

NSF 21-045

Dear Colleague Letter: Pilot Projects to Integrate Existing Data and Data-Focused Cyberinfrastructure to Enable Communitylevel Discovery Pathways

February 2, 2021

Dear Colleagues:

This Dear Colleague Letter (DCL) replaces NSF 20-085: DCL: Pilot Projects to Integrate Existing Data and Data-Focused Cyberinfrastructure to Enable Community-level Discovery Pathways.

Many research communities supported by the National Science Foundation (NSF) are challenged by the need to manage, integrate, access, and use ever larger and diverse scientific datasets to conduct research. NSF accordingly invests in the creation of a wide range of data-focused cyberinfrastructure (CI) tools, resources, and solutions for use by the various disciplinary communities that it supports in order to transform data into knowledge and discovery.

Scientific endeavors are increasingly collaborative, cross-disciplinary, and convergent. NSF thus recognizes the importance of promoting holistic CI approaches to address the growing and evolving data lifecycle and workflow challenges both within and across research fields. This holistic view is articulated in NSF's recent vision¹ for an *agile CI ecosystem*, and is predicated on harmonization, integration and interoperability among CI resources, tools, services and expertise to achieve accessible, seamless and flexible end-to-end discovery pathways that drive new thinking and enable transformative discoveries.

Through this Dear Colleague Letter (DCL), NSF encourages proposals to the Cyberinfrastructure for Emerging Science and Engineering Research (CESER) program² within the Office of Advanced Cyberinfrastructure for **pilot** projects that bring together researchers and CI experts to develop the means of combining existing community data resources and shared data-focused CI into new integrative and highly performing data-intensive discovery workflows that empower new scientific pathways. Aims of such pilot

projects can include, but are not limited to:

- improving the end-to-end process of accessing, integrating and transforming research and education data to knowledge and discovery for one or more communities;
- creating new workflows and new usage modes to address multi-disciplinary and crossdomain scientific objectives;
- addressing emerging community-scale scientific data challenges such as real-time, streaming and on-demand data access; data discovery through knowledge networks and intelligent data delivery; enabling access to data with privacy concerns; and data fusion, integration and interoperability;
- enhancing the performance and robustness of community-scale data integration and discovery workflows such as through automated curation, end-to-end performance monitoring, provenance tracking, and means of assuring data trustworthiness; and
- federating learner data to empower innovative assessment tools for large-scale modeling of learning gains.

NSF welcomes submissions of proposals for pilot projects that address one or more of these aims in **all areas of science and engineering (S&E) research and education supported by NSF**. Within this array of aims, NSF encourages proposers to address, where appropriate, community-scale scientific data challenges stemming from the ongoing pandemic, whether technical in nature or related to broadening participation by, and increasing benefit to, diverse audiences, including groups underrepresented and underserved in STEM. Proposals are particularly encouraged from minority-serving institutions. Proposals from organizations in Established Program to Stimulate Competitive Research (EPSCoR) jurisdictions are also particularly encouraged.

NSF also encourages proposals for pilots involving international collaborations and partnerships aimed to advance global scientific data integration and sharing in science and engineering research and education.

The following NSF directorates emphasize interest in specific topical areas for proposals:

- Directorate for Computer and Information Science and Engineering (CISE):
 Proposals are encouraged on enabling accessibility, integration, discovery,
 management and analysis of community-scale research data in support of identified
 science objectives or use cases, such as those related to wireless networking,
 cybersecurity, machine learning applications, and related performance monitoring and
 assessment. CISE particularly welcomes proposals that aim to enable community-scale
 integration of, and access to, data sets from individual investigators and/or those
 generated by industry to enable new research and discovery broadly for the CISE and
 other research communities.
- Directorate for Education and Human Resources (EHR): Proposals are encouraged

that bring together CI experts and STEM education researchers to explore approaches to merging fine-grained "digital footprints" of learner interaction within disparate digital educational resources, tools, and platforms into a federated suite of interoperable data repositories. Existence of such a federated system would enable deep probing of individual conceptual learning gains that can support both generalizable conclusions about populations of learners and the creation of personalized learning opportunities. Such a corpus of data, including assessments of learning gains, can also be leveraged to inform not only the improvement of existing educational resources and tools, but also the creation of new ones. Proposers are also encouraged to envision the creation of a services layer residing on top of the data.

