

An update from the MaRDA LIMS Working Group

Joshua Taillon, Eric Stach, & the WG members

2024 MaRDA Virtual Annual Meeting

Wednesday, Feb 21, 2024 - 3:10 EST



NIST Disclaimer

Certain commercial equipment, instruments, materials, vendors, and software are identified in this talk for example purposes and to foster understanding. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

Any opinions expressed are my own, and not a statement on behalf of the U.S. Government.

NSF FAIROS RCN on Materials (MaRCN) - FAIR DATA Theme

(Findable Accessible Interoperable Reusable Open Science Research Coordination Networks)

MaRCN Project Goals:

- **Convene** the community to develop metadata standards and shared tooling to enable FAIR materials research
- **Connect** the efforts of critical stakeholders in materials science and engineering research to support national goals

FAIR Data Theme Objectives:

Jointly Hosted Virtual Seminars: Dec. 8, 2022

1. “Microscopy & FAIR Data”, Mitra Taheri, Johns Hopkins University
2. “Electron microscopy facility data management & NexusLIMS”, June Lau, NIST

Two Working Groups: 18 months – (1) Microscopy & (2) LIMS

Co-chairs and WGs consist of recognized MSE leaders & experts

Face-to-face Kickoff meetings in May 2023 & Vendor meeting Oct. 2023

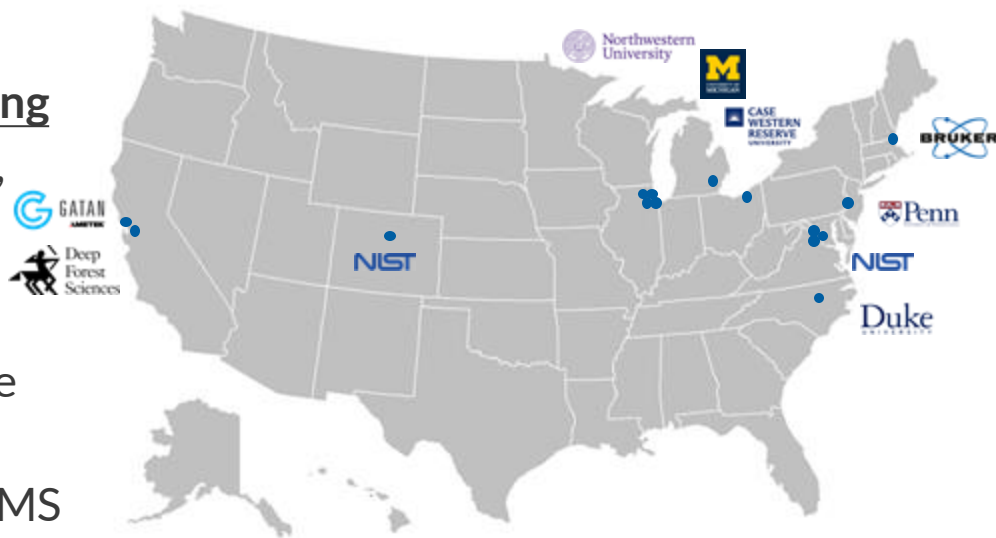


Northwestern

Introducing the FAIR LIMS Data Working Group

Brings together nationwide experts in materials science and engineering from across academia, government, and industry

Primary aim is to make recommendations to facilitate the use of LIMS in materials research and engineering



Co-Chairs

Eric Stach *University of Pennsylvania*

Josh Taillon *NIST*

Ex Officio

June Lau, *NIST*

Laura Bartolo, *Northwestern*

Members

John Allison *University of Michigan*

Jennifer Carter

Case Western Reserve University

Carelyn Campbell *NIST*

Kamal Choudhary *NIST*

Cory Czarnik *Gatan, Inc.*

Dieter Isheim *Northwestern University*

Derk Joester *Northwestern University*

Bharath Ramsundar *Deep Forest Sciences*

Roberto dos Reis *Northwestern University*

Richard Sheridan *Duke University*

Doug Stauffer *Bruker Corporation*

What do we mean by LIMS?

