



HYPERION RESEARCH



# Measuring and Assessing the Value and Scientific ROI of NERSC's Leadership Computing in Advancing Science

## Key Findings

October 4<sup>th</sup>, 2024

[www.HyperionResearch.com](http://www.HyperionResearch.com)  
[www.hpcuserforum.com](http://www.hpcuserforum.com)

Mark Nossokoff, Jaclyn Ludema, and  
Earl Joseph

# About Hyperion Research

([www.HyperionResearch.com](http://www.HyperionResearch.com) & [www.HPCUserForum.com](http://www.HPCUserForum.com))



## Hyperion Research mission:

- Hyperion Research helps organizations make effective decisions and seize growth opportunities
  - *By providing research and recommendations in high performance computing and emerging technology areas*

## HPC User Forum mission:

- To improve the health of the HPC/AI/QC industry
  - *Through open discussions, information sharing and initiatives involving HPC users in industry, government and academia along with HPC vendors and other interested parties*

# The Hyperion Research Team

## Analysts

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Andrew Rugg, Certus Insights

Jie Wu, China and Technology Trends

Mara Jacob, HPC User Forum Support

# Agenda

- **Project Goals**
- **Methodology**
- **Demographics**
  - Study participants
  - NERSC Office, Program, & Science Category profiles
  - Additional projects included
- **Key Findings**
  - Notable research conducted at NERSC
  - Overview
  - Innovation Return on Research (RoR)
- **Other Findings**

# Project Goals

- **Measure and convey the impact, value and scientific ROI of investments in leadership computing centers**
- **Show the value and returns from scientific research, R&D, discoveries and other accomplishments made through the use of large-scale advanced computing**
- **Provide the ability to articulate the value that comes from investments in leadership computing**
- **Focus of the assessment will be projects conducted at NERSC, including projects over the last few decades**



# Methodology

- **Used the Hyperion Research framework that measures the value of scientific computing projects to fit NERSC's unique mission:**
  - Advancing Science, Advancing Engineering, Economic Growth, Saving Lives, National Security
- **Measured the historical value by surveying individual projects and accomplishments**
  - NERSC provided researchers' contact information, research topics
  - NERSC introduced Hyperion Research and requested support for the project
  - Hyperion Research invited researchers to participate and schedule 30-minute phone conversations
- **Analyzed the results and compare the results to other sites**

# Study Research Projects

| Principal Investigator (PI) | Organization                          | Research Title  |
|-----------------------------|---------------------------------------|---|
| Aluie, Hussein              | University of Rochester               | Computational Studies Across Time and Length Scales of Multifunctional Ionic Polymers Membranes   |
| Austregesilo, Alexander     | Jefferson Lab                         | Analysis and Simulation for the GlueX Detector: studying the strong nuclear force and searching for exotic configurations of quarks and gluons  |
| Bajdich, Michal             | SLAC National Accelerator Laboratory  | SUNCAT-FWP CATALYSIS PROJECT: focusing on CO2 reduction, nitrogen reduction, and water splitting  |
| Baron, Edward               | University of Oklahoma                | High performance computing in support of the DIII-D National Fusion Facility  |
| Baron, Edward               | University of Oklahoma                | Synthetic Spectra of Astrophysical Objects  |
| Burrows, Adam               | Princeton University                  | Three-Dimensional Simulations of Core-Collapse Supernovae: to understand how supernova explosions occur, resulting in the formation of neutron stars or black holes.                            |
| Calafiura, Paolo            | Lawrence Berkeley National Laboratory | Detector Simulation of the CERN ATLAS Detector on NERSC HPCs  |
| Car, Roberto                | Princeton University                  | Chemistry in Solution and at Interfaces: to fit the potential energy of interaction among atoms.  |
| Ching, Wai-Yim              | University of Missouri - Kansas City  | Structure refinement of Spike-protein of SARS-COV-2: This approach allows them to analyze the entire complex structure of the virus, rather than breaking it down into smaller separate pieces. |
| Christ, Norman              | Columbia Univeristy                   | High Energy Particle Physics - Symmetry of Nature. The equivalence of particles and antiparticles. Right-handed vs. left-handed   |
| DeTar, Carleton             | University of Utah                    | Flavor physics: the focus is on understanding physics beyond the Standard Model   |
| Fagnan, Kjersten            | DOE Joint Genome Institute (JGI)      | Joint Genome Institute - Production Sequencing and Genomics: researching areas such as nutrient cycling, biofuels, microbial communities, and plant genomics.                                   |
| Galli, Giulia               | University of Chicago                 | First Principles Simulations of Nanostructures: to study matter at the atomic level   |
| Gavini, Vikram              | University of Michigan                | PRISMS: Integrated multiscale modeling of Mg structural alloys: The goal is to understand and improve the mechanical properties of magnesium alloys   |



# Study Research Projects (continued)

| PI   | Organization                          | Research Title   |
|--|---------------------------------------|--|
| Glezakou, Vassiliki                                  | Oak Ridge National Laboratory         | Carbon management and energy efficiency through multifunctional catalysis  |
| Gottlieb, Ore,<br>Tchekhovskoy,<br>Alexander (Sasha) | Northwestern University               | Effects of remnant neutron star lifetime on compact object merger outflows, nucleosynthesis, and emission: The goal is to connect the merger event itself with the observable electromagnetic signatures, allowing scientists to extract valuable physics information from these observations. |
| Gupta, Rajan   | Los Alamos National Laboratory        | High Precision Calculations of the Nucleon Structure for Fundamental Symmetries: to create a better understanding the properties of neutrons and protons.  |
| Gupta, Rajan   | Los Alamos National Laboratory        | Lattice QCD search for physics beyond the standard model   |
| Hoffman, Forrest                                     | Oak Ridge National Laboratory         | Reducing Uncertainties in Biogeochemical Interactions through Synthesis and Computation (RUBISCO): to study the interactions between biogeochemistry and the climate system.   |
| Howard, Dr. Nathan                                   | Massachusetts Institute of Technology | Computational Studies in Plasma Physics and Fusion Energy: Multi-scale Turbulence in Tokamak Reactors: to reduce heat and particle losses in fusion plasmas.   |
| Jardin, Stephen                                      | Princeton Plasma Physics Laboratory   | 3D Extended MHD simulation of fusion plasmas: for tokamak fusion reactors.   |
| Jena, Puru   | Virginia Commonwealth University      | Cluster and Nanostructure for Energy and Bio Applications: for improved energy production and storage.   |
| Leung, Lai-Yung Ruby                                 | Pacific Northwest National Laboratory | Water Cycle and Climate Extremes Modeling (WACCEN): to understand how various aspects of the water cycle, particularly precipitation, have changed in the past and how they might change in the future.  |
| Leung, Lai-Yung Ruby                                 | Pacific Northwest National Laboratory | Energy Exascale Earth System Modeling (E3SM): improving the understanding of how energy use contributes to climate change and how climate change may affect future energy use and infrastructure.  |
| Mavrikakis, Manos                                    | University of Wisconsin - Madison     | First-Principles Catalyst Design for Environmentally Benign Energy Production: to uncover why certain materials are effective catalysts while others are not.  |
| Mccallen, David                                      | Lawrence Berkeley National Laboratory | High Performance Simulations for Regional Scale Earthquake Hazard and Risk Assessments   |
| Monzani, Maria Elena                                 | SLAC National Accelerator Laboratory  | LZ - LUX ZEPLIN experiment, which aims to detect dark matter.  |
| Perahia, Dvora                                       | Clemson University                    | Computational Studies Across Time and Length Scales of Multifunctional Ionic Polymers Membranes: The focus is on polymers with ionic groups that can conduct ions, generate electricity, and trap nanoparticles.   |



# Study Research Projects (continued)

| PI                            | Organization                          | Research Title  |
|-------------------------------|---------------------------------------|---|
| Petreczky, Peter              | Brookhaven National Lab               | Quarkonia in Hot Medium: the properties of matter under extreme conditions.   |
| Qian, Jin                     | Lawrence Berkeley National Laboratory | From Molecules to Continuum: Developing a Universal Approach for Accurate Description of X-ray Photo: for nanoscale phenomena.  |
| Qiu, Diana                    | Yale University                       | Electronic and Optical Properties of Layered Materials for Energy Applications: to develop new theoretical and computational tools for understanding how materials interact with light. |
| Radice, David                 | The Pennsylvania State University     | Nuclear Astrophysics with Numerical Relativity: the collision between neutron stars   |
| Ryne, Robert                  | Lawrence Berkeley National Laboratory | Frontiers in Accelerator Design: Advanced Modeling for Next-Generation BES Accelerators: the design and development of particle accelerators.   |
| Sako, Masao                   | University of Pennsylvania            | The Dark Energy Survey Supernova Search: The project aimed to measure the properties of around 300 million galaxies and discover thousands of new supernova explosions.                 |
| Sankaranarayanan, Subramanian | Argonne National Laboratory           | Development of New Force Fields using Machine Learning and First Principles Physics   |
| Sharifzadeh, Sahar            | Boston University                     | Large-Scale Many-Body Perturbation Theory Simulations of Optoelectronic Materials: to understand the electronic properties of materials at the atomic scale.                            |
| Smith, Sterling               | General Atomics                       | Computing in support of the DIII-D National Fusion Facility: the goal is to study how to confine and heat plasma efficiently enough to achieve fusion                                   |
| Trebotich, David              | Lawrence Berkeley National Laboratory | Advanced Simulation of Pore Scale Flow and Transport Processes in Nanoporous Materials: examining how fluids interact with materials at a microscopic level (around 1-100 microns).     |
| Ullrich, Paul                 | University of California Davis        | A Framework for Improving the Analysis and Modeling of Earth System and Intersectoral Dynamics at Regional Scales   |
| Vermaas, Josh                 | Michigan State University             | Large Scale Molecular Simulations to Support Photosynthesis and Carbon Fixation   |
| Wang, Hailong                 | Pacific Northwest National Laboratory | High-Latitude Application and Testing (HiLAT) of Earth System Models & Regional Arctic System Model   |
| Wu, Xifan                     | Temple University                     | Theoretical spectra calculations of liquid water and ion solutions  |

