

OSTI Update to ASCAC – Moving Toward a More “Unified” Scientific Record: Software, Data, Publications



U.S. DEPARTMENT OF
ENERGY

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Science



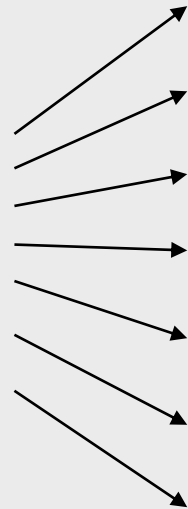
Brian Hitson, Director

December 21, 2017

DOE Invests \$12B per Year in R&D

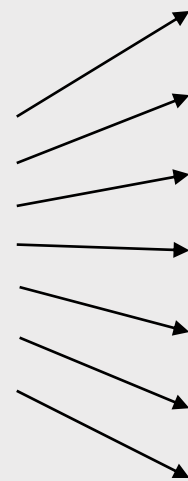


U.S. DEPARTMENT OF
ENERGY
R&D Funding



NATIONAL LABS

Ames
Argonne
Brookhaven
Fermi
Idaho
Los Alamos
Lawrence Berkeley
Lawrence Livermore
NETL
NREL
Oak Ridge
Pacific Northwest
Princeton
SLAC
Sandia
Savannah River
Thomas Jefferson



SCIENTIFIC & TECHNICAL INFORMATION (STI/R&D Results)

Text

- Journal articles/accepted manuscripts
- Technical reports
- Conference papers
- Patents

Data

- Large and small datasets
- Images
- Visualizations

Software/Code

≥ 50,000 STI “products” annually

OSTI’s mission: make R&D results accessible and useful in the modern science landscape.

GRANTEES

Review of the ASCAC-STI Subcommittee Charge

- Are OSTI products and services best in class?
- What is the national and international standing of OSTI?
- In what areas must OSTI be a clear leader?
- Recommendations for OSTI's future direction.

ASCAC established STI Subcommittee in early 2015, chaired by Dr. Tony Hey. ASCAC-STI Subcommittee performed on-site review and issued report (May-Sept. 2015).

Summary of Subcommittee Answers and Recommendations

- OSTI products have a number of “best in class” capabilities
 - SciTech Connect’s semantic search
 - Data ID Service (providing DOIs for datasets)
 - ScienceCinema’s speech indexing for multimedia
 - Federated search engines Science.gov and WorldWideScience.org
 - NOT best in class: Energy Science and Technology Software Center
- OSTI’s “standing” nationally and internationally
 - “OSTI is in a leadership position among Federal agencies”
 - “OSTI services employ a range of innovative technologies not uniformly available from their peer international scientific information organizations”
- OSTI must be a clear leader in providing public access to DOE-funded scholarly publications

Summary of Subcommittee Answers and Recommendations (cont'd)

- While there is significant uptake of OSTI services by the public and commercial services, OSTI needs to have a better understanding of researcher needs and should “initiate a vigorous outreach program with the DOE Lab researchers.”
- OSTI needs to “re-invent the ESTSC software service.”
- OSTI should continue to work “toward a unified user environment with a limited number of clearly delineated, non-redundant tools.”
- DOE and OSTI need to effectively implement public access, address publication content gaps, and incentivize labs and grantees to support DOE’s Public Access Plan.
- The Office of Science should consider “defining a useful role for OSTI . . . in managing DOE data.”

OSTI Actions and Progress

1. Outreach to DOE research community
 - Four lab workshops in 2016 (ORNL, BNL, SLAC, LBNL)
 - Data and software “roundtables” 2016-2017 (NREL and INL)
 - 9 software re-invention project requirements teams, comprising 51 lab and DOE stakeholders
 - Data ID Service workshops at SLAC (2016) and OSTI (2017)
 - Workshop scheduled at LLNL in March 2018

Feedback incorporated to develop product roadmaps and to improve Data ID Service, DOE Data Explorer, “unified” product features, and new software dissemination model.

OSTI Actions and Progress (cont'd)

2. Reinvent the Energy Science and Technology Software Center (ESTSC) service – DOE's software submission and dissemination tool
 - × Not comprehensive
 - × Not modern
- Defined requirements for a reinventing ESTSC, incorporating feedback from DOE researchers, developers, policy, legal, and technical communities – in all, 9 requirements teams
- Renamed DOE CODE – (launched November 2017) open source code and requirements posted to GitHub.



