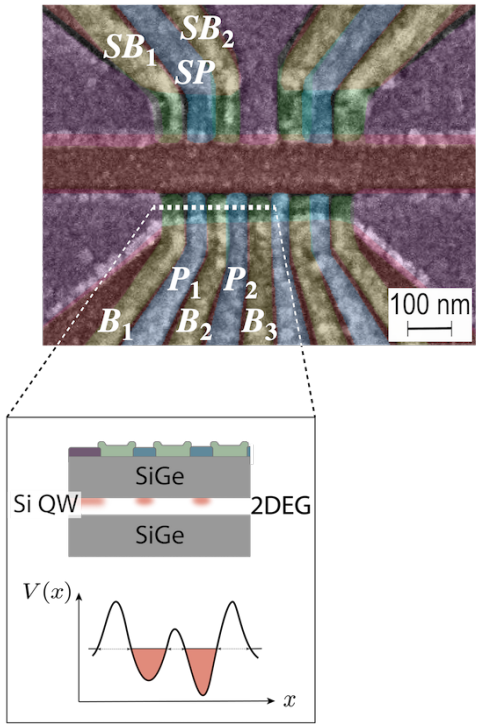
National Institute of Standards and Technology
U.S. Department of Commerce

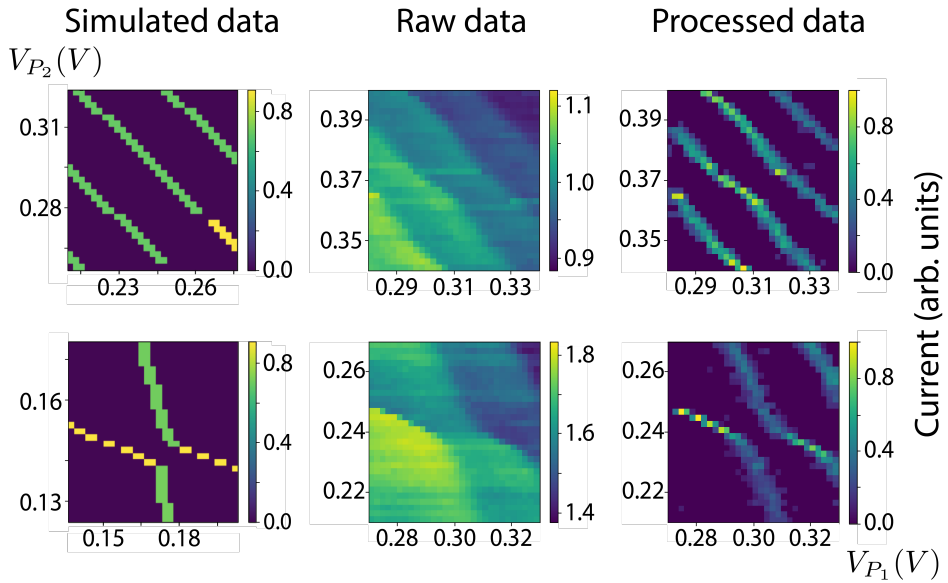
S. S. Kalantre, J. P. Zwolak, S. Ragole, X. Wu, N. M. Zimmerman, M. D. Stewart, and J. M. Taylor. npj Quantum Inf., 5(1), 1-10 (2019).

Automation of Quantum Dots Experiments

$\boldsymbol{p}_{\text{target}} = [0, 0, 1]$ (double dot)

Step 1:
Measurement





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

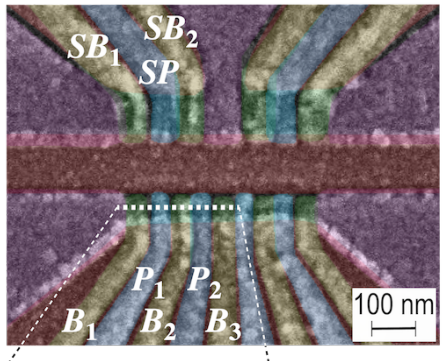
J. P. Zwolak, T. McJunkin et al. Auto-tuning of double dot devices *in situ* with machine learning. Phys. Rev. Applied 13, 034075 (2020).