# Collaborating Organizations

*The PIs were supported by many research organizations and utilized supporting computational computing facilities*

- **Supporting research organizations**

- Brookhaven National Lab
- CERN
- Indiana University
- MIT
- Pittsburgh Supercomputer Center
- Sandia National Lab
- UC-Berkeley
- UC-Davis
- University of Arizona
- University of Bristol
- University of Connecticut
- University of Edinburgh

- **Supporting computational facilities**

- PI host/local organization clusters
- Argonne National Lab
- Hamburg University
- HLRN
- Jefferson Lab
- Jülich
- Oak Ridge National Lab
- Lawrence Livermore National Lab
- NCAR
- NCSA
- TACC
- University of Chicago
- University of Georgia

# Additional Projects Included

- **6 Nobel Prize winners utilized NERSC resources**

| Year | Category  | Principal Investigator (PI)  | Research Title  | Organization   |
|------|-----------|------------------------------|---|--|
| 2017 | Chemistry | Frank Joachim, Eva Nogales   | Correlative Cryo-EM and Molecular Dynamics Simulations of Ribosomal Structure             | Lawrence Berkeley National Laboratory                    |
| 2015 | Physics   | Takaaki Kajita, Art McDonald | Sudbury Neutrino Experiment   | Tokyo University; Queen's University (Kingston, Ontario) |
| 2013 | Chemistry | Martin Karplus, Paul Bash    | Multiscale Chemical Modeling  | Harvard; Northwestern                                    |
| 2011 | Physics   | Saul Perlmutter              | Supernova Cosmology Project   | Lawrence Berkeley National Laboratory                    |
| 2007 | Peace     | Warren Washington, et al     | Fourth Report of the Intergovernmental Panel on Climate Change (IPCC) (climate modelling) | NERSC  |
| 2006 | Physics   | George Smoot                 | Birth of Precision Cosmology  | Lawrence Berkeley National Laboratory                    |

- **Other notable leadership site accomplishments**
  - First large-scale application to achieve Tflop performance
  - Global repository for LHC raw data and ensuing analysis enable worldwide collaboration

# NERSC Office, Program, and Science Category Profiles of Participants

| Office                                | #  |
|---------------------------------------|----|
| Basic Energy Sciences                 | 16 |
| High Energy Physics                   | 7  |
| Nuclear Physics                       | 7  |
| Biological and Environmental Research | 6  |
| Fusion Energy Sciences                | 4  |
| NERSC Directors Reserve               | 2  |

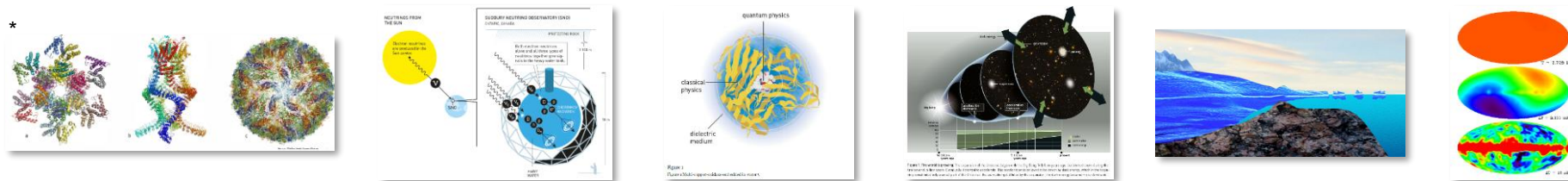
| Program   | # |
|---|---|
| Chemical Sciences, Geosciences, & Biosciences (CSGB)      | 9 |
| Nuclear Physics   | 7 |
| High Energy Physics                                       | 6 |
| Materials Sciences and Engineering                        | 6 |
| Earth and Environmental Systems Sciences Division (EESSD) | 5 |
| Fusion Energy Sciences                                    | 4 |
| Biological Systems Science                                | 1 |
| DDR Campaign  | 1 |
| DDR Scale   | 1 |
| Scientific User Facilities                                | 1 |

| Science Category                             | # |
|--|---|
| Physics : Astrophysics                       | 4 |
| Chemistry : Catalysis                        | 3 |
| Chemistry : Chemical Physics                 | 3 |
| Earth Systems : Coupled Systems              | 3 |
| Energy : Fusion                              | 3 |
| Physics : High Energy Physics (Theory)       | 3 |
| Physics : Nuclear Physics (Theory)           | 3 |
| Earth and Environmental Systems              | 2 |
| Materials Science : General                  | 2 |
| Physics : Condensed Matter                   | 2 |
| Physics : High Energy Physics (Experimental) | 2 |
| Biosciences : Genomics                       | 1 |
| Biosciences : Molecular Science              | 1 |
| Chemistry : Physical Chemistry               | 1 |
| Energy : General                             | 1 |
| Geoscience : Geochemistry                    | 1 |
| Materials Science : Biomolecular Materials   | 1 |
| Materials Science : Energy Storage           | 1 |
| Materials Science : Soft Matter              | 1 |
| Physics : Accelerator Science                | 1 |
| Physics : Cosmology                          | 1 |
| Physics : Nuclear Physics (Experimental)     | 1 |
| Physics : Plasma Physics                     | 1 |

# Key Findings

# Notable Research Conducted at NERSC

| Nobel Prize Winners |           |                              |   |
|---------------------|-----------|------------------------------|---|
| Year                | Category  | PI                           | Research Title  |
| 2017                | Chemistry | Frank Joachim, Eva Nogales   | Correlative Cryo-EM and Molecular Dynamics Simulations of Ribosomal Structure             |
| 2015                | Physics   | Takaaki Kajita, Art McDonald | Sudbury Neutrino Experiment   |
| 2013                | Chemistry | Martin Karplus, Paul Bash    | Multiscale Chemical Modeling  |
| 2011                | Physics   | Saul Perlmutter              | Supernova Cosmology Project   |
| 2007                | Peace     | Warren Washington, et al     | Fourth Report of the Intergovernmental Panel on Climate Change (IPCC) (climate modelling) |
| 2006                | Physics   | George Smoot                 | Birth of Precision Cosmology  |



| Select Highlighted NERSC Research |   |
|-----------------------------------|---|
| PI                                | Research Title  |
| Robert Ryne                       | Frontiers in Accelerator Design: Advanced Modeling for Next-Generation BES Accelerators                       |
| Ruby Leung                        | Energy Exascale Earth System Modeling   |
| Subramanian Sankaranarayanan      | Development of New Force Fields using Machine Learning and First Principles Physics                           |
| Puru Jena                         | Cluster and Nanostructure for Energy and Bio Applications   |
| Paul Ullrich                      | A Framework for Improving Analysis and Modeling of Earth System and Intersectoral Dynamics at Regional Scales |
| Wai-Yim Ching                     | Structure refinement of Spike-protein of SARS-COV-2   |
| Kjiersten Fagnan                  | Joint Genome Institute - Production Sequencing and Genomics   |
| Sterling Smith                    | High performance computing in support of the DIII-D National Fusion Facility                                  |
| Jin Qian                          | From Molecules to Continuum: Developing a Universal Approach for Accurate Description of X-ray Photo          |
| Michal Bajdich                    | SUNCAT-FWP Catalysis  |
| Giulia Galli                      | First principles simulations of nanostructures  |

# Key Findings Overview

*Inclusive of 6 Nobel Prize awards, 42 interviews with leading researchers and notable research from annual reports*

- **Research performed at NERSC touches most scientific areas**
  - Fusion energy as an alternative fuel source
  - Astrophysics for understanding matter and the origins of the universe
  - Climate and weather for earlier, more accurate predictions
  - Water splitting for harvesting hydrogen for fuel
  - Earth sciences for mitigating impacts from earthquakes
  - Genomics to address challenges in agriculture, environmental science, and sustainable energy production
- **Advancing Science is the clear mission of most researchers**
  - Outcomes also heavily contribute to Advancing Engineering, Saving Lives, Economic Growth and National Security (non-defense-related)
- **NERSC accomplishments go beyond scientific discovery**
  - Enables collaborations with global research institutions
  - First demonstration of Tflop performance at scale
- **Glowing reviews/praise for NERSC**
  - Research would not have been possible without NERSC
  - Performance and continued roadmap of resources
  - Quality and knowledge of support personnel
  - Response timeliness of support personnel
  - Simplicity of process to submit grants & secure time on the infrastructure



# Innovation Return on Research (ROR) Results

# The Innovation Return on Research (ROR) Metrics Used in the Study

In order to properly quantify the innovation from HPC projects, Hyperion Research uses a rating system that measures both the importance and the impact of each innovation in this study.

