

#### EarthCube Town Hall: Evolution of the Geosciences /

#### Cyberinfrastructure Community

Christine Kirkpatrick SDSC-UCSD

December 13, 2022

This work is supported through the NSF award #1928208.

# J-EDI Justice, Equity, Diversity, and Inclusion

The heart of EarthCube is people. We put people first and do our best to recognize, appreciate, and respect the diversity of our global contributors. EarthCube welcomes contributions from everyone who shares our interests and wants to contribute in a healthy and constructive manner within our community.

We acknowledge that for millennia, Indigineous peoples have been a part of the land where this venue and our respective institutions' reside. This land has nourished, healed, and protected people for many generations in a relationship of balance and harmony.





## **Town Hall Overview**

- EarthCube Retrospective C. Kirkpatrick
- Sustainability Mike Daniels
- NSF Update Eva Zanzerkia
- Key Projects for Continued EC Involvement
  - DeCODER Kenton McHenry
  - FARR Christine Kirkpatrick
- Funded Project Lightning Talks
  - OpenMindat Marshall Ma
  - Project Raijin John Clyne





## EarthCube Retrospective Highlights

- November 8-9, 2022 @AGU in DC wonderful hosts
- Met and exceeded expectations
  - EarthCube history by Cliff Jacobs, NSF (retired)
- Great impact
  - EC-funded publications have 2x the citations as the average papers in the same journal
  - EC scholarship impactful in altmetrics, e.g.picked up by news outlets, social media, usage
- Vibrant and interconnected community network
- Can't be all volunteer
  - EC found just the right combination of governance, staffing, and incentives to keep work moving and the community flowing
     thCube



#### Top 10 Altmetric scores

- full (114) Altmetric scores [csv (download)] | [markdown (.md) (download)]
- top 10 Altmetric scores [markdown (.md) (download)]





Impact figure source: Maull, K., and M. Mayernik, 2022: EarthCube Program Metrics Analysis 2013-2022. https://doi.org/10.5065/VMFJ-QY55.

## EarthCube Retrospective Highlights ct.

- Contributed to positive culture change
  - emphasis on cooperation, collective effort, and inclusivity
  - more work to do
- What's Next?
  - strong signals from the community that new opportunities like EC are needed







**Progress:** The balance between cooperation and competition in the culture of your field or discipline.

**Progress:** Degree to which success is primarily a product of individual effort or a product of collective effort.

**Progress:** EarthCube initiative is inclusive in the way it operates.



**Pain Point:** Trusting that shared data, tools, models, notebooks, and software will be well-documented and reliable.

2015 14% Agree/Strongly Agree

Pain Point: Tenure, promotion, and rewards in my organization recognize and value sharing research data.





## **Additional Reflections**

- EarthCube contributed significantly to progress & leadership in intl FAIR data efforts
- In addition to NSF, NASA, NOAA, USGS recognize value of EC community and tools

opportunities for community post-EC

 EarthCube's legacy includes robust sustainability models









#### **EarthCube Sustainability**

#### Mike Daniels Ronin Institute December 13, 2022

## EarthCube Sustainability Timeline

January-March 2021: Discussions with NSF Program Managers June-July 2021: Listening Sessions at the 2021 EarthCube Annual Meeting September 2021: EarthCube Sustainability Panel (ECSP) Convened October-December 2021: CDF and CFP Sustainability Working Groups formed December 2021: Draft ECSP Report Announced at Fall 2021 AGU January 2022: Community feedback incorporated into the ECSP Report February 2022: Final ECSP Report Released June 2022: Sunset/Reshaping of Earthcube Governance Committees May 2022: CDF Sustainability Working Group Report Completed July 2022: CFP Sustainability Working Group Report Completed July 2022: First meeting of the EarthCube Transition Leadership Team November 2022: EarthCube Retrospective in Washington, D.C. December 2022: Final Wrap-up of EarthCube Governance and the Office

#### <u>https://tinyurl.com/E3-Sustainability</u>



## The EarthCube Transition Leadership Team



Mike Daniels **Ronin** Institute



Stephen Kuehn Concord University



Christine Kirkpatrick ECO/SDSC



**Dave Fulker OPeNDAP** 



**Denise Hills** Advanced Resources International



Leah LeVay Texas A&M



Kenton McHenry ECO/NCSA



Lynne Schreiber ECO/SDSC



**Karen Stocks** ECO/UCSD



https://tinyurl.com/EC-Transition



### CDF is reshaping itself as an ESIP Cluster

ABOUT V NEWS & EVENTS V PROGRAMS V RESOURCES V GET INVOLVED V

ACTIVE

**ESIP** 

Join CDF discussions every second Friday of the month at noon Eastern.