• **Directorate for Geosciences (GEO)**: Proposals in the geosciences are encouraged to improve the accessibility of existing data in order to mitigate novel coronavirus 2019-(COVID-19-) related impacts on research. GEO recognizes that field and laboratory research has been delayed, modified and/or cancelled because of the pandemic creating significant challenges for the geosciences and the need to pursue other avenues for continuing research in these impacted areas. Projects will make data reuse possible and facile through the development and improvement of data infrastructure and workflows, including simpler formats, adoption of open source software and common standards. This is intended to maximize usage in the general scientific community for data that already exist but are not easy to access or integrate. Investigators will need to provide compelling scientific cases for any targeted data. Investigators will need to identify how students and early-career scientists will be involved in the work, what skills they will develop, and/or what community training will be available. Investigators supporting research in the areas covered by the Division of Atmospheric and Geospace Sciences, Office of Polar Programs, Division of Earth Sciences and Division of Ocean Sciences are welcome to submit.

Directorate for Mathematical and Physical Sciences (MPS):

The Division of Astronomical Sciences (AST) encourages proposals for pilot projects that will test a) approaches to common user-friendly interfaces optimized for data access and discovery by diverse inquiries, and b) ways to archive and curate the long tail of smaller value-added datasets. Innovative ideas in these and other areas are welcome, especially where they build on prior NSF support for astronomical data, software, and interfaces.

The Division of Materials Research (DMR) encourages proposals that bring together materials researchers and cyberinfrastructure specialists to identify and address scientific challenges that could be advanced through the innovative use of digital data, but for which barriers exist in combining existing data resources and data cyberinfrastructure into an effective data-intensive materials research approach. Data

resources and data-focused computational tools, including but not limited to, those supported through Cyberinfrastructure for Sustained Scientific Innovation (CSSI), together with Materials Innovation Platforms (MIP), National Facilities and Instrumentation (NaFI), Designing Materials to Revolutionize and Engineer our Future (DMREF) projects, Materials Research Science and Engineering Centers (MRSEC), and Partnerships in Research and Education in Materials (PREM), form a network of data resources and computational tools to support a broad range of research that utilizes digital data. DMR seeks to i) fill gaps that hinder the effective use of digital data and computation to engage challenging problems at the frontiers of materials research, including the discovery of new materials in concert with the goals of the Materials Genome Initiative, and ii) stimulate the creation of new workflows and paradigms that will lead to the effective use of digital data and computation to accelerate materials research and transform the way it is done. A successful proposal will address an important and potentially transformative materials research problem through the application of a data-intensive research approach; it will identify barriers to combining existing data resources and data cyberinfrastructure, which include resources within and possibly outside the network outlined above, it will develop missing cyberinfrastructure to forge an effective data-intensive research workflow, and engage the problem.

The Division of Chemistry (CHE) encourages proposals for pilot projects in response to this DCL that aim to explore the scientific and technical challenges facing big data standardization, storage, dissemination and repurposing in electrochemistry, including electrosynthesis, electrocatalysis, electrochemical sensor and battery development. The research areas in electrochemistry have seen growing interest in recent years for their potential in renewable energy, chemical manufacturing, environmental remediation and sensing. The large volumes and heterogeneity of data generated in experimental and computational design of electrode materials, catalysts, and synthetic pathways provide a natural testbed to develop data workflows and identify common needs across different areas for full-scale deployment of data-driven CI in chemistry. Proposals are welcome for data CI pilot projects in electrochemistry that can serve as an initial proving ground for the development of wider chemistry community data CI, and that address best practices and scalable approaches for areas including, but not limited to, acquisition, storage, accessibility, dissemination, transparency and openness applied to both legacy and new large-scale data. The successfully competed pilot projects will facilitate exploration of new research areas, reuse of legacy data for emerging applications, (re)evaluation of new and previous findings, and comparison of data with future models. In preparing their proposals, proposers are encouraged to consult the findings and recommendations from the 2017 NSF-funded workshop on Framing the Role of Big Data and Modern Data Science in Chemistry³ and the 2019 National Academies of Science, Engineering, and Medicine (NASEM) Workshop on Advances, Challenges, and Long-Term Opportunities of Electrochemistry: Addressing Societal Needs - A

Chemical Sciences Roundtable Workshop⁴.

