Materials Data Science for Stockpile Stewardship Biannual Meeting

May 8th and 9th, 2023

Case Western Reserve University

Cleveland, OH

Event Program

MDS3 CENTER OF EXCELLENCE

Case Western Reserve University EST. 1826

UCF University of Central Florida

Los Alamos National Laboratory

NNSA

Lawrence Livermore National Laboratory

Kansas City NSC National Security Campus

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DAY 1, Monday, May 8th	
Tinkham Veale University Center | Ballroom A	
START TIME	**TITLE**
9:00 – 9:30 AM	**Check-in and Breakfast**
9:30 – 9:45 AM	**Welcome and Opening Remarks –** Director, Prof. Roger French
9:45 – 9:55 AM	**Senior Vice President for Research Welcome –** Dr. Michael Oakes
9:55 – 10:05 AM	**Case School of Engineering Dean's Welcome –** Dean Balakrishnan
10:05 – 10:15 AM	**State of the Center –** Managing Director, Jonathan Steirer
10:15 – 10:45 AM	**Keynote:** *Accelerating Discovery: AI for Applied Science*, Dr. Brian Spears
10:45 – 12:35 PM	**Morning Technical Session**
12:35 – 1:05 PM	**Lunch**
1:05 – 5:05 PM	**Afternoon Technical Session**
5:05 – 6:05 PM	**Technical Discussion**
The Fairmount Cocktail Bar – 2448 Fairmount Boulevard	
7:00 – 9:00 PM	**Dinner –** RSVP Required, Invitation Only

DAY 2, Tuesday, May 9th		
Tinkham Veale University Center | Ballroom A		
START TIME	**TITLE**	
9:00 – 9:30 AM	Breakfast	
9:30 – 11:00 AM	Group Research Discussion	
11:00 – 12:00 PM	Collaborator, Sponsor, & Faculty Workshop	Advisory Meeting with Dir. French (invite only)
12:00 – 12:30 PM	**Lunch**	
12:30 – 2:00 PM	Collaborator, Sponsor, & Faculty Workshop	Sponsor Meeting with Dir. French (invite only)
2:00 – 2:15 PM	Closing Remarks	

Technical Sub-Agenda

Day 1 Morning Technical Session, 10:45 AM – 12:35 PM			
START	**DURATION**	**TITLE**	**SPEAKER(S)**
10:45 AM	0:20	AISC and HPC Data Science	Prof. Vipin Chaudhary
11:05 AM	0:10	CRADLE Distributed Compute Clusters	Arafath Nihar
11:25 AM	0:10	FAIRification of PV Systems	Dr. Mengjie Li
11:35 AM	0:10	Simulation-based Digital Twins	Prof. Robert Gao
11:45 AM	0:20	ddDT case Subsurface, SunSmart, LPBF	Prof. Roger French
12:05 PM	0:10	Deep Learning for XRD of Ti-6AI-4v	Weiqi Yue
12:15 PM	0:20	Federated Learning on XRD	Prof. Erman Ayday

Day 1 Afternoon Technical Session, 1:05 PM – 5:15 PM			
START	**DURATION**	**TITLE**	**SPEAKER(S)**
1:05 PM	0:20	LANL real-time data analysis needs	Dr. Dan Savage (LANL)
1:25 PM	0:20	Robust Statistical Learning	Prof. Anirban Mondal
1:45 PM	0:20	Materials Study Protocols and Spatiotemporal Cross-correlation	Prof. Laura Bruckman
2:05 PM	0:10	Service Life Prediction of Acrylic	Hein Htet Aung
2:15 PM	0:10	GLM Modeling for Additive Manufacturing	Dr. Erika Barcelos
2:25 PM	0:20	C-V, Interdigitated Combs, FAIR	Prof. Alp Sehirlioglu
2:45 PM	0:20	Graph-based Deep Learning	Prof. Yinghui Wu
3:05 PM	0:10	Image Proc. Pipeline for FE Crystallization	Mingjian Lu
3:15 PM	0:10	FE Crystallization Kinetics	Sameera Nalin Venkat
3:25 PM	0:10	LPBF High Speed Camera Meltpool	Kristen Hernandez
3:35 PM	0:20	Fractography B sprint	Prof. John Lewandowski
3:55 PM	0:10	XCT Stress Corrosion Cracking	Tommy Ciardi
4:05 PM	0:10	Bond Wire Corrosion	Dr. Pawan Tripathi
4:15 PM	0:20	Forward Model	Prof. Frank Ernst
4:35 PM	0:10	Near Subsurface Temperatures	Deepa Bhuvanagiri
4:45 PM	0:10	Surveillance at the scale of US	Olatunde Akanbi
4:55 PM	0:20	Geospatial	Prof. Jeffrey Yarus

Visitors

Erin Barker

Pacific Northwest National Laboratory
Math, Statistics, and Data Science Group Leader

Daniel Bowen

DOE Kansas City National Security Campus
Chief Scientist – Senior Science Fellow

Kerri Blobaum

Group Leader, *Lawrence Livermore National Laboratory*
Material Characterization, Thermodynamics,
Kinetics of solid-solid phase transformations

Ian Brookes

Principal Solutions Engineer, Cloudera

Col. David Coy

National Nuclear Security Administration
Federal Program Manager for the Capability Based Investments Program

John Carpenter

Scientist, *Los Alamos National Laboratory*
Manufacturing Science

Douglas Allen Dalton

National Nuclear Security Administration
Office of Research, Development, Test, and Evaluation

Mahantesh Halappanavar

Chief Data Scientist, *Pacific Northwest National Laboratory*
Combinatorial and Graph Algorithms, Parallel Computing,
Artificial Intelligence and Machine Learning

Stephan C Hwang

Engineer, *Sandia National Laboratory*

Jay Jimenez

Postdoc, *Lawrence Livermore National Laboratory*
AM, Data Science

Bob (Robert) Maxwell

Program Leader*, Lawrence Livermore National Laboratory*
3D printing, AM, NMR, Aging and degradation

Dario Perez

Federal Account Manager, Cloudera

Dan Savage

Scientist, *Los Alamos National Laboratory*
XRD analysis (Don Browns' team)

David Schrock

National Nuclear Security Administration
Dep. Director for Non-Nuclear Capabilities
Office of Production Modernization, NA-194
Program Management, Nuclear Weapon Logistics

Brian Spears

Physicist, *Lawrence Livermore National Laboratory*
Deep learning for inertial confinement fusion

Mike Steinkamp

Manager*, Sandia National Laboratory*

Keynote Speaker

Brian Spears
Physicist, *Lawrence Livermore National Laboratory*
Deep learning for inertial confinement fusion
spears9@llnl.gov

Accelerating Discovery: AI for Applied Science

Modern science has grown so data rich that traditional approaches struggle to make use of this wealth of information. However, the convergence of high-performance computing (HPC), artificial intelligence (AI), and automated experimentation is allowing a new way to conceive of scientific operations. We describe a general framework to incorporate AI in science applications that focuses on the discovery of materials, the design of systems and components, the manufacturing of those designs, and the deployment and observation of those systems. We will demonstrate aspects of this framework on a variety of science efforts including fusion ignition, advanced manufacturing, and more. We will highlight new opportunities for "self-driving facilities" that emerge from the application of these AI methods to automated and high-repetition rate facilities from energy production to biology. We will also cover the emerging infrastructural requirements for facilities that hope to capitalize on this revolution in scientific investigation.