## Council of Data Facilities (CDF)

What we do: Connect data facilities, especially those that include Earth science datasets, and provide a collective voice for CDF members.

Why we do it: Geoscience data standards and stewardship require collaboration and communication.

Nick Jarboe (Oregon State University), Karen Stocks (Scripps Institution of Oceanography) Cluster Co-Chairs







#### https://www.esipfed.org/get-involved/collaborate/council-of-data-facilities-cdf

#### Notebooks as Scholarly Objects

**Notebooks Now!** 

HOME ABOUT POSTS CONTACT

# Notebooks Now!

Elevating Computational Notebooks as Primary Elements of the Scientific Record





https://data.agu.org/notebooks-now/



#### Sustainability models for integrated digital Earth Science

Virapongse, Arika; Gallagher, James; Tikoff, Basil; Cornillon, Peter: Koskela, Rebecca: Shingledecker, Susan; Trabant, Chad; Hanson, Brooks (2022). Sustainability models for integrated digital Earth Science. In EarthCube Organization Materials. UC San Diego Library Digital Collections. https://doi.org/10.6075/ **JOJH3MBN** 

EarthCube



## Sustainability of the EarthCube Community





Please stay tuned as discussions are underway for support of a Summer 2023 workshop which will serve as a bridge from EarthCube to new NSF initiatives for CI and Earth Science!



## Thank you!







# **NSF Opportunities 2023**

Eva Zanzerkia, NSF/GEO

The National Academies of SCIENCES • ENGINEERING • MEDICINE

#### CONSENSUS STUDY REPORT

#### NEXT GENERATION EARTH SYSTEMS SCIENCE NATIONAL SCIENCE FOUNDATION



#### National and community reports call for future R&D investments in cyberinfrastructure and open science

#### National Research Infrastructure plans (NITRD)

- National Discovery Cloud
- Open Science Data Commons
- Future Advanced Computing
- National AI Research Resource

#### Key Characteristics for NSF Earth Systems Sciences (NASEM 2022 report)

- Advance both curiosity-driven and use-inspired basic research
- Use observational, computational, and modeling capabilities synergistically to accelerate discovery and convergence.
- Educate and support a workforce with the skills and knowledge

#### Interagency Collaborations

- NSF-NOAA partnership team on Earth System Modeling and AI/ML
- ICAMS (Interagency Council for Advancing Meteorological Services) Subcommittee on Earth Systems ML/AI and Advanced Technology

### Growing importance of open, accessible, and reproducible science at NSF

- **OSTP Memo**: Ensuring Free, Immediate, and Equitable Access to Federally Funded Research (Aug. 25, 2022)
- FAIROS RCNs (NSF 22-553)
  - New NSF program supporting Research Coordination Networks (RCNs) that advance FAIR principles (findable, accessible, interoperable, reusable) and open science (OS) practices
- Reproducibility & Replicability DCL (NSF 23-018)

\*\* Public Access Listen and Learn Session for NSF Stakeholders November 30, 2022, 2 PM EST via Zoom \*\* <u>https://nsf.zoomgov.com/webinar/register/WN\_nKHJhfl4RJGWQnEXqFiaLQ</u> Dear Colleague Letter: Reproducibility and Replicability in Science

October 25, 2022

#### Dear Colleagues:

A 2019 consensus study report published by the National Academies of Sciences, Engineering, and Medicine (NASEM) discussed the meaning of the terms replicability and reproducibility and identified approaches for researchers, academic institutions, journals, and funders to improve reproducibility and replicability in science <sup>[1]</sup>. In July 2021, at NSF's request, NASEM convened an expert meeting focused on National Science Foundation (NSF) policies and investments to make reproducible and replicable science easier for scientific communities to understand and execute and to embed reproducibility and replicability within the fundamental scientific method.

Through this Dear Colleague Letter (DCL), NSF reaffirms its commitment to advancing reproducibility and replicability in science. NSF is particularly interested in proposals addressing one or more of the following topics:

- Advancing the science of reproducibility and replicability. Understanding current
  practices around reproducibility and replicability, including ways to measure reproducibility
  and replicability, what reproduction and replication means in practice, the right degree of
  replicability to target, quantitative measures of progress to understand the effectiveness of
  interventions to improve reproducibility and replicability, and exploration of reasons why
  studies may fail to replicate.
- Research infrastructure for reproducibility and replicability. Developing and facilitating adoption of cyberinfrastructure tools and/or research methods that enable use of reproducible and replicable practices across one or more science and engineering communities.
- 3. Educational efforts to build a scientific culture that supports reproducibility and replicability. Enabling training in science and engineering communities to identify and encourage best practices for reproducibility and replicability, providing community-building and institutional support, and supporting broad public outreach about rigor, reproducibility, and replicability in science.

