U.S. DEPARTMENT OF ENERGY | Office of Science

View from Germantown
Advanced Scientific Computing Research

Presented to the
ASCAC

by

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Associate Director

March 26, 2019

ASCR FY 2019 Enacted
in thousand

	FY 2018	FY 2019	
	Enacted Approp.	President's Request	Enacted
Mathematical, Computational, and Computer Sciences Research			
Applied Mathematics	30,104	40,316	28,206
Computer Science	29,508	38,296	22,000
Computational Partnership	49,910	62,667	75,667
Artificial Intelligence and Big Data (Non Add)	*(3.500)*	*(…)*	*(13,000)*
SBIR/STTR	4,301	5,352	4,768
Total, Mathematical, Computational, and Computer Sciences Research	117,823	146,631	130,641
High Performance Computing and Network Facilities			
High Performance Production Computing (NERSC)	94,000	80,000	104,000
Leadership Computing Facility at ANL (ALCF)	*110,000*	*140,000*	*140,000*
Exascale	*(…)*	*(100,000)*	*(140,000)*
Leadership Computing Facility at ORNL (OLCF)	*162,500*	*200,000*	*199,000*
Exascale	*(62,500)*	*(100,000)*	*(100,000)*
Total, Leadership Computing Facilities	272,500	340,000	339,000
Research and Evaluation Prototypes	24,260	24,452	24,452
High Performance Network Facilities and Testbeds (ESnet)	79,000	56,435	84,000
SBIR/STTR	17,417	18,786	20,701
Total, High Performance Computing and Network Facilities	487,177	519,673	572,153
Exascale Computing			
17-SC-20 Office of Science Exascale Computing Project (SC-ECP)	205,000	232,706	232,706
Total, Advanced Scientific Computing Research	**647,000**	**899,010**	**935,500**

Advanced Scientific Computing Research *(ASCR: FY 2018 $810M; FY 2019 $935.5M)*

FY 2018 Enacted Highlights

- Expanded QIS efforts with additional investments in Quantum Testbed Pathfinder and initiation of 2 new programs:
  - Quantum Computing Application Teams (QCATs): interdisciplinary teams of QIS experts, applied mathematicians, and computer scientists with expanded focus on algorithms, software stack and verification & validation methods. Two teams led by ORNL and SNL were funded.
  - Quantum Testbeds for Science: these quantum computing testbed laboratories will provide external researchers with access to novel, early-stage quantum computing resources not available through other means. A trapped ion testbed was funded at SNL and a superconducting qubit testbed was funded at LBNL.
- Funded two additional Mathematical Multifaceted Integrated Capability Centers (MMICC) to address fundamental mathematical challenges within the DOE mission that require new integrated efforts; the FY 2017 MMICC call for proposals was limited to National Laboratories.
- Funded four new Scientific Data Management, Analysis, and Visualization projects and an Artificial Intelligence and Machine learning project, titled *Co-design for Artificial Intelligence coupled with computing at scale for extremely large, complex datasets*, to advance DOE's capabilities in cognitive computing – coupling Artificial Intelligence and computing at scale.
- Increased funding that permitted the Exascale Computing Project (ECP) to fully fund four of the five seed projects ASCR was supporting and to initiate a co-design center focused on Artificial Intelligence. The software technology integration activity developed software development kits to promote use of their software by the facilities and larger computing community. ECP also fully funded proposed vendor milestones in the Hardware Integration activity and completed initial engagement plans with the ASCR facilities.

