QUANTUM, AI, AND EXASCALE:

BES-ASCR COLLABORATIONS

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For Basic Energy Sciences

26 March 2019

Basic Energy Sciences

The Program:

Materials sciences & engineering—exploring macroscopic and microscopic material behaviors and their connections to various energy technologies

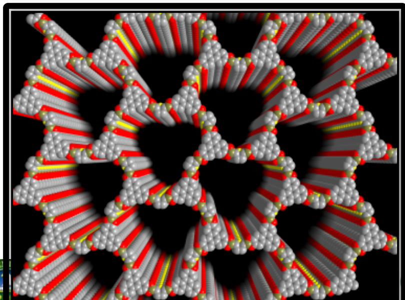
Chemical sciences, geosciences, and biosciences—exploring the fundamental aspects of chemical reactivity and energy transduction over wide ranges of scale and complexity and their applications to energy technologies

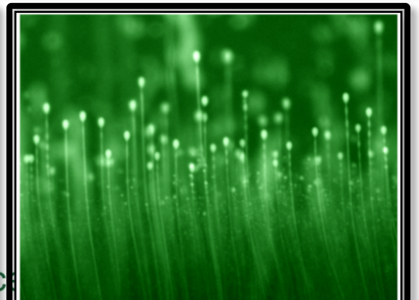
Scientific User Facilities
The largest collection of facilities for x-ray and neutron scattering and nanoscience tools in the world

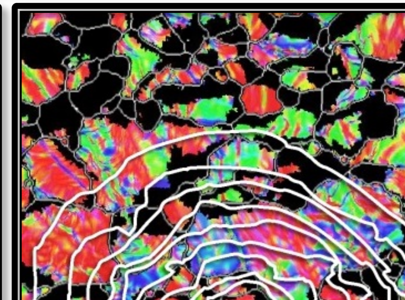
The Scientific Challenges:

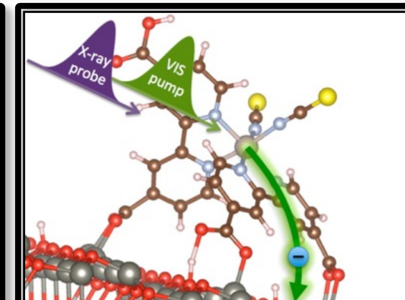
- Synthesize, atom by atom, new forms of matter with tailored properties, including nano-scale objects with capabilities rivaling those of living things
- Direct and control matter and energy flow in materials and chemical assemblies over multiple length and time scales
- Explore materials & chemical functionalities and their connections to atomic, molecular, and electronic structures
- Explore basic research to achieve transformational discoveries for energy technologies

Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels









Basic Energy Sciences At a Glance (2018)

BES RESEARCH SPANS

MORE THAN **150** ACADEMIC, NONPROFIT, AND INDUSTRIAL INSTITUTIONS

15 DOE NATIONAL LABORATORIES

45 STATES AND WASHINGTON, D.C.

25 CORE RESEARCH AREAS

46 ENERGY FRONTIER RESEARCH CENTERS

SUPPORTED RESEARCHERS

~6,200 Ph.D. SCIENTISTS

~2,100 STUDENTS SUPPORTED

BES | BY THE NUMBERS

FY 2018

BES supports fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels.

2 ENERGY INNOVATION HUBS

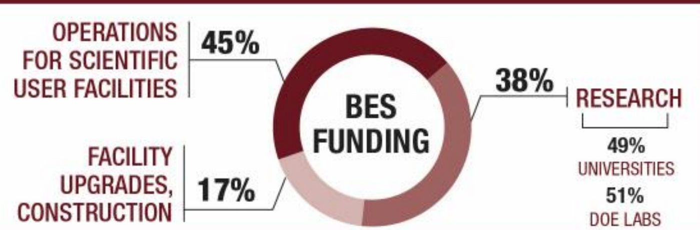
$787 MILLION RESEARCH BUDGET

~26% AVERAGE NEW GRANT SUCCESS RATE

OVER **1,100** CORE RESEARCH PROJECTS

MORE THAN **16,000** USERS AT 12 BES FACILITIES

$934 MILLION SCIENTIFIC USER FACILITY OPERATING BUDGET



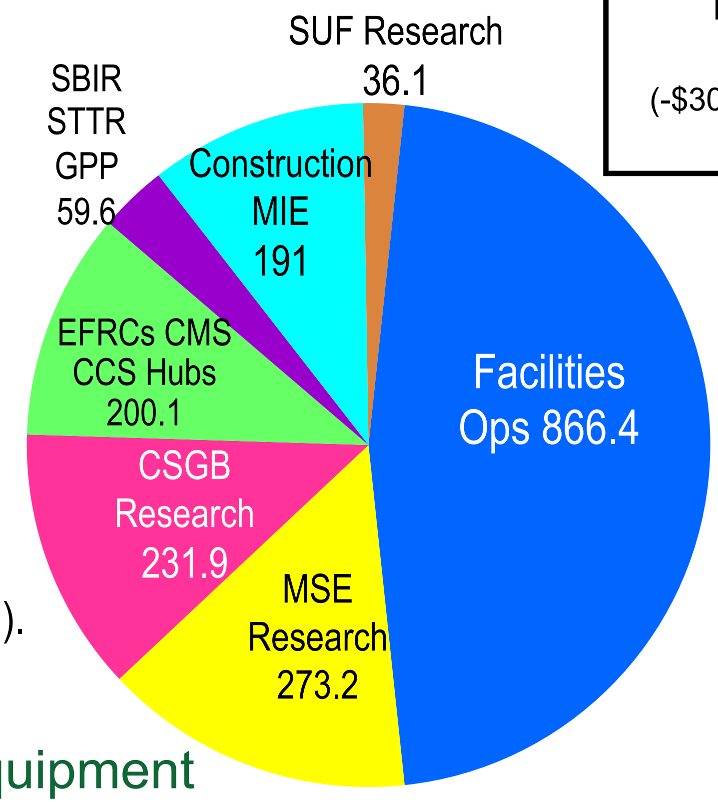
$369 MILLION FACILITY UPGRADES, CONSTRUCTION BUDGET

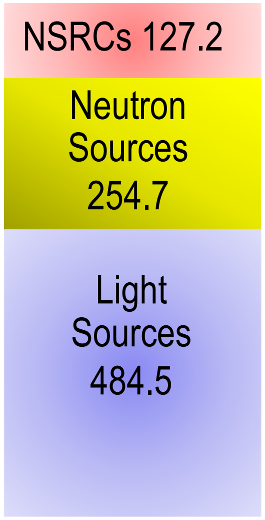
FY 2020 BES Budget Request

FY 2020 Request:
$1,858.3M
(-$307.7M or -14% from FY 2019 Enacted)