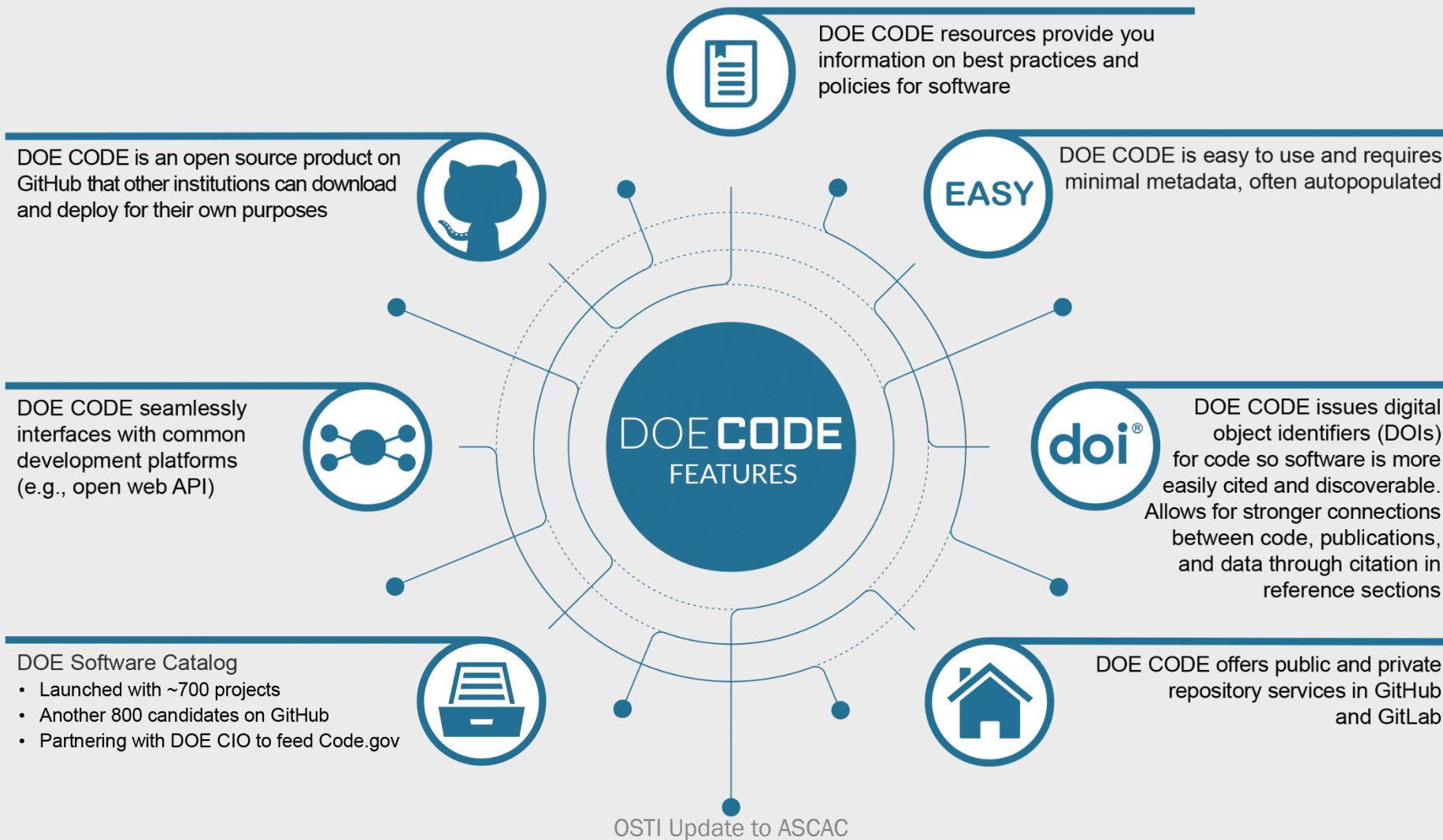
DOE CODE repository on GitHub

◦ github.com/doecode/

DOE CODE landing page

◦ www.osti.gov/doecode/

DOE CODE



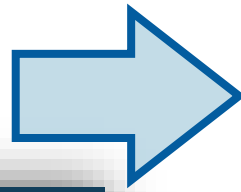
OSTI Actions and Progress (cont'd)

3. Toward a unified user environment

- Product streamlining and consolidation
 - Consolidated/eliminated 10 standalone web products since 2014
 - January 2018 consolidation of OSTI.gov website and umbrella product SciTech Connect to make OSTI.gov synonymous with search of DOE R&D results.