Investigators who wish to submit proposals on any of these topics, or others related to advancing reproducibility and replicability in research, are encouraged to reach out to programs and program officers to discuss the fit of their ideas to existing funding opportunities. Definitions of the terms replicability and reproducibility may be found in Reference <sup>[1]</sup>.

#### NSF's FY 2023 Budget Request: Major GEO Investments



#### GEO Cyberinfrastructure Goals

- Advance geoscience research
- Promote openness and participation through Open Science
- Pursue AI/ML innovation in the geosciences



## **Office of Advanced Cyberinfrastructure (OAC) opportunities**

- **Cyberinfrastructure for Sustained Scientific Innovation (CSSI)** (NSF 22-632): Support for robust, reliable, and sustainable data and software cyberinfrastructure (*Deadline:* December 16, 2022)
- **CyberTraining (NSF 23-520):** Supports efforts toward broad adoption of CI tools, methods, and resources; and integration of CI literacy into curriculum / instructional materials (*Deadline:* Feb. 23, 2023)
- **SCIPE (NSF 23-521):** "Strengthening the Cyberinfrastructure Professionals (CIP) Ecosystem" (*Deadline:* Feb. 23, 2023)
- OAC CI Resource Ecosystem:
  - ACCESS: Coordinates allocations for advanced computing, visualization, and data resources for researchers and educators (follow-on to XSEDE) (<u>https://access-ci.org</u>)
  - **CloudBank:** Enabling access to commercial cloud service resources
  - **Partnership to Advance Throughput Computing (PATh):** Pilot support for high-throughput computing (HTC) resources (see NSF 22-051)

*More information here:* <u>https://www.nsf.gov/geo/geo-ci</u>

# **Relevant CI-Related Programs**

What will your project focus on?	Develop software or data repository	Perform research that will enable future CI	Support research that uses CI, foster CIP careers	Provide training
What gap will you fill?	Increase community CI for research or education	Increase knowledge needed for CI	Increase support for CIP career & research by underserved groups	Increase research workforce to leverage CI
What will your project deliver?	Community-sustained Cl	Techniques that will enable CI and a CI prototype	Research support in CI, CIP career paths	Scalable and sustainable training program
	CSSI	OAC CORE	SCIPE	CyberTraining

Programs have specific purposes, however, are not necessarily mutually exclusive



# Technology, Innovation, and Partnerships (TIP) opportunities

**TIP is NSF's newest directorate.** Supports use-inspired research, accelerating development of key technologies, and expanding the STEM workforce

- Convergence Accelerator: phased funding model to accelerate solutions toward societal impact (RFI for topics => Workshops => topic selection for project cohorts)
  - 2022 workshop examples: Ethical Design of AI, Computing Solutions for Climate-Driven Extreme Events
  - Past cohort examples: Open Knowledge Networks, Al-driven Innovation via Data & Model Sharing
- Pathways to Enable Open-Source Ecosystems (POSE) (NSF 22-552)
  - Supports efforts toward harnessing open-source development approaches for new technology solutions to problems of national and societal importance
  - Applicable to a wide range of "open-source" development (including software and other products)





## Student Training in Al



NSF's Convergence Accelerator is funding a use-inspired training opportunity to tackle climate challenges with AI

The Institute's theme for the 2023 CORE Fellows is "Tackling Climate-Induced Challenges with AI"

Due: January 8, 2023

https://www.sdsc.edu/education\_and\_training/core\_institu te.html?utm\_medium=email&utm\_source=govdelivery



### At AGU

- **NSF Booth** (#1313 in Exhibit Hall): lightning talks (times are tentative)
  - Data Management & Public Access: 12/12 at 4:50 PM CST and 12/14 at 11:50 AM CST
  - Antarctic & Arctic Sciences New Data Policy: 12/13 at 3:00 PM CST, 12/14 at 3:00 PM CST
  - The Evolving Landscape of Open Science in Federally funded Research: 12/14 at 4:50 PM CST
  - *Mid-Scale Infrastructure Funding Opportunities*: 12/15 10:20 AM CST

GEO Cyberinfrastructure Opportunities



#### Decoder Democratized Cyberinfrastructure for Open Discovery to Enable Research

#### Kenton McHenry University of Illinois Urbana-Champaign

December 13, 2022

This work is supported through the NSF award #2209863.