Research programs

- Core Research will emphasize quantum information science (QIS), including co-sponsoring QIS center with ASCR and HEP, microelectronics ($505.1M).
- Computational Materials and Chemical Sciences continue ($26M)
- Energy Frontier Research Centers continue ($130M)
- Energy Innovation Hubs, including re-competition for Solar Fuels Hub ($44.1M).
- Data analytics for BES facilities ($10M)





Construction/Major Items of Equipment

- No funding for LCLS-II (Δ = -$135.4M)
- APS-U (Δ = +20M), ALS-U (Δ = -$47M), LCLS-II-HE (Δ = -$16M), PPU (Δ = -$55M)
- Three new projects: NEXT-II ($1M), NSRC Recap ($1M), and STS ($1M)

Scientific user facilities

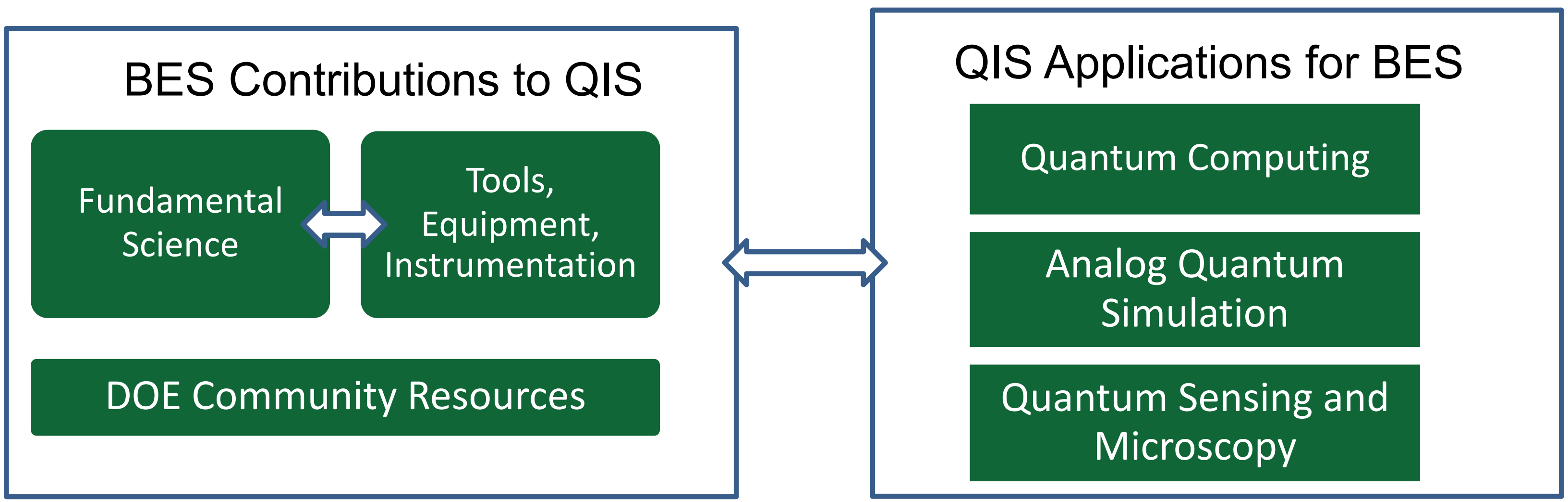
- Operations of 12 facilities at ~87% optimal level
- LCLS resumes operations starting 2Q FY 2020

BES Research Priorities

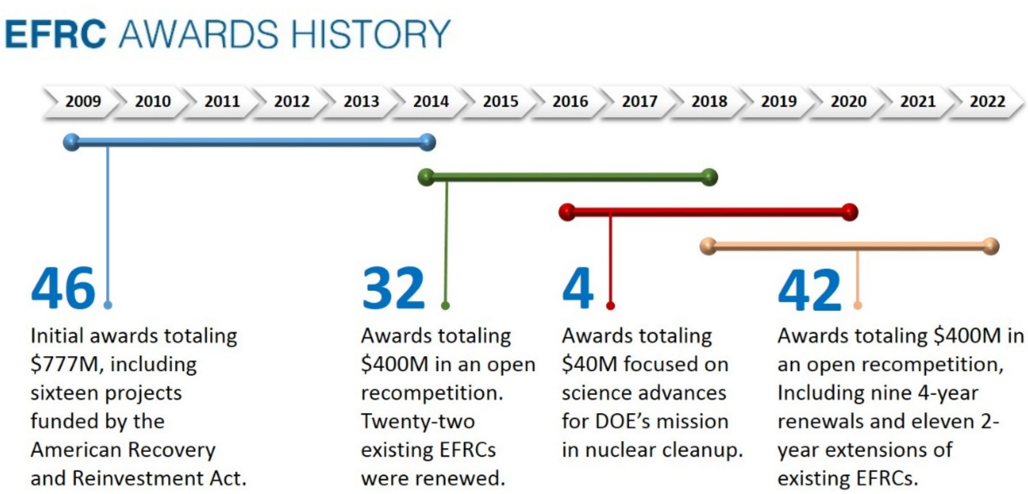
- **Quantum Information Science**
  - New investments in QIS research will exploit quantum phenomena to allow new ways to measure, process, and transmit information in novel ways and for numerous application areas including computing/simulations, sensing and metrology, and communication. A new QIS Center investment will be initiated in FY 2020.
- **Energy Frontier Research Centers**
  - The Request increases funding for the EFRCs with a planned solicitation in FY 2020 to expand the EFRC portfolio in high priority topical areas, including QIS, microelectronics, and other program priorities. This EFRC solicitation will also recompete funding for science relevant to the Department's environmental management mission.
- **Energy Innovation Hubs**
  - With the completion of the second 5-year term of the Fuels from Sunlight Energy Innovation Hub, an open competition in FY 2020 will solicit research to address emerging new directions and long-standing challenges in early-stage fundamental research on solar fuels generation that builds on the Hub's unique capabilities and accomplishments.
- **Computational Materials and Chemical Sciences**
  - The Request continues support for computational materials and chemical sciences to deliver shared software infrastructure to the research communities as part of the Exascale Computing Initiative.
- **Microelectronics**
  - New efforts in materials and chemical sciences for next generation microelectronics will focus on critical scientific challenges for future computing, sensors, and detectors to meet national needs. Research priorities are guided by the Basic Research Needs workshop held in October 2018.
- **Data Analytics and Machine Learning for BES Facilities**
  - The increase will be used to explore data analytics and machine learning techniques for accelerator optimization, control, prognostics, and data analysis.

