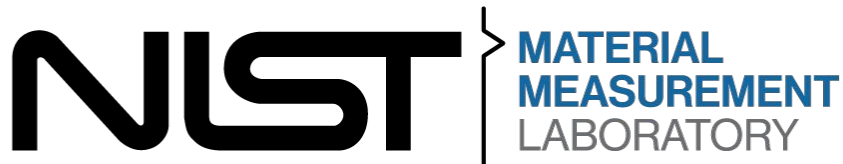


Introducing the MaRDA LIMS Working Group: LIMS Schema Development

Joshua A. Taillon

RDA P21 Breakout Session 3

Tuesday, Oct 24, 2023 - 16:25 CEST



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

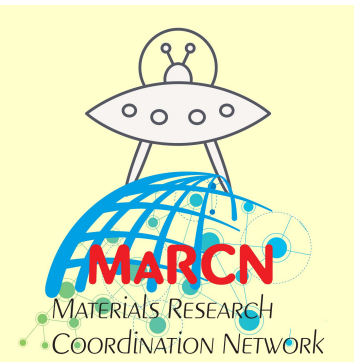
Co-chairs and WGs consist of recognized MSE leaders & experts

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

Northwestern

Two New MaRDA Working Groups

(Materials Research Data Alliance: <https://www.marda-alliance.org>)



Northwestern

Microscopy Metadata Working Group

Co-Chairs

Mitra Taheri

Johns Hopkins University

Edward Barnard

Lawrence Berkeley Lab

Maria Chan

DOE Argonne National Lab

Ex Officio

June Lau, NIST

Peter Voorhees, Northwestern

Cate Brinson, Duke

Members

Jotham Austin

University of Chicago

Eva Campo

Campostella R+C

Miaofang Chi

DOE ORNL

Anthony DiGiovanni

US Army Research Lab

Leanne Friedrich

NIST

Robert Klie

University of Illinois-Chicago

Thomas Isabell

JEOL USA, Inc.