OLD



NEW

The old website features a dark blue header with the U.S. Department of Energy logo and navigation links for 'Office of Science' and 'Office of Scientific and Technical Information'. A search bar is located in the top right. Below the header is a navigation menu with links for 'HOME', 'ABOUT OSTI', 'SCIENCE SEARCH TOOLS', 'DOE PAGES / PUBLIC ACCESS', 'COMMUNICATIONS', and 'DOE STI PROGRAM'. The main content area has a large search bar with the text 'Find DOE R&D Results' and a red 'GO' button. Below the search bar, it says 'SciTech Connect'. A section titled 'DOE Scientific and Technical Information...and more' contains two featured tiles: 'SciTech Connect' and 'DOE PAGES' (Public Access Gateway for Energy & Science).

The new website has a clean, modern design with a blue background. It features the OSTI.GOV logo and the U.S. Department of Energy logo. A search bar at the top right contains the text 'Search 2.9+ million Department of Energy research results'. Below the search bar is a grid of icons for 'Submit Research Results', 'Search Tools', 'Public Access Policy', 'Data Services & Dev Tools', 'About', 'FAQs', and 'News'. The footer includes the U.S. Department of Energy logo and navigation links for 'Website Policies / Important Links', 'Contact Us', and social media icons for Facebook, Twitter, Google+, and YouTube.

OSTI Actions and Progress (cont'd)

3. Toward a unified user environment

- Product streamlining and consolidation
 - Consolidated/eliminated 10 standalone web products since 2014
 - January 2018 consolidation of OSTI.gov website and umbrella product SciTech Connect to make OSTI.gov synonymous with search of DOE R&D results
- Improved product features responsive to researcher feedback

Nudged-elastic band method with two climbing images: Finding transition states in complex energy landscapes

Article Details

References: 9

Cited by: 9

Reference / Citation Traversal

The nudged-elastic band (NEB) method is modified with concomitant two climbing images (C2-NEB) to find a transition state (TS) in complex energy landscapes, such as those with a serpentine minimal energy path (MEP). If a single climbing image (C1-NEB) successfully finds the TS, then C2-NEB finds it too. Improved stability of C2-NEB makes it suitable for more complex cases, where C1-NEB misses the TS because the MEP and NEB directions near the saddle point are different. Generally, C2-NEB not only finds the TS, but guarantees, by construction, that the climbing images approach it from the opposite sides along the MEP. In addition, C2-NEB provides an accuracy estimate from the three images: the highest-energy one and its climbing neighbors. C2-NEB is suitable for fixed-cell NEB and the generalized solid-state NEB.

Authors: Zarkevich, Nikolai A. ^[1]; Johnson, Duane D. ^[2]

[+ Show Author Affiliations](#)

Publication Date: 2015-01-09

Report 4. Nudged-elastic band method with two climbing images: Finding transition states in complex energy landscapes

Zarkevich, Nikolai A.; Johnson, Duane D. January 2015 - American Institute of Physics (AIP)

The nudged-elastic band (NEB) method is modified with concomitant two climbing images (C2-NEB) to find a transition state (TS) in complex energy landscapes, such as those with a serpentine minimal energy path (MEP). If a single climbing image (C1-NEB) successfully finds the TS, then C2-NEB finds it too. Improved stability of C2-NEB makes it suitable for more complex cases, where C1-NEB misses the TS because the MEP and NEB directions near the saddle point are different. Generally, C2-NEB not only finds the TS, but guarantees, by construction, that the climbing images approach it from the opposite sides along the MEP. [more »](#)

 Cited by 9

[Full Text Available](#)

Publisher: American Institute of Physics (AIP)

REFERENCES: 9

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Zarkevich, Nikolai A.; Johnson, Duane D.
PHYSICAL REVIEW B 2014

A generalized solid-state nudged ...

Sheppard, Daniel; Xiao, Penghao; ...
JOURNAL OF CHEMICAL PHYSICS 2012

Crystal structures and shape-me...

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Nudged-elastic band method with two climbing images: Finding transition states in complex energy landscapes

Zarkevich, Nikolai A.; Johnson, Duane D.
JOURNAL OF CHEMICAL PHYSICS 2015

10.1063/1.4905209

< 9 references

9 citing articles >

CITED BY: 9

Reliable and Efficient Reaction Pa...

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JOURNAL OF COMPUTATIONAL C... 2017

Potential Energy Surface-Based A...

Satoh, Hiroko; Oda, Tomohiro; Nak...
JOURNAL OF CHEMICAL THEORY ... 2016

Free-end adaptive nudged elastic ...