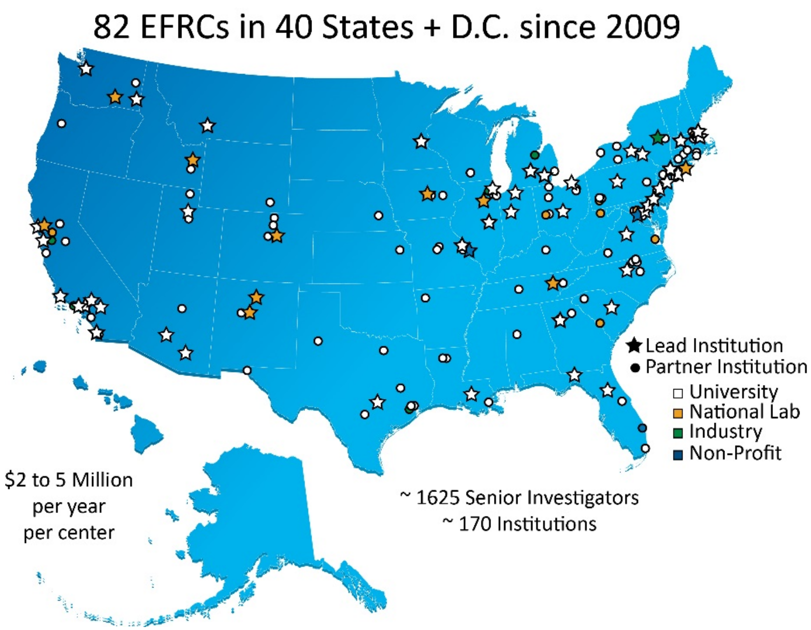
Quantum Information Science Activities in BES

- **NEXT GENERATION QUANTUM SYSTEMS**: Develop understanding leading to control of quantum phenomena in chemical and materials systems to advance quantum-based science and technology.
- **QUANTUM COMPUTING**: Develop quantum computing algorithms and utilize emerging quantum computing capabilities to address major scientific problems in chemical and materials sciences.
- **USER CAPABILITIES:** Research and infrastructure at the Nanoscale Science Research Centers, enabling next-generation qubit concepts, innovative quantum and classical architectures.



Energy Frontier Research Centers
FY 2020 Request: $130M (+$20M)





Accomplishments (Aug 2009 – May 2018)

- Over 10,500 peer-reviewed scientific publications
- ~100 companies have benefited from EFRC research
- At least 160 patents issued

Current EFRC Members

- ~670 senior investigators and ~1,100 postdoctoral associates, graduate students, undergraduate students, and technical staff at 115 institutions

FY 2020 Funding Opportunity Announcement (~$40M)

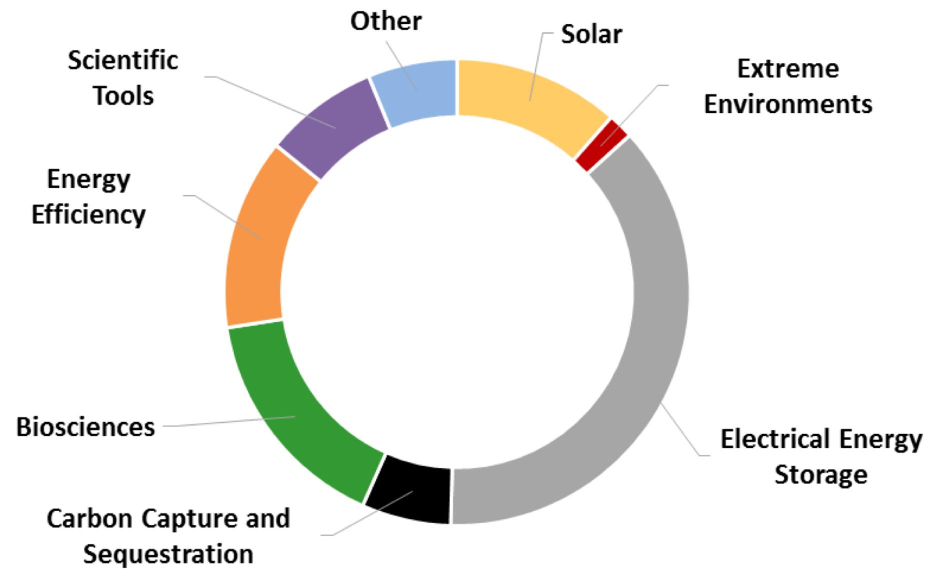
- Recompetition of four-year EFRC awards made in FY2016, which focused on science relevant to DOE's environmental management mission.
- Solicitation of proposals for new EFRCs that are responsive to recent BES workshop reports, including use-inspired science relevant to advanced microelectronics and quantum information science (QIS).

EFRC Impact – Publications, IP, Interactions (May 2018)

EFRC IMPACT BY THE NUMBERS

- Over **10,500** Peer-reviewed publications
- Over **550** Invention disclosures
- Over **160** Patents Issued
- Over **375** Foreign patent applications
- Over **500** U.S. patent applications
- At least **100** Licenses Reported
- About **100** Companies benefited from EFRC research

DISTRIBUTION OF COMPANIES THAT HAVE BENEFITTED FROM EFRC RESEARCH



~34% Start-ups
~20% Mid-sized companies
~46% Large companies

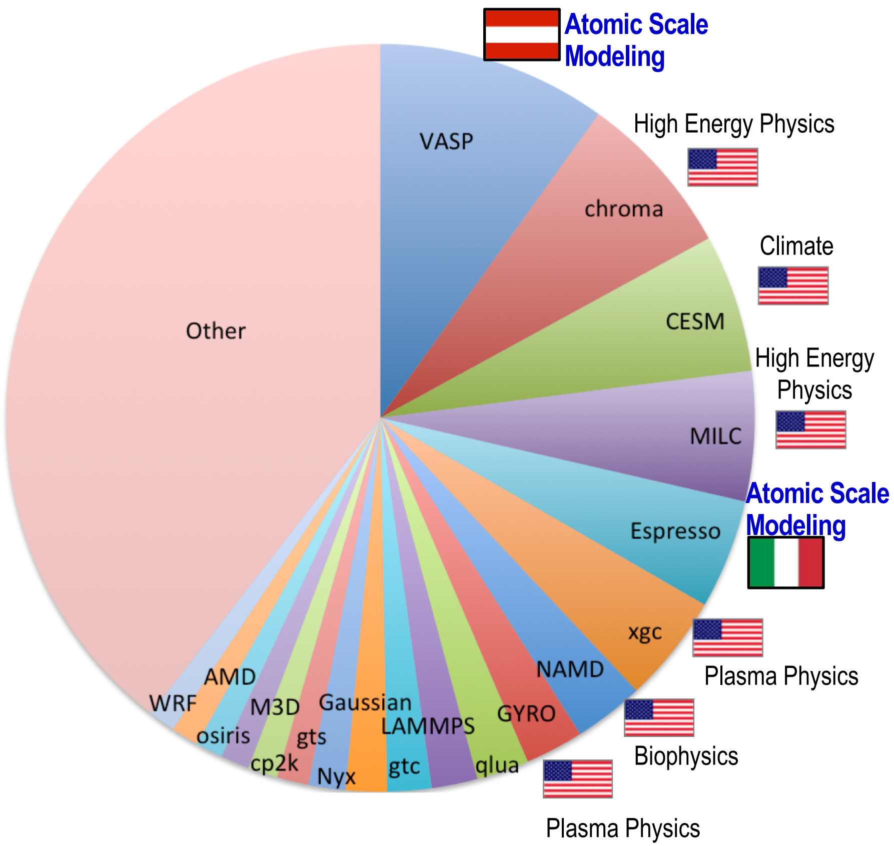
General criteria for claiming company's benefits from EFRCs:
Licensed EFRC IP; Established CRADA; Used EFRC ideas in their business; Provided follow-on funding; Substantial interactions, involving personnel or sample exchange