- Directorate for Social, Behavioral and Economic Sciences (SBE): Proposals are encouraged that focus on CI tools, resources, and/or solutions related to any of the directorate's core programs. Example areas of emphasis include:
 - Combination of diverse brain data the collection of which varies in technology, methodology, and context – in order to make useable such data by a broader research community and to enable novel kinds of brain-behavior computational modeling.
 - Integration of heterogeneous human data neural, cognitive, behavioral, economic, spatial – in ways that foster large-scale behavioral modeling. This could also incorporate networking tools into many aspects of human data analysis, including population migration and disaster response.
 - Linkage among social, behavioral, or economic datasets in ways that accommodate the imputation of ambiguous or nonexistent metadata and address the tradeoff between privacy and accuracy. Because of the transient complexity of human behavior, solutions are needed to account for data aggregation when researchers are unable to make observations or perform experiments more than once under identical circumstances. Specific challenges for solution include identifying co-factors, specifying models, sampling strategies, checking robustness, triaging data, and drawing causal inferences.

Other NSF science and engineering directorates and offices not listed above (Directorate for Biological Sciences, Directorate for Engineering, Office of Integrative Activities,⁵ Office of International Science and Engineering) encourage proposals in any of the areas that they support.

Please note that the CESER program supports creation of CI for the benefit of research, but does not support activities aimed at conducting the targeted discovery-oriented research activities themselves including but not limited to creation of datasets or creation or maintenance of databases or repositories; proposers are discouraged from including these activities in their proposals beyond a limited degree of data collection that is necessary to verify the performance of the CI.

This DCL encourages proposals for exploratory pilot projects that specifically aim to integrate diverse existing scientific data sources and enable novel end-to-end discovery pathways through close collaboration of domain science researchers and CI experts and through sharing of approaches and solutions among the eventual supported projects (see below). This DCL is complementary to a number of existing disciplinary and cross-cutting NSF programs, such as the cross-cutting NSF CSSI program (https://www.nsf.gov/funding/pgm_summ.jsp?pims_id=505505), which support a wide range of data and software infrastructure projects, and which may be alternative

avenues for prospective proposers whose project ideas do not align with the crossdisciplinary and data-integration expectations of this DCL. Proposals previously submitted to, or otherwise designed for, those other CI programs may not be submitted to the CESER program in response to this DCL.

PI teams of successful proposals responding to this DCL should plan to engage regularly with one another, including attending one or more related workshops sponsored by NSF, to exchange approaches and envisaged solutions towards cross-domain harmonization and collective adoption of similar or compatible CI solutions.

HOW TO RESPOND TO THIS DCL

Proposers must follow the guidance and instructions provided under "GUIDANCE TO POTENTIAL PROPOSERS" in the CESER program description.

Per the CESER program description, in advance of submitting a proposal in response to this DCL, interested proposers are strongly encouraged to discuss their project idea with cognizant Program Directors in the CESER program and with the relevant NSF disciplinary research program(s). To initiate discussion of a project idea, prospective proposers are encouraged to send an email to CESERQueries@nsf.gov.

For planning purposes, projects funded through the CESER program are typically in the \$300,000 to \$1,500,000 budgetary range.

Proposals responsive to this DCL and received on or before March 23, 2021 will be considered for FY 2021 funding.

The proposal title should begin with "Data CI Pilot:"

Awards for projects responsive to this DCL will be funded through OAC's CESER program with co-funding from the relevant directorate/office programs.

Proposals that fail to address the objectives and guidance described in this DCL and in the CESER program description may be returned without review.

Questions should be directed to CESERQueries@nsf.gov; do not contact the signatories to this DCL.

Sincerely,

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REFERENCES

https://www.nsf.gov/mps/che/workshops/data_chemistry_workshop_report_03262018.pdf.

¹Transforming Science Through Cyberinfrastructure, NSF's Blueprint for a National Cyberinfrastructure Ecosystem for Science and Engineering in the 21st Century, https://www.nsf.gov/cise/oac/vision/blueprint-2019/.

²CESER program description: https://nsf.gov/funding/pgm_summ.jsp?pims_id=505385.

³Workshop report link:

⁴NASEM Report link: https://www.nap.edu/catalog/25760/advances-challenges-and-long-term-opportunities-in-electrochemistry-addressing-societal.

⁵Subject to availability of funds, OIA's Established Program to Stimulate Competitive

Research program (EPSCoR) is interested in providing co-funding support for EPSCoReligible institutions.