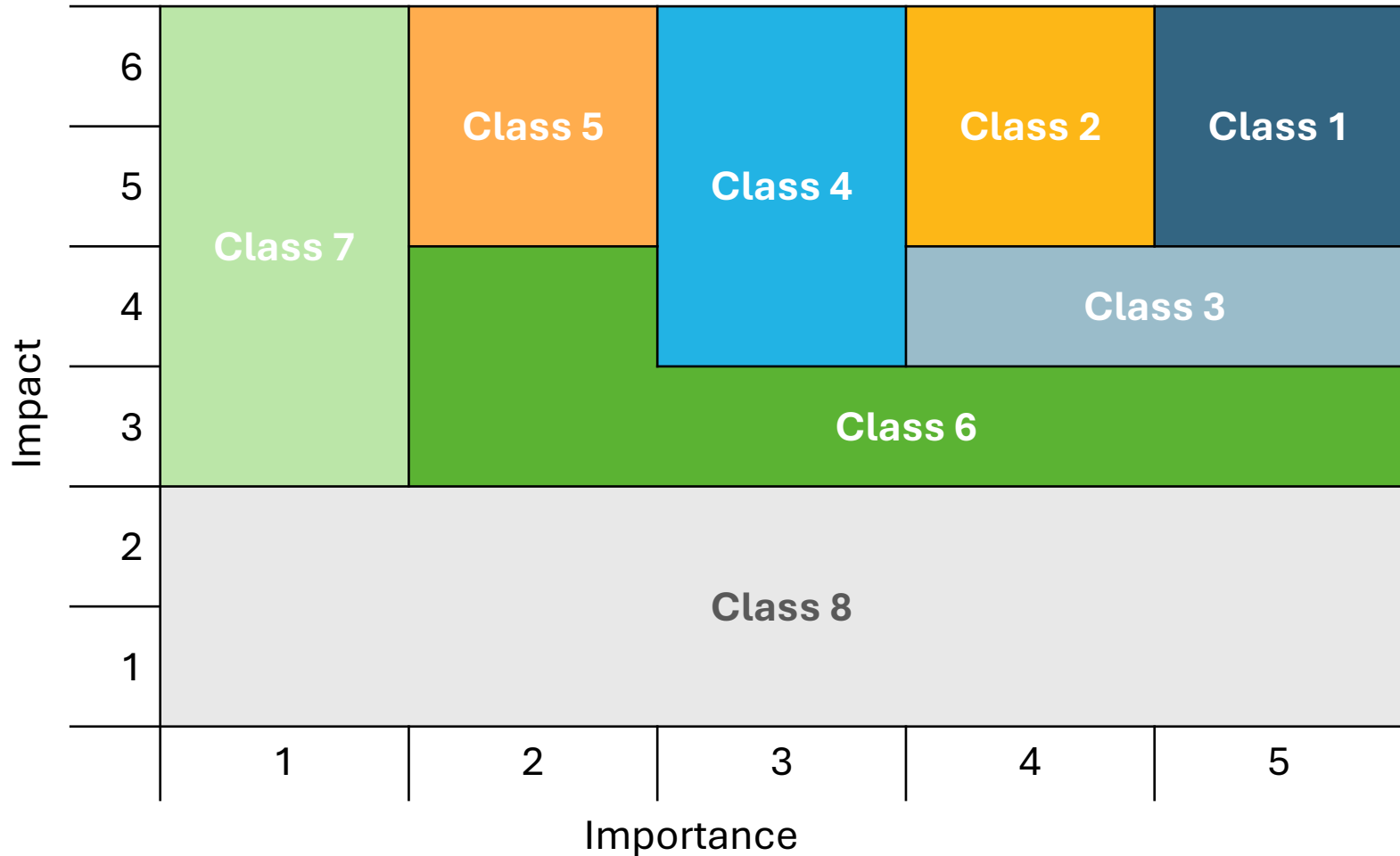
- **The IMPORTANCE of this innovation compared to all other innovations in the specific field over the last ten years:**
  - 5 (One of the top 2 to 3 innovations in the last decade)
  - 4 (One of the top 5 innovations in the last decade)
  - 3 (One of the top 10 innovations in the last decade)
  - 2 (One of the top 25 innovations in the last decade)
  - 1 (One of the top 50 innovations in the last decade)
- **The IMPACT of this innovation to multiple organizations:**
  - 6 (It is useful to over 50 organizations)
  - 5 (It is useful to 10 to 49 organizations)
  - 4 (It is useful to 6 to 9 organizations)
  - 3 (It is useful to 2 to 5 organizations)
  - 2 (It is only useful to 1 organization)
  - 1 (It is recognized ONLY by experts in the field)

# The Innovation Class Index

Combining these two measures, Hyperion Research creates an overall **INNOVATION CLASS** rating for these projects:

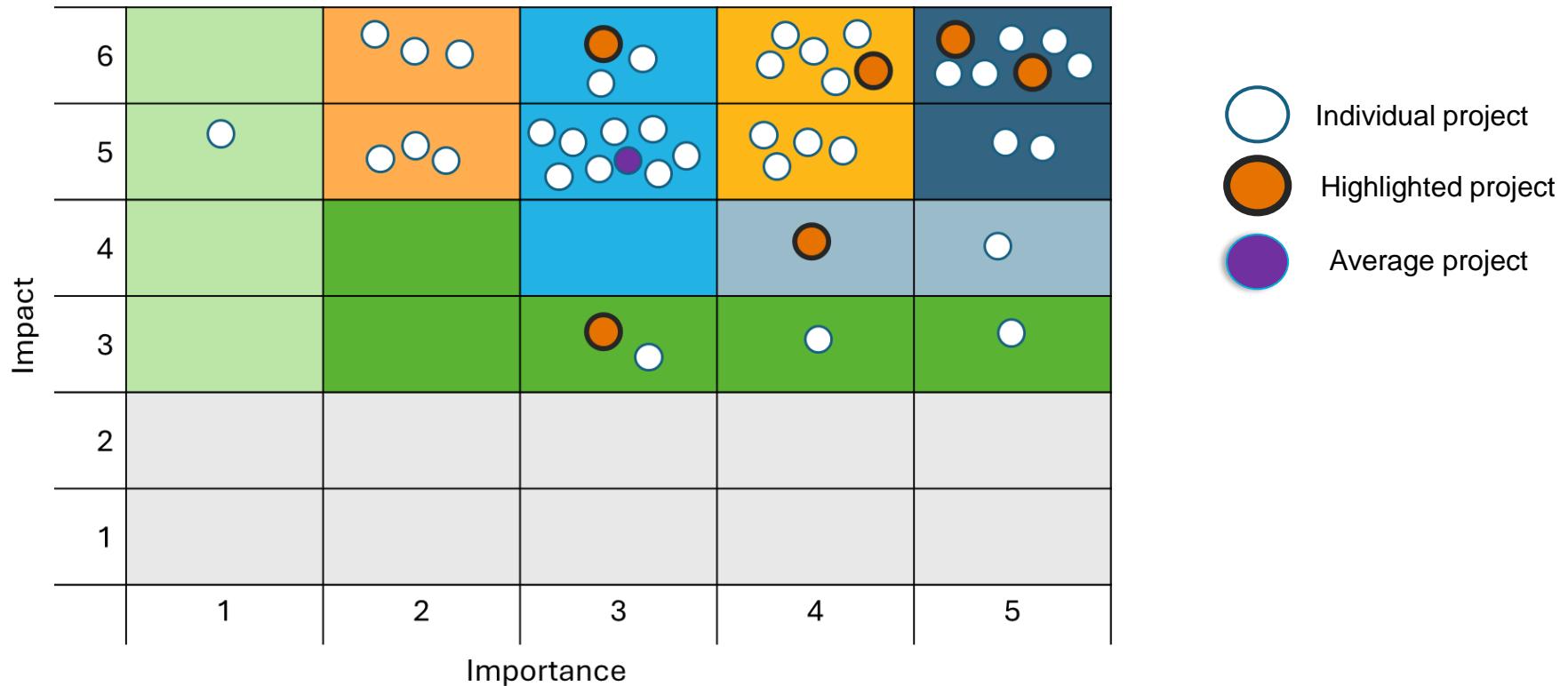
1. Class 1 innovations – One of the top 2 to 3 innovations in the last decade PLUS useful to over 10 organizations
2. Class 2 innovations – One of the top 5 innovations in the last decade PLUS useful to over 10 organizations
3. Class 3 innovations – One of the top 5 innovations in the last decade PLUS useful to over 5 organizations
4. Class 4 innovations – One of the top 10 innovations in the last decade PLUS useful to over 5 organizations
5. Class 5 innovations – One of the top 25 innovations in the last decade PLUS useful to at over 10 organizations
6. Class 6 innovations – One of the top 25 innovations in the last decade PLUS useful to at least 2 organizations
7. Class 7 innovations – One of the top 50 innovations in the last decade PLUS useful to at least 2 organizations
8. Class 8 innovations – All other innovations

# Innovation Class Research Mapping



# Innovation Class Research Mapping

*Majority of research from the study has high potential for substantial impact on society*



# Energy Exascale Earth System Modeling (E3SM): improving understanding of how energy use contributes to current and may affect future climate change

*Ruby Leung, Pacific Northwest National Lab (PNNL)*

- **Summary Description**

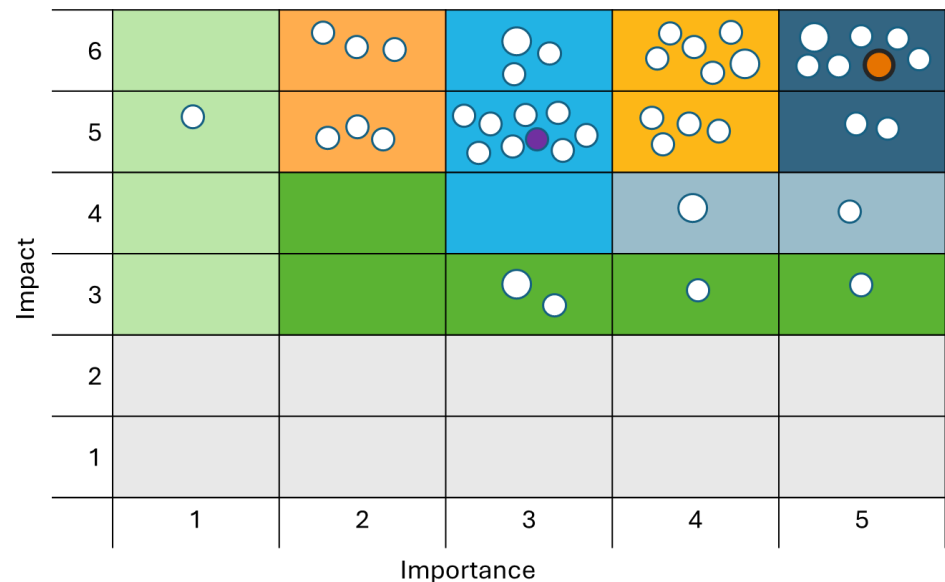
- Create a sophisticated earth system model that can take advantage of exascale computing capabilities.