Industry Interactions with EFRCs

AltaDevices, Anellotech, Blue Current, chromation, mc10, activated research company™, UbiQD, Unite to Light, Synopsys, Asylum Research (an Oxford Instruments company), Fulcrum BioEnergy, American Lithium Energy, Dioxide Materials™, Washington Diamonds (Quality Diamonds, Genuine Value), American Aerogel (Revolutionary materials. Superior products.), amsc, electroninks, Global Thermostat, ubiquitous energy, Trinity Industries, Inc., UNIFI, AstraZeneca, Universal Display Corporation, Samsung, framergy™, Philips Lumileds, P&G, Applied Materials, mosaic materials, Photon Spot, Milliken, SuperPower Inc. (A Furukawa Company), SINTEF, Schlumberger, WFC Watt Fuel Cell, Solid Power, Saft, Sigma-Aldrich, Air Liquide, ConocoPhillips, Evident Thermoelectrics, iBeam Materials, Voxel8, NanoFlex Power Corporation, intel, DuPont, GE, GM, Exxon, Mobil, Reliance Industries Limited, LioNano, thermaura, REG (Renewable Energy Group), Pioneer, Dow, IBM, Toray (Innovation by Chemistry), QuesTek Innovations LLC, Millifluidica, Spero (Pioneering A Greener Future), Xerion Advanced Battery Corp., uraniumone (investing in our energy), Ford, Toyota, Stora Enso, Delphi, ADA Technologies, Inc., Corning, IHI, Bridgestone, Gentherm, PEC Point Engineering, Micromidas, X-Celeprint, Murata (Innovator in Electronics), Konica Minolta, Sharp, Invista™, NanoIntegris, Sironix Renewables, Proton OnSite, Flexterra, alpha-En (pure lithium metal - clean technology), Oorja, LanzaTech, NuMat Technologies, SiNode Systems, Remylop Structured Materials™, QuantumScape™, Soft Robotics, Primet Precision Materials, Orthogonal, LiOx, nohms Technologies, NEXT

Computational Materials and Chemical Sciences

2015 Top Application Codes at NERSC

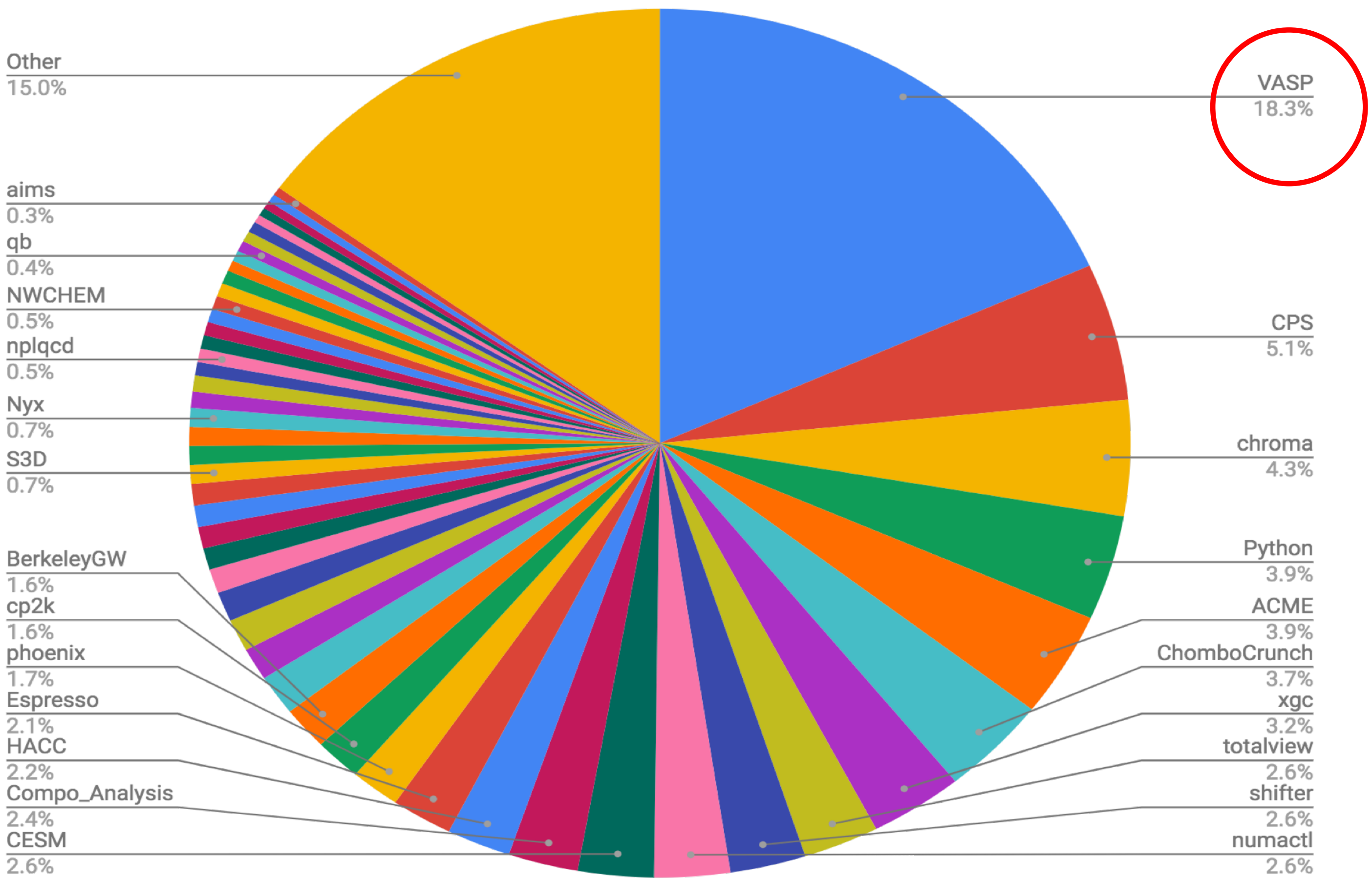


The U.S. trails other countries in development of computational codes in chemistry and materials sciences.

- High-accuracy software is needed to understand how the behavior of atoms and molecules (or quantum effects) impacts energy conversion and materials synthesis.
- Open-source, experimentally validated software, based on advanced quantum mechanical methods, is needed for accelerated prediction of functional materials and molecular assemblies.
- At NERSC, the most used code is VASP, a commercial Austrian atomic scale modeling code requiring purchase of license. Development of Espresso, a materials sciences code, is led by Italy.
- Top codes used at NERSC for other fields (e.g., particle physics and plasma physics) were developed in the U.S. and are all free, open-source community codes.
- A dedicated effort to support Computational Materials and Chemical Sciences was initiated starting in 2015 to ensure U.S. leadership in computing for BES key scientific disciplines and in support of the DOE Exascale Computing Initiative.