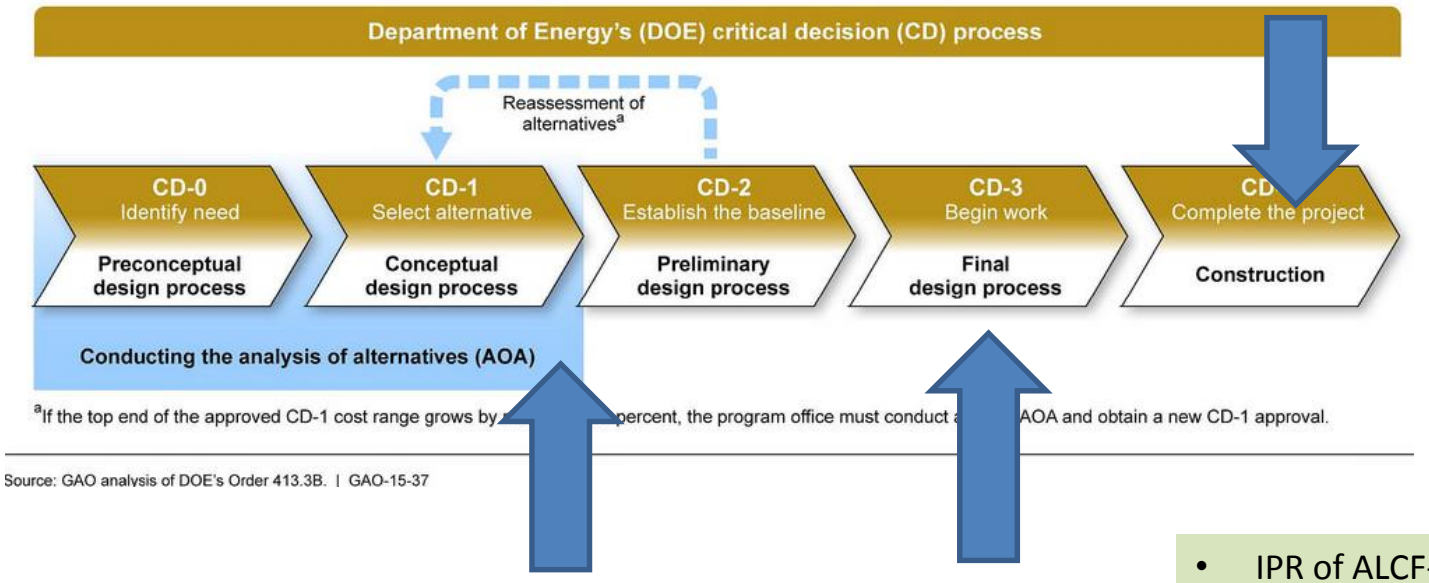
Facility Operations:

- Facilities operated at over 97% of scheduled availability

ASCR Facilities Project Update

CD-4

OLCF-4, 3/2019,
9 months ahead of schedule,
$13.5M below cost



CD 1/3A

Esnet 7/2018

CD 2/3

NERSC- 9 –Perlmutter 9/2018

ALCF-3 – Aurora rebaselined, 3/2018

OLCF-5 -- Frontier, 3/2019

- IPR of ALCF-3(Aurora) scheduled for April 9-10, 2019
- Esnet CD-2 IPR scheduled for Fall, 2019
- ECP CD-2 review scheduled for December 10-12, 2019

Advanced Scientific Computing Research
FY 2019 Appropriation Enables

Research

Proposed funding opportunity announcements

- Quantum algorithms and other crosscutting quantum technologies
- Quantum networking
- Scientific Machine Learning and Uncertainty quantification – High Risk, High Reward
- Artificial Intelligence, Machine Learning and Data Analytics CoDesign

Facilities

- Maintain facility operations at >95%, operating Cori at NERSC, Summit and Titan (9 months) at OLCF and Theta and Mira at ALCF

Project funding supports

- Larger power upgrade at NERSC
- Long lead time procurements for Esnet-6 in preparation for CD-2/CD-3 in Fall, 2019
- Exascale upgrades at the ALCf and OLCF
- ECP
  - Fund last Path forward milestones with Vendors
  - Release Software Development Kits for use by Facilities and larger community
  - Continue testing application and system software on pre-exascale systems at DOE facilities

FY 2020 President's Budget Priorities

FY 2018 Enacted: $6.260B

FY 2019 Enacted: $6.585B

FY 2020 President's Request: $5.546B

Priorities:

