

Office of Science Update

Basic Energy Sciences Advisory Committee

Dr. Harriet Kung Deputy Director for Science Programs Office of Science U.S. Department of Energy July 30, 2020

Outline

- Office of Science Reorganization
- FY 2021 Budget Update
- DOE COVID-19 Response
- SC Program Activities

Office of Science Reorganization

- Better aligns the organization to achieve strategic goals
- Mostly affects top levels of the organization
- Establishes the Principal Deputy Director position
- Eliminates the Deputy Director for Resource Management
- Minimal changes below the Deputy Director level
- Effective 4/12/2020

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Effective 04/12/2020



Office of the Principal Deputy Director (SC-2)

Office of Engineering and Technology

- Office of Accelerator R&D and Production
 - Established in recognition of the central importance of accelerators and related technologies to the current and future scientific capabilities stewarded by SC programs. Related technologies to be considered may include, e.g., next-generation magnets, control systems, and high-power lasers. Activities will be tightly integrated with those in BES, FES, HEP, and NP.
- Office of Isotope R&D and Production
 - The DOE Isotope Program is transferred in its entirety from the Office of Nuclear Physics. The scope of the Isotope Program is unchanged.

Office of Strategic Planning & Interagency Coordination

Develop and maintain a Strategic Plan for the Office of Science. Planning process is currently underway. This
Office will also track and coordinate interactions across and between other Federal Agencies and the White
House Office of Science and Technology (OSTP) and the National Science Technology Council.

• Office of Diversity, Inclusion & Research Integrity

 Established to recognize the importance diversity and inclusion across all aspects of the SC programs and national laboratories.



Deputy Director For Science Programs

Deputy Director for Science Programs (SC-3) Harriet Kung **Office of Advanced Scientific** Office of Basic Energy Office of Biological & **Office of Fusion Energy** Office of High Energy Office of Communications & **Office of Nuclear** Computing Research (SC-31) Sciences (SC-32) **Environmental Research (SC-33)** Sciences (SC-34) Physics (SC-35) Physics (SC-36) Public Affairs (SC-3.1) Timothy Hallman Barbara Helland Sharlene Weatherwax Linda Horton James Van Dam James Siegrist Rick Borchelt **Office of Scientific & Technical** Computational Chemical Earth & Facilities, **Research & Physics** Information (SC-3.2) Science Research & Sciences, Environmental **Operations &** Technology Research Brian Hitson Partnerships Geosciences, & **Systems Science** (SC-35.1) Projects (SC-36.1) (SC-33.1) (SC-31.1) **Biosciences** (SC-34.1) Glen Timothy Laura Biven (A) (SC-32.1) Gerald Geernaert Joseph May Crawford Hallman (A) Office of Workforce Bruce Garrett **Development for Teachers &** Facilities **Biological Systems** Research Facilities Facilities & Scientists (SC-3.3) Materials (SC-31.2) Science (SC-34.2) (SC-35.2) Proiect Ping Ge (A) Sciences & Barbara Helland (A) (SC-33.2) Michael Management John Engineering Robert Anderson Mandrekas (A) (SC-36.2) Procario (SC-32.2) Jehanne **Office of Grants & Contracts** Linda Horton (A) Advanced Gillo Support (SC-3.4) Computing Michael Zarkin Technology Scientific User (SC-31.3) Facilities Barbara Helland (A) (SC-32.3) Linda Horton (A)



Effective

04/12/2020

Office of Science at a Glance FY 2020 Enacted: \$7.0B + \$99.5M (CARES Act)



Largest Supporter of Physical Sciences in the U.S.