NERSC System Utilization (Aug 2017 - July 2018)

Breakdown of Hours at NERSC

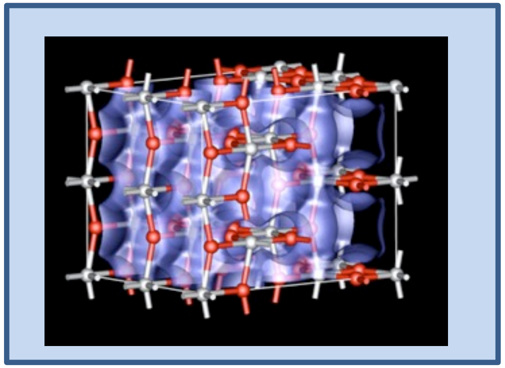


- 3 codes > 25% of the workload
- 10 codes > 50% of the workload
- 29 codes > 75% of the workload
- Over 600 codes comprise the remaining 25% of the workload.

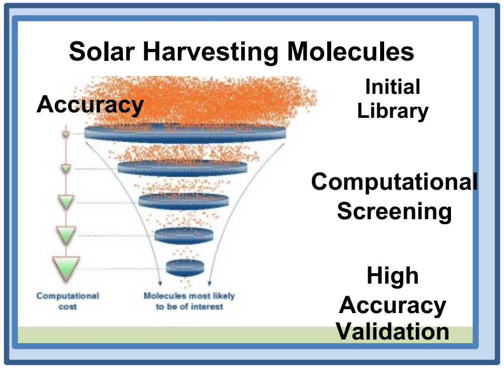
Computational Materials & Chemical Sciences
FY 2020 Request: $26M

Deliverable: Robust, open-source community software and databases for predictive design of functional materials and chemical systems for global competitiveness and in support of DOE's Exascale Computing Initiative

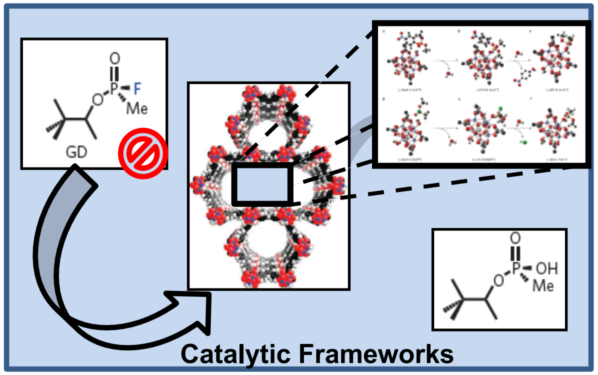
- Support began for CMS in 2015 and for CCS in 2017 to deliver research codes and data for design of functional materials and chemical systems to communities in academia, labs, and industry
- Use integrated teams combining expertise in theory, modeling, computation, synthesis, characterization, and processing/fabrication
- Use facilities and tools for synthesis, characterization, simulation, and computation, relying especially on the SC scientific user facilities and leadership class computing



Strongly Correlated Electron Systems



High-Accuracy Design of Catalysis



Artificial Photosynthesis

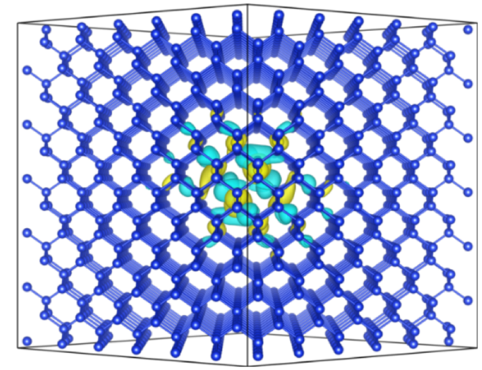
Computational Materials Sciences
FY 2020 Request: $13M

Accomplishments to date: over 16 new or enhanced open-source software packages add community capabilities for predictive design of materials and simulation of atomic interactions. For example:

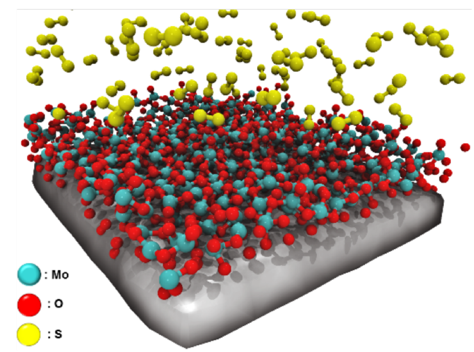
- QMCPACK: new release of quantum Monte Carlo methods for electronic structure calculations in strongly correlated solids and chemicals
- BerkeleyGW and StochasticGW: new releases of many-body perturbation theory for excited state calculations of energy materials
- West, Qbox, SSAGES and COPPS: new releases of interoperable codes at multiple length and time scales relevant to heterogeneous materials, solids and interfaces in semiconductors, batteries, and thermoelectric materials

In FY 2020, a funding opportunity will:

- Consider applications for new and renewal awards
- Focus on applications on topics identified as basic research needed for specific energy technologies, quantum information sciences, and next generation electronics, as well as consideration of advanced data techniques, including data mining.



Atomic arrangement in commonly observed 2-atom vacancy in silicon for semiconductor applications



Computational synthesis of MoS_2 layers with potential for future electronics applications

Computational Chemical Sciences
FY 2020 Request: $13M

Complex Chemical Transformations:

Complex chemical are common in energy applications and require new approaches from electronic to mesoscales for chemical separations and conversions

Functional Transition Metals:

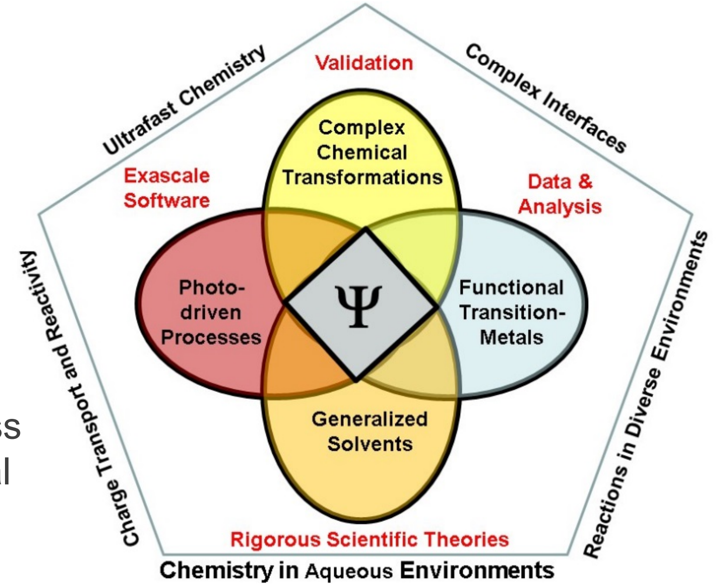
The multiple oxidation states transition metals require new approaches to accurately treat spin states (e.g., spin ordering) and their processes

General Solvents:

Accurate modeling of solvents requires the development across a ranges of approaches from electronic structure and statistical mechanic to multiscale modeling, and the creation of an integrated software suite

Photodriven Processes:

Quantitatively describing how electromagnetic radiation interacts non-linearly with matter at energy scales that accurately describe electronic transitions and their impact on dynamical process in molecular systems



Organization of projects into 4 interacting teams advances computational approaches and tools in important areas of BES chemical sciences

FY 2020 funding will support projects started in FY 2017 and FY 2018.

