U.S. DEPARTMENT OF ENERGY | Office of Science

ASCR Research Update

Ceren Susut, Computational Science Research & Partnerships Division Director

September 30, 2022

FY2022 At-A-Glance: 11 Solicitations, 157 New Awards

Early Career Research Program	11 new projects
SciDAC-5 Partnership in Earth System Science (BER)	7 new projects*
SciDAC-5 Partnership in High Energy Physics (HEP)	5 new projects*
SciDAC-5 Partnership in Nuclear Physics (NP)	3 new projects*
SciDAC-5 Partnership in Nuclear Energy (NE)	1 new project*
Randomized Algorithms for Combinatorial Scientific Computing	4 new projects
2022 Mathematical Multifaceted Integrated Capability Centers (MMICCs)	4 new projects
Data Visualization for Scientific Discovery, Decision-Making, and Communication	5 new projects
Management and Storage of Scientific Data	5 new projects
Advancing Computer Modeling and Epidemiology for Biopreparedness and Response	3 new projects
EXPRESS: Federated Scientific Machine Learning, Differentiable Programming, Explainable Artificial Intelligence, Parallel Discrete Event Simulation, Quantum Algorithms & Mathematical Methods, Quantum Computing at the Edge	22 new projects

* Indicates partnerships with other SC offices

FY2022 At-A-Glance: 10 Community Events

Artificial Intelligence for Earth System Prediction (AI4ESP) Workshop*	October 25, 26, 2021; November 1, 2, 8, 9, 12, 30, 2021; December 3, 2021, February 14, 2022
ASCR Workshop on Cybersecurity and Privacy for Scientific Computing Ecosystems	November 3-5, 2021
Basic Research Needs for the Science of Scientific-Software Development and Use	December 13-15, 2021
Quantum Computing Testbeds Stakeholder Workshop	December 2, 6, 15, 17, 2021
Visualization for Scientific Discovery, Decision-Making, and Communication	January 18-20, 2022
Basic Research Needs for Management and Storage of Scientific Data	January 24, 25, 27, 2022
AI@DOE*	December 8-9, 2021; January 12-13, 2022; February 24, 2022
Foundational Science for Biopreparedness and Response*	March 8, 15, 22, 2022
RENEW Networking Workshops	June 29-July 1 and July 13-15, 2022
Virtual Roundtable on Foundational Science to Accelerate Nuclear Energy Innovation	July 20-21, 2022

* Indicates in collaboration with other DOE offices

https://science.osti.gov/ascr/Community-Resources/Program-Documents

Submodular Matchings for Balancing Data and Computations

A scalable parallel algorithm and a case study in Chemistry

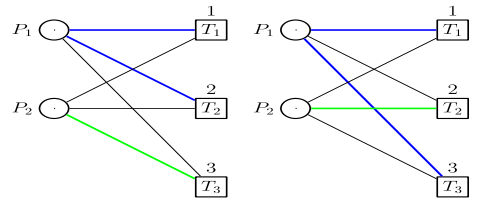
ASCR research tackles long standing problems

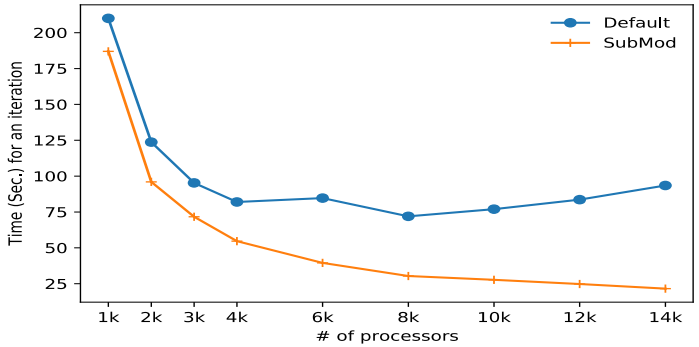
Scalable Quantum Chemistry via Submodular Matching

- Computing electronic properties of molecules via density functional theory involves the data intensive and compute intensive Fock matrix, whose elements consist of multidimensional integrals. The computation scales as $O(n^4)$, where n is the number of basis functions.
- We provide a scalable parallel algorithm for computing the Fock matrix within the NWChemEx software from Pacific Northwest National Lab.
- The algorithm assigns blocks of Fock submatrix computations to processors in order to balance the data and work load among the processors, and also the number of messages each processor is involved in.
- This is accomplished by computing a *b*-matching in the block-processor graph, with a nonlinear (submodular) objective function, to satisfy both objectives mentioned above.
- A submodular function balances the load on the processors, whereas a linear function cannot distinguish between unbalanced and balanced task assignments.
- Although the submodular *b*-matching problem is computationally intractable, we design fast approximation algorithms that provide constant-factor approximations to the optimal matching.