Laboratory Information Management Systems



LIMS are key resources supporting collaboration, scientific integrity, and transfer of knowledge over time [and can] empower a research community by establishing common tools providing access to laboratory data resources [1]



Some example functions of LIMS:

Workflow
Management

Data Repositories

Creation of Data
Products

Organization for
Data Queries

[1] "A Roadmap for LIMS at NIST Material Measurement Laboratory" NIST Technical Note 2216 (2022), National Institute of Standards and Technology, Gaithersburg, MD, [online], <https://doi.org/10.6028/NIST.TN.2216>

Working group goals

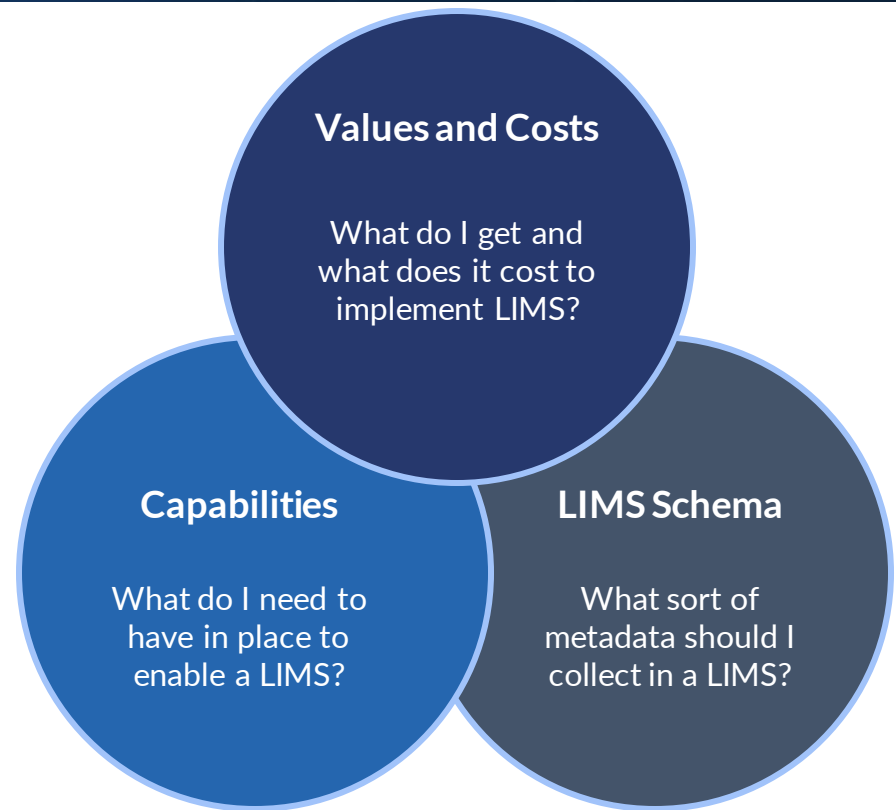
- Document best practices for recording experimental metadata in materials analysis (both research and engineering)
- Foster awareness of existing recognized schemas used in LIMS
- Identify (any) key gaps in existing schemas and metadata recording methods in current materials research practices
- Document how LIMS can benefit individuals, institutions, and the community as a whole through better practices in recording and sharing of data

Deliverables

- Documentation of various capabilities required for implementation of a LIMS
- Description of value added by LIMS, together with associated costs for various stakeholders (researchers, project leaders, facility managers, vendors, etc.)
- Review of existing recognized metadata practices in materials science and cognate disciplines (with references and links)
- Development and publication of an extensible schema appropriate for use in a LIMS to support materials research and engineering

Working group focus areas

- Working group divided into three focus areas depending on member interests
- Sub-groups work independently and periodically report back to the larger group
- Outputs of each group will be collected into a set of recommendations for final publication to the community



Progress to date and expected timeline

Early 2023	May 2023	Oct 2023	Early 2024	Spring 2024	Fall 2024
Working Groups Founded	In-person meetings to finalize proposal	Instrument vendor WG meeting	Preparation of draft recommendations	Gather feedback	Publish final recommendations
Members and chairs identified, initial in-person meeting scheduled, virtual meetings, WG proposal drafted	Working groups met at Northwestern University to hone working group proposals and expected outcomes	Working groups meet to gather feedback from instrument vendors Vendor representatives added to working groups	Working groups will prepare drafts of their recommendations and request feedback from MaRDA membership and interested parties	Drafts will be presented at MRS Spring Meeting and other venues Feedback will be gathered and incorporated to generate final recommendations	Final recommendations will be published online and in a suitable journal by August 2024

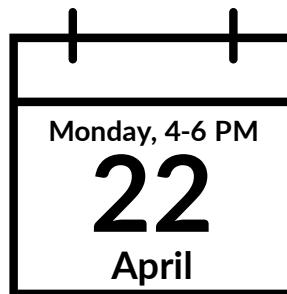
How to learn more

MaRDA Working
Groups Website

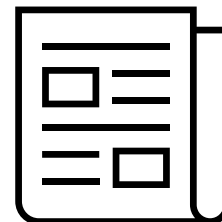


<https://www.marda-alliance.org/working-groups/>

Townhall event at 2024
Spring MRS Meeting



Publication of
Recommendations



Late 2024