- **Impact to the World**

- Latest version can run at very high resolutions (down to 3 km globally), incorporating both natural earth systems and human activities.
- Allows for complex interactions between climate change and human energy use.
- Features variable resolution capabilities, enabling researchers to focus computational resources on specific areas of interest, such as North America or Antarctica.

| Office   | Program | Category                          |
|----------|---------|-----------------------------------|
| Research | EESDD   | Earth Systems:<br>Coupled Systems |

| Advances Science | Advances Engineering | Saving Lives | Economic Growth | National Security |
|------------------|----------------------|--------------|-----------------|-------------------|
| x                | x                    | x            | x               | x                 |



# Joint Genome Institute - Production Sequencing and Genomics: researching areas such as nutrient cycling, biofuels, microbial communities, and plant genomics.

*Kjiersten Fagnan, DOE Joint Genome Institute (JGI)*

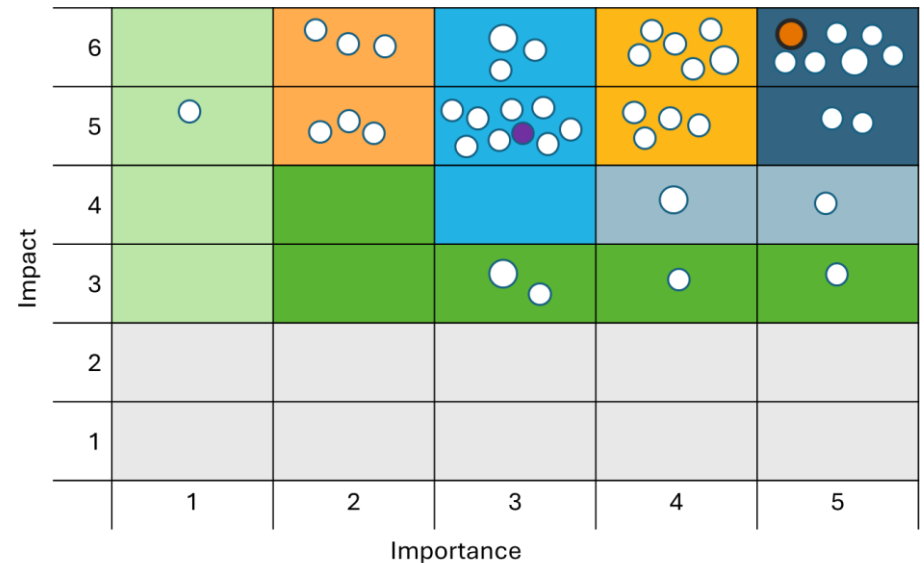
## • Summary Description

- Contribute to better understanding of nutrient cycling, the development of improved biofuels, and insights into how microbial communities work.

## • Impact to the World

- Addressing challenges in agriculture, environmental science, and sustainable energy production.
- Support a large community of scientists (around 2000) who use this information for their research. The ability to process and analyze complex metagenomic samples has opened up new avenues of research.

| Office                                |                      | Program                    |                 | Category              |  |
|---------------------------------------|----------------------|----------------------------|-----------------|-----------------------|--|
| Biological and Environmental Research |                      | Biological Systems Science |                 | Biosciences: Genomics |  |
| Advances Science                      | Advances Engineering | Saving Lives               | Economic Growth | National Security     |  |
| x                                     | x                    |                            |                 |                       |  |





# Computing in support of the DIII-D National Fusion Facility: the goal is to study how to confine and heat plasma efficiently enough to achieve fusion

*Sterling Smith, General Atomics*

## • Summary Description

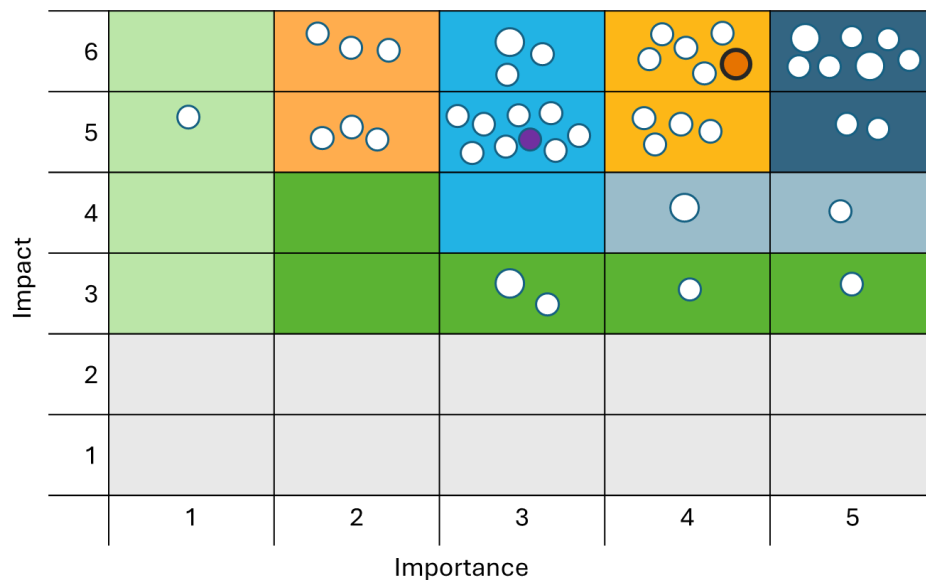
- Fusion research the D3D tokamak device, a donut-shaped vacuum chamber that uses powerful magnetic fields to confine and heat plasma to extremely high temperatures.
- Study how to confine and heat plasma efficiently enough to achieve fusion, where atomic nuclei combine to release energy.

## • Impact to the World

- Seeks to understand, control, and mitigate turbulence and heat transport within the plasma.
- Scientists used NERSC's real-time queue and Superfacility API to perform rapid analysis between plasma experiments, every 15 minutes during operational days.

| Office                 | Program                | Category       |
|------------------------|------------------------|----------------|
| Fusion Energy Sciences | Fusion Energy Sciences | Energy: Fusion |

| Advances Science | Advances Engineering | Saving Lives | Economic Growth | National Security |
|------------------|----------------------|--------------|-----------------|-------------------|
| x                |                      |              |                 |                   |



# SUNCAT-FWP Catalysis Project: focusing on CO2 reduction, nitrogen reduction, and water splitting

Michal Bajdich, SLAC National Accelerator Lab

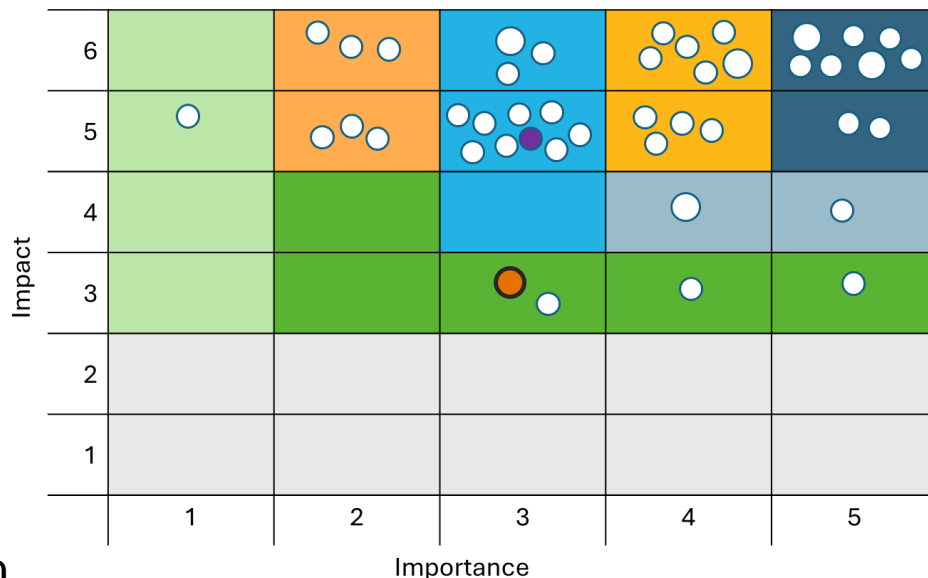
## • Summary Description

- Electrocatalysis, thermal catalysis, and application of machine learning and AI.
- Development of an iridium-based catalyst for water splitting, crucial for enabling a hydrogen economy.