## NSF EarthCube Program

- NSF Program started around 2012 to advance cyberinfrastructure in support of geoscience research
  - Develop tools, data resources, infrastructure, standards
    - Data sharing, data interface standards, data wrangling, workflows, analytics, reproducibility
  - Funded roughly 95 efforts to date

![](_page_25_Picture_5.jpeg)

![](_page_25_Picture_6.jpeg)

![](_page_25_Picture_7.jpeg)

## **Council of Data Facilities**

![](_page_26_Picture_1.jpeg)

```
<html>
                                              Science on Schema
<head>
 <title>NCDC Storm Events Database</title>
 <script type="application/ld+json">
   "@context":"https://schema.org/",
   "@type":"Dataset",
   "name": "NCDC Storm Events Database",
   "description": "Storm Data is provided by the National Weather Service (NWS) and contain statist
   "url": "https://catalog.data.gov/dataset/ncdc-storm-events-database",
   "sameAs": "https://gis.ncdc.noaa.gov/geoportal/catalog/search/resource/details.page?id=gov.noaa.
   "identifier": ["https://doi.org/10.1000/182",
                  "https://identifiers.org/ark:/12345/fk1234"],
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      "ATMOSPHERE > ATMOSPHERIC PHENOMENA > CYCLONES",
      "ATMOSPHERE > ATMOSPHERIC PHENOMENA > DROUGHT",
      "ATMOSPHERE > ATMOSPHERIC PHENOMENA > FOG",
      "ATMOSPHERE > ATMOSPHERIC PHENOMENA > FREEZE"
   ],
   "license" : "https://creativecommons.org/publicdomain/zero/1.0/",
   "hasPart" : [
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       "name": "Sub dataset 01",
       "description": "Informative description of the first subdataset...",
       "license" : "https://creativecommons.org/publicdomain/zero/1.0/"
     },
       "@tvpe": "Dataset",
```

https://github.com/ESIPFed/science-on-schema.org

![](_page_27_Picture_2.jpeg)

## GeoCODES

- Work with repositories to adopt standard means of sharing metadata
- Pilot crawler and demonstration portal for geoscience data

![](_page_28_Picture_3.jpeg)

EarthCube GeoCODES	× +		
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CSDCO_Data	LinkedEarth	Neotoma	IEDA
BALTO	MagIC	Open Topography	IRIS
OpenCore	UNAVCO		
🌒 Get	t Top Results For Each Selected Provider Submit Text i	Get Top Results Across All Selected Pro	viders

![](_page_28_Picture_5.jpeg)

![](_page_28_Picture_6.jpeg)

## Repositories Using Science on Schema

- 23 repositories: AquaDocs, OpenTopography, IRIS, Environmental Data Initiative, Biological and Chemical Oceanography Data Management Office, Consortium of Universities for the Advancement of Hydrologic Science, Inc.(CUAHSI), IEDA (Integrated Earth Data Applications), UNAVCO, IODP Site Survey Databank, Balto, Linked Earth, Linked PaleoData, IRIS, UCAR, opencoredata, Magnetics Information Consortium (MagIC), Neotoma, earthchem, xdomes, National Ecological Observatory Network (NEON), Resource Registry, UNIDATA, Rolling Deck to Repository Program (R2R), Geocodes Demo Datasets, U.S. Antarctic Program Data Center
- Currently working with 3 others: Decade, CReSIS, and DesignSafe
- Engaging with Google to support analytics within Data Commons

![](_page_29_Picture_4.jpeg)

![](_page_29_Picture_5.jpeg)

![](_page_30_Picture_0.jpeg)

#### **Call for Notebooks - Abstracts Due April 15**

As scientific studies become more data intensive and software dependent, reproducibility principles and other factors increase the importance of citable publications that include reusable workflows, software, and data-access procedures. This importance is reflected in new academic journals, such as the Journal of Open Source Software, whose peer reviewed articles highlight the software itself, and often can include executable notebooks (Jupyter, R Studio, etc.). In this spirit, EarthCube is issuing its first call for Notebooks as primary, peer-reviewed submissions to a digital proceedings for this year's EarthCube Annual Meeting. Submitted notebooks should highlight a tool (i.e. software, service, library, dataset, standard), explaining—and demonstrating interactively—how the tool may be used to address a significant problem in geoscience.