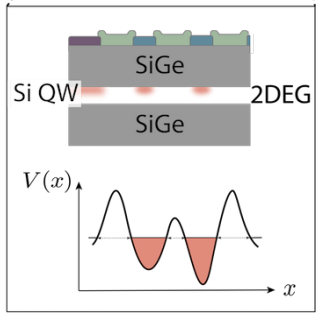
Automation of Quantum Dots Experiments

$\boldsymbol{p}_{\text{target}} = [0, 0, 1]$ (double dot)

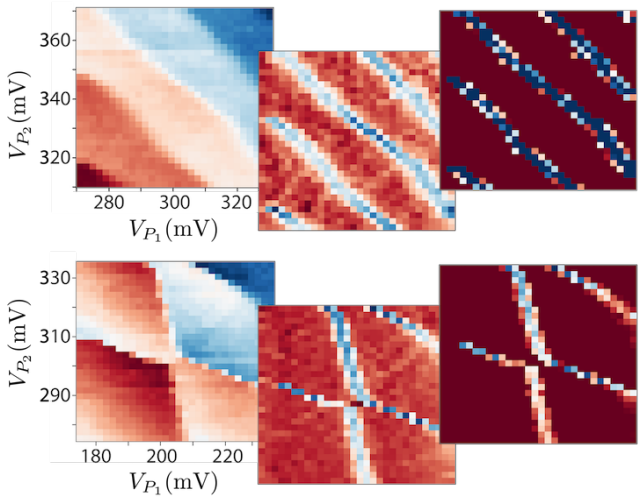
Success rate: 85.7 %
N = 14 runs

Step 1:
Measurement

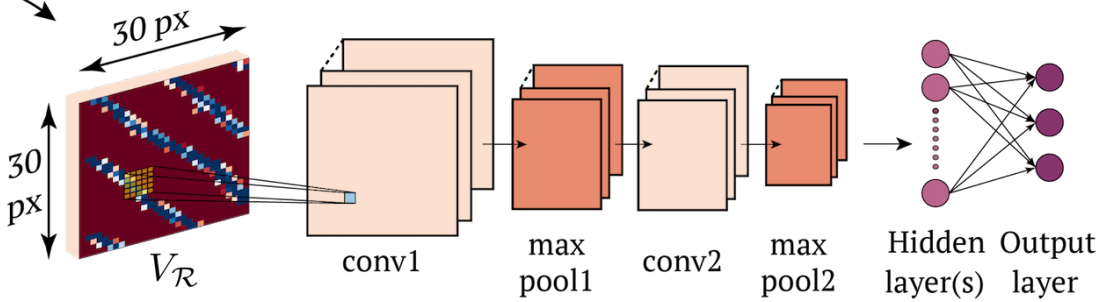




Step 2:
Data processing



Step 3:
Network analysis



State recognition
for region $V_{\mathcal{R}}$

$$\boldsymbol{p}(V_{\mathcal{R}}) = [p_{none}, p_{SD}, p_{DD}]$$