Funding at >300 Institutions, including 17 DOE Labs



Over 23,000 Researchers Supported



Over 33,000 Users of 27 SC Scientific Facilities



~38% of Research to Universities



Research: 38.8%, \$2.7B



Facility Operations: 36.4%, \$2.5B



Projects/Other: 24.9%, \$1.7B



Office of Science Guiding Principles

FY 2019 Enacted: \$6.585B FY 2020 Enacted: \$7.000B FY 2021 Request: \$5.838B

Guiding Principles:

- The Office of Science's (SC) mission is to deliver scientific discoveries and major scientific tools to transform our understanding of nature and advance the energy, economic and national security of the United States.
- The FY 2021 Request supports a balanced research portfolio, focused on cutting edge, early stage research and development, probing some of the most fundamental questions in areas such as: high energy, nuclear, and plasma physics; materials and chemistry; biological and environmental systems; applied mathematics; next-generation high-performance computing and simulation capabilities; and basic research for advancement in new energy technologies.
- The future of the Office of Science includes:
 - New research investments

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• Reduce deferred maintenance with upgrades/improvements to infrastructure

FY 2021 SC President's Budget Request

(Dollars in Thousands)

	FY 2019		FY 2020	FY 2021 President's Request		
	Enacted	Current	Enacted	President's	President's Request vs.	
	Approp.	Approp.	Approp.	Request	FY 2020 Enacted	
ıtists	935,500	910,031	980,000	988,051	+8,051	+0.8%
	2,166,000	2,105,873	2,213,000	1,935,673	-277,327	-12.5%
	705,000	680,246	750,000	516,934	-233,066	-31.1%
	564,000	549,181	671,000	425,151	-245,849	-36.6%
	980,000	955,905	1,045,000	818,131	-226,869	-21.7%
	690,000	669,888	713,000	653,327	-59,673	-8.4%
	22,500	22,500	28,000	20,500	-7,500	-26.8%
	232,890	232,890	301,000	174,110	-126,890	-42.2%
	106,110 183,000	106,110 183,000 169,376	112,700 186,300 	115,623 190,306 	+2,923 +4,006 	+2.6% +2.2%
nce	6,585,000	6,585,000	7,000,000	5,837,806	-1,162,194	-16.6%
		123,254				
	6,585,000	6,708,254	7,000,000	5,837,806	-1,162,194	-16.6%

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Advanced Scientific Computing Research **Basic Energy Sciences Biological and Environmental Research** Fusion Energy Sciences High Energy Physics Nuclear Physics Workforce Development for Teachers and Scien Science Laboratories Infrastructure Safeguards and Security Program Direction SBIR/STTR (SC) Total Budget Authority and Obligations, Office of Scien SBIR/STTR (DOE) Total, Office of Science



Office of Science - FY 2021 Research Initiatives

New Research Initiatives

- 1. Integrated Computational and Data Infrastructure for Scientific Discovery
- 2. Next Generation Biology Initiative
- 3. Rare Earth / Separation Science Initiative
- 4. Revolutionizing Polymer Upcycling
- 5. Strategic Accelerator Technology Initiative
- 6. Data and Computational Collaboration with NIH

Ongoing Research Initiatives

- 1. Artificial Intelligence and Machine Learning
- 2. Biosecurity
- 3. DOE Isotope Initiative
- 4. Exascale Computing Initiative
- 5. Microelectronics Innovation
- 6. Quantum Information Science
- 7. U.S. Fusion Program Acceleration

Office of Science Request vs. Appropriation History*



Basic Energy Sciences Request vs. Appropriation History



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FY 2021 House Mark

- House Energy and Water Subcommittee Mark Up: Tuesday July 7, 2020
- House Appropriations Full Committee Mark Up: Monday July 13, 2020
- Six-bill minibus proposed for House vote by next week before House leaves for August recess
- Office of Science The bill provides \$7.05 billion, an increase of \$50 million above the FY 2020 level and \$1.2 billion above the request.
- Emergency funding The bill provides \$6.25 billion for Office of Science national laboratories, scientific user facilities, and universities to accelerate ongoing construction projects across the country.
 - \$75M for equipment and infrastructure for QIS Research Centers
 - \$214M for LCLS-II-HE
 - \$207.3M for STS
 - \$200M for Ames Main Building modernization
 - \$170M for ALS-U
 - \$151M for APS-U

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- \$75M for LCLS-II
- \$73M for CRMF
- \$60M for NSRC Recap
- \$59.5M for NEXT-II

COVID-19 Flexibilities

 Investigators, staff, and students may continue to charge salaries and benefits to SC awards if the recipient institution permits salaries to continue to be paid in the event of emergencies or disasters.