- Drew Camron (UNIDATA)
- Julien Chastang (UNIDATA)
- Jeff Dozier (UCSB)
- David Fulker (OPeNDAP)
- Ryan Gooch (NREL)
- Joseph Hardin (PNNL)
- Keith Maull (NCAR)
- Kenton McHenry (NCSA)
- Chris Olson (UCSD)
- Stephen Richard (U.S. Geoscience Information Network)
- Bradley Spitzbart (Stony Brook University)
- Lisa Tauxe (Scripps Institution of Oceanography)
- Carol Willing (Project Jupyter)
- Ilya Zaslavsky (UCSD)

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![](_page_31_Picture_17.jpeg)

![](_page_31_Picture_18.jpeg)

![](_page_31_Picture_19.jpeg)

# CfN'20

- <u>https://github.com/earthcube2020</u>
   <u>https://www.essoar.org</u>
- 21 submissions
  - 2-3 reviewers per notebook
  - 12 accepted, 5 as oral presentations
  - Published through AGU ESSOAr system

#### • Insights

- Types of notebooks
- Runnability
- An emphasis on testing
- Science Tool focused vs Science focused submissions
- Formatting Guidelines

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Diego Calderon   See all authors   Published Online: Wed. 2 Sec 2020   https://doi.c	ec20_havlin_etal	G earthcube2020/ec20_havlin_etal O Code ◯ Issues I? Pull requests ◯ Actions  Projects III Wild ◯ Security 낟 Insights	0	
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annotate, connect, integrate, and reas framework allows the semantic enrich heterogeneous geoscience resources, s This notebook provides examples on h	ec20_hamman_etal ● Jupyter Notebook 4 CC-BY-4.0 ♀1	README.md ec20_havlin_etal.ipynb	(2) I = 2) I = 2) I = 2) 9 cont 1 monthin 1 monthi	
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vocabularies using SKOS, and how to a definitions pro- vided by these endpoir the IML Critical Zone Observatory data (https://data.imlczo.org/). By supporti	Compare indexides the provided of the pro			

![](_page_32_Picture_13.jpeg)

on tomographic models of North America and the Western U.S., where high resolution models and rapidly varying seismic properties provide a rich dataset to explore systematically at a range of lengthscales. The notebook demonstrates loading and rendering of IRIS netcoff models, highlighting interesting 3D features of the Western U. upper mantile, and goes on to demonstrate how having direct control of the transfer functions used in creating the set of the

final volume rendering allows for a more systematic exploration of the role of the visualization method in our interpretation of 3D volumetric data. Finally, we conclude by demonstrating some of the semantically-aware capabilities of yt for analysis purposes, and demonstrate how these tools have cross-disciplinary functionality

@ launch binder

## GeoCODES Data + Tools

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	Specification 3	36 M	Improve knowledge of the relationship beto repositories and online access to data to su			
	Catalog/Registry 1 Interface/API 1	16 15	links: https://docs.google.com/document/d			
	Service 1 Platform 1	13	Details			
	Use Case	5	Along Track Scanning Radiometer series (ATSR-1,			
	Name		Along Track Scanning Radiometer ser			
	Date		ATSR (the Along Track Scanning Radiomete	rsion: 0.9.5 Date: 2022-04-13 staging		
	Keywords		third instrument, AATSR (the Advanced Along t the ca	track Scanning Radiometer), these are known as	(A)ATSR. This product contains	
	Maturity/status		links: https://earth.esa.int/documents/700255/	/2482719/PO-TN-RAL-	4640.200	
	License		Details	01112330611.7/CC003770-3207-7172-0787-83200	u110303	
			Apache Parquet format			

![](_page_33_Picture_2.jpeg)

![](_page_34_Figure_0.jpeg)

### Recommended Standards and Specifications for EarthCube Projects

K. Rubin, M. Daniels, D. Fulker, J. Brown, S. Richard, O. Meier, I. Zaslavsky, C. Willis, K. McHenry, C. Kirkpatrick, **"Recommended Standards and Specifications for EarthCube Projects**", 2020

https://doi.org/10.6075/J0QR4VMG

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→ Best Practices! F.A.I.R.

- Schema.org
- GitHub,
- Markdown,
- Docker,
- Binder,
- Jupyter,

...

Recommended Standards and Specifications for EarthCube Projects Authors: Ken Rubin, Mike Daniels, Dave Fulker, Jed Brown, Stephen Richard, Oulda Meier, Ilya Zaslavsky, Craig Willis, Kenton McHenry, Christine Kirkpatrick. Approved by EarthCube Leadership Council: 7M 2020, DOI: https://doi.org/10.6075/J0QR4VMG

This living document describes minimal and optimal recommended practices for NSF EarthCube projects, proposed in 2020 and beyond, with the hope that prior funded EarthCube projects voluntarily conform too. The contents of this document are informed by several prior efforts within EarthCube Community Governance to describe programmatic goals (including component architecture and interoperability), open community conditions for standards development, and the needs of EarthCube affiliated data repositories and existing Earthcube projects. Three such efforts are noted and linked in the acknowledgments section.

