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Making the Major Facilities Data Lifecycle FAIR

To provide AI ready data

USC Viterbi School of Engineering Information Sciences Institute

INDIANA UNIVERSITY

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TEXAS TECH UNIVERSITY

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Agenda

- Introduction (5 min) - Charles Vardeman
- FAIR Data and the MF Data Lifecycle (10 min) - Donald Brower
- Wikidata: A knowledge graph for the earth sciences (10 min) - Charles Vardeman
- ESIP Schema.org cluster: Utilizing the Schema.org vocabulary for FAIR Earth Science Data (15 min) - Adam Shepherd and Doug Fills
- NEON's first data releases: challenges and opportunities to provide FAIR data Draft Description (10 min) - Christine Laney
- Questions for first group of talks (5 min)
- AI strategies for improving data management components and preparing AI-ready data that meets FAIR and data provenance (15 min) - Giri Prakash
- Application of FAIR Principles in Astronomy (10 min) - Bruce Berriman

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Agenda

- Questions for second set of talks (5 min)
- Break - Close Poll at end of break
- Group Discussion over

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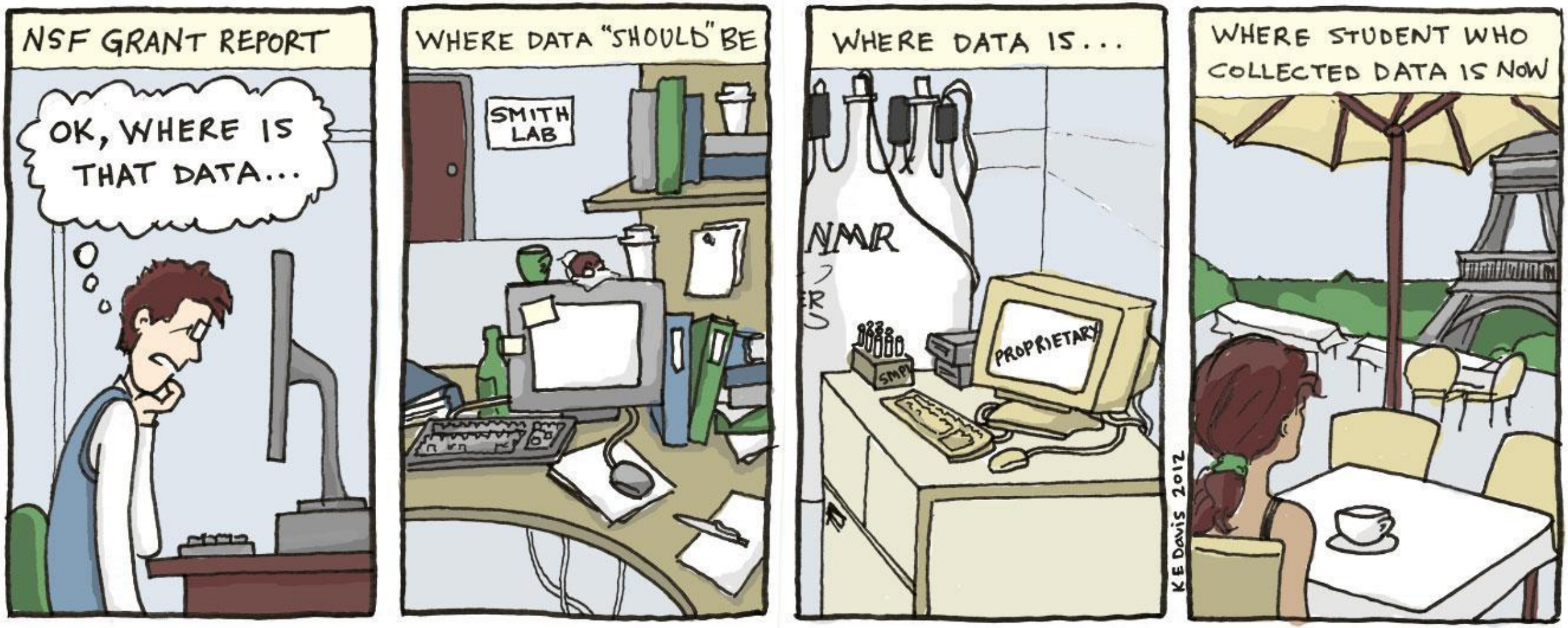