Robust and Synthesizable Photocatalysts for CO_2 Reduction: A Data-Driven Materials Discovery

Scientific Achievement

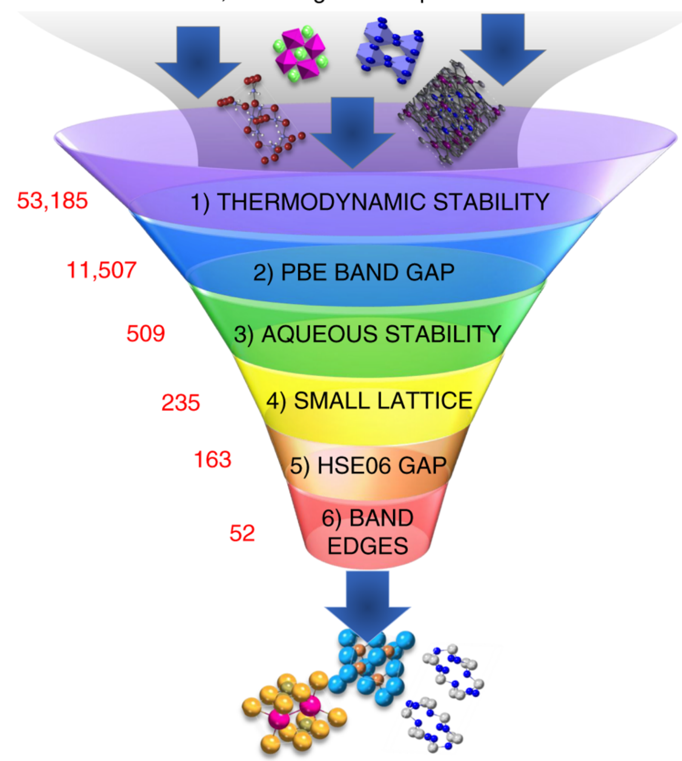
JCAP identified 39 new materials that satisfy the requirements for a CO_2 reduction photocathode by executing a first-principles computation-based screen of 68,860 candidates.

Significance and Impact

This computational discovery will accelerate the targeted experimental synthesis, characterization, and testing of new CO_2 reduction photocathodes.

Research Details

- A tiered computational screening strategy – using the Materials Project database and data science tools at NERSC – was developed to evaluate synthesizability, corrosion resistance, visible-light absorption, and electronic structure compatibility with fuel synthesis.
- Results were compared to materials reported in the literature as experimentally active photocathodes to highlight scope of the screening strategy and show its viability in identifying suitable, durable photocathodes.



The photocathode materials identified by the tiered computational screening include 9 materials previously reported as CO_2 photocathodes, as well as a discovery of 39 new candidate photocathodes.

Arunima K. Singh, Joseph H. Montoya, John M. Gregoire, and Kristin A. Persson. *Nature Communications* 10, no. 1 (2019): 443.

Basic Research Needs for Microelectronics Workshop
Co-sponsored by ASCR, BES, HEP; October 23–25, 2018

Workshop Chair: Cherry Murray (Harvard Univ.)
Associate Chairs: Supratik Guha (ANL)
Dan Reed (Univ. of Utah)

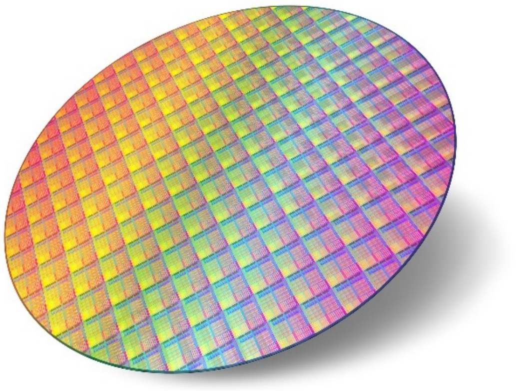
SC Technical Lead: Andy Schwartz (BES)



CHARGE:

- Conduct a thorough assessment of critical scientific challenges, fundamental research opportunities, and priority research directions that require further study as a foundation for future advances in microelectronics over the next decade and beyond.
- Emphasize energy-relevant applications and those areas that are aligned with the missions and needs of the DOE Offices of Advanced Scientific Computing Research (ASCR), Basic Energy Sciences (BES), and High Energy Physics (HEP) including data management and processing, power electronics, and high performance computing.
- Examine research that is relevant to both the extension of CMOS and beyond CMOS technologies; however topics of direct relevance to Quantum Information Science and Quantum Computing are outside the scope of this workshop.
- Focus on a co-design innovation ecosystem in which materials, chemistries, devices, systems, architectures, and algorithms are researched and developed in a closely integrated fashion.

BES Microelectronics Research



- Semiconductor-based microelectronics are critical to the U.S. economy, scientific advancement, and national security.
- High-performance computing underpins DOE missions and future computing technologies (e.g., quantum, neuromorphic, probabilistic, etc.) hold promise for next-generation DOE mission applications.
- The multi-decade success of Moore's Law has been driven by innovation.
- Additional innovation is needed to keep up with dramatic market growth and to meet future national needs; alternative materials, devices, fabrication techniques and architectures are likely to result.

FY 2020 Plans

- BES will expand core research and the EFRCs in 2020, placing an emphasis on materials and chemical science challenges that are relevant to advanced microelectronics.
- Research priorities will be guided by the Basic Research Needs for Microelectronics workshop.