- Continue operations of all the national laboratories
- Focus on the development of foundational Artificial Intelligence (AI) and Machine Learning (ML) capabilities
- Continue exascale computing research for delivery in FY 2021
- Expand quantum computing and quantum information science efforts
- Provide sufficient funding to ensure robust cybersecurity program
- Focus on cutting edge, early stage research and development
- Maintain interagency and international partnerships

FY 2020 Priority #1 Research Initiatives

- Machine Learning/Artificial Intelligence
- Bio (security, materials, manufacturing)
- Quantum Information Science - includes quantum sensing, computing, networking, and isotope production
- Exascale Computing
- Microelectronics Innovation
- National Isotopes Strategy
- U.S. Fusion Program Acceleration

FY 2020 Priority #1 Research Initiatives

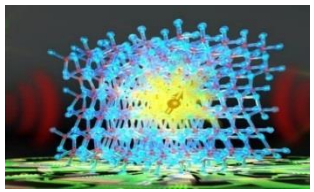
Dollars in Thousands

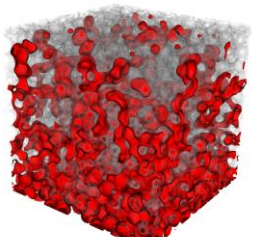
Research Initiative	ASCR	BES	BER	FES	HEP	NP	Total
Machine Learning / Artificial Intelligence	36,000	10,000	3,000	7,000	15,000		**71,000**
Biosecurity			20,000				**20,000**
Quantum Information Science	51,161	52,503	12,000	7,520	38,308	7,000	**168,492**
Exascale Computing	463,735	26,000	10,000				**499,735**
Microelectronics		25,000					**25,000**
Isotope Development and Production for Research and Applications						47,500	**47,500**
U.S. Fusion Program Acceleration				4,000			**4,000**
Total	**550,896**	**113,503**	**45,000**	**18,520**	**53,308**	**54,500**	**835,727**

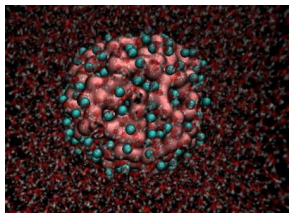
Advanced Scientific Computing Research

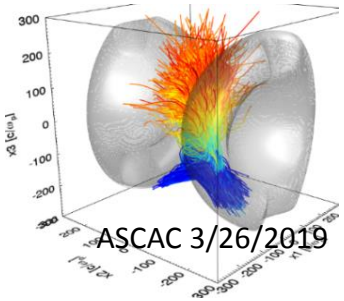
Computational and networking capabilities and tools to extent the frontiers of science and technology

- **Exascale:** The FY 2020 Request fully supports ASCR's commitment to the Exascale Computing Project (ECP), in partnership with NNSA. The FY 2020 Request also supports additional facility investments at the ALCF and OLCF to deploy at least one exascale system in the calendar year 2021-2022 timeframe.
- **Facilities:** The FY 2020 Request maintains facility operations and supports the ESNET-6 upgrade, and final site preparations for the NERSC-9 upgrade.
- **Computational Partnerships:** The FY 2020 Request continues support for SciDAC partnerships and institutes, and partnerships in "beyond Moore's law" applications such as quantum information systems, artificial intelligence, and data intensive science.
- **Applied Mathematics research** continues to provide the fundamental building blocks (algorithms, mathematical models, and methods) for describing complex physical systems computationally. Increase in FY 2020 requested to provide vital investments in fundamental research in artificial intelligence (AI)/machine learning (ML) and other ML activities based on Priority Research Needs identified at the Basic Research Needs Workshop on Scientific Machine Learning (SciML) (1/2018)
- **Computer Science** increase supports: development of adaptive software tools based on AI/ML techniques for future extremely heterogeneous HPC and to meet data-intensive science challenges, the collaboration and workflow tools to support the increasing data needs of the DOE scientific user facilities, and continues research into quantum networking.
- **Research and Evaluation Prototypes** continues to explore technologies "beyond Moore's law," increasing investments in quantum testbeds and Centers in support of the National Quantum Initiative in partnership with BES and HEP.
- The **Computational Sciences Graduate Fellowship** is funded at $10,000K.