Performance of NWChemEx on Summit

- We designed a submodular matching algorithm and incorporated it with the NWChemEx library.
- The code speeded up the Fock matrix computation for the ubiquitin protein molecule by a factor of four over the current task assignment.
- It also scaled the NWChemEx code to 14000 processors on Summit, from 4000 processors.
- More work could be done to reduce the size of the data even further by means of matrix factorizations.
- We collaborated with colleagues at PNNL from the ExaGraph and NWChemEX projects.





Top Fig. : A submodular matching balances the work in assigning tasks T to processors P (left), while a linear matching does not (right).
Bottom Fig.: Submodular assignment balances the load in computing the energy levels of the Ubiquitin protein, reducing the time on 14K Summit processors four-fold over the default.

PI: Alex Pothen
Collaborating Institutions: Purdue University, PNNL

ASCR Program: Computer Science
ASCR PM: Hal Finkel
Publication(s) for this work: S M Ferdous et al., "A parallel approximation algorithm for submodular b-matching," Proceedings SIAM Applied Computational Discrete Algorithms, (2021): pp. 45-56, . Doi: 10.1137/1.9781611976830.5

Stochastic Learning for Binary Optimal Design of Experiments

ASCR research enables new approaches

Scientific Achievement

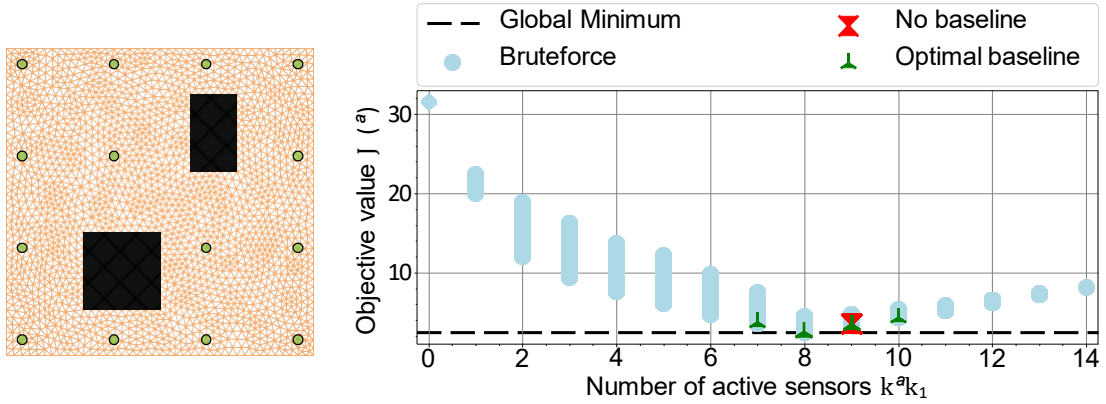
New stochastic approach to binary optimization for optimal experimental design (OED) for Bayesian inverse problems governed by mathematical models such as partial differential equations.

Significance and Impact

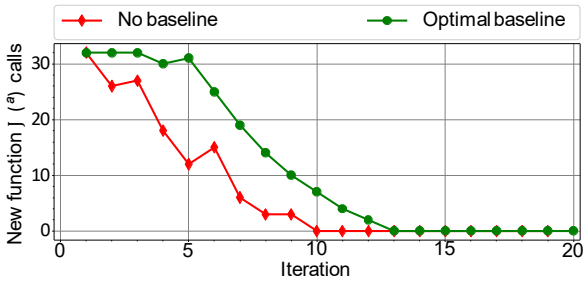
Binary OED problems are crucial for designing optimal data acquisition schemes, such as sensor placement or spatiotemporal data collection, in inverse problems in order to improve inversion accuracy (e.g., identifying the source of a contaminant) and long-term predictability of data assimilation systems.

