Data Science and Optimal Learning for Materials Discovery and Design

Agenda

Hilton Santa Fe Historic Plaza
100 Sandoval Street
Santa Fe, NM 87501
505-988-2811

May 16 – 18, 2016

Day 1: Monday, May 16, 2016

8:00 ***Breakfast***

Welcome Remarks: 8:30AM—9:30AM

8:30 **Welcome, Program Overview, Logistics** ..... Turab Lookman, Frank Alexander, Stephan Eidenbenz
.....Workshop Organizers, Los Alamos National Laboratory (LANL)

8:40 **Frontiers of Mesoscale Science with Opportunities for Co-Design** ..... John Sarrao
.....Associate Director Theory, Simulation, Computation, LANL

9:00 **MaRIE Perspectives on Information Science and Learning** ..... Cris W. Barnes
.....MaRIE Capture Manager, LANL

SESSION 1: Learning from Data in Material Science: 9:30AM—12:30PM

9:30 **Designing Novel Multifunctional Materials via Inverse Optimization Techniques** .....
.....Salvatore Torquato, Princeton University

10:00 **Quantifying Uncertainties in First Principles Alloy Thermodynamics** .....
..... Nicholas Zabaras, University of Warwick

10:30 ***BREAK***

11:00 **Forward Modeling of Electron Scattering Modalities for Microstructure Quantification** .....
.....Marc DeGraef, Carnegie Mellon University

11:30 **The Potential of Network Analysis Strategies to HEDM Data: Classification of Microstructures and Prediction of Incipient Failure** .....
..... Joel Bernier, Lawrence Livermore National Laboratory

12:00 ***DISCUSSION*** .....
.....Lead: Jack Shlachter, LANL

12:30 ***LUNCH (On Your Own)***

SESSION 2: Data and Inference: 2:00PM—5:30PM

2:00 **TBD** ..... Barbara Jones, IBM Research Almaden

2:30 **Integration of Computational Reasoning, Machine Learning, and Crowdsourcing for Accelerating Materials Discovery** ..... Carla Gomes, Cornell University

3:00 ***BREAK***

3:30 **Computational Creativity for Materials Science** ..... Lav Varshney, University of Illinois at Urbana Champaign

4:00 **Optimal Experimental Design Based on Uncertainty Quantification** ..... Edward Dougherty, Texas A&M University

4:30 ***DISCUSSION*** ..... Lead: Frank Alexander, LANL

POSTER SESSION - GALLERY: 5:30PM—7:30PM

5:45 **Lightning Round** ..... Poster Presenters, 3 minutes per poster

6:30 **Poster Presentation – Light Hors D'Oeuvres Provided**

Day 2: Tuesday, May 17, 2016

8:00 ***Breakfast***

SESSION 3: High-Throughput Calculations and Experiments: 8:30AM—12:30PM

8:30 **Functionality-Driven Design and Discovery** ..... Alex Zunger, University of Colorado, Boulder

9:00 **The Use of Proxies and Data for Guiding Materials Synthesis: Examples of Phosphors and Thermoelectrics** ..... Ram Seshadri, UC Santa Barbara

9:30 **TBD** ..... Sergei Kalinin, Oak Ridge National Laboratory

10:00 ***BREAK***

10:30 **Data Driven Approaches to Combinatorial Materials Science** .....

.....Ichiro Takeuchi, University of Maryland

11:00 **Invariant Representations for Robust Materials Prediction** .....
.....Gus Hart, Brigham Young University

12:00 ***DISCUSSION*** .....
.....Leads: Blas Ueberagua, James Gubernatis, LANL

12:30 ***LUNCH (On Your Own)***

SESSION 4: Data Optimization/Challenges in Analysis of Data for Facilities: 2:00PM—6:30PM

2:00 **The MGI Data Infrastructure** .....
..... James Warren, National Institute of Standards and Technology

2:30 **Is Rigorous Automated Materials Design and Discovery Possible?** .....
.....Mike McKerns, California Institute of Technology

3:00 **Improve your Monte Carlo: Learn a Control Variate and Correct it with Stacking** .....
.....David Wolpert, Santa Fe Institute

3:30 ***BREAK***

4:00 **X-ray Free Electron Laser Studies of Shock-Driven Deformation and Phase Transitions** .....
.....Cindy Bolme, LANL

4:30 **Coherent Diffraction Imaging Techniques at 3rd and 4th Generation Light Sources**.....
.....Edwin Fohtung, New Mexico State University

5:00 **3D Data Challenges from X-ray Synchrotron Tomography** .....
.....Brian Patterson, LANL

5:30 ***DISCUSSION*** .....
..... Leads: Mark Bourke, LANL

BANQUET: 6:30—8:00PM

6:30 ***Materials Future at Los Alamos*** .....Speaker: Alan Bishop
..... Principle Associate Director Science, Technology, and Engineering, LANL

Day 3: Wednesday, May 18, 2016

8:00 ***Breakfast***

SESSION 5: Interference/HPC/Software Integration: 8:30AM—12:30PM

8:30 **Optimal Bayesian Experimental Design: Formulations and New Computational Strategies**.....
.....Youssef Marzouk, Massachusetts Institute of Technology

Agenda Continued

9:00 **Optimal Bayesian Inference with Missing Data** ..... Lori Dalton, Ohio State University

9:30 **Applying an Experimental Design Loop to Shape Memory Alloys** ..... John Hogden, LANL

10:00 ***BREAK***

10:30 **Big Data Need Big Theory Too** ..... Peter Coveney, University College London

11:00 **Combining Experiments, Simulation and Machine Learning in a Single Materials Platform - A Materials Informatics Approach** ..... Gary Delaney, Commonwealth Scientific and Industrial Research Organization, Melbourne

11:30 **Rethinking the HPC Programming Environment, what can we learn from Big Data and Cloud** ..... Galen Shipman, LANL

12:00 ***DISCUSSION*** ..... Leads: Stephan Eidenbenz, Turab Lookman, LANL

12:30 **ADJOURN**