$$= [0, 1, 0]$$

Step 4:
Optimization

$$\min \delta(\boldsymbol{p}_{target}\ ,\ \boldsymbol{p}(V_{\mathcal{R}}))$$

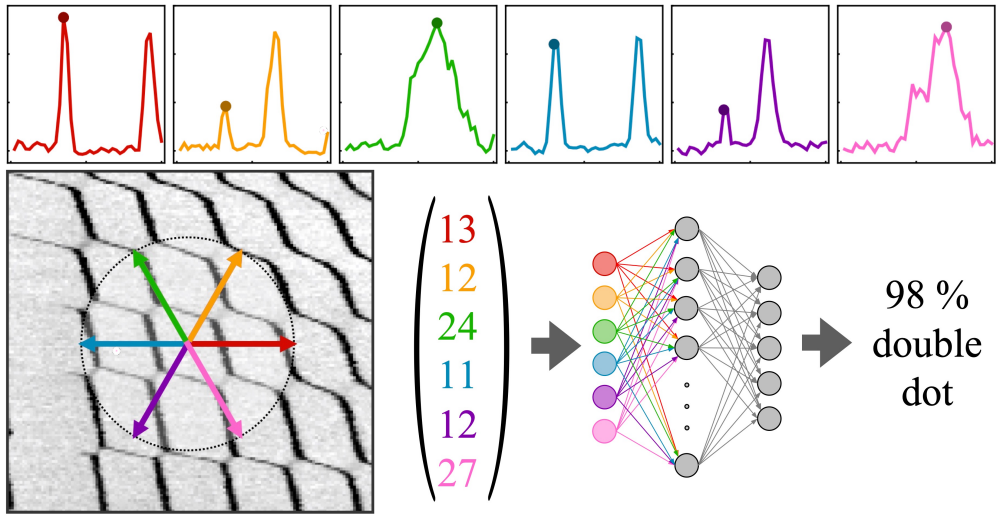
Step 5:
Gate voltages
adjustment

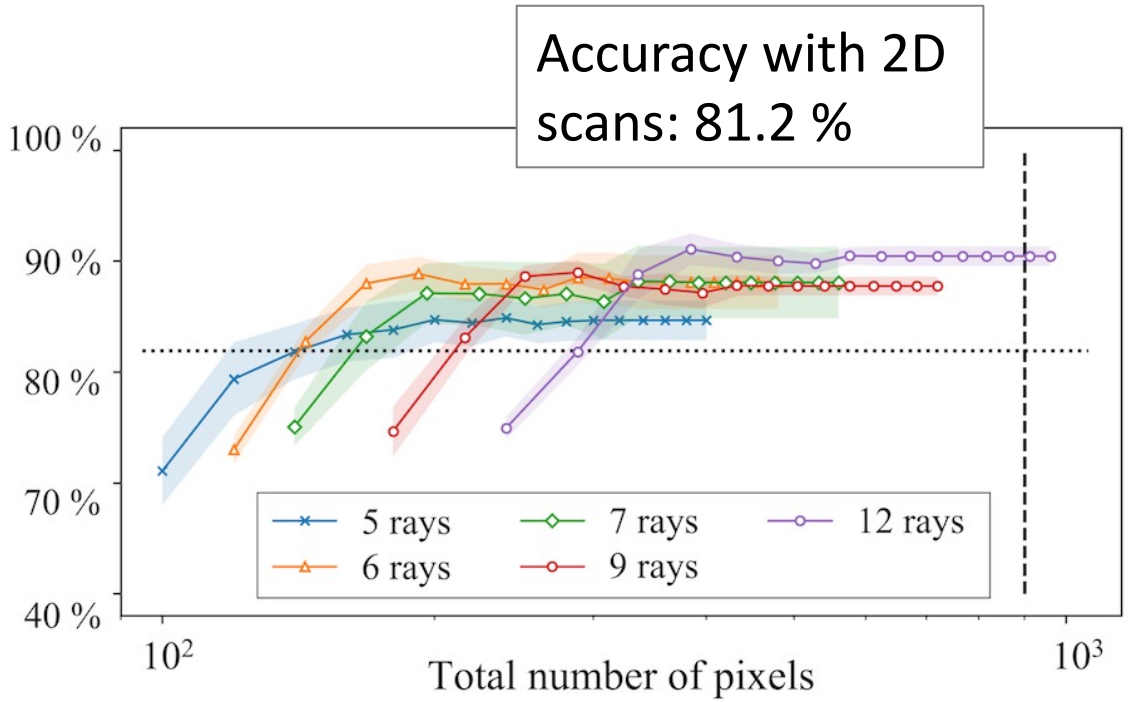
Termination

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

J. P. Zwolak, T. McJunkin et al. Auto-tuning of double dot devices *in situ* with machine learning. Phys. Rev. Applied 13, 034075 (2020).