Research Details

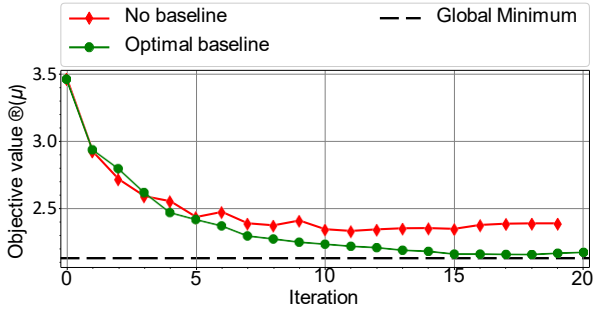
- We have developed a new probabilistic approach to efficiently solving binary OED optimization problems, without needing to relax the design, or carry out heuristic rounding techniques.
- The stochastic approach does not require differentiability of the utility function with respect to the design, and is directly interpretable:
  - Enable employment of sparsity-enforcing penalty functions such as $l_!$,
  - Massively reduce the computational cost compared with traditional OED,
  - Sample efficient observational policies in a small number of optimization steps.
- Computationally efficient policy gradient (reinforcement learning) optimization algorithms, with convergence guarantees.



Sensor placement for parameter identification in an Advection-Diffusion experiment to locate contaminant source. Results of the policy gradient procedures, compared with the brute-force search of all candidate binary designs.



The value of the objective function at each iteration of the optimization procedures.



Number of new function evaluations at each optimization step

References:

[1] Attia, Ahmed, Sven Leyffer, Todd Munson. Stochastic Learning Approach for Binary Optimization: Application to Bayesian Optimal Design of Experiments. SIAM Journal on Scientific Computing, 2022.

ANL: Ahmed Attia, Sven Leyffer, Todd Munson

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Argonne NATIONAL LABORATORY

Giant leap toward quantum internet realized with Bell state analyzer

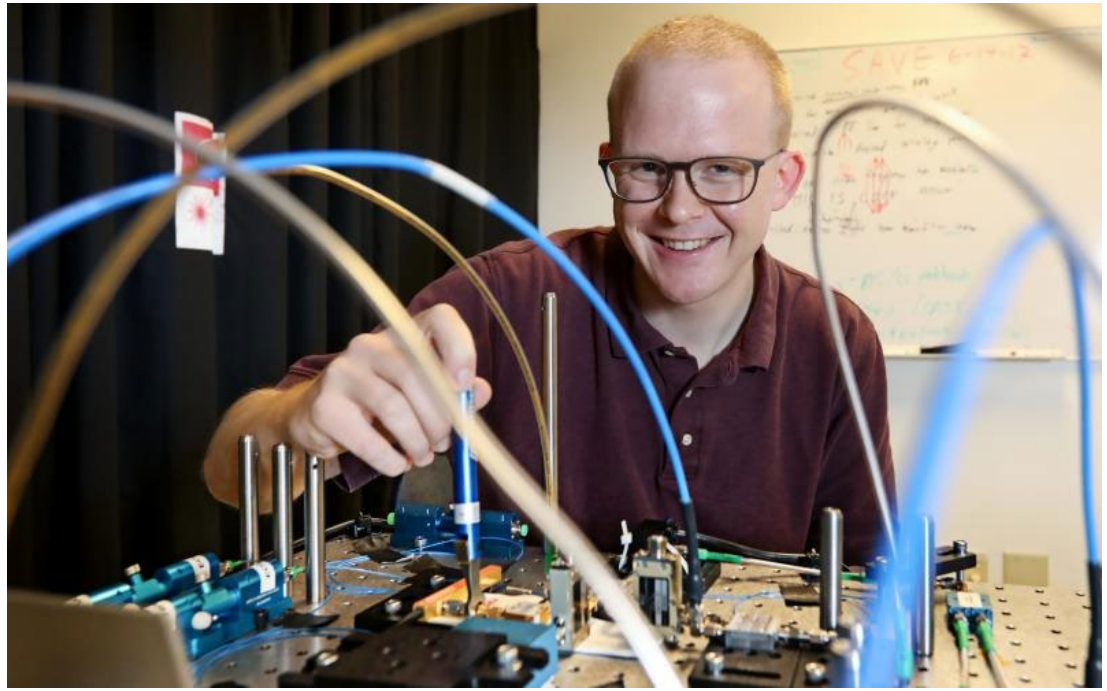
ASCR research advances future technologies

The Science

A multi-institutional team featuring ORNL's Joe Lukens has made strides toward a fully quantum internet by designing and demonstrating the first ever Bell state analyzer for frequency bin coding. Measuring Bell states is critical to performing many of the protocols necessary to perform quantum communication and distribute entanglement across a quantum network. The team's method represents the first Bell state analyzer developed specifically for frequency bin coding, a quantum communications method that harnesses single photons residing in two different frequencies simultaneously.