Credit: Kristina Furse and Charles Vardeman, University of Notre Dame, Center for Research Computing, NSF DASPOS: Data and Software Preservation for Open Science (2012)

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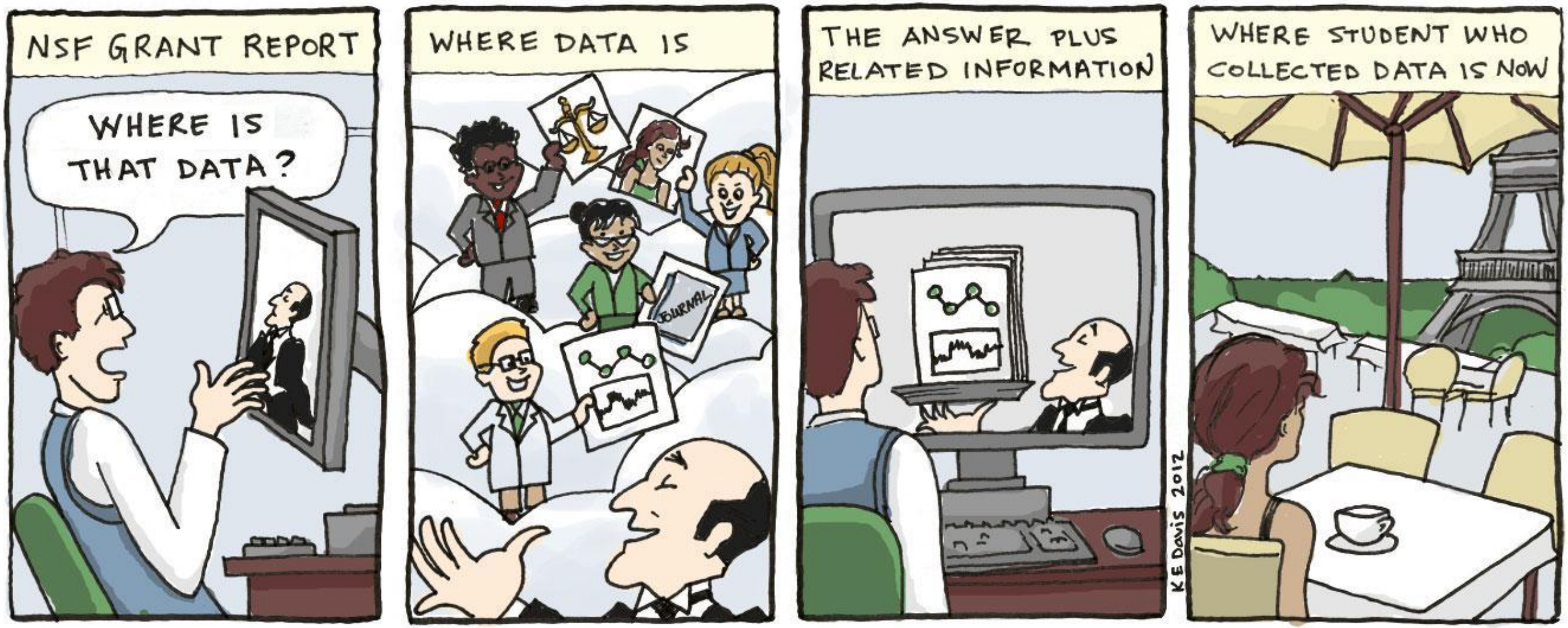

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Wilkinson et al.
https://www.nature.com/articles/sdata201618

scientific data

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Open Access | Published: 15 March 2016

The FAIR Guiding Principles for scientific data management and stewardship

Mark D. Wilkinson, Michel Dumontier, ... Barend Mons + Show authors

Scientific Data 3, Article number: 160018 (2016) | Cite this article

423k Accesses | 3576 Citations | 1934 Altmetric | Metrics

An Addendum to this article was published on 19 March 2019

Abstract

There is an urgent need to improve the infrastructure supporting the reuse of scholarly data. A diverse set of stakeholders—representing academia, industry, funding agencies, and scholarly publishers—have come together to design and jointly endorse a concise and measureable set of principles that we refer to as the FAIR Data Principles. The intent is that these may act as a guideline for those wishing to enhance the reusability of their data holdings. Distinct from peer initiatives that focus on the human scholar, the FAIR Principles put specific emphasis on enhancing the ability of machines to automatically find and use the data, in addition to supporting its reuse by individuals. This Comment is the first formal publication of the FAIR Principles, and includes the rationale behind them, and some exemplar implementations in the community.