Automation of Quantum Dots Experiments

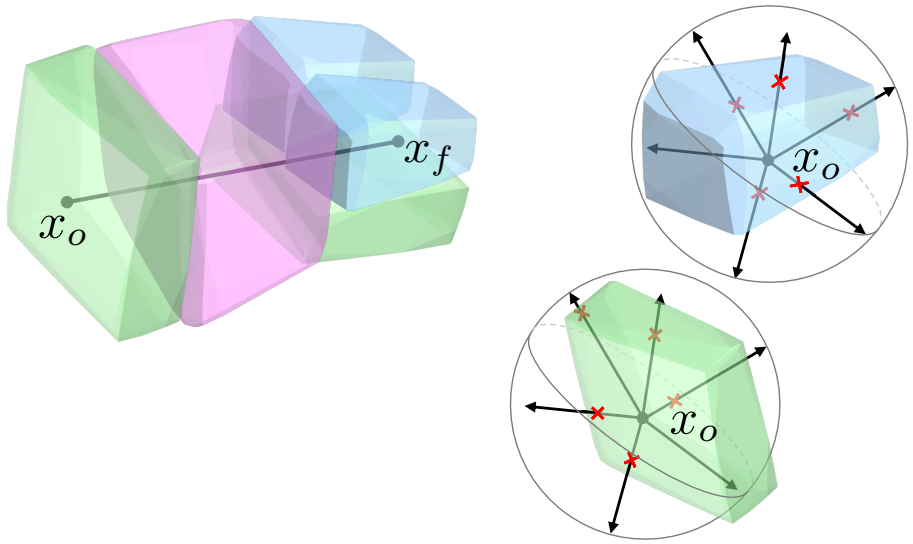


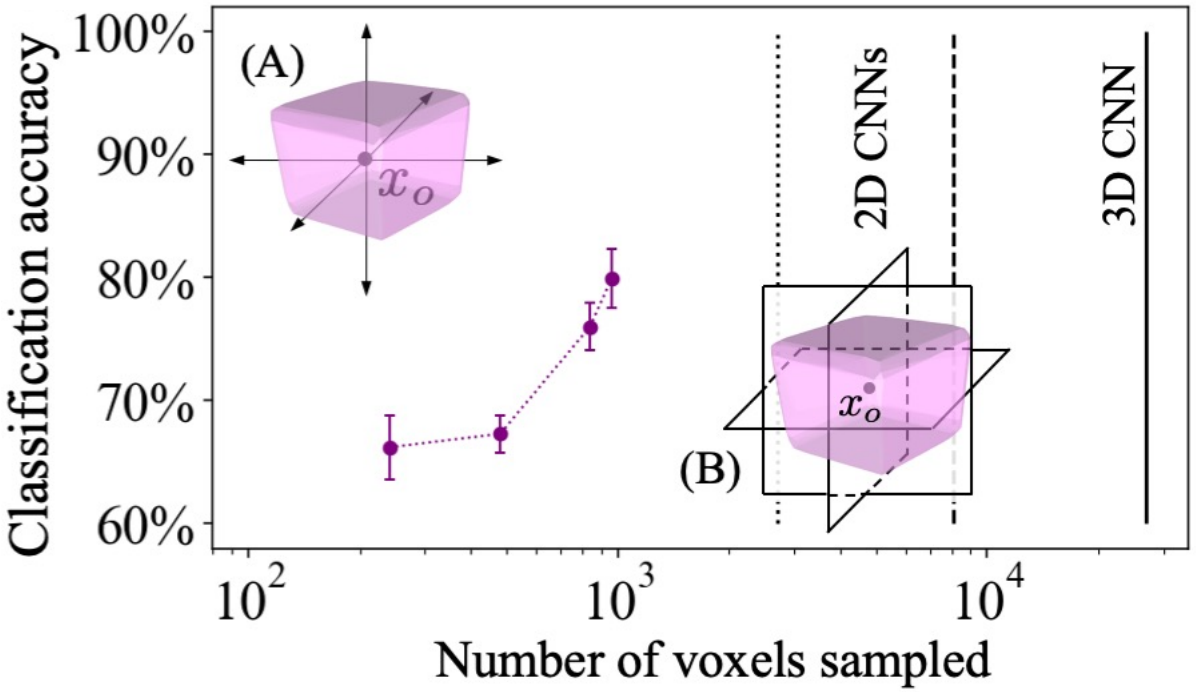


6 rays of length 22 mV (44 pixels) → 70 % data reduction

J. P. Zwolak, T. McJunkin *et al*. Ray-Based Framework for State Identification in Quantum Dot Devices. PRX Quantum **2**, 020335 (2021).