The Impact

The analyzer was designed with simulations and has experimentally demonstrated 98% fidelity for distinguishing between two distinct frequency bin Bell states. This incredible accuracy is expected to enable new fundamental communication protocols necessary for frequency bins.



ORNL's Joseph Lukens runs experiments in an optics lab. Credit: Jason Richards/ORNL, U.S. Dept. of Energy

PI(s)/Facility Lead(s): Joe Lukens (ORNL)
ASCR Program/Facility: N/A
ASCR PM: Lali Chatterjee
Funding: Office of Science through the Early Career Research Program
Publication for this work: Navin B. Lingaraju, Hsuan-Hao Lu, Daniel E. Leaird, Steven Estrella, Joseph M. Lukens, and Andrew M. Weiner. "Bell state analyzer for spectrally distinct photons," Optica Vol. 9, Issue 3, pp. 280-283 (2022).
Date submitted to ASCR: Spring 2022

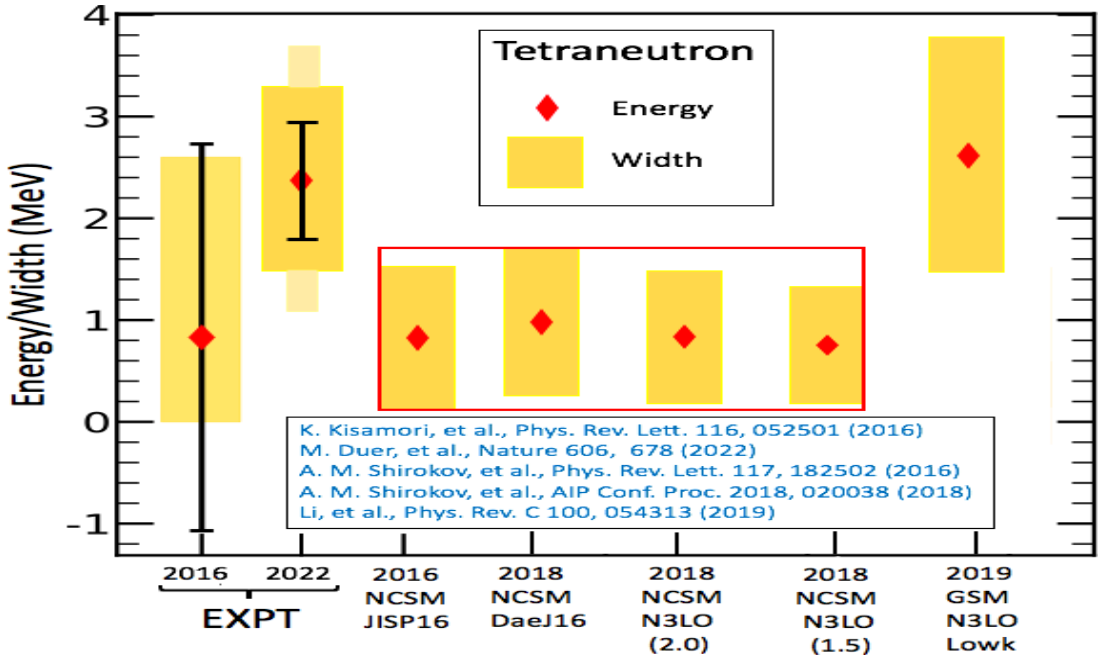
Tetraneutron Discovery Confirms Prediction

ASCR research has long lasting impact

NUCLEI Nuclear Computational Low-Energy Initiative

Objectives

- *Ab initio* nuclear theory aims for parameter-free predictions of nuclear properties with controlled uncertainties using supercomputer simulations.
- Specific goal is to predict if the tetraneutron (4-neutron system) has a bound state, a low-lying resonance or neither



Experiment and theory for the tetraneutron's resonance energy and width. *Ab initio* No-Core Shell Model (NCSM) and Gamow Shell Model (GSM) predictions use different neutron-neutron interactions and different basis function techniques.