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DeepMind › Blog › AlphaFold: a solution to a 50-year-old grand challenge in biology

BLOG POST
RESEARCH

30 NOV 2020

AlphaFold: a solution to a 50-year-old grand challenge in biology

Article | Open Access | Published: 22 July 2021

Highly accurate protein structure prediction for the human proteome

Kathryn Tunyasuvunakool, Jonas Adler, ... Demis Hassabis + Show authors

Nature **596**, 590–596 (2021) | Cite this article

184k Accesses | **200** Citations | **1413** Altmetric | Metrics

Abstract

Protein structures can provide invaluable information, both for reasoning about biological processes and for enabling interventions such as structure-based drug development or targeted mutagenesis. After decades of effort, 17% of the total residues in human protein sequences are covered by an experimentally determined structure[1]. Here we markedly expand the structural coverage of the proteome by applying the state-of-the-art machine learning method, AlphaFold[2], at a scale that covers almost the entire human proteome (98.5% of human proteins). The resulting dataset covers 58% of residues with a confident prediction, of which a subset (36% of all residues) have very high confidence. We introduce several metrics developed by building on the AlphaFold model and use them to interpret the dataset, identifying strong multi-domain predictions as well as regions that are likely to be disordered. Finally, we provide some case studies to illustrate how high-quality predictions could be used to generate biological hypotheses. We are making our predictions freely available to the community and anticipate that routine large-scale and high-accuracy structure prediction will become an important tool that will allow new questions to be addressed from a structural perspective.

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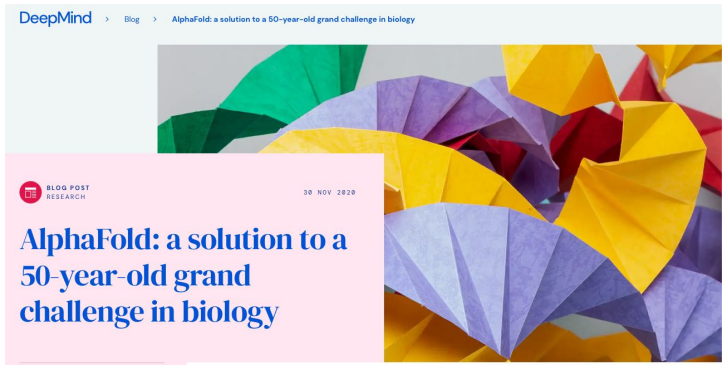
Model confidence and added coverage

We predicted structures for the UniProt human reference proteome (one representative sequence per gene), with an upper length limit of 2,700 residues[6]. The final dataset covers 98.5% of human proteins with a full chain prediction.



The dataset adds high-quality structural models across a broad range of Gene Ontology (GO) terms[36,37], including pharmaceutically relevant classes such as enzymes and membrane proteins[38] (Fig. 1d). Membrane proteins, in particular, are generally underrepresented in the PDB because they have historically been challenging experimental targets. This shows that AlphaFold is able to produce confident predictions even for protein classes that are not abundant within its training set.

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The Question?

Where are we in terms of FAIR adoption in the MF community and where do we need/want to go with FAIR?

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FAIR Data and the MF Data Lifecycle

Donald Brower

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FAIR

- Domain-independent, high-level principles that can be applied to a wide range of scholarly outputs
- Acronym for Findable, Accessible, Interoperable, Reusable.
- Proposed by Wilkinson et al. (2016)
- Not a standard or a specification
- May be applied in any combination and incrementally
- Recognizes the importance of "computational agents"

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F — Findable

- F1: (meta)data are assigned a globally unique and persistent identifier
- F2: data are described with rich metadata (as defined by R1)
- F3: metadata clearly and explicitly include the identifier of the data it describes
- F4: (meta)data are registered or indexed in a searchable source

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A — Accessible

- A1: (meta)data are retrievable by their identifier using a standardized communications protocol
  - A1.1: the protocol is open, free, and universally implementable
  - A1.2: the protocol allows for an authentication and authorization procedure, where necessary
- A2: metadata are accessible, even when the data are no longer available

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I — Interoperable

- I1: (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation
- I2: (meta)data use vocabularies that follow FAIR principles
- I3: (meta)data include qualified references to other (meta)data