Zhang, Jiayong; Zhang, Hongwu; Y...
JOURNAL OF CHEMICAL PHYSICS 2016

10.1063/1.4905209

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Citation Impact by Journal:	2.49
Citation Impact by Field:	1.95
% Rank by Field / Year:	10.96

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Modern Science Demands Reproducibility

End state goal: interlink all related research outcomes (e.g., from publication to related data to related software).

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OSTI.GOV / Journal Article: An architecture for consolidating multidimensional time-series data onto a common coordinate grid

An architecture for consolidating multidimensional time-series data onto a common coordinate grid

Full Record References (5) Cited by (0) Reference / Citation Traversal Similar

JOURNAL ARTICLE:

Free Publicly Available Full Text
Accepted Manuscript (Publisher)

Publisher's Version of Record at
10.1007/s12145-016-0285-z

Copyright Statement

RELATED DATASETS:

ARM: Surface Radiation Measurement Quality Control testing, including climatologically configurable limits

RELATED SOFTWARE:

ARM Data Integrator

OTHER AVAILABILITY

Search WorldCat to find libraries that may hold this journal

Abstract

In this paper, consolidating measurement data for use by data requires transforming the data onto a common grid. Standard are often not appropriate for data with non-homogenous dimensions for different datastreams. In addition, these challenges procedures necessary for use with continuous, operational applying a series of one-dimensional transformations to measurement of ensuring consistent application of data consolidation methods challenges, and describe the implementation of such a framework (ARM) program.

Authors: Shippert, Tim [ORCID]; Gaustad, Krista [ORCID]
+ Show Author Affiliations

Publication Date: 2016-12-16

Research Org.: Pacific Northwest National Lab. (PNNL), Richland, WA (United States)

Sponsoring Org.: USDOE Office of Science (SC), Biological and Environmental Research (BER) (SC-23)

OSTI Identifier: 1336507

OSTI Update to ASCAC

ARM DATA DISCOVERY

CLIMATE RESEARCH FACILITY

HOME DATA SEARCH DATASTREAM SEARCH

SEARCH

Search Text:

Start Date: End Date:

[Expand All] [Close All] Clear » Apply »

CATEGORIES

Radiometric 217

DATASTREAMS 31

SUBCATEGORIES 2

MEASUREMENTS 6

SITES 13

FACILITIES 31

DATA LEVELS 1

SOURCE 1

DATA PRODUCTS 1

1996-10-01 2015-12-01 Applies to this time

Showing 1-20 of 217 measurements

	1997	1998	1999	2000	2001	2002
acrad1long c1 @ nsa C2 // Surface Radiation Measurement Quality Control						
★1 Shortwave broadband total downwelling irradiance // Best Estim						
★1 Longwave broadband downwelling irradiance // Downwelling Li						
acrad1long c1 @ mao M1 // Surface Radiation Measurement Quality Control						
★1 Shortwave broadband total downwelling irradiance // Best Estim						
★1 Longwave broadband downwelling irradiance // Downwelling Li						
acrad1long c1 @ nim M1 // Surface Radiation Measurement Quality Control						
★1 Shortwave broadband total downwelling irradiance // Best Estim						
★1 Longwave broadband downwelling irradiance // Downwelling Li						
acrad1long c1 @ fkb M1 // Surface Radiation Measurement Quality Control						
★1 Shortwave broadband total downwelling irradiance // Best Estim						
★1 Longwave broadband downwelling irradiance // Downwelling Li						

ARM-DOE / ADI

Code Issues (1) Pull requests (0) Projects (0)

ARM Data Integrator

57 commits 1 branch 0 releases 2 contributors

Branch: master New pull request Find file Clone or download

kgaustad Update README.md Latest commit a36e98 on Apr 13

File	Commit	Time
ADI_source.zip	clean up	2 years ago
LICENSE	clean up	2 years ago
README.md	Update README.md	8 months ago
Vagrantfile	weituos modification	a year ago

ADI

ARM Data Integrator, ADI, is an open source framework that automates the process of retrieving and preparing data for analysis, simplifies the design and creation of output data products produced by the analysis, and provides a modular, flexible software development architecture for implementing algorithms. These capabilities are supported through the use of a workflow for data integration, a source code generator that produces C, IDL and Python templates, and a graphical interface through which users can efficiently define their data input, preprocessing, and output characteristics.