## • Impact to the World

- The iridium catalyst, optimized through computational methods, showed exceptional performance in transforming oxygen from water.
- Demonstrated the highest activity among iridium catalysts.
- Led to a collaboration with the largest hydrogen electrolyzer in the US.

| Office                |                      | Program  |                 |                   | Category             |
|-----------------------|----------------------|--|-----------------|-------------------|----------------------|
| Basic Energy Sciences |                      | Chemical Sciences, Geosciences, & Biosciences (CSGB) |                 |                   | Chemistry: Catalysis |
| Advances Science      | Advances Engineering | Saving Lives   | Economic Growth | National Security |                      |
| x                     | x                    |  |                 |                   |                      |



# First Principles Simulations of Nanostructures: to study matter at the atomic level

*Guilia Galli, University of Chicago*

- **Summary Description**

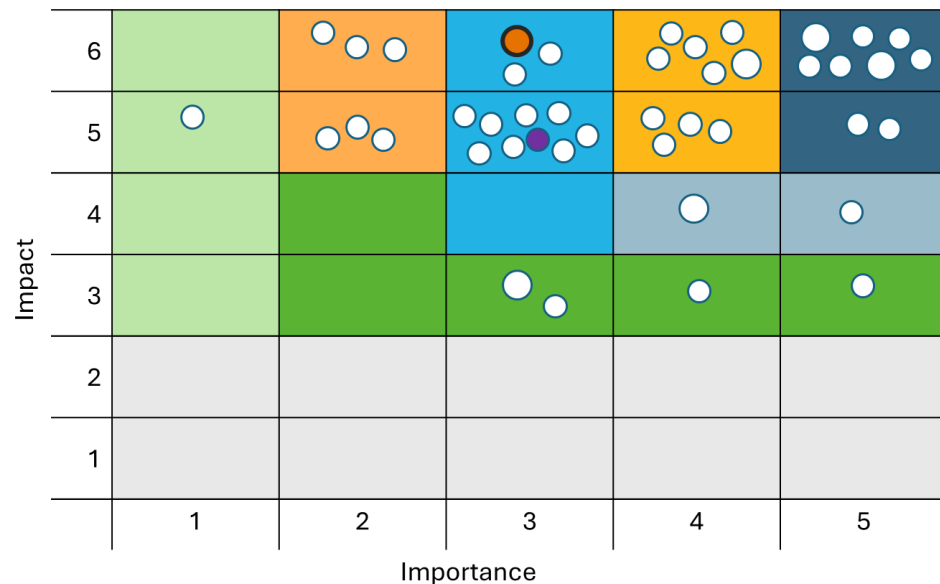
- Simulating materials at the quantum mechanical level to identify and design materials with properties suitable for quantum applications
- Development of more efficient materials for energy harvesting and conversion.

- **Impact to the World**

- Contribute to more powerful computers, ultra-sensitive sensors, and secure communication systems
- Potential to accelerate the transition to clean energy technologies and reduce reliance on fossil fuels.

| Office       | Program                            | Category                   |
|--------------|------------------------------------|----------------------------|
| Basic Energy | Materials Sciences and Engineering | Materials Science: General |

| Advances Science | Advances Engineering | Saving Lives | Economic Growth | National Security |
|------------------|----------------------|--------------|-----------------|-------------------|
| x                | x                    |              |                 |                   |



# From Molecules to Continuum: Developing a Universal Approach for Accurate Description of X-ray Photo: for nanoscale phenomena

Jin Qian, Lawrence Berkeley National Lab (LBNL)

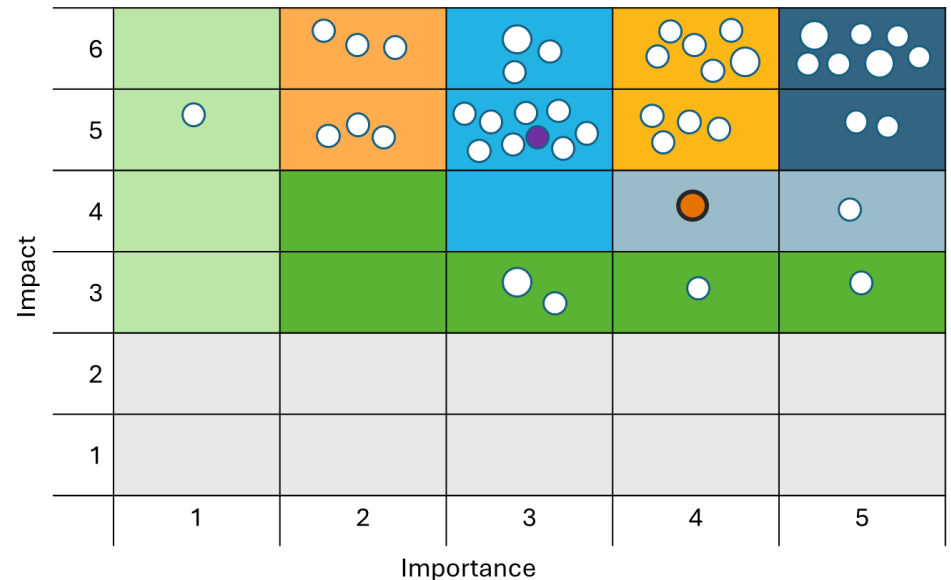
## • Summary Description

- Developing tools to predict spectroscopic signatures, particularly X-ray Photo Electron Spectroscopy (XPS), for nanoscale phenomena
- using a specialized form of Density Functional Theory (DFT) called real space Kohn-Sham DFT.

## • Impact to the World

- Achieved simulation of systems with 10,000s of atoms, up from 100s prior.
- Addressing chemistry and material science problems, with potential applications in catalysis and battery research.

| Office                |                      | Program   |                 | Category                    |  |
|-----------------------|----------------------|---|-----------------|-----------------------------|--|
| Basic Energy Sciences |                      | Chemical Sciences, Geosciences & Biosciences (CSGB) |                 | Chemistry: Chemical Physics |  |
| Advances Science      | Advances Engineering | Saving Lives  | Economic Growth | National Security           |  |
| x                     | x                    |   |                 |                             |  |

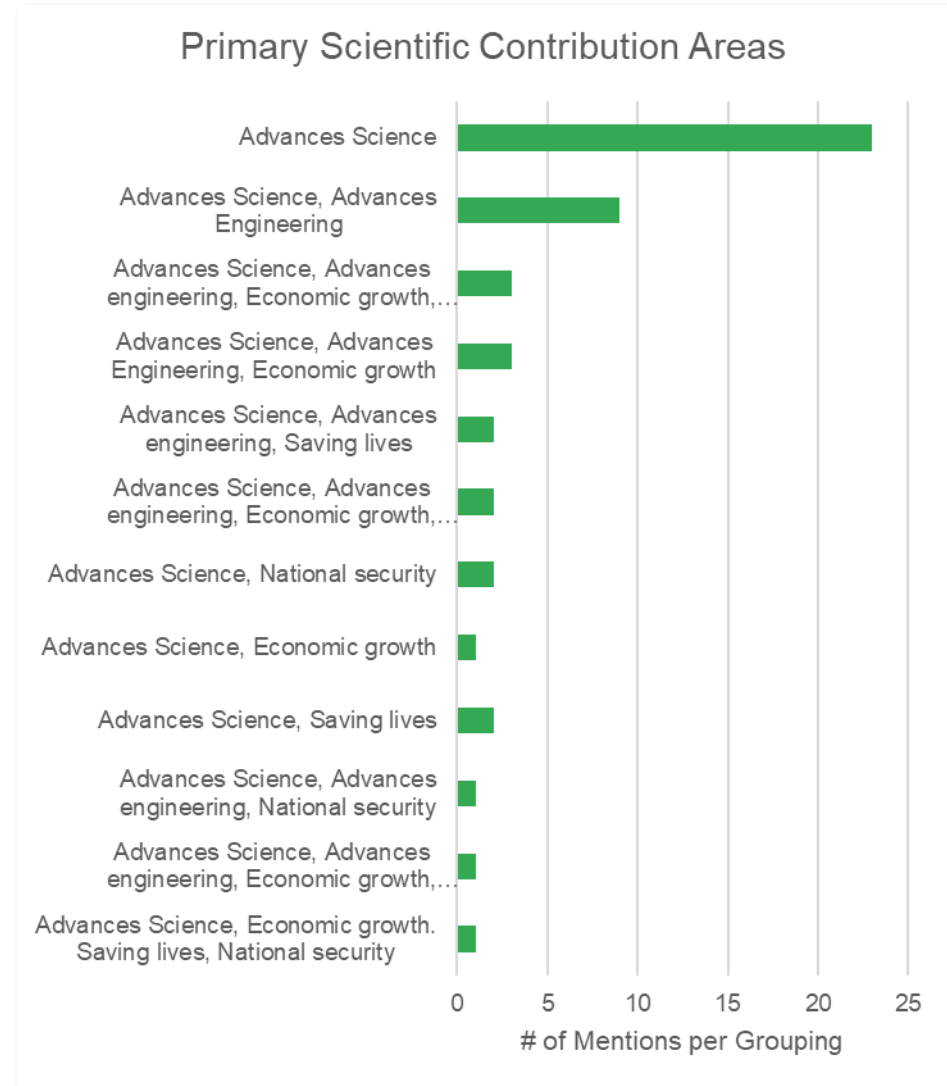
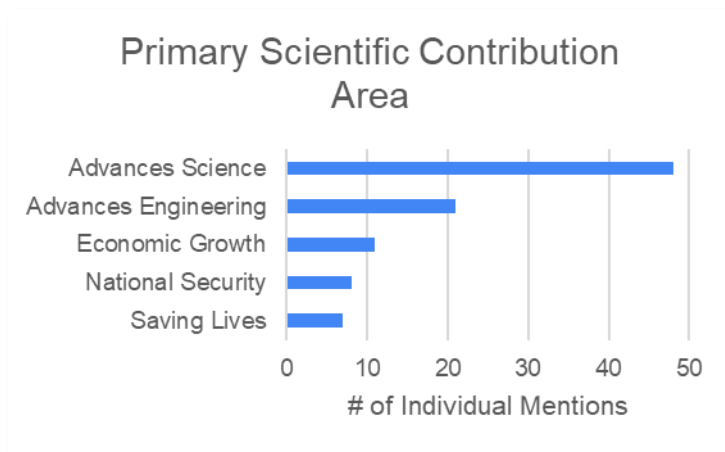