Automation of Quantum Dots Experiments





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

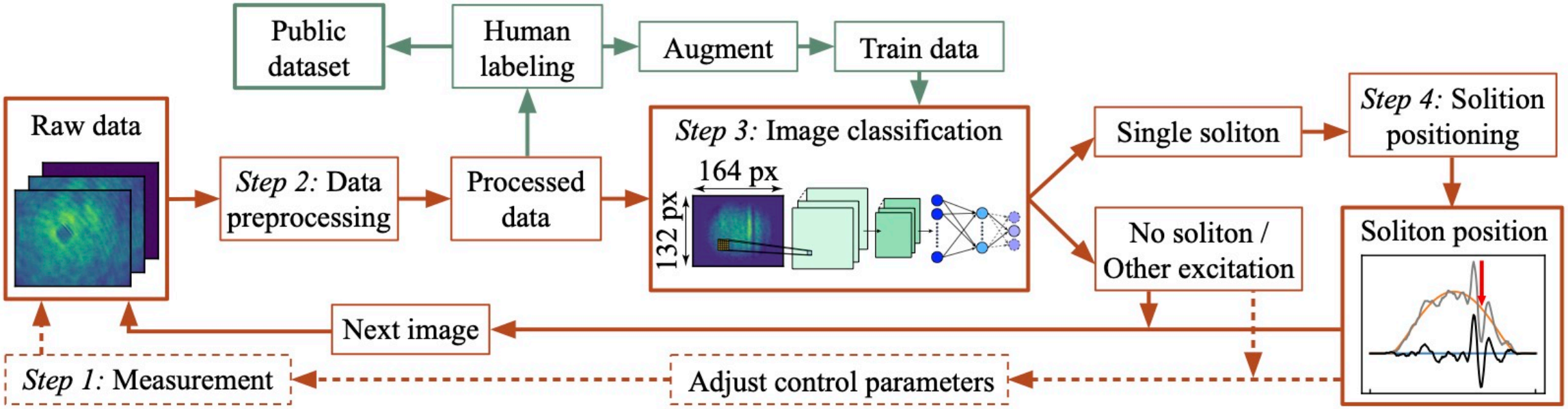
J. P. Zwolak, S. S. Kalantre et al. Ray-based classification framework for high-dimensional data. Proceeding of ML4PS @ NeurIPS 2020.

Enhancement of Cold-atom Experiments

- Most data in cold-atom experiments comes from images
- The analysis of images is limited by our preconceptions of the patterns that could be present in the data
- Studying such systems over a wide range of parameters requires the analysis of large datasets
- The existing human-inspection-based methodology a significant bottleneck

Guo, S., Fritsch, A. R., Greenberg, C., Spielman, I. B., & Zwolak, J. P. (2021). Machine-learning enhanced dark soliton detection in Bose-Einstein condensates. Mach. Learn.: Sci. Technol. **2** (3): 035020 (2021).