OSTI Actions and Progress (cont'd)

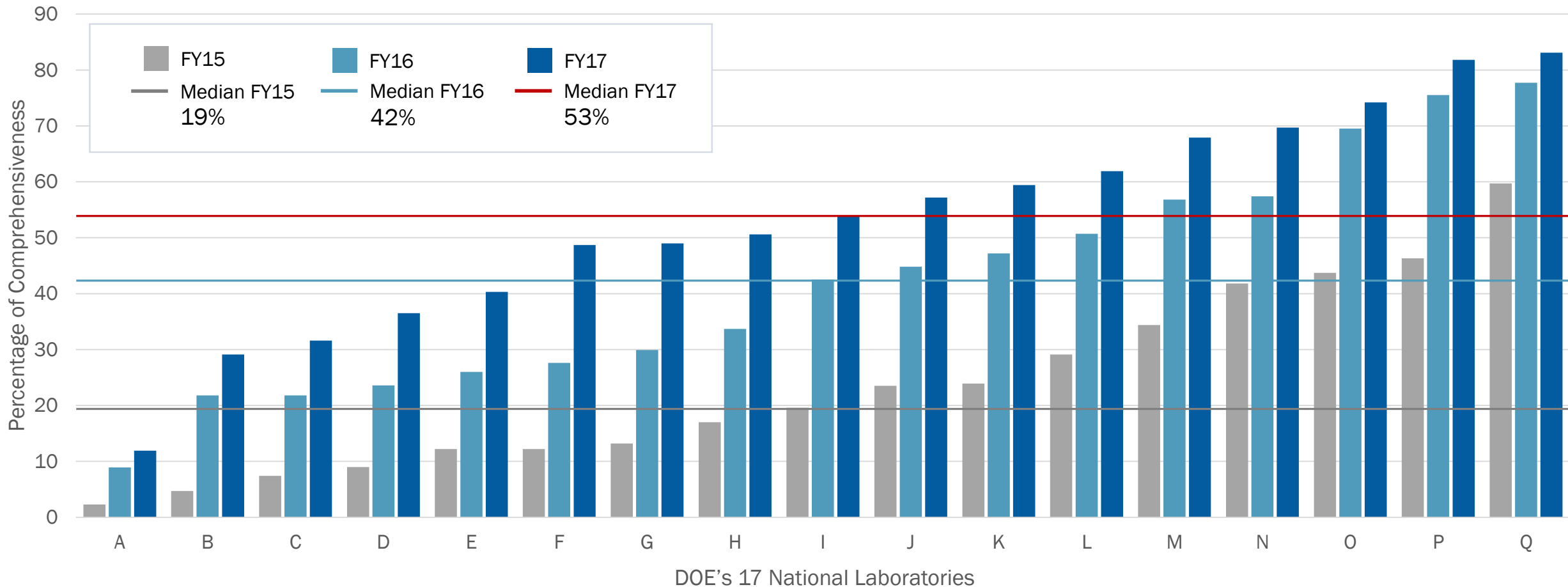
4. Effectively implement public access
 - Address publication content gaps. OSTI uses Web of Science to establish “denominator” for articles authored by lab researchers, and labs collect accepted manuscripts.
 - Incentivize labs and grantees to support DOE public access efforts. SC and all DOE program offices established public access as a measurable in labs’ annual performance plans.



<https://youtu.be/mZky964Lef8>

Public Access Progress

Lab Comprehensiveness



OSTI Actions and Progress

5. OSTI's role in DOE's data landscape
 - Primary contribution is the DOE Data ID Service:
 - Enabled by OSTI's membership in DataCite
 - Issued >70,000 DOIs to 21 DOE data clients
 - Makes datasets discoverable through OSTI products and indexing by Google and other common search engines
 - OSTI also provides this service to 7 other federal agency data clients on cost-reimbursable basis
 - Implementing supplemental material submission with publications in 2018
 - Exploring image, graph, table extraction from publications. Investigating both automated and human curation techniques; possibly a candidate for machine learning
 - Workshop feedback identified needs for data repository services; DMP guidance and best practices; and hierarchical relationships among datasets

Conclusions

As a result of ASCAC-STI recommendations and support from SC and individual subcommittee members, OSTI:

- Initiated ongoing, active outreach efforts to DOE lab research community to inform product improvements;
- Modernized scientific software dissemination model with launch of DOE CODE;
- Further unified and streamlined OSTI product environment, moving toward increased interlinking of research objects;
- Increased DOE's comprehensiveness in providing public access to scholarly publications through DOE PAGES;
- Broadened the DOE Data ID Service to improve discoverability of DOE datasets.

OSTI appreciates SC and ASCAC support and is committed to continued progress.

Thank you,

Brian A. Hitson, hitsonb@osti.gov