# Other Findings

# Primary Scientific Contribution Area

*“Advances Science” was the predominant area*

- **Q: Which of the following areas best describes the primary scientific contribution of your research (select all that apply):**
  - Advances Science
  - Advances Engineering
  - Economic Growth
  - Saving Lives
  - National Security

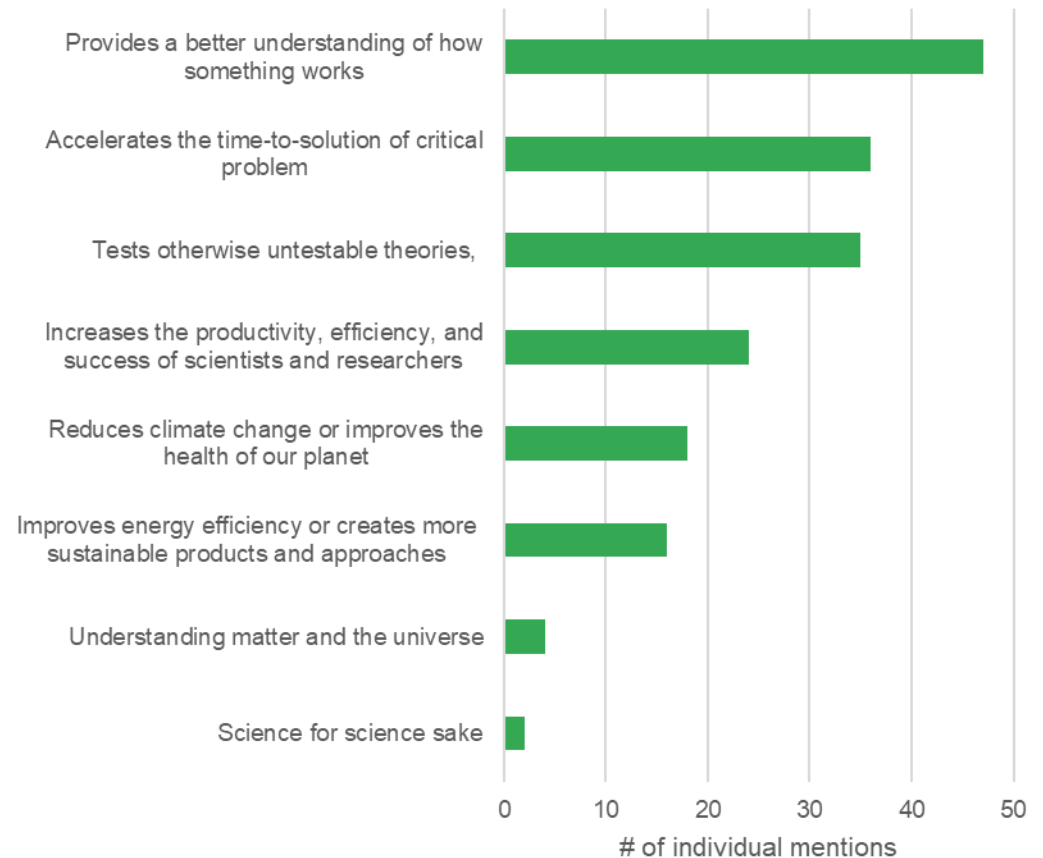


# Primary Research Outcomes for Advancing Science

*“Providing a better understanding of how something works” was the top Advancing Science outcome*

- **Q: Which of the following best reflects the outcome of your research: (select all that apply)**
  - Provides a better understanding of how something works
  - Accelerates the time-to-solution of critical problem
  - Tests otherwise untestable theories,
  - Reduces climate change or improves the health of our planet
  - Improves energy efficiency or creates more sustainable products and approaches
  - Increases the productivity, efficiency, and success of scientists and researchers
  - Other (please specify)
- **Other:**
  - Understanding matter and the universe
  - Science for science's sake

Primary Research Outcomes for Advancing Science

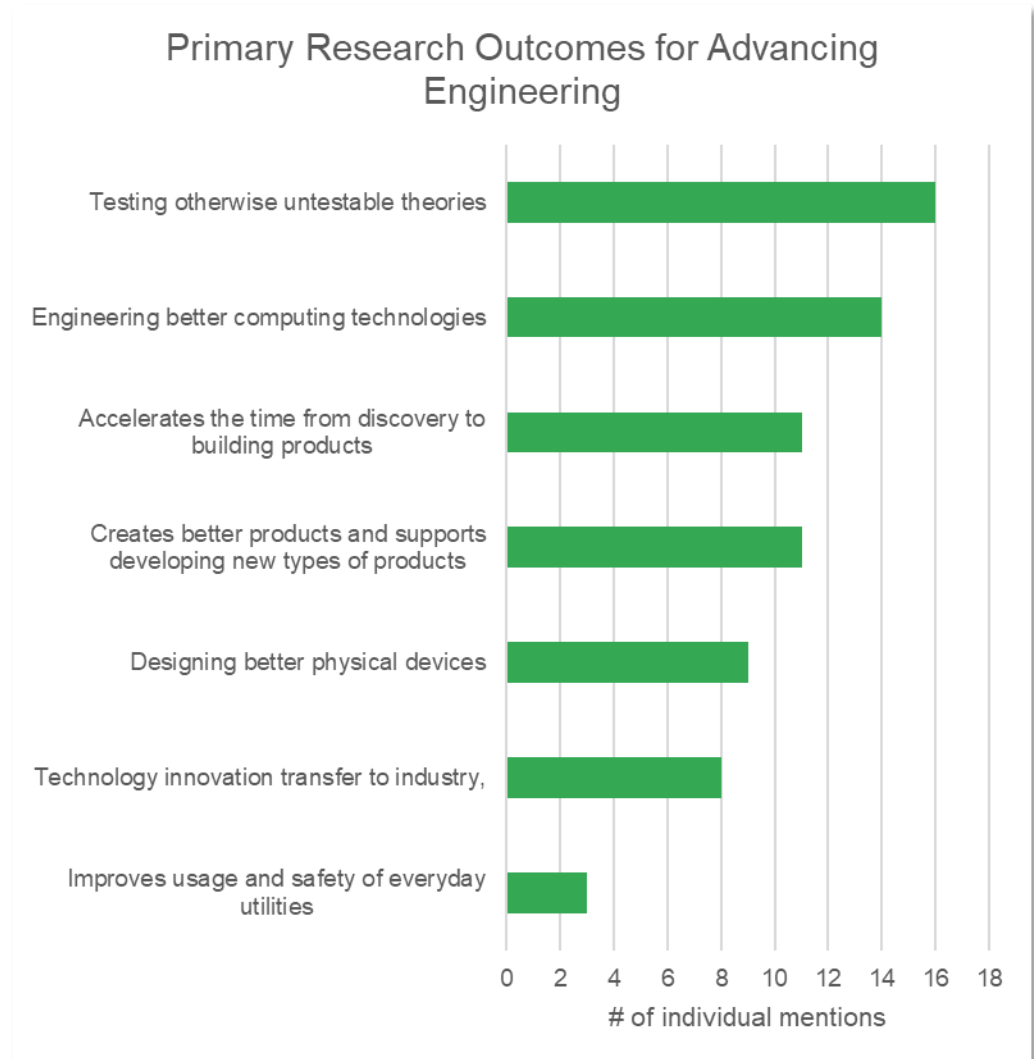




# Primary Research Outcomes for Advancing Engineering

*“Testing otherwise untestable theories” was the top Advancing Engineering outcome*