Office of Science Actions

- Deadlines extended for proposals, preproposals, letters of intent, and progress reports
- No-cost extensions awarded promptly
- Supplemental requests considered, subject to availability of funds

OMB Memos on Administrative Relief: M-20-11 (March 9), M-20-17 (March 19), M-20-20 (April 9), and M-20-26 (June 18)

- Salaries and wages may continue to be charged to awards through September 30 if other sources of funding are exhausted (*if relying on this flexibility*)
- No-cost extensions on expiring awards
- Extension of financial, performance, and other reporting
- *Flexibility with application deadlines

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- *Allowability of costs not normally chargeable to awards (eg. canceled events, travel)

*rescinded under M-20-26

DOE broad capabilities for addressing COVID-19 crisis

- Light and neutron sources
- Nanoscience centers
- Computational resources
- People with deep expertise relevant to:
 - Testing
 - Antiviral drug discovery
 - Vaccine discovery

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- Supply chain bottlenecks
- Modeling and understanding disease spread
- Molecular and structural biology

HOW DOE AND OUR LABS ARE COMBATING COVID-19



UNDERSTANDING THE STRUCTURE -

DOE scientists are studying the components of the virus so we can determine how to fight it.

MODELING EPIDEMICS -

DOE scientists use previous experience they gained modeling Smallpox, Arithrax and Ebola spread to understand how COVID-19 might behave.





SCREENING DRUGS -

Our supercomputers are allowing us to expedite testing, screen more than 8,000 drug compounds and found 77 have potential to fight against COVID-19... what took days on Summit would take months with a MacBook.

COORDINATING AND EXPANDING ACCESS FOR COVID-19 RESEARCH – DOE made a nationwide call to the scientific community to utilize our state-of-the-art facilities and technologies to understand and combat COVID-19 together.



ENERGY.GOV



About

DOE User Facilities

NVBL Structure

NVBL Coordination Team

https://science.osti.gov/nvbl

National Virtual Biotechnology Laboratory (NVBL)

- Consortium of 17 DOE National laboratories
- Takes advantage of DOE user facilities
- Initial activities include:

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- Epidemiological and logistical support
- Addressing supply chain bottlenecks by harnessing advanced manufacturing
- Medical therapeutics: computational drug discovery and structural biology
- Innovations in testing capabilities
- New project in understanding fate and transport of virus in the environment

Epidemiology: Modeling COVID-19 Spread

Lead: Budhu Bhaduri Laboratories: ANL, LANL, ORNL, SNL

- Developing an integrated COVID-19 pandemic monitoring modeling and analysis capability
- Taking advantage of DOE's leadership computing capabilities

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 Builds on scalable data and computing, spatial demography/ human dynamics research, and economic and risk modeling



Where are people located? With whom?





infected?

Where are people going, coming from?

Advanced Manufacturing for Medical Supplies Lead: Lonnie Love Laboratories: All 17

- The rapid spread of COVID-19 has resulted in significant supply chain issues
- DOE leadership in materials, manufacturing, modeling, and characterization is being leveraged to design and prototype products
 - Addressing alternative materials and approaches for rapid mass production, including new processing and tooling approaches

• NVBL focus areas:

- Masks/respirators (ORNL lead)
- Ventilators (INL lead)
- Consumables (LLNL lead)

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Tubes and swabs



Testing plates: ~500,000 needed per week



Molecular Design to Inform Medical Therapeutics

Lead: Marti Head Laboratories: ANL, BNL, LANL, LBNL, LLNL, ORNL, PNNL, SLAC, SNL

- COVID-19 has no approved medical therapeutic interventions beyond palliative care
- DOE capabilities are being applied to accelerate scientific discovery for therapeutics targeting SARS-CoV-2
 - Supercomputing and AI
 - Materials characterization at light and neutron sources

