Conference Agenda October 4, 2021: General Topics in Machine Learning	
9:00 - 10:00 am	*Subtle quantum physics probed by STM: Examples and Lessons* Plenary Talk - Mikhail Katsnelson - Radboud University
10:00 - 10:40 am	*Generative Models and Symmetries* Invited Talk - Danilo Rezende – Google
10:40 - 11:20 am	*Towards Autonomous Experimentation for Nanomechanics with Scanning Probes* Invited Talk – Keith Brown – Boston University
11:20 am - 12:00 pm	*Quantitative Digital Microscopy with Deep Learning* Invited Talk - Giovanni Volpe - University of Gothenburg
12:00 -12:40 pm	*Dynamical systems and machine learning: combining in a principled way data-driven models and domain-driven models* Invited Talk – Michael Mahoney – University of California Berkeley
12:40 – 2:00 pm	Lunch Break
2:00 – 3:00 pm	Tutorial – Multivariate Methods *Chad Parish*
3:00 – 4:00 pm	*Tutorial – Pycroscopy: SPM in the Cloud* *Rama Vasudevan*
4:00 – 5:00 pm	Tutorial - Supervised machine learning of imaging data: DCNNs go ELIT *Ayana Ghosh and Maxim Ziatdinov*

October 5, 2021: Machine Learning in Force Based Scanning Probe Microscopies	
9:00 - 10:00 am	*Digital Chemistry and Chemputation* Plenary Talk - Lee Cronin - University of Glasgow
10:00 - 10:40 am	*Time-Frequency Analysis and Multimodal Imaging of Energy Materials Using Scanning Probe* Invited Talk - Rajiv Giridharagopal – University of Washington
10:40 - 11:20 am	*Machine Learning for Sparse Nonlinear Modeling and Control* Invited Talk – Steven Brunton – University of Washington
11:20 am - 12:00 pm	*Enabling autonomous scanning probe microscopy imaging of single molecules with deep learning* Invited Talk - Juan F. Gonzalez-Martinez – Malmö University
12:00 - 12:20 pm	*Random and sparse mixed-scale convolutional neural networks with pyMSDtorch* Contributed Talk – Eric Roberts – Lawrence Berkeley National Laboratory
12:20 – 12:40 pm	*Fast Label-Free Nanoscale Composition Mapping of Eukaryotic Cells Via Scanning Dielectric Force Volume Microscopy and Machine Learning* Contributed Talk - Martí Checa – Oak Ridge National Laboratory
12:40 – 2:00 pm	Lunch Break
2:00 – 3:00 pm	*Tutorial – Variational Autoencoders: applications and physical invariances* Maxim Ziatdinov
3:00 – 4:00 pm	*Tutorial – Mapping structure-property relationships with the encoder-decoder architectures* Maxim Ziatdinov
4:00 – 5:00 pm	*Tutorial - Rapid Unsupervised Fitting using Physics Constrained Neural Network Approximates* Joshua C. Agar

October 6, 2021: Piezoresponse Force Microscopy	
9:00 - 10:00 am	***Machine Learning for Microscopy: from Imaging to Autonomous Experiments*** Plenary Talk – Sergei Kalinin - Oak Ridge National Laboratory Automated Experiments in Electron Microscopy
10:00 - 10:40 am	*Reinforcement learning: improving behavior through evaluative feedback* Invited Talk – Michael Littman – Brown University
10:40 - 11:20 am	*"Intelligent" and Practical Machine Learning in Scanning Probe Microscopy* Invited Talk – Joshua C. Agar – Lehigh University
11:20 am - 12:00 pm	*Automated experimentation in piezoresponse force microscopy* Invited Talk – Kyle Kelley – Oak Ridge National Laboratory
12:00 - 12:20 pm	*Hystorian: A Processing Tool for Scanning Probe Microscopy and Other n-Dimensional Datasets* Contributed Talk – Ralph Bulanadi and Loïc Musy – University of Geneva
12:20 – 12:40	*The applications of novel machine-learning approaches to the laser-selective integrated additive/subtractive manufacturing of ceramics* Contributed Talk - Fei Peng – Clemson University
12:40 – 2:00 pm	Lunch Break
2:00 – 3:00 pm	*Tutorial – Gaussian Processes and Bayesian Optimization* Rama Vasudevan
3:00 – 4:00 pm	*Tutorial – Adding Physics into Bayesian Optimization* Maxim Ziatdinov
4:00 – 5:00 pm	*Tutorial – Physics Driven Multi-objective Bayesian Optimization* Arpan Biswas