ASCR FY 2020 President's Request

(Dollars in thousands)

	FY 2018		FY 2019	FY 2020 Request		
	Enacted Approp.	Current Approp.	Enacted Approp.	President's Request	Request vs. FY 2019 Enacted	
Mathematical, Computational, and Computer Sciences Research						
Applied Mathematics	34,104	34,720	28,206	41,500	+13,294	+47.1%
Computer Science	29,508	27,342	22,000	38,700	+16,700	+75.9%
Computational Partnerships (SciDAC)	49,910	51,402	75,667	60,959	-14,708	-19.4%
SBIR/STTR	4,301		4,768	5,347	+579	+12.1%
Total, Mathematical, Computational, and Computer Sciences Research	**117,823**	**113,464**	**130,641**	**146,506**	**+15,865**	**+12.1%**
High Performance Computing and Network Facilities						
High Performance Production Computing (NERSC)	94,000	94,000	104,000	85,000	-19,000	-18.3%
Leadership Computing Facilities						
Leadership Computing Facility at ANL (ALCF)	110,000	110,000	140,000	150,000	+10,000	+7.1%
Leadership Computing Facility at ORNL (OLCF)	162,500	162,500	199,000	210,000	+11,000	+5.5%
Total, Leadership Computing Facilities	272,500	272,500	339,000	360,000	+21,000	+6.2%
Research and Evaluation Prototypes	24,260	24,260	24,452	39,453	+15,001	+61.3%
High Performance Network Facilities and Testbeds (ESnet)	79,000	79,000	84,000	80,000	-4,000	-4.8%
SBIR/STTR	17,417	...	20,701	21,194	+493	+2.4%
Total, High Performance Computing and Network Facilities	**487,177**	**469,760**	**572,153**	**585,647**	**+13,494**	**+2.4%**
Subtotal, Advanced Scientific Computing Research	**605,000**	**583,224**	**702,794**	**732,153**	**+29,359**	**+4.2%**
Exascale Computing						
17-SC-20, Office of Science Exascale Computing Project (SC-ECP)	205,000	205,000	232,706	188,735	-43,971	-18.9%
Total, Advanced Scientific Computing Research	**810,000**	**788,224**	**935,500**	**920,888**	**-14,612**	**-1.6%**

Artificial Intelligence and Machine Learning

FY2020: President's request: $36M

To address the Administration's priority and the basic research needs in scientific machine learning and extremely heterogeneous systems in the FY2020 President's request, ASCR is investing in:

- Foundational research in machine learning and artificial intelligence to improve the reliability, robustness and interpretability of big data and AI technologies and to develop new algorithms, methods and software tools for extracting information from scientific and engineering data. (Applied Math)
- Co-design of a Distributed Computing Ecosystem (DCE), including vendor partnerships, and collaboration tools to ensure the seamless integration of Big Data with computing resources to support the large-scale computing and data requirements for machine learning; (Computer Science)
- Partnerships to broaden the applicability of AI and big data solutions across a broad range of DOE applications. (Computational Partnerships)

National Quantum Initiative

- **National Quantum Initiative Act – Public Law 115-368, signed by President Trump 12/21/2018**
- **Established National Quantum Coordination Office and through the National Science and Technology Council a Subcommittee on Quantum Information Science**
- **DOE roles**
  - Provide support for National Quantum Coordination Office
  - Serve as co-chair on QIS Subcommittee
  - Leverage the collective body of knowledge from existing quantum information science research
  - Provide research and training for additional undergraduate and student students in QIS
  - Establish at least 2 but no more than 5 National Quantum Information Science Research Centers.