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Nanoscience research



COVID-19 Testing R&D Lead: Pat Fitch

Laboratories: Ames, ANL, LBNL, LLNL, LANL, NREL, ORNL, PNNL, SNL, SLAC

- No effective COVID-19 vaccine drives needs for improved testing accessibility and for new tests of infection and host response/immune status
- DOE capabilities in biology, bioinformatics, structural biology, bioengineering, computing, and light source and genome user facilities are being applied to accelerate COVID-19 Testing R&D

• NVBL focus areas:

- Establishing alternative instruments and reagents
- Developing affinity reagents for diagnostics
- Providing structure-based protein designs for diagnostics
- Accelerating R&D through novel data science

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https://covid19.edgebioinformatics.org/#/home



Viral Fate and Transport Lead: Katrina Waters

Laboratories: Ames, ANL, BNL, LANL, LBNL, LLNL, ORNL, PNNL, SNL, SLAC, SRNL

- Major public health questions remain about what dictates the prevalence and mobility of viable SARS-CoV-2 virus indoors and outdoors under a variety of environmental conditions
- Enhancing the potential to predict SARS-CoV-2 viability in varied environments will inform continued quarantine measures and/or abatements of infections, as well as inform strategies that guide society's resumption of normal activities
- Controlling spread within our community and workplaces requires an understanding of factors regulating COVID-19 viability, transmission, and transport as well as the prevalence of infectious virus in the environment
- NVBL focus areas:

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- Prioritized administrative and engineering controls that reduce the risk of SARS-CoV-2 transmission within the built environment
- Chemical and physical properties of materials that influence binding of SARS-CoV-2 to abiotic surfaces, which can be used to design new materials for desired applications
- Contribution of environmental reservoirs and conditions on transmission and resurgence of SARS-CoV-2

High Performance Computing Consortium Website: <u>https://covid19-hpc-consortium.org/</u>

Laboratories: ANL, INL, LANL, LBNL, LLNL, ORNL, SNL

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- Mission: Provide COVID-19 researchers worldwide with access to the world's most powerful high-performance computing resources that can significantly advance the pace of scientific discovery in the fight to stop the virus.
- A unique public-private consortium between government, industry, and academic leaders to aggregate free compute time and resources on their machines initiated in 10 days (March 11-March 22, 2020). First project started March 26.
- Over 40 members including resources from the United Kingdom, Switzerland, Sweden and Japan
- To date: the Consortium has received 148 proposals and approved 78, declined 51 and were awaiting further information on 19 and 2 projects have completed. Out of the 78 approved projects, 68 were enabled.

SC Program Activities

- Quantum Internet Blueprint Workshop report released.
 - https://www.energy.gov/sites/prod/files/2020/07/f76/QuantumWkshpRpt20FINAL_Nav_0.pdf
- FESAC Long Range Planning Subcommittee is drafting a strategic plan to be delivered by Dec 2020.
 - <u>https://sites.google.com/view/fesac-lrp-public/home</u>
- Impact of COVID-19 on HEP Research

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- <u>https://science.osti.gov/-/media/hep/hepap/pdf/202007/07-Hildreth_Narain-Community_Gathered_COVID-</u>
 <u>19 Impacts for HEP.pdf</u>
- Electron Ion Collider project received CD-0, Approve Mission Need, and BNL selected as host
 - <u>https://www.energy.gov/articles/us-department-energy-selects-brookhaven-national-laboratory-host-major-new-nuclear-physics</u>
 <u>new-nuclear-physics</u>
 and https://www.bnl.gov/eic/
- DOE Explains offers straightforward explanations of key words and concepts in fundamental science.
 - <u>https://www.energy.gov/science/science-innovation/doe-explains</u>