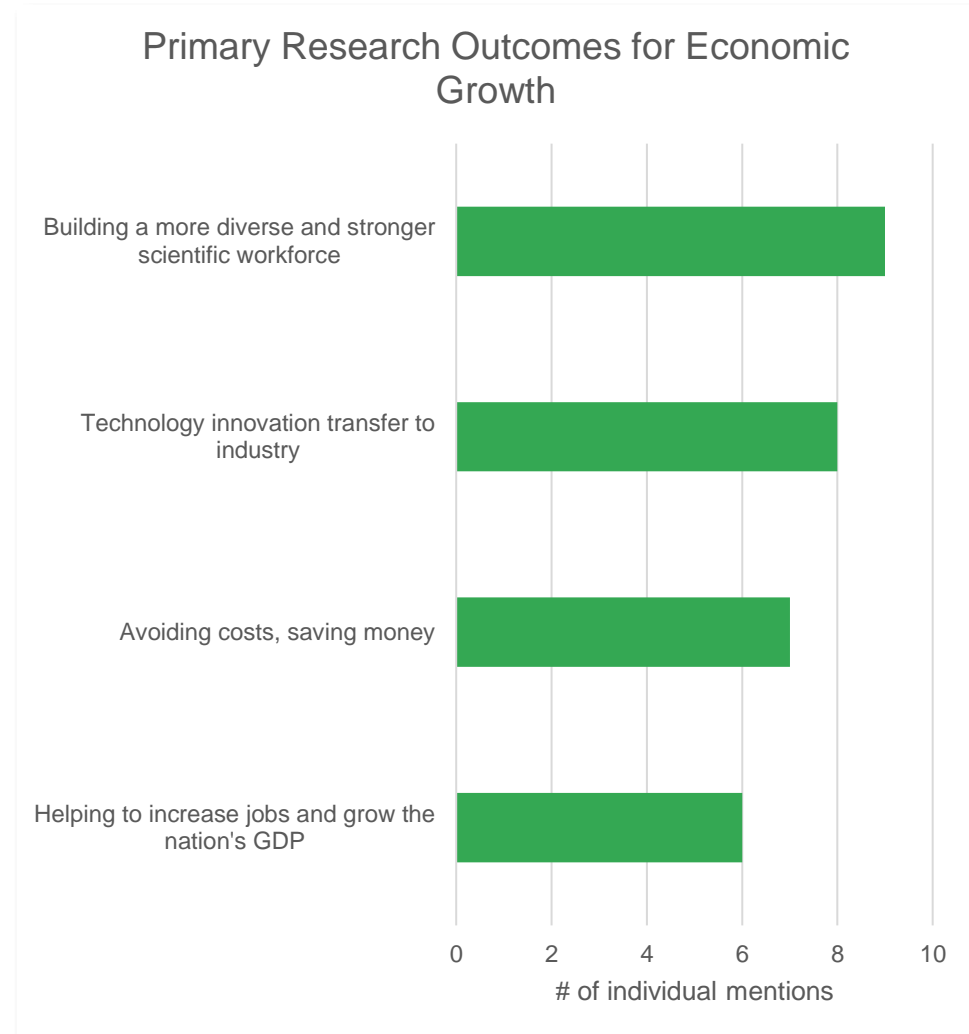
- **Q: Which of the following best reflects the outcome of your research: (select all that apply)**
  - Creates better products and supports developing new types of products
  - Designing better physical devices
  - Accelerates the time from discovery to building products
  - Testing otherwise untestable theories
  - Technology innovation transfer to industry
  - Engineering better computing technologies
  - Improves usage and safety of everyday utilities



# Primary Research Outcomes for Economic Growth

*“Building a more diverse and stronger scientific workforce” was the top Economic Growth outcome*

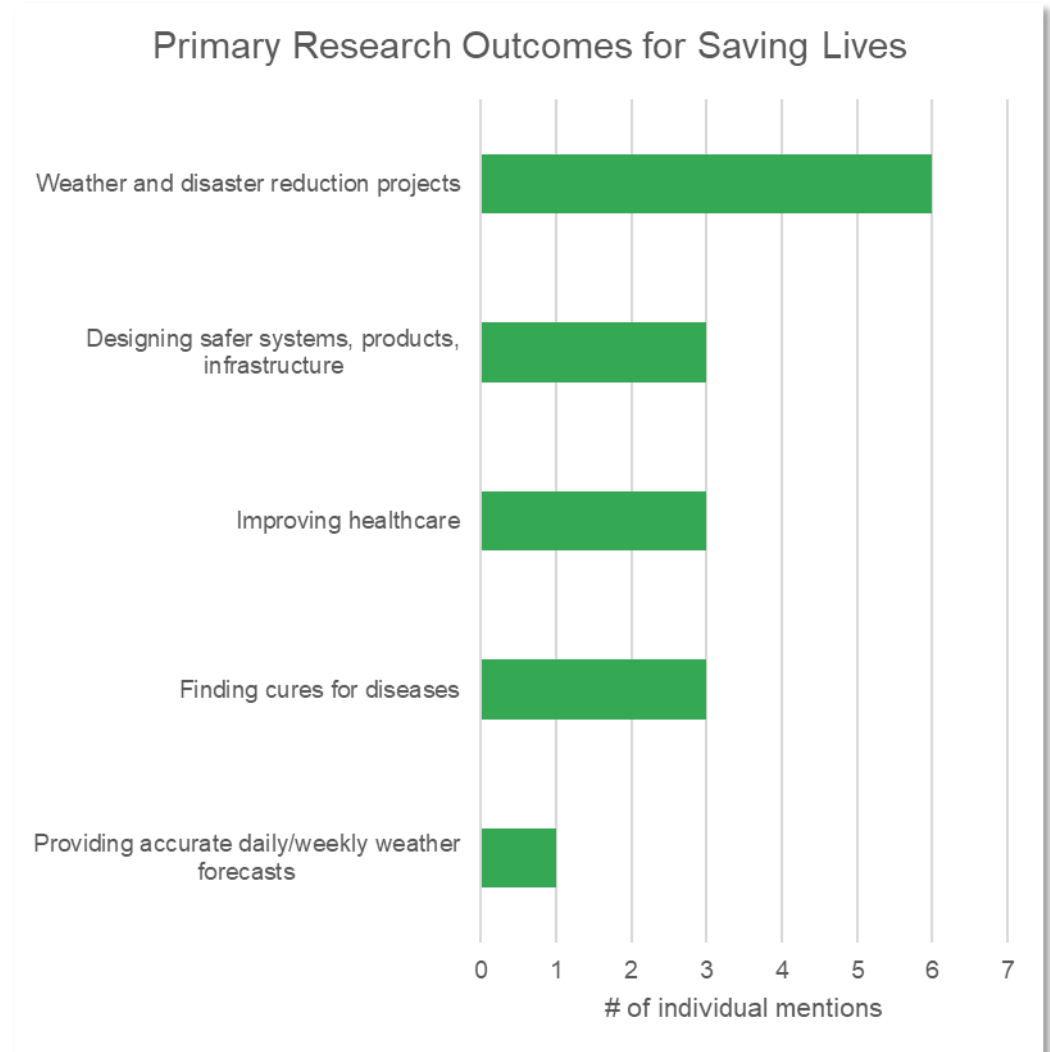
- **Q: Which of the following best reflects the outcome of your research: (select all that apply)**
  - Helping to increase jobs and grow the nation’s GDP
  - Technology innovation transfer to industry
  - Avoiding costs, saving money
  - Building a more diverse and stronger scientific workforce



# Primary Research Outcomes for Saving Lives

*“Weather and disaster reduction projects” was the top Saving Lives outcome*

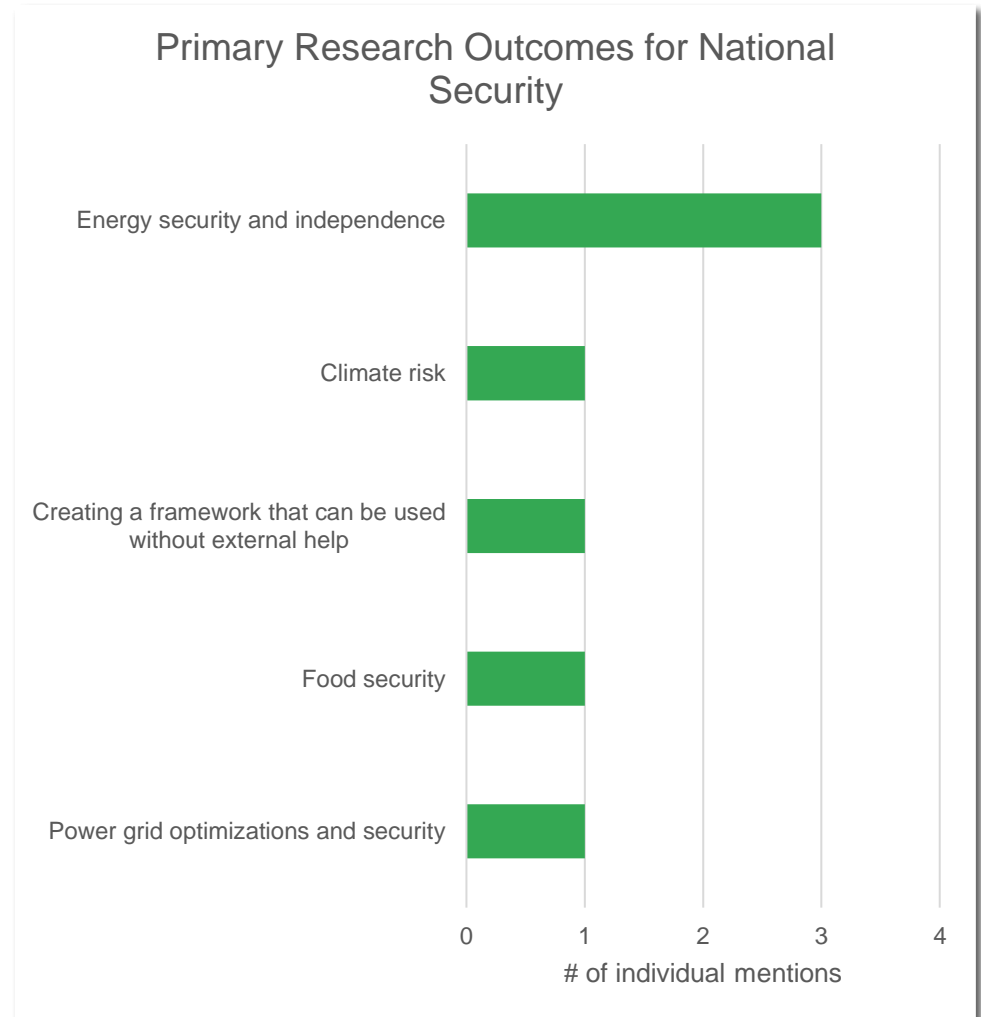
- **Q: Which of the following best reflects the outcome of your research: (select all that apply)**
  - Weather and disaster reduction projects
  - Finding cures for diseases
  - Providing accurate daily/weekly weather forecasts
  - Improving healthcare
  - Designing safer systems, products, infrastructure