Quantum Information Science (QIS) in ASCR

- **FY 2020 President's Request: $51.1M (Enacted Appropriations: FY2018 $20.6M; FY 2019 $33.7M)**

- **FY 2020 Objectives:**
  - Continue the SC-wide Partnership program with a focus on interdisciplinary teams that tackle basic research needs in quantum computing, including advances required in quantum algorithms and software tools for applications targeting identified grand challenge problems and support for cross-cutting research themes.(Computational Partnerships)
  - Expand the Quantum Networking program to develop robust and scalable theory, technologies, and communication software stack enabling wide-area distributed quantum information processing in support of open science. (Computer Science)
  - Continue the Quantum Testbeds program to the develop of hardware testbeds that will be available to the research community and to provide decision support for future investments in quantum computing hardware. (Research and Evaluation Prototypes)
  - **In support of the National Quantum Initiative, partner with BES and HEP to establish at least one QIS center.** (Research and Evaluation Prototypes)

ASCR's New Applied Mathematics Program Manager

William Spotz

BS, MS and PhD in Aerospace Engineering from the University of Texas at Austin

Research Interests: High-order accuracy numerical approximation methods, global atmosphere and climate modeling, linear and nonlinear solver techniques, multiphysics coupling techniques, graph algorithms, high-performance computing for high-level languages, uncertainty quantification, and performance portability.

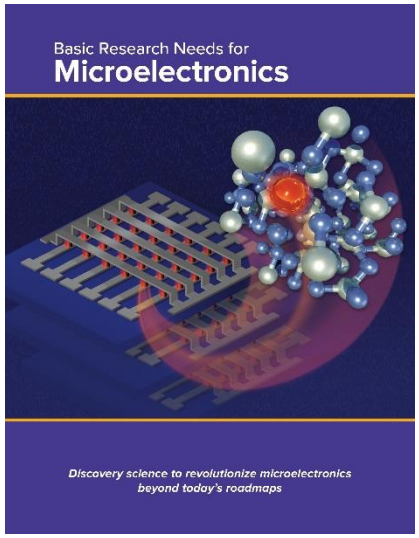
Current Projects: Overseeing the implementation of new verification tests for the Energy Exascale Earth System Model (E3SM), starting with the atmospheric component; implementing advanced nonlinear solvers into a aerodynamics code; and collaborating with UTEP to implement Trilinos solvers into MFiX, a multiphase flow solver.

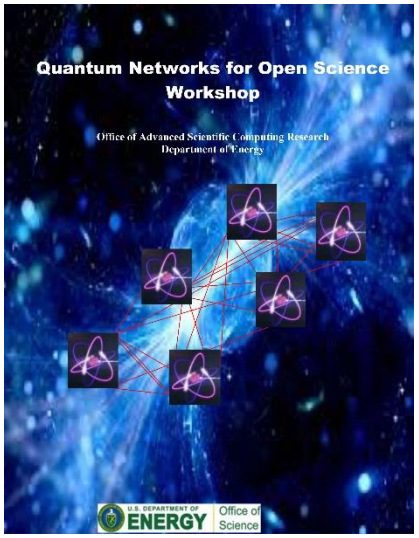
Bill also did a tour of duty in ASCR from 2008-2010

Some ASCAC Agenda Details

- **VIEW FROM WASHINGTON,** *Paul Dabbar, Under Secretary for Science*
- **INTERNATIONAL COLLABORATIONS IN SC PROGRAMS** -- *Steve Binkley, Deputy Director of the Office of Science for Programs*
- **QUANTUM, AI, AND EXASCALE – ASCR-BES COLLABORATIONS –** *Harriet Kung, Associate Director for Basic Energy Science*
- **OVERVIEW OF THE AMERICAN AI INITIATIVE:** *Lynne Parker, Office of Science and Technology Policy*
- **SEXUAL HARASSMENT: CLIMATE, CULTURE, AND CONSEQUENCES IN ACADEMIA** -- *Frazier Benya, the National Academies of Sciences, Engineering, and Medicine*
- **SSIO WORKSHOP UPDATE –** *Rob Ross, ANL*
- **QUANTUM NETWORKING WORKSHOP UPDATE,** *Nicholas Peters, ORNL*
- **UPDATE ON THE EXASCALE COMPUTING PROJECT –** *Terri Quinn and Lori Diachin, LLNL*
- **UPDATE ON CURRENT CHARGES**
  - *ASCR 40th Anniversary Impacts – Bruce Hendrickson, LLNL*
  - *Transitioning from Exascale project – Roscoe Giles, Boston University*
  - *Technologies from Beyond Moore's law – Vivek Sarkar, ASCAC*
- **OVERVIEW OF DATA SCIENCE EFFORTS AT THE ASCR FACILITIES –** *Elise Jennings, ANL; Debbie Bard, LBNL; Bonson Messer, ORNL; Bill Johnston, LBNL*
- **UPDATE FROM ASCR'S APPLIED MATH PROGRAM:** *Steven Lee, ASCR*