Expected Partnership with ASCR & HEP

DOE Office of Basic Energy Sciences: Scientific User Facilities

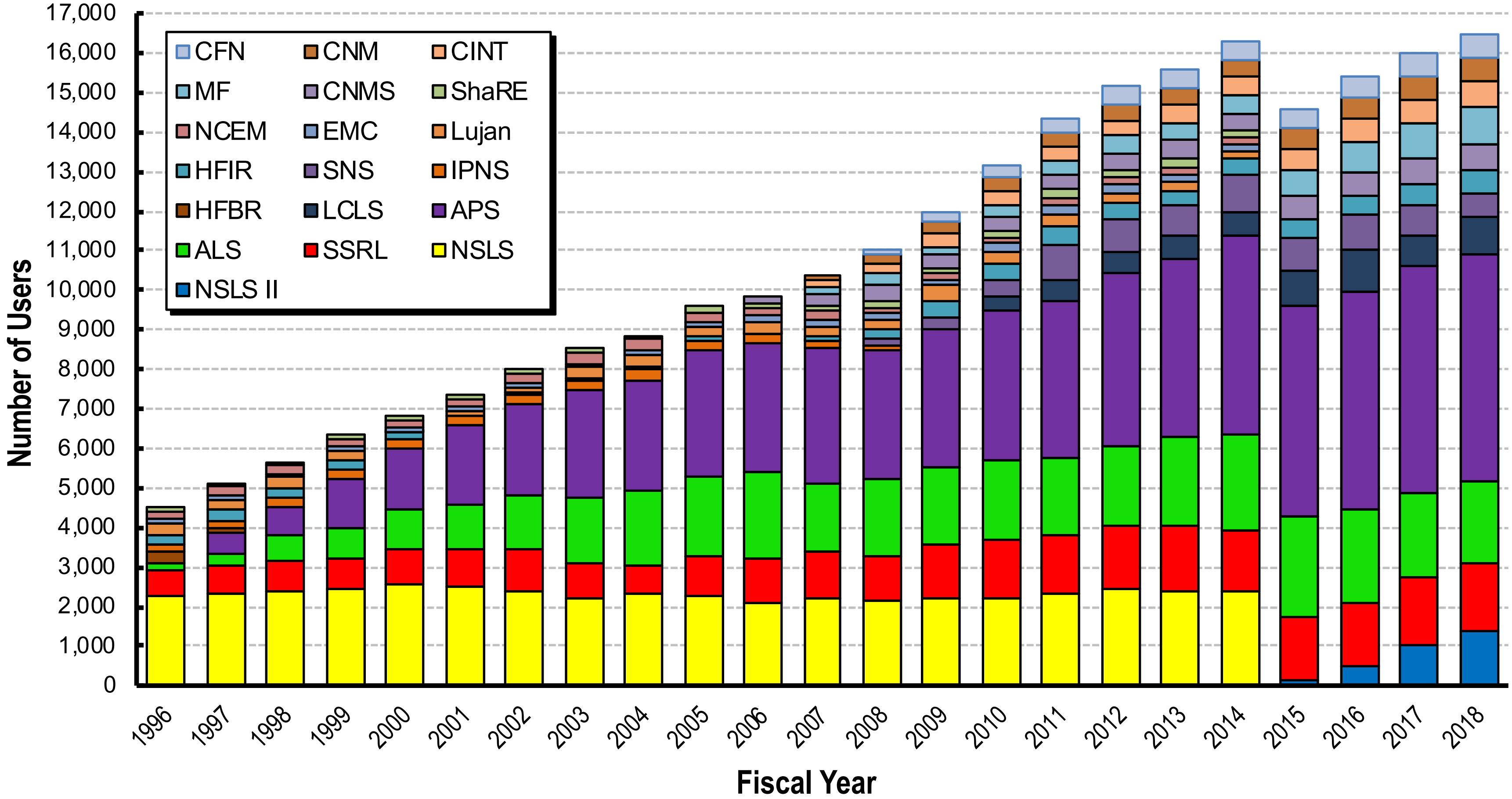
- Available to all researchers ***at no cost*** for non-proprietary research, regardless of affiliation, nationality, or source of research support
- Access based on external peer merit review of brief proposals
- Coordinated access to co-located facilities to accelerate research cycles
- Collaboration with facility scientists an optional potential benefit
- Instrument and technique workshops offered periodically
- A variety of on-line, on-site, and hands-on training available
- Proprietary research may be performed at full-cost recovery

Light Sources
- Advanced Light Source (LBNL)
- Advanced Photon Source (ANL)
- Linac Coherent Light Source (SLAC)
- National Synchrotron Light Source-II (BNL)
- Stanford Synchrotron Radiation Lightsource (SLAC)

Neutron Sources
- High Flux Isotope Reactor (ORNL)
- Spallation Neutron Source (ORNL)

Nanoscale Science Research Centers
- Center for Functional Nanomaterials (BNL)
- Center for Integrated Nanotechnologies (SNL & LANL)
- Center for Nanophase Materials Sciences (ORNL)
- Center for Nanoscale Materials (ANL)
- Molecular Foundry (LBNL)

BES User Facilities Hosted >16,000 Users in FY 2018



More than 300 companies from various sectors of the manufacturing, chemical, & pharmaceutical industries conducted research at BES scientific user facilities. Over 30 companies were Fortune 500 companies.

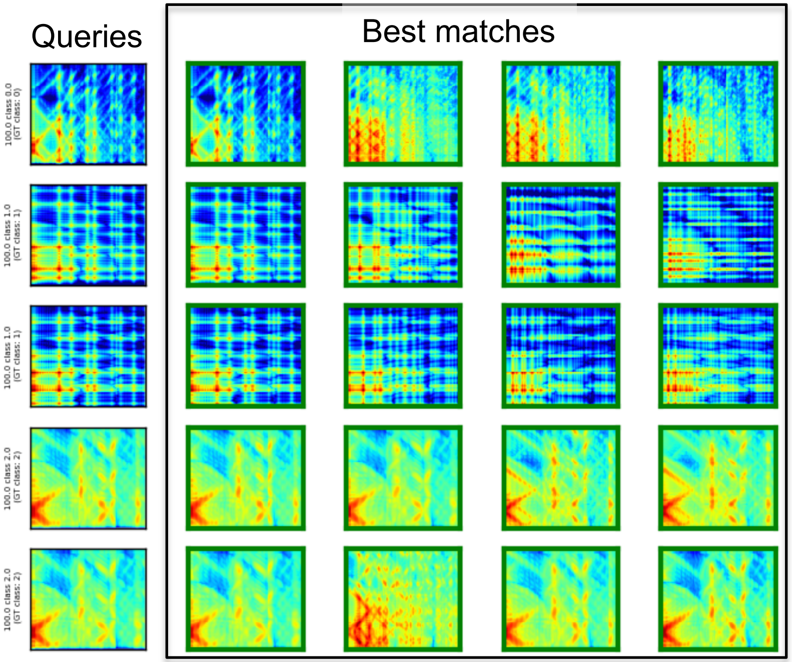
Data Analytics and Machine Learning
Deep Learning for X-ray Diffraction and Materials

Scientific Achievement

- Search and ranking materials using X-ray diffraction data
- Recognize crystal structure from images without feature design

Significance and impact

- Devise algorithms to bridge the gap between theoretical models and experimental observational data
- X-ray diffraction prototypes with accuracy above 98%



Developing algorithms to categorize millions of grazing-incidence small-angle scattering (GISAXS) patterns and recognize the possible crystal structure(s) and orientation(s) on the surface (or interface) based on the simulation.