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R — Reusable

- R1: meta(data) are richly described with a plurality of accurate and relevant attributes
  - R1.1: (meta)data are released with a clear and accessible data usage license
  - R1.2: (meta)data are associated with detailed provenance
  - R1.3: (meta)data meet domain-relevant community standards

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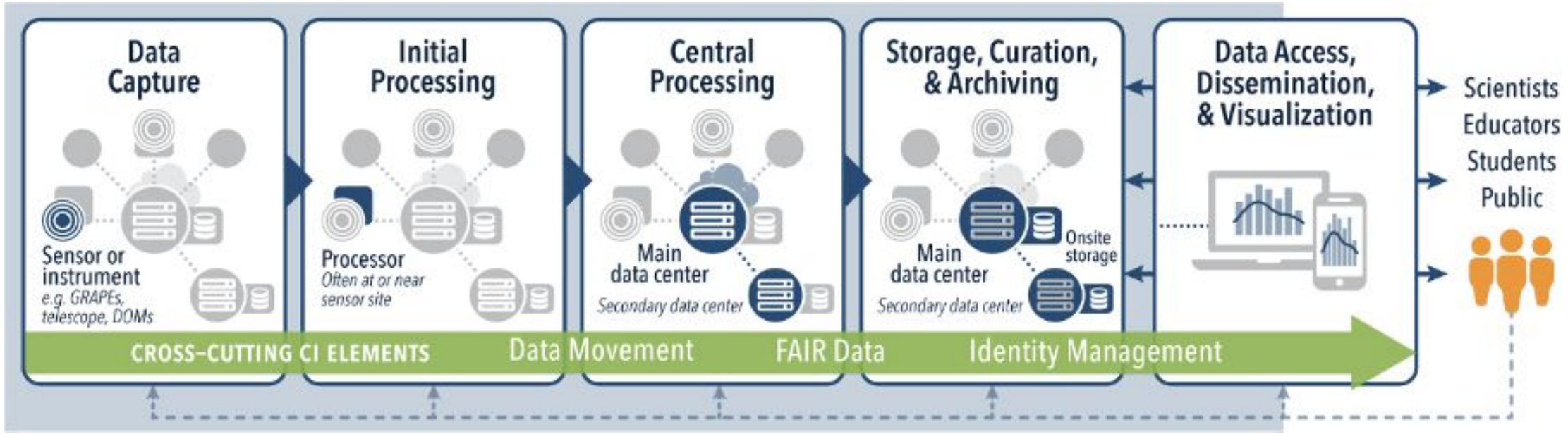
Data Lifecycle



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- Identifiers are essential at each step of lifecycle to identify and describe data
- Need ability to add metadata and provenance at each step
- Metadata/provenance helps with further reuse, eg. AI-ready data
- Some domain specific efforts to "FAIR"-ify data https://www.go-fair.org/

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- "good data management and stewardship is not a goal in itself, but rather a pre-condition supporting knowledge discovery and innovation" (Wilkinson 2016)
- Data management is a cross-cutting concern and not limited to the archiving and dissemination phases of the data lifecycle

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References

- Wilkinson, Mark D., et al. “The FAIR Guiding Principles for Scientific Data Management and Stewardship.” Scientific Data 3, no. 1 (December 2016): 160018. https://doi.org/10.1038/sdata.2016.18.
- McMurry, Julie A, et al. “Identifiers for the 21st Century: How to Design, Provision, and Reuse Persistent Identifiers to Maximize Utility and Impact of Life Science Data”. https://doi.org/10.1101/117812.

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Extra: Persistent Identifiers

- URI schemes. Difference from URLs.
- Opaque identifiers
- DOI, ORCID, ARK

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Wikidata: A knowledge graph for the earth sciences

Charles F Vardeman II

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ESIP Schema.org cluster: Utilizing the Schema.org vocabulary for FAIR Earth Science Data

Adam Shepherd and Doug Fills

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[Link to slides]

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NEON's first data releases: challenges and opportunities to provide FAIR data

Christine Laney

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AI strategies for improving data management components and preparing AI-ready data that meets FAIR and data provenance

Giri Prakash

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Application of FAIR Principles in Astronomy

Bruce Berriman

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Discussion…

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Explain

1. Which FAIR principle are you farther along with regarding implementation, and how would you evaluate your progress towards being FAIR? (check all that apply)
    a. Findable
    b. Accessible
    c. Interoperable
    d. Reusable
    e. Very good progress
    f. Some progress
    g. A little progress
    h. No progress