October 7, 2021: Advanced Machine Learning in Microscopy	
9:20 - 10:20 am	*Plenary Talk – Eun Ah Kim – Cornell University*
10:20 - 11:00 am	*Variational Autoencoders for Physics Extraction: Latent View of Complex Processes* Invited Talk – Maxim Ziatdinov – Oak Ridge National Laboratory
11:00 - 11:40 am	*Reinforcement learning for sequential decision tasks: A novel approach for microscopy optimization and design?* Invited Talk – Matthew Taylor – University of Alberta
11:40 am - 12:20 pm	*Sifting Self-Organisation: Automated Classification of Far-From-Equilibrium Nanostructures* Invited Talk – Philip Moriarty – University of Nottingham
12:20 - 12:40 pm	*Machine-Driven Characterization and Classification over Au and WS2* Contributed Talk – John C. Thomas – Lawrence Berkeley National Laboratory
12:40 – 1:00 pm	*Characterizing possible failure modes in physics-informed neural networks* Contributed Talk – Aditi Krishnapriyan – University of California Berkeley
1:00 – 2:00 pm	Lunch Break
2:00 – 3:00 pm	*Tutorial – Deep Kernel Learning* Maxim Ziatdinov
3:00 – 4:30 pm	*Tutorial - Reinforcement Learning* *Rama Vasudevan*

Abstracts

Subtle quantum physics probed by STM: Examples and Lessons

Mikhail Katsnelson

Institute for Molecules and Materials, Radboud University, Nijmegen, Netherlands

I will discuss some examples of efficient interaction between theory and experiment in scanning probe microscopy. The first is on the discovery of "orbital Kondo resonance" on Cr(001) surface [1]; the related theoretical work is still continuing [2,3]. A very general and nontrivial issue on the role of essentially many-body physics in STM is clearly manifested in this case.
The second one is a direct observation of Berry phase in graphene by STM [4] following the theoretical prediction [5]. This is a nice opportunity to discuss topological effects observable by scanning probe microscopy.
The third one is a discovery of self-induced spin-glass state in elemental Nd via spin-polarized STM [6] following theoretical predictions of this new magnetic state of matter [7]. This illustrates the role of STM in studying general issues of statistical physics and in particular the origin of complexity.

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Generative Models and Symmetries

Invited Talk - Danilo Rezende – Google

Abstract:
The study of symmetries in physics has revolutionised our understanding of the world. Inspired by this, I will focus on our recent work on equivariant generative models and its applications to fundamental physics and molecular dynamics simulations.

Towards Autonomous Experimentation for Nanomechanics with Scanning Probes

Keith A. Brown

Department of Mechanical Engineering, Boston University, Boston, MA

Nature realizes extraordinary material properties through the hierarchical organization of polymers from the molecular scale to the macroscopic scale. However, designing polymers for desired nanomechanical performance is a grand challenge as not only are these experiments challenging to perform, but there are an overwhelming number of potential materials and processing conditions to consider. In this talk, we describe our recent progress addressing this challenge by transforming scanning probes into autonomous experimentation (AE) systems that accelerate the pace and value of experiments.

First, we discuss our efforts to use scanning probes to understand size effects in nanoscale polymers through an approach that combines finite element analysis and nanoindentation. We find that elastomeric thin films are stiffer than bulk samples in a manner consistent with enhanced crosslinking at the surface. Subsequently, in an effort to accelerate the rate at which novel materials can be studied, we describe our recent realization of a closed-loop process for using scanning probes to pattern fluids and polymers at the sub-femtoliter scale. The ability of scanning probes to both pattern and characterize polymers could enable materials research on the nanometer scale using a single instrument. To explore the degree to which such a system could accelerate research, we discuss AE systems, or automated platforms in which experiments are iteratively chosen by machine learning to maximize progress towards a chosen goal. To test the merits of AE, and study the mechanics of macroscopically structured polymers, we present an AE system that combines additive manufacturing, robotics, and mechanical characterization to rapidly print, test, and study mechanical structures. In addition to developing an understanding of the non-linear mechanics of a family of mechanical structures, we also use these studies to determine how simulation can be incorporated into AE to provide a transferable path to optimizing non-linear mechanical properties. AE systems that span additive manufacturing, machine learning, and advanced characterization have the potential for transformatively advancing the pace of research to meet the challenge of designing and understanding hierarchical materials.