Ying Jia

Northwestern University

Prashant Singh

DOE Ames Lab

Maureen Williams

NIST

FAIR LIMS Data Working Group

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

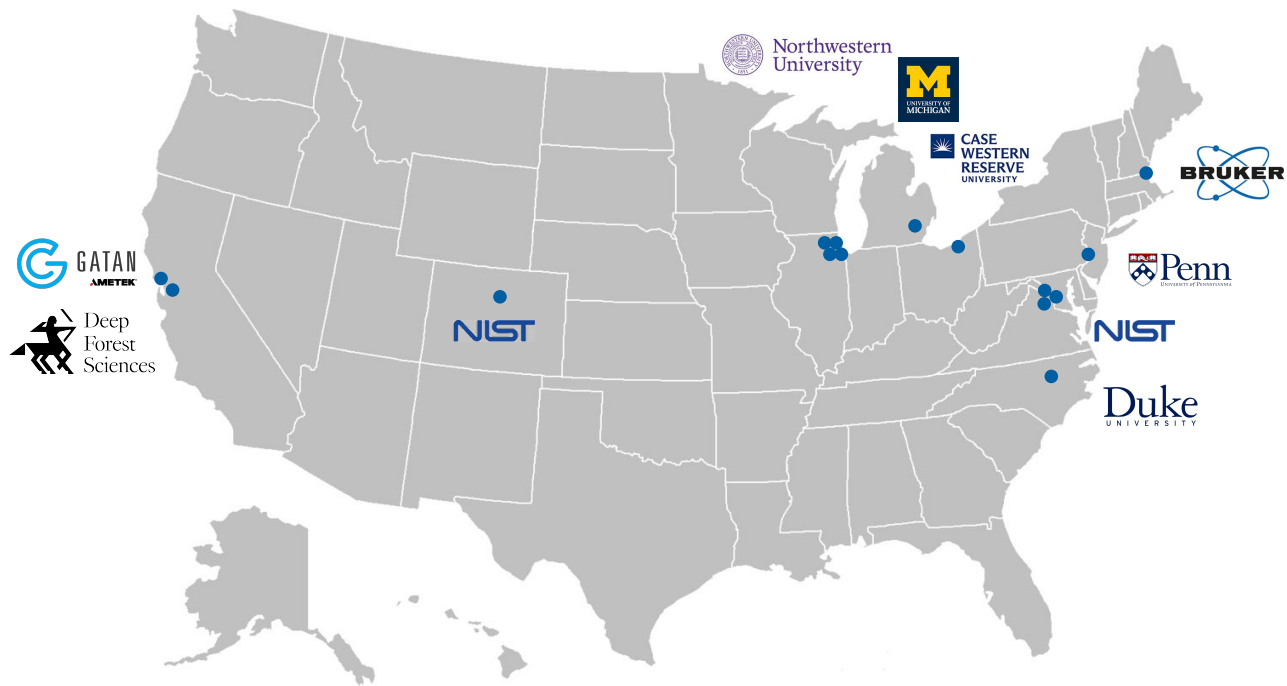
Doug Stauffer

Bruker Corporation

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



Working group goals

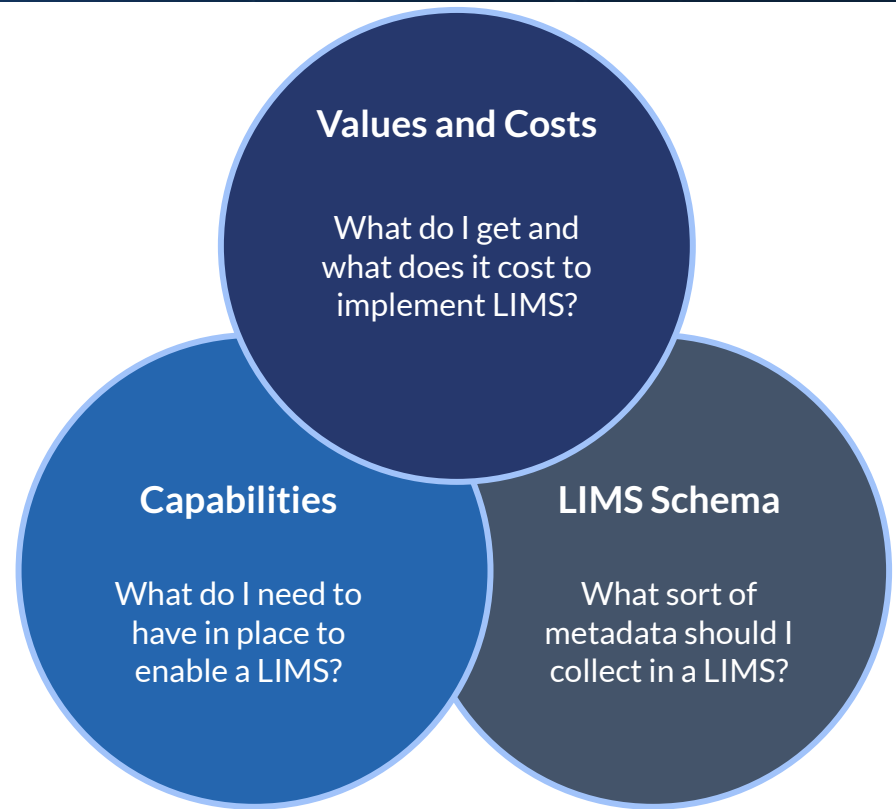
- Document best practices for recording experimental metadata in materials analysis (both research and engineering)
- Foster awareness of existing recognized schemas
- Identify (any) key gaps in existing schemas and metadata recording methods in current materials research practices
- Document how LIMS can benefit individuals, institutions, and the community as a whole through better procedures for the 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 Members and chairs identified, initial in-person meeting scheduled, virtual meetings, WG proposal drafted	In-person meetings to finalize proposal Working groups met at Northwestern University to hone working group proposals and expected outcomes	Instrument vendor WG meeting Working groups meet to gather feedback from instrument vendors Vendor representatives added to working groups	Preparation of draft recommendations Working groups will prepare drafts of their recommendations and request feedback from MaRDA membership and interested parties	Gather feedback Drafts will be presented at MaRDA annual meeting and other venues Feedback will be gathered and incorporated to generate final recommendations	Publish final recommendations Final recommendations will be published online and in a suitable journal by August 2024