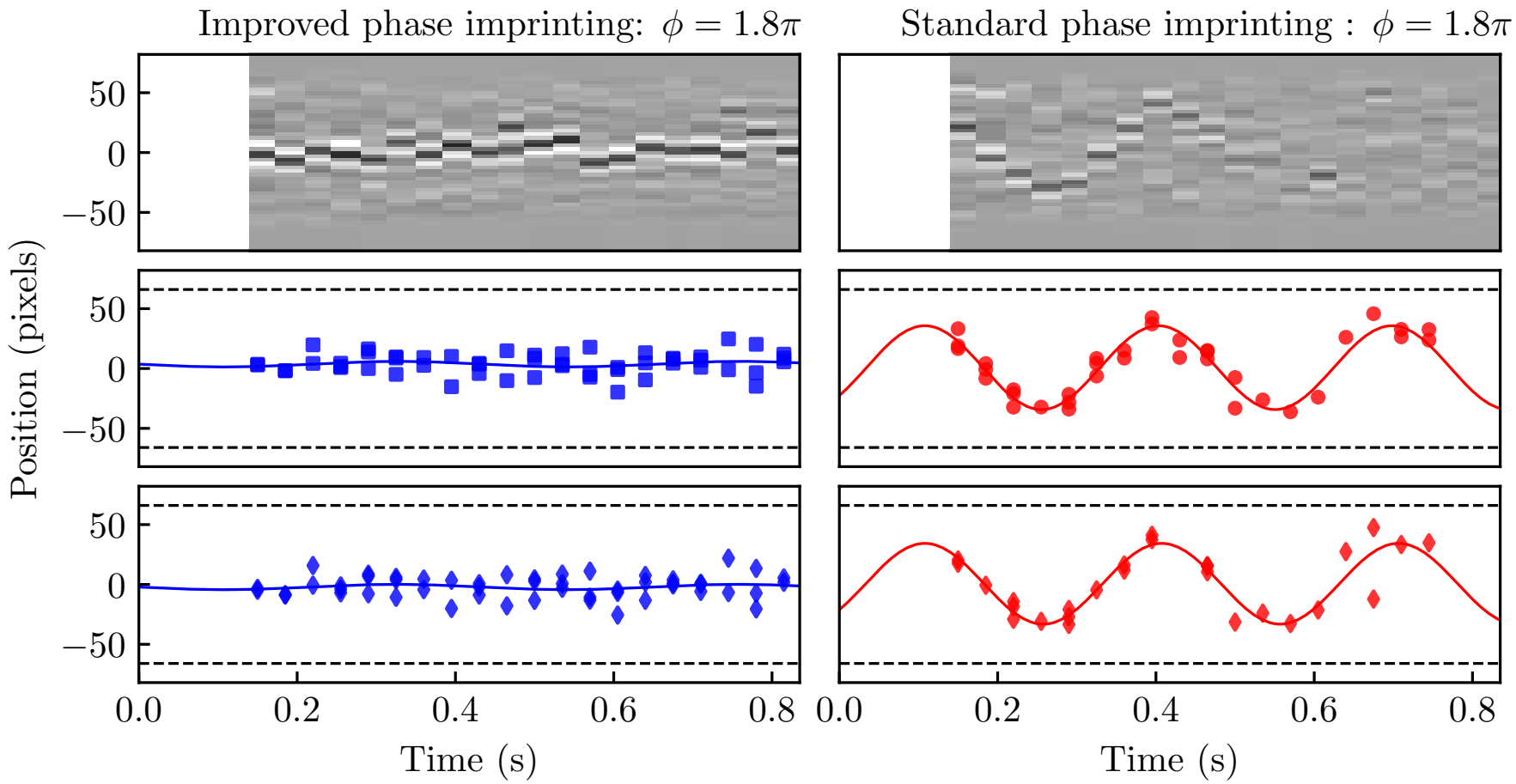
Enhancement of Cold-atom Experiments



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

Guo, S., Fritsch, A. R., Greenberg, C., Spielman, I. B., & Zwolak, J. P. (2021). Machine-learning enhanced dark soliton detection in Bose-Einstein condensates. Mach. Learn.: Sci. Technol. **2** (3): 035020 (2021).

Enhancement of Cold-atom Experiments



Guo, S., Fritsch, A. R., Greenberg, C., Spielman, I. B., & Zwolak, J. P. (2021). Machine-learning enhanced dark soliton detection in Bose-Einstein condensates. Mach. Learn.: Sci. Technol. **2** (3): 035020 (2021).

What's next?