Quantitative Digital Microscopy with Deep Learning

Video microscopy has a long history of providing insights and breakthroughs for a broad range of disciplines, from physics to biology. Image analysis to extract quantitative information from video microscopy data has traditionally relied on algorithmic approaches, which are often difficult to implement, time consuming, and computationally expensive. Recently, alternative data-driven approaches using deep learning have greatly improved quantitative digital microscopy, potentially offering automatized, accurate, and fast image analysis. However, the combination of deep learning and video microscopy remains underutilized primarily due to the steep learning curve involved in developing custom deep-learning solutions. To overcome this issue, we introduce a software, DeepTrack 2.0, to design, train and validate deep-learning solutions for digital microscopy. We use it to exemplify how deep learning can be employed for a broad range of applications, from particle localization, tracking and characterization to cell counting and classification. Thanks to its user-friendly graphical interface, DeepTrack 2.0 can be easily customized for user-specific applications, and, thanks to its open-source object-oriented programming, it can be easily expanded to add features and functionalities, potentially introducing deep-learning-enhanced video microscopy to a far wider audience.

Dynamical systems and machine learning: combining in a principled way data-driven models and domain-driven models

Michael W. Mahoney
ICSI and Department of Statistics, UC Berkeley

Data-driven machine learning (ML) models tend to be relatively domain-agnostic and thus are widely-applicable across many domains. A fundamental challenge in scientific machine learning (SciML) involves combining such data-driven models with fine-scale domain-driven scientific models that make strong use of domain-specific insight and that are common in physics and other natural sciences. Among other things, a domain-informed model formulation should encode some degree of stability or robustness or well-conditioning (in that a small change of the input will not lead to drastic changes in the output), characteristic of the underlying scientific problem. Here, we describe recent work on using techniques from dynamical systems theory to combine these two types of models in a principled way. We'll describe how to develop physics-informed autoencoders using Lyapunov stability, leading to novel domain-driven regularization and to models that improve the generalization error and reduce prediction uncertainty for fluid flow problems. We'll also describe ContinuousNet, a variant of the popular residual neural network (ResNet) model that is meaningfully continuous-in-depth. By embedding discrete neural network models into higher-order numerical integration schemes, e.g., Runge Kutta schemes, ContinuousNet can learn to represent continuous dynamical systems (which ResNets and other nominally-continuous models cannot); and, by exploiting ideas from numerical integration theory, ContinuousNet have improved robustness properties as well as improved training and inference properties on standard (non-scientific) ML tasks and initial SciML tasks. These results point to directions for SciML more generally.

Tutorial – Pycroscopy: SPM in the Cloud

Rama Vasudevan

Collecting, storing, processing, analyzing and visualizing microscopy data is a standard workflow for most scientists in microscopy; yet the choices available at each step, and the lack of coherence and standardization in this process leads to sub-optimal workflows with low efficiency, high redundancy and poor reproducibility.

Here, in this tutorial, we will discuss our solution: the pycroscopy ecosystem of packages, starting out with the base input/output tools with standardized data models for imaging and spectral data, and discuss how microscopy data can be read into these formats through the SciFiReaders package. Once read into sidpy dataset objects, this allows users full access to the visualization and processing capabilities of the sidpy package, which is itself built on top of dask arrays. Further processing is also possible with more domain-specific packages, including AtomAI and pyTEMLib and STEMTools, which users are encouraged to visit. Data can then be saved via the pyNSID package for completeness.

Digital Chemistry and Chemputation

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Today it is possible to design and synthesize many of the physically allowed molecules and materials conceivable if practical, yet paradoxically