Impact

- Discovery announced in Nature [1] confirms *ab initio* theory predictions from 2016 [2] of a short-lived tetraneutron resonance at low energy and the absence of a tetraneutron bound state
- Demonstrates the predictive power of *ab initio* nuclear theory since theory and experiment are within their combined uncertainties
- Sets stage for further experimental and theoretical research on new states of matter formed only of neutrons
- Shows need to anticipate a long wait time for experimental confirmation of such an exotic phenomena, ~ 6 years in this case
- Emphasizes the value of DOE supercomputer allocations (NERSC) and support for multi-disciplinary teamwork (SciDAC/NUCLEI)

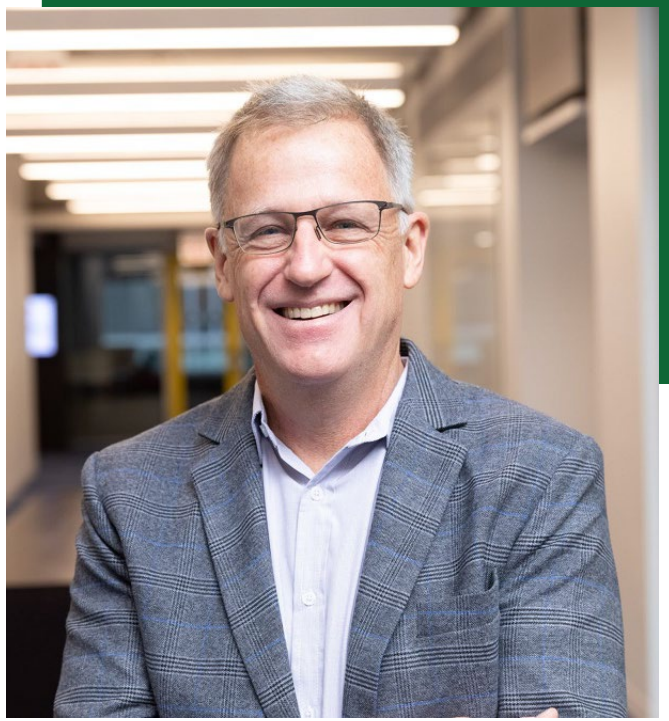
Publications

[1] M. Duer, et al., Nature 606, 678 (2022)

[2] A.M. Shirokov, G. Papadimitriou, A.I. Mazur, I.A. Mazur, R. Roth and J.P. Vary, "Prediction for a four-neutron resonance," Phys. Rev. Lett. 117, 182502 (2016)