Quantum dots

- Full automation of tuning for quantum dot devices
- Ray-based learning: going beyond two dots (learning high-dimensional volumes)

Cold-atoms

- Adding heuristics to complement the ML techniques
- Developing tools for more complex systems

What about uncertainty?

- Developing framework for UQ for ML methods in physics

Guo, S., Fritsch, A. R., Greenberg, C., Spielman, I. B., & Zwolak, J. P. (2021). Machine-learning enhanced dark soliton detection in Bose-Einstein condensates. Mach. Learn.: Sci. Technol. **2** (3): 035020 (2021).

Opportunities

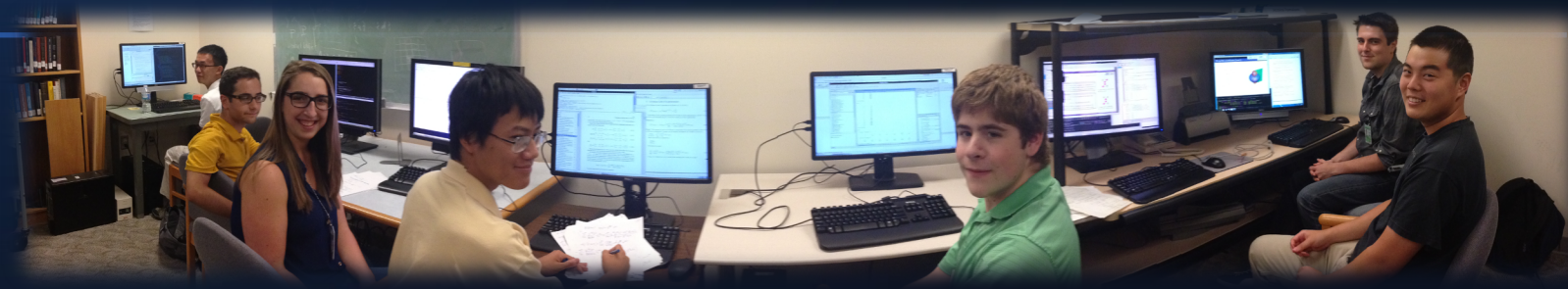
Summer Undergraduate Research Fellowship (SURF)

- Competitive; US citizenship required
- 9 or 11 weeks: work with mentor on research project
- Gaithersburg, MD or Boulder, CO
- Housing allowance ($4,500), travel ($600), stipend ($6,000)
- Seminar series; Student symposium; Social program

  http://www.youtube.com/watch?v=wMFMqMMGGrg
- Application deadline: February 21

https://www.nist.gov/surf

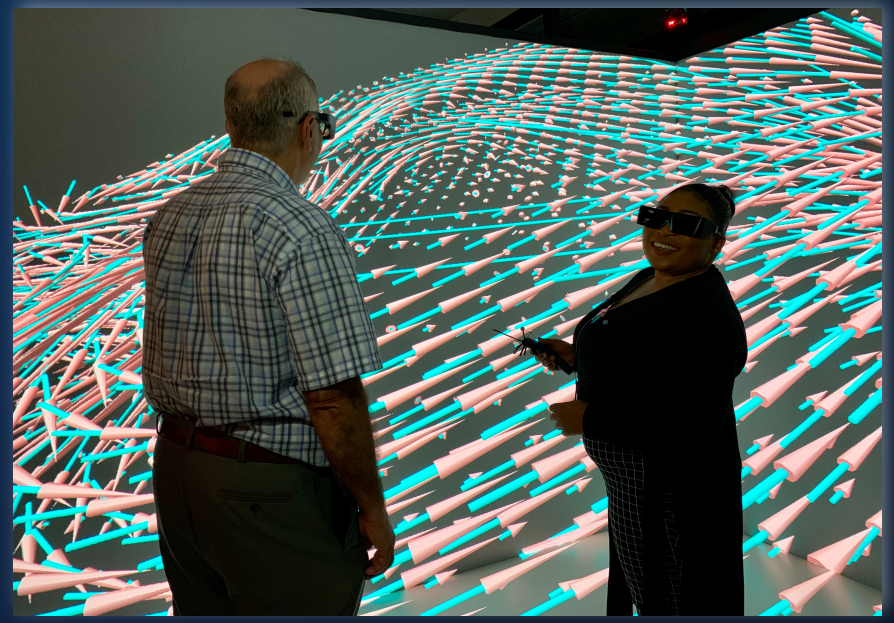
NIST National Institute of Standards and Technology
U.S. Department of Commerce