# Primary Research Outcomes for National Security

*“Energy security and independence” was the top National Security outcome*

- **Q: Which of the following best reflects the outcome of your research: (select all that apply)**
  - Creating a framework that can be used without external help
  - Improvements in cybersecurity, making AI safer, tracking bad players
  - Other
- **Other**
  - Climate risk
  - Energy security and independence
  - Food security
  - Power grid optimizations and security



# NERSC Utilization

# Computationally Demanding Scientific Workloads Require NERSC

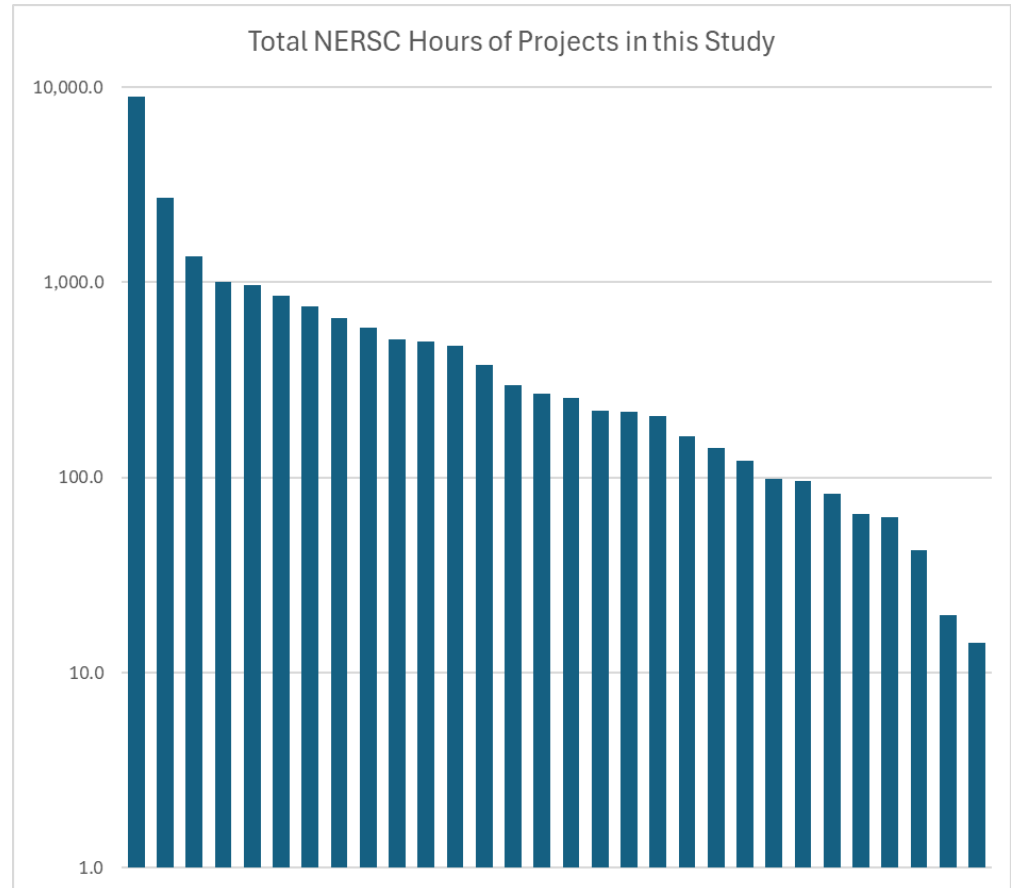
*Surveyed 42 projects consume on average 20% of “NERSC” hours*

- **What is a NERSC hour?**
  - Normalized utilization metric for computational usage
  - Allows comparison across time and architectures
  - Example: if a project used 1/365 of all the hours available at NERSC, then it would get credit for 24 NERSC Center Hours (1 day)
- **Current snapshot of total NERSC utilization**
  - > 10,000 users
  - > 1,000 projects
- **Study participant utilization**
  - 42 projects or “users”
  - Average NERSC hours of all projects would consume almost 20% of total NERSC hours

# NERSC Hour Utilization for Included Research

*Includes utilization across multiple years*

- **Projects ranged from 3-24 years, with many still in progress**
- **Top 3 included projects:**
  - Advanced Simulation of Pore Scale Flow and Transport Processes in Nanoporous Materials (Trebotich)
  - Computational Studies in Plasma Physics and Fusion Energy (Howard)
  - Quarkonia in Hot Medium (Petreczky)



# Quotes from Researchers

| Quote   | Attribution  |
|---|--|
| <i>The insights we gained into multi-scale turbulence in fusion plasmas would not have been possible without the use of NERSC resources.</i>  | Nathan Howard, a Fusion Energy researcher from MIT Plasma Science and Fusion Center      |
| <i>NERSC is an extremely valuable resource for researchers supported by the DOE because it's accessible for any researcher. Continuous access to HPC resources is critical and they provide extremely good support. I really like to work with NERSC and without them, the research would not have been possible.</i> | A researcher from Brookhaven National Lab  |
| <i>NERSC is best partner for energy science. I'm very happy with the NERSC allocation process and continued support over the years.</i>   | A research from SLAC National Accelerator Lab at Stanford                                |
| <i>The application process is nicely streamlined and pretty straightforward. We complement NERSC for making a system that is not a huge burden on users.</i>  | Alexander Austregesilo, a researcher from Thomas Jefferson National Accelerator Facility |
| <i>Our experience with NERSC has been very positive and the impact of NERSC on our scientific research has been critical; without NERSC, our publications would not have been possible.</i>   | A research from University of Chicago  |
| <i>We appreciate what a super-efficient organization NERSC is for supporting world-class research. It's amazing to see how such a complex enterprise can facilitate world-class research. It's a real jewel for the computational sciences and engineering community.</i>   | Manos Mavrikakis, a Chemical Engineering researcher                                      |



# Quotes from Researchers (continued)

| Quote  | Attribution  |
|--|--|
| <i>NERSC will remain a really important resource for us.</i>   | Ruby Leung, an Earth Systems researcher from PNNL                                |
| <i>NERSC provides very powerful and accessible capabilities for research, successful support for using the machines, and is a very effective place to work.</i>  | A researcher from Columbia University  |
| <i>Perlmutter and NERSC have been a tremendous asset to our project both from the standpoint of code development on GPU systems as well as running large regional cases of ground motion and infrastructure response.</i>      | David McCallen a researcher from the Energy Geosciences Division at Berkeley Lab |
| <i>I cut my teeth in HPC on NERSC allocations that in retrospect helped to launch me as a computational astrophysicist.</i>  | Adam Burrows a researcher from Princeton   |
| <i>I am beyond grateful - we honestly could not have done this research without NERSC.</i>   | A researcher from ORNL   |
| <i>I am extremely grateful for the support provided by NERSC. Much of what we have done would not have been possible.</i>  | Puru Jena, a Chemical Physics researcher from Virginia Commonwealth University   |
| <i>What makes NERSC different from other global HPCs, it's not run just as a research facility but is the easiest to use. Documentation is excellent and support is good. It's HPC being run with the researchers in mind.</i> | Paolo Calafiura, a researcher from LBNL  |

# Quotes from Researchers (continued)

| Quote  | Attribution  |
|--|--|
| <i>NERSC has been a stable computing platform for my entire career and has been phenomenal in terms of consistency and increasing capabilities.</i>  | Stephen Jardin, a Fusion researcher from the Princeton Plasma Physics Laboratory |
| <i>I cannot overstate how important NERSC has been to my career and my research. From establishing the research, performing the work, and providing training, NERSC has been invaluable to my career. It's such a well-run organization and a pleasure to work with.</i>   | Eddie Baron, an Astrophysics researcher from the University of Oklahoma          |
| <i>NERSC by far, of all the HPC resources used in conjunction with this research, has the best infrastructure and the most responsive staff. The research couldn't have been done without NERSC.</i>   | Diana Qiu, a physics researcher from Yale  |
| <i>By far NERSC is the best HPC resource I've worked with for my research in terms of on-line documentation, performance of the computing systems and the unbelievable staff who provide help whenever I need it - and they do it quickly. I've never had to wait more than half a day to get some problem resolved.at NERSC</i> | Masao Sako, a cosmology physics researcher from University of Pennsylvania       |
| <i>NERSC has constantly provided incredibly useful resources and support to my research in climate modeling and analysis for the past 15 years</i>   | Hailong Wang, an Earth Scientist from PNNL                                       |
| <i>I had a great experience with NERSC. NERSC has enabled research that I couldn't do anywhere else. I'm a big fan of NERSC.</i>   | Anonymous  |

# Constructive feedback (paraphrased)

- **Sometimes difficult to identify and connect with correct researcher for support on how to get older Fortran codes re-compiled to run on GPUs**
- **Difficulty managing queue time (which can be up to a week) to run multi-day jobs, and then wait up to another week to re-run**

# The Next 50 Years...



**...looking forward to what a century's worth of NERSC accomplishments and impact!**

# Questions?

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