Workshop Report Updates



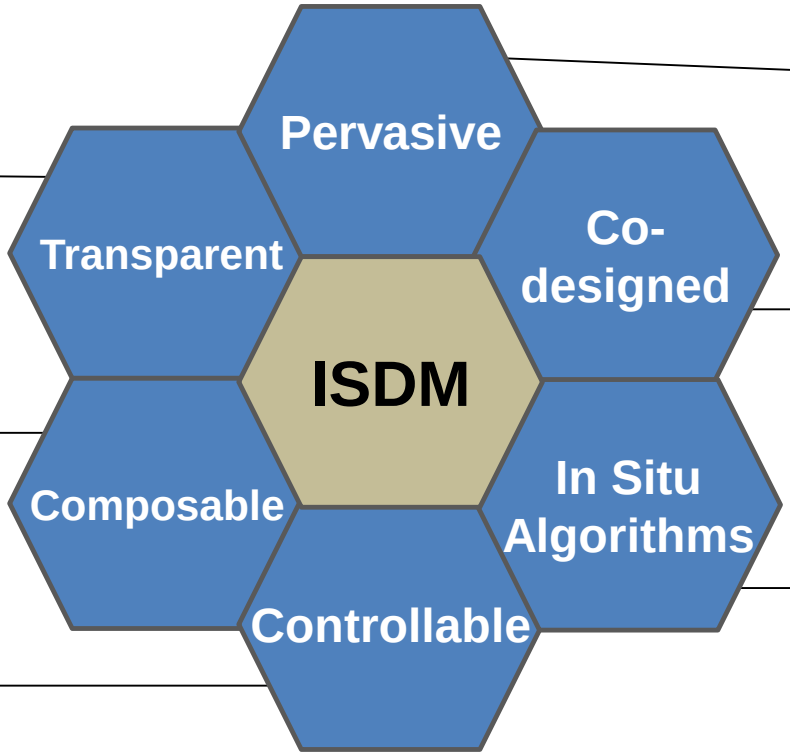


Report and/or Brochures posted at
https://science.energy.gov/ascr/community-resources/program-documents/

ASCR Workshop on In Situ Data Management

January 28-29, 2019 POC: Laura Biven

Priority Research Directions: Components and Capabilities Needed for Successful ISDM



Increase confidence in reproducible science, repeatable performance, and feature discovery through provenance.

Develop interoperable ISDM components for agile and sustainable programming.

Understand the design space of autonomous decision-making and control of in situ workflows.

Apply ISDM and in situ workflows at a variety of platforms and scales.

Coordinate ISDM development with underlying system software.

Redesign analysis algorithms for the in situ paradigm.