Professional Research and Education Program (PREP)

- 13 participating universities
- US Citizenship not required
- Placement within NIST research group

  Matches made through contact with researchers, funded by NIST Division
- Undergrads: hourly
- Graduate assistantships
- **Full-time postdocs**
- Faculty sabbaticals



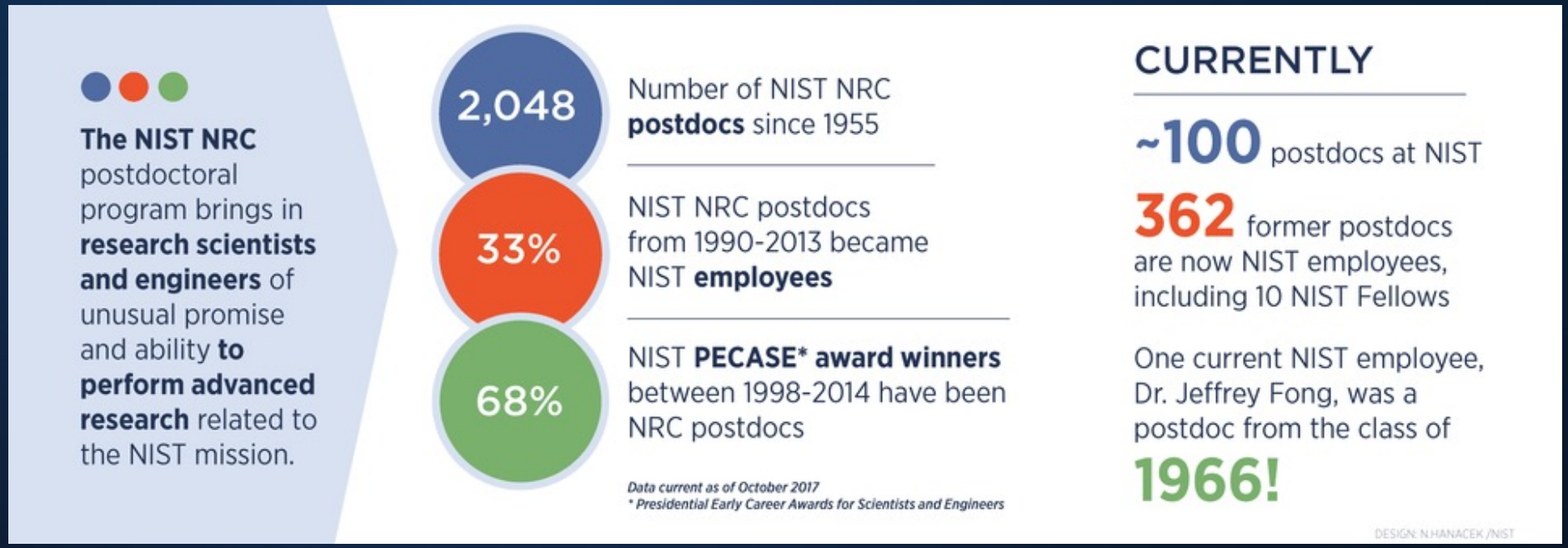
Nicos Martys (NIST Engineering Lab) and Rukayat Aiori (Morgan State)

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

https://www.nist.gov/iaao/academic-affairs-office/nist-professional-research-experience-program-prep

NRC Postdoc Program

- Competitive; US citizenship required; 2-year Fed appointment
- Currently 26 opportunities in ACMD, 50 across ITL



https://www.nist.gov/itl/how-work-us/nrc-postdoctoral-research-fellowships-itl

Diverse and Exciting Opportunities of Research in Applied & Computational Math @ NIST

Any questions?