Recognition of Our Community Members

2022 ACM-IEEE CS Ken Kennedy Award



Ian Foster, ANL
SC Distinguished Scientist

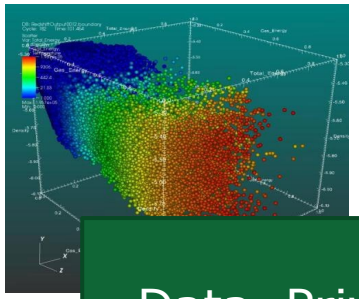
2022 AGU William Bowie Lecturer

Bridget Scanlon,
UT Austin, ICDI PI

ASCR Research Enables DOE and SC Scientific Enterprise

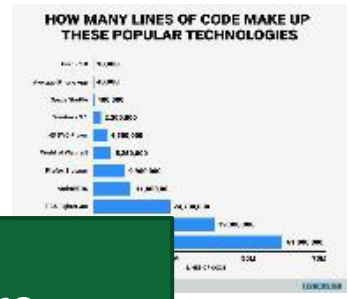
Thriving in the Exascale Era

Revolutionizing Future of Computing

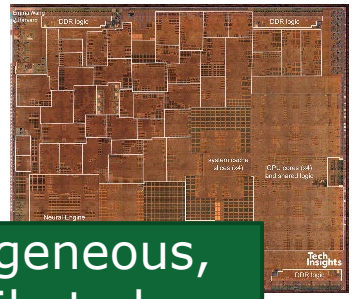


Data, Privacy & Scientific Integrity

Artificial Intelligence & Machine Learning



Software Complexity



Heterogeneous, Distributed, Special-Purpose, Energy-Efficient

Critical Trends Motivating ASCR Research

FY2023: A Preview

- **Scientific Machine Learning for Complex Systems**
- **Distributed, Resilient Systems**
- **Codesign for Scientific Continuum Computing**
- **Software Sustainability**
- **SciDAC Partnerships**
- **Quantum Communications & Network Research**
- **Quantum Computing & Internet**
- **EXPRESS: Future Computing Systems, Programming Techniques, Uncertainty Quantification, Quantum Algorithms**
- **RENEW: Reaching a New Energy Sciences Workforce**
- **Funding for Accelerated, Inclusive Research (FAIR)**
- **Accelerate Innovations in Emerging Technologies (ACCELERATE)**
- **Energy Earthshots**
- **Biopreparedness Research Virtual Environment (BRaVE)**

Leveraging and Building our Core Strengths

Innovative Basic Research
Inspired by Science Drivers
Strategic Partnerships
Smart Sustainability
Agility
Next-Generation Workforce

(*) Subject to congressional appropriations.

ASCR Software Sustainability: FY23 Opportunities

- ASCR-supported software technologies are critical to DOE scientific software on *all* platforms.
- In the CHIPS and Science Act, congress explicitly added *Exascale Ecosystem Sustainment* to ASCR's portfolio balance, "**It is the sense of Congress that** the Exascale Computing Project has successfully created a broad ecosystem that provides shared software packages, novel evaluation systems, and applications relevant to the science and engineering requirements of the Department, and that **such products must be maintained and improved in order that the full potential of the deployed systems can be continuously realized**."
- ASCR expects to convene a review panel in January 2023 for sustainability applications submitted through the "open call."
- Applications for sustainability collaborations should **articulate a long-term vision for sustaining a substantial part of the ecosystem** of software for scientific and high-performance computing, and should describe **how their efforts might be rapidly scaled up in the future**.
- Applicants should think creatively about how to meet the long-term needs of the software ecosystem, including stakeholders who may need paid commercial support, and about potential partners, including national laboratories, academic institutions, nonprofit organizations, and businesses of all sizes.
- For more information on community needs, please see results from ASCR's Software-Stewardship RFI (https://science.osti.gov/-/media/ascr/ascac/pdf/meetings/202203/ASCAC_202203_Finkel-RFI-Codesign-PDES.pdf).
- For more information, please contact Hal Finkel, William Spotz, and Robinson Pino.

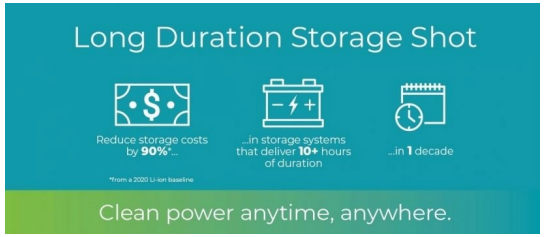
(*) Subject to congressional appropriations.

SC Energy Earthshots Initiative
FY 2023 $204M

https://www.energy.gov/policy/energy-earthshots-initiative

- Accelerates breakthroughs to realize abundant, affordable, and reliable clean energy solutions within the decade
- Addresses key research challenges at the interface of basic and applied research to bridge the R&D gap
- Initiates new research modality, Energy Earthshot Research Centers (EERCs)
  - Advances foundational knowledge and state-of-the-art capabilities in experimental, theoretical, and computational sciences needed to realize new approaches and solutions
  - Brings together large, multi-investigator, multi-disciplinary teams
  - Coordinates closely with the Energy Technology Offices and existing research consortia/demonstration projects for a new era of cross-office research cooperation
- EERCs will be complemented by small group awards focused on use-inspired fundamental research to address knowledge gaps that limit achievement of the Energy Earthshot goals

Hydrogen Shot



Carbon Negative Shot

Enhanced Geothermal Shot

(*) Subject to congressional appropriations.