Research details

- Exploration of ALS data, including simulation performed @NERSC using machine learning (ML) prototype from CAMERA;
- Test ability to categorize millions of GISAXS patterns without manual interaction;
- Core codes: HipGISAXS simulation @NERSC, ML TensorFlow @CAMERA GPU test-bed.

Data Analytics and Machine Learning

Recommendation System for Scientific Images

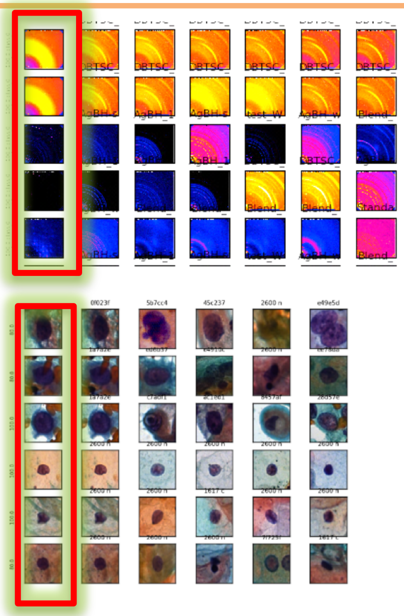
CAMERA Applied Math

Scientific Achievement

- New visual search engine: pyCBIR, for scientific image retrieval based on pictorial similarity
- Tool capable of retrieving relevant images using datasets across science domains
- Convolutional Neural Nets (CNN)

Significance and impact

- Real-time image retrieval using compact data representation
- Enable investigation of abstract patterns, by leveraging historical data, gathered by domain experts at a high cost
- Improve collaboration among researchers across scientific communities



Developing a pattern recognition algorithm to retrieve relevant images from a database based on pictorial similarity

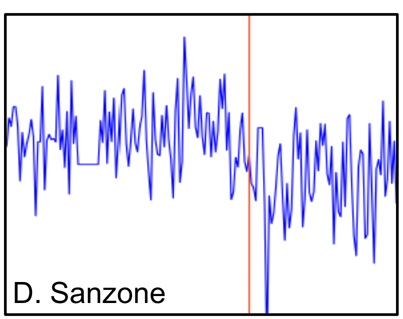
Research details

- Deployed CNN-based tools for pattern recognition using optimized libraries, such TensorFlow, cuDNN, cuFFT;
- Delivered quantitative analytics to recover data and respective confidence associated to recommendation;
- Tested pyCBIR with data varying from nano to km scale;
- Upcoming developments: promote guided data explorations and new discoveries among scientists through enhanced collaborative environments.

- As the complexity and performance requirements of accelerators continue to grow, the need for more dynamic and adaptive control systems becomes essential. Particle accelerators are ideal for applications of data analytics and machine learning algorithms to improve performance.

- The FY 2020 Request includes $10M to apply data analytics and machine learning techniques to accelerator optimization, control, prognostics, and data analysis.

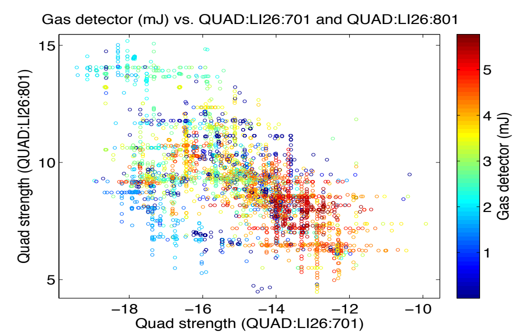
Error prediction



Time

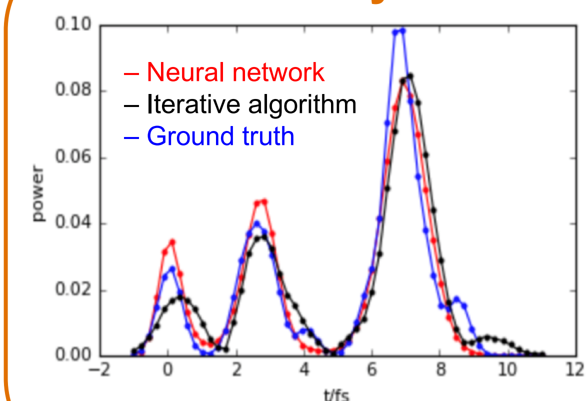
Learning from experience

Quad 2



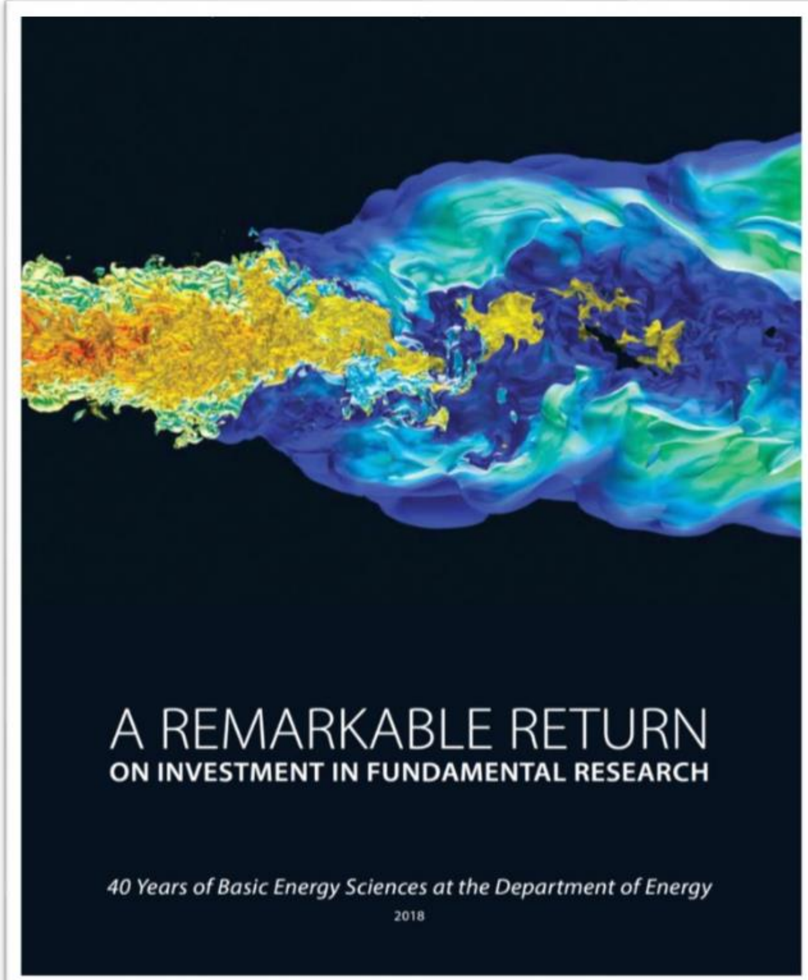
Quad 1

Fast analysis



Time (arb. Units)

40 Years of Basic Energy Sciences at the Department of Energy (BES40) – a BESAC Subcommittee Study



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