Standards and Specifications for cyberinfrastructure to support cross-disciplinary science will continue to change as technologies evolve and new science domains join the effort. The ideas expressed here focus on current and future NSF-funded efforts to create new EarthCube and related cyberinfrastructure that promotes interoperability, sustainability, useability and repurposing (othen via open-source software).

The Standards and Specifications listed here focus on basic principles and are not comprehensive (i.e., they do not at this time address coding practice, testing, human interfaces, product stability, or other attributes that are currently up to developers to define). Project developers building software are encouraged to engage with the EarthCube Community Office (ECO) Technology Team to take advantage of and incorporate the latest features and recommendations.

This document draws from a recent White paper [LINK] describing some of the rationale for, and nuance of, many of the specifications listed here, as well as additional, options and recommendations regarding licensing, reuse of existing components, use of notebooks, version control, information exchange procedures (e.g., APs), and vocabularies/ontologies.

#### Primary Guidelines:

- EarthCube seeks to have all data and data resources produced by and for EarthCube to be FAIR Compliant, in keeping with its status as a co-signatory of the US FAIR data effort. See <u>http://earthcube.org/fair</u> for additional details.
- Products require producer attribution and contact, version control, hardware and operating system requirements, and notation of any data format or data resource dependencies.
- Products shall be properly registered in the EarthCube registries documented at: <u>https://www.earthcube.org/geocodes</u>. Currently there are two paths to registration.

 For datasets employed in EarthCube: should be made accessible from a data repository whose metadata is exposed and formatted for harvesting by EarthCube's GeoCODES [LINK], via a repository that is (or easily can be) recorded in the EarthCube Resource Registry [LINK], or- via an existing alternate and interoperable resource

![](_page_35_Picture_22.jpeg)

## Potential of GeoCODES

![](_page_36_Figure_1.jpeg)

rthCube

![](_page_36_Picture_2.jpeg)

Computers & Geosciences 157 (2021) 104933

The future low-temperature geochemical data-scape as envisioned by the U. S. geochemical community

Susan L. Brantley<sup>a,o,\*</sup>, Tao Wen<sup>b</sup>, Deborah A. Agarwal<sup>c</sup>, Jeffrey G. Catalano<sup>d</sup>, Paul A. Schroeder<sup>e</sup>, Kerstin Lehnert<sup>f</sup>, Charuleka Varadharajan<sup>8</sup>, Julie Pett-Ridge<sup>h</sup>, Mark Engle<sup>1</sup>, Anthony M. Castronova<sup>1</sup>, Richard P. Hooper<sup>k</sup>, Xiaogang Ma<sup>1</sup>, Lixin Jin<sup>1</sup>, Kenton McHenry<sup>m</sup>, Emma Aronson<sup>n</sup>, Andrew R. Shaughnessy<sup>o</sup>, Louis A. Derry<sup>p</sup>, Justin Richardson<sup>q</sup>, Jerad Bales<sup>j</sup>, Eric M. Pierce

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ABSTRACT

#### ARTICLE INFO

Keywords Data managemen Data repositories Geochemistry Metadata

Data sharing benefits the researcher, the scientific community, and the public by allowing the impact of data to be generalized beyond one project and by making science more transparent. However, many scientific communities have not developed protocols or standards for publishing, citing, and versioning datasets. One community that lags in data management is that of low-temperature geochemistry (LTG). This paper resulted from an initiative from 2018 through 2020 to convene LTG and data scientists in the U.S. to strategize future management of LTG data. Through webinars, a workshop, a preprint, a townhall, and a community survey, the group of U.S. scientists discussed the landscape of data management for LTG - the data-scape. Currently this data-scape includes a "street bazaar" of data repositories. This was deemed appropriate in the same way that LTG scientists publish articles in many journals. The variety of data repositories and journals reflect that LTG scientists target many different scientific questions, produce data with extremely different structures and volumes, and utilize copious and complex metadata. Nonetheless, the group agreed that publication of LTG science must be accompanied by sharing of data in publicly accessible repositories, and, for sample-based data, registration of samples with globally unique persistent identifiers. LTG scientists should use certified data repositories that are either highly structured databases designed for specialized types of data, or unstructured generalized data systems. Recognizing the need for tools to enable search and cross-referencing across the proliferating data repositories, the group proposed that the overall data informatics paradigm in LTG should shift from "build data repository, data will come" to "publish data online, cybertools will find". Funding agencies could also provide portals for LTG scientists to register funded projects and datasets, and forge approaches that cross national