Workshop brochure: https://science.energy.gov/ascr/community-resources/program-documents/
Workshop report: to follow

DOE/SC QIS PI Meeting

- **Held January 31-February 1, 2019**
- **267 attendees with PIs and observers from all SC programs and observers from other Federal Agencies**
- **Plenary speakers included Jake Taylor, OSTP; John Preskill, Caltech; Irfan Siddiqi, LBNL; and David Awschalom, ANL/University of Chicago**
- **Topical Breakout Discussion sessions**
    - Quantum computing for application-specific research: Machine learning, data analysis, and related topics
    - Foundational quantum physics and information theory
    - Quantum qubits and computing platforms
    - Advanced synthesis and characterization tools (including validation)
    - Computer science and applied math challenges for quantum computing
    - Quantum sensors and detectors
    - Quantum computing for application-specific research: Chemistry, materials, variational techniques, field theories
    - Analog simulations and quantum simulation experiments
- **SC Program Office Breakout discussions**
- **Lightning round of Quantum Center Pitches**

Verified Quantum Information Scrambling Algorithm and Experiment Published in Nature

Scientific Achievement

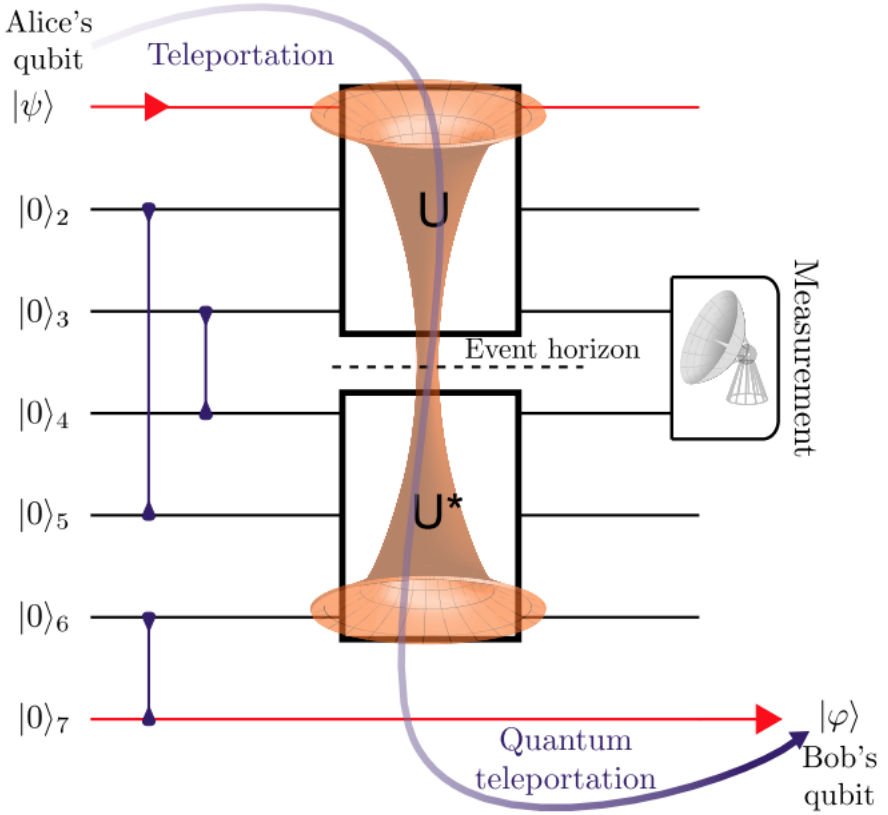
Monroe Group at UMD experimentally implemented the recent proposal from Yao and Yoshida to distinguish between decoherence and scrambling via quantum teleportation

Significance and Impact

First demonstration of verified quantum information scrambling in a quantum system
Experimental data can be used to bound the value of OTOC correlation functions

Research Details

7-qubit all-to-all connected quantum simulation of black hole scrambling. Required a gate depth > 24 to initialize EPR pairs and perform the maximally scrambling three-qubit circuit



Caption: Schematic of the 7-qubit circuit, which uses quantum teleportation to detect information scrambling. The underlay depicts an analogy between our protocol and information propagation through a traversable wormhole.

"Verified quantum information scrambling", Landsman, Figgatt, Schuster, Linke, Yoshida, **Yao**, Monroe, **Nature 567, 61 (2019)**

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Work was a collaboration between UC Berkeley (QAT4Chem PI: Norman Yao) and the Monroe group (UMD)

BERKELEY LAB