

### **Polymer Pilot Project Discussion Session**

September 27, 2017, 1-5 PM, IBBR (room TBA)

A discussion session will be held for the Polymer Pilot Project Planning Group and prospective participants to see a presentation about the project and to discuss details of the project.

For more information contact: Laura Bartolo (Center for Hierarchical Materials Design), [laura.bartolor@northwestern.edu](mailto:laura.bartolor@northwestern.edu), 847-467-6244

### **Tutorials and hands-on demonstrations to cover various tools in greater depth**

September 27, 2017

1-5 PM in 2 sessions: 1-3 PM and 3-5 PM to allow attendees to participate in up to two tutorials

IBBR (various rooms, TBA)

For more information contact: Chandler A Becker (NIST Office of Data and Informatics), [cbecker@nist.gov](mailto:cbecker@nist.gov), 301-975-5344

### **Participating projects (see below for more information)**

MATIN: Materials e-Collaboration, Data Sciences and Informatics

Materials Data Facility (MDF)

Materials Knowledge System (MKS)

Cloud of Reproducible Records (CoRR)

Materials Data Curation System (MDCS) and Materials Resource Registry (MRR)

### **MATIN: Materials e-Collaboration, Data Sciences and Informatics**

**Aleksandr Blekh**

<http://materials.gatech.edu/MatIN>

This tutorial will include:

1. Using MATIN platform for managing research projects (core functionality, including Groups and Projects).
2. Using MATIN for computational materials science (simulation/modeling tools, Jupyter, HPC integration).
3. Using MATIN for managing materials data sets (Project Files, adapters, metadata management, MDCS integration).
4. MATIN roadmap / future plans.
5. Brief Q&A session (time permitting).

### **Materials Data Facility (MDF)**

**Logan Ward**

<https://materialsdatafacility.org>

The Materials Data Facility (MDF) is set of data services built specifically to support materials science researchers. MDF consists of two synergistic services, data publication and data discovery (in development). The production-ready data publication service offers a scalable repository where materials scientists can publish, preserve, and share research data. The repository provides a focal point for the materials community, enabling publication and discovery of materials data of all sizes.

### **Materials Knowledge System (MKS)**

**Daniel Wheeler**

The Materials Knowledge Systems (MKS) is a novel data science approach for solving multiscale materials science problems. It uses techniques from physics, machine learning, regression analysis, signal processing, and spatial statistics to create processing-structure-property relationships. The tutorial will explore the MKS approach using the PyMKS package. The primary focus will be on demonstrating how PyMKS is used to create process-structure-property relationships. The tutorial will try to cover some of the following (time permitting),

- Decomposing microstructure into a digital signal
- Quantifying microstructure using 2 point statistics
- Learning from a Cahn-Hilliard simulation
- Running PyMKS work in a threaded or multiprocessing environment
- Creating machine learning pipelines to cross-validate results

See <https://github.com/materialsinnovation/mks-tutorial> for more details.

Links:

- PyMKS: <http://pymks.org/en/latest/rst/README.html>
- PyMKS Paper: <http://dx.doi.org/10.1007/s40192-017-0089-0>.

### **Cloud of Reproducible Records (CoRR)**

**Faical Yannick P. Congo**

CoRR is a cloud based platform for storing, disseminating and collaborating on reproducible record objects. The hands-on demo will present use cases involving CoRR interacting with automated simulation management tools. The demo will show how to use the CoRR platform including:

- overview of CoRR components
- setting up an account,
- running a simple scientific simulation using two simulation management tools,
- setting up the simulation management tools to communicate with CoRR
- viewing and searching simulation records
- downloading record archives
- sharing and collaborating using CoRR

The demo will conclude with a discussion about the future direction of CoRR and how it might become a more widely used and eventually a fully federated platform across multiple institutions.

Please see the MGI Website [1], the CoRR Github source code repository [2] and the CoRR Github deployment repository [3] for further details.

[1]: <https://mgi.nist.gov/cloud-reproducible-records>

[2]: <https://github.com/usnistgov/corr>

[3]: <https://github.com/usnistgov/corr-deploy>

### **Materials Data Curation System (MDCS) and Materials Resource Registry (MRR)**

**Zachary Trautt**

This tutorial will present an overview of two codes to support the interoperable exchange of materials data and to enable finding and sharing of materials data resources. The first tool presented will be the Materials Data Curation System, a web-based data curation tool that is based modular community-developed data standards. The Materials Resource Registry will be demonstrated as a tool that allows materials researchers to find and share their data in a decentralized way. Both platforms support NIST's efforts in the Materials Genome Initiative.