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https://doi.org/10.1016/j.cageo.2021.104933 Received 31 January 2021; Received in revised form 26 July 2021; Accepted 3 September 2021 Available online 7 September 2021 0098-3004/© 2021 Elsevier Ltd. All rights reserved

# NSF CSSI Frameworks: DeCODER

![](_page_37_Picture_1.jpeg)

![](_page_37_Picture_2.jpeg)

![](_page_37_Picture_3.jpeg)

Christine Kirkpatrick Cyberinfrastructure UCSanDiego

![](_page_37_Picture_5.jpeg)

Karen Stocks Ocean Science

Tao Wen Hydrochemistry Syracuse University

![](_page_37_Picture_9.jpeg)

Shuang Zhang

**Biochemical Cycles** 

Thomas Quinn

Ecology

![](_page_37_Picture_11.jpeg)

Carl Boettiger Ecology Berkeley

![](_page_37_Picture_13.jpeg)

Lynne Schreiber Coordinator <u>UC San Diego</u>

![](_page_37_Picture_15.jpeg)

Geoscience Cyberinfrastructure for Open Discovery in the Earth Sciences (GeoCODES)

Democratized Cyberinfrastructure for Open Discovery to Enable Research (DeCODER)

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**CSSI: Democratized Cyberinfrastructure for Open Discovery to Enable Research** - \$3,199,896

https://nsf.gov/awardsearch/showAward?AWD\_ID=2209863 - \$900,640 (UIUC) https://nsf.gov/awardsearch/showAward?AWD\_ID=2209864 - \$460,281 (Syracuse) https://nsf.gov/awardsearch/showAward?AWD\_ID=2209865 - \$1,303,971 (UCSD) https://nsf.gov/awardsearch/showAward?AWD\_ID=2209866 - \$535,004 (Virginia) Oct 1, 2022 - Sept. 30, 2026 (4 years)

RCN: Disciplinary Improvements: AI Readiness, Reproducibility, and FAIR: Connecting Computing and Domain Communities Across the ML Lifecycle <u>https://nsf.gov/awardsearch/showAward?AWD\_ID=2226453</u> - \$1,260,000 (UCSD) August 15, 2022 - July 31, 2025 (3 years)

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## Tasks

- Gleaner community
- Extending Schema.org
  - Depth, horizon, ...
- Portal customization and deployments
- Graph Search
  - Data Integration
- Linking tools with data
  - Notebooks as scholarly objects
  - Crawling tools
- Community Support & Engagement
  - Support for smaller repositories

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![](_page_39_Picture_13.jpeg)

#### Opportunities for EarthCube Projects & Community

- Advice and jump start help on adopting schema.org for repositories
- Register your geo CI resources and associate with data sets and notebooks
- Provide use cases for our continual UI/UX process
  - test DeCODER against your own scientific questions and use cases
- Get credit for other types of scholarship with our annual notebook competition
  - encourage your students to take part!
  - be a reviewer

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## **FARR:**

#### FAIR in ML, AI Readiness, & Reproducibility Research Coordination Network

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Christine Kirkpatrick SDSC, UC San Diego Date: December 13, 2022

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This work is supported through the NSF award #2226453.

## Motivation

- If 80% of time with data is wrangling, can FAIR principles increase efficiency of people and machines?
- What does it mean to be AI ready as a repository or organization?
- What roles can repositories play in AI readiness?
- What are best practices in AI reproducibility and what are the gaps in current knowledge?

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AI Readiness

Reproducibility

FAIR in ML

## FARR Goals and Activities

We welcome individual researchers, institutions/organizations, CI providers, repositories/facilities, and networks of facilities in Computer Science, Geosciences, and the 'Research Data' Community. FARR provides a neutral and novel meeting place for bridging multiple networks.

- Building communities to
  - promote better practices for AI
  - harness community efforts
  - improve efficiency and reproducibility
  - stimulate and enhance new research

- Activities will include
  - workshops
  - assessing community needs
  - fostering new collaborations (proposals)
  - setting research agendas
  - community-led reports

Incorporating EarthCube's sustainability lessons from the beginning.