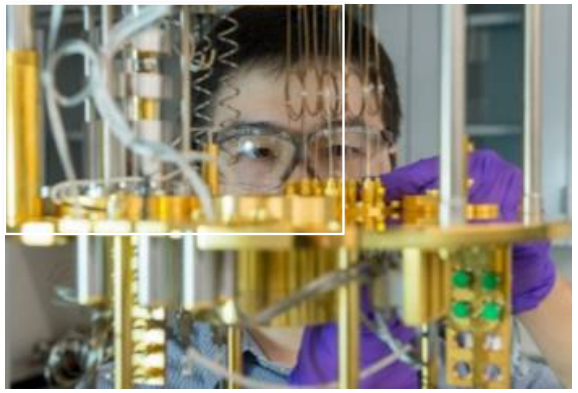
Floating Offshore Wind Shot

Industrial Heat Shot

Funding to Accelerate Inclusive Research (FAIR)
FY 2023 $36M

FAIR will enhance research on clean energy, climate, and related topics at minority serving institutions (MSIs), including underserved and environmental justice regions

- Builds research capacity, infrastructure, and expertise at MSIs
- Develops mutually beneficial relationships between MSIs and DOE national laboratories and user facilities
- Complements the RENEW initiative
- Provides support of single PI or research teams, and includes an equipment or infrastructure element
- Majority of funds will go directly to HBCUs/MSIs, a portion will fund the partnering institution (Lab, university)



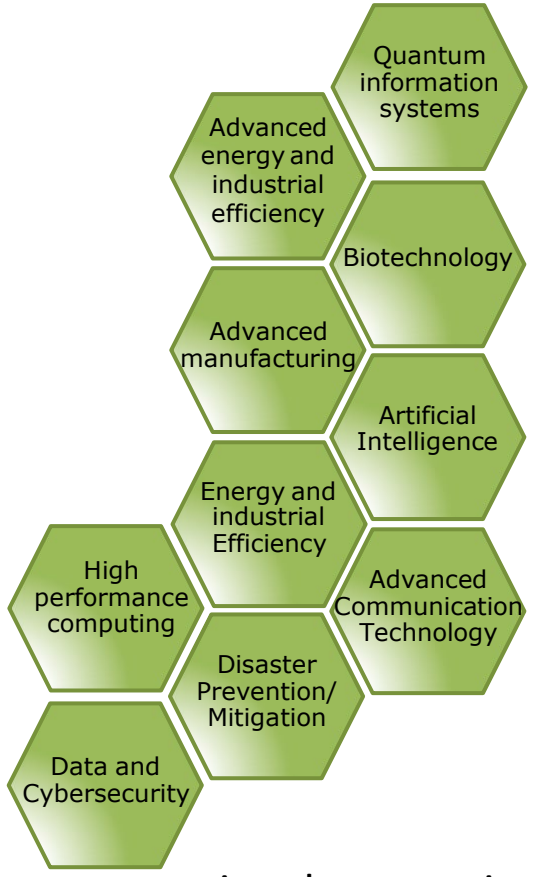
(*) Subject to congressional appropriations.

Accelerate Innovations in Emerging Technologies
FY 2023 $40M

Highly integrated research teams to accelerate the discovery, creation, production, and commercialization of new technologies to form the basis of future industries with public and economic impact

Initiative goals:

- To drive scientific discovery for sustainable production of new technologies across the innovation continuum
- To train a STEM workforce to support industries of the future
- To meet the nation's needs for abundant clean energy, a sustainable environment, and national security



(*) Subject to congressional appropriations.

New ASCR Program Manager Position Now Open

GS-15 Interdisciplinary Physical Scientist/Computer Scientist Position in the Research Division, Computer Science Group

- Manage the computer science and networking research portfolios that include quantum communications and advanced wireless communications such as 6G and related Artificial Intelligence (AI) technologies, workflows, and cybersecurity systems

- Open between September 29 and October 12

- Two parallel announcements in USAJobs.gov
  - To be considered as a computer scientist, the applicants should apply to: https://www.usajobs.gov/job/679121400
  - To be considered as a physical scientist, the applicants should apply to the Open Continuous Direct Hire Announcement CY-22-OCDH-1301-11434839-DH posted in: https://www.usajobs.gov/job/646322700

HAPPY RETIREMENT!

Randall Laviolette
Ph.D. Chemistry, U.C. Berkeley
ASCR Program Manager for SciDAC Partnerships w/ SC Offices BES, BER, FES, HEP, NP and Office of Nuclear Energy.
Previously at Sandia National Laboratory, Idaho National Laboratory, Rockwell Science Center, and Bell Laboratories