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![](_page_43_Picture_15.jpeg)

#### **FARR Team**

![](_page_44_Picture_1.jpeg)

PI, Christine Kirkpatrick

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Co-PI, Karen Stocks

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Co-PI, Yuhan (Douglas) Rao

![](_page_44_Picture_7.jpeg)

Co-PI, Daniel Katz

![](_page_44_Picture_9.jpeg)

Project Director, Lynne Schreiber

![](_page_44_Picture_11.jpeg)

![](_page_44_Picture_12.jpeg)

Sr. Personnel, Kevin Coakley

> **NC STATE** UNIVERSITY **I ILLINOIS** NCSA | National Center for Supercomputing Applications

![](_page_44_Picture_15.jpeg)

Project Manager, Julie Christopher

![](_page_44_Picture_17.jpeg)

![](_page_44_Picture_18.jpeg)

Communications,

Kim Mann Bruch

![](_page_44_Picture_19.jpeg)

![](_page_44_Picture_20.jpeg)

#### **Opportunities for EarthCube Projects & Community**

- Interviews with CDF members and other data repositories on AI readiness topics
- Input on community needs, gaps, and roadmap
- FARR network meetings and early career travel scholarships
- Connect with FARR via
  - ESIP's Data readiness and ML clusters ESIP Winter (virtual)
  - Research Data Alliance (RDA) FAIR4ML interest group RDA P20 (Sweden/virtual)
  - o FARR hosted webinars
  - Sign up for our **newsletter**
- Suggest use cases and let us promote your project's use of AI and FARR-related practices
- Let us feature you in a science story

For more info, contact us at community@farr-rcn.org

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# Funded Project Lightning Talks

- John Clyne (Project Raijin)
- Marshall Ma (OpenMindat)

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#### Community Geoscience Analysis Tools for Unstructured Grids

John Clyne<sup>1</sup>, Orhan Eroglu<sup>1</sup>, Brian P. Medeiros<sup>1</sup>, Colin Zarzycki<sup>2</sup> <sup>1</sup> National Center for Atmospheric Research (NCAR) <sup>2</sup> Pennsylvania State University

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NSF Earth Cube Town Hall December 13, 2022

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![](_page_48_Figure_0.jpeg)

After nearly two decades of development and evaluation, the climate and global weather modeling communities are transitioning from more simple structured grids to more complex, but scalable unstructured grids upon which governing equations of state are solved.

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### **Problem?**

![](_page_49_Picture_2.jpeg)

- 1. No widely used convention for the storage of unstructured grid data
  - UGRID conventions: https://ugrid-conventions.github.io
- 1. Few analysis tools capable of working directly with unstructured data
  - Resampling to structured grids has numerous pitfalls
- 1. Global storm resolving resolution models are capable of generating LOTS of data
  - Further exacerbating problems with limited set of tools that

operate directly on unstructured meshes

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## **Project Raijin Goals**

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#### Community developed software for analysis on unstructured grids

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#### Community Geoscience Analysis Tools for Unstructured Grids

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#### UXarray for visualization

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#### Get involved!

Send us email projectraijin@googlegroups.com

Start a discussion https://github.com/UXARRAY/uxarray/discussions

Find out more <u>https://raijin.ucar.edu</u>

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### Acknowledgements

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NSF Earth Cube program (award #2126458)

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Collaborators: Ryan Abernathy, Falko Judt, David Randall, Niklas Röber, and Bjorn Stevens

Pangeo community

Our growing list of contributors on GitHub!

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#### OpenMindat: machine interface to the world's largest database in mineralogy

Xiaogang (Marshall) Ma Associate Professor, University of Idaho Visiting Scientist, Carnegie Institution for Science max@uidaho.edu | @MarshallXMa

![](_page_54_Picture_4.jpeg)

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#### Citations to "mindat.org" on Google Scholar

![](_page_56_Figure_1.jpeg)

# Challenges

## Massive needs on data sharing vs No machine interface for data access

#### **Designed Structure of OpenMindat**

![](_page_58_Figure_1.jpeg)

#### Work Towards Semantic Harmonization

- Semantics of General Subjects: For spatial and temporal information and metadata elements for dataset, we refer to existing standards such as those developed by OGC, W3C, and DataCite
- **Community-level Standards/Guidelines**: For geoscience subjects, such as name list and attributes of mineral species and rock classification, we refer to scientific societies' guidelines and widely used standards and vocabularies
- Leverage Schema.org: We are designing a metadata schema for annotation of dataset webpages, by following the Schema.org guidelines and best practices shared by ESIP and EarthCube
- **Persistent Identifiers**: We are discussing the possibility of deploying persistent and resolvable identifiers, such as the International Generic Sample Number, for mineral species
- Collaboration amongst Stakeholders: We are working together with scientific societies and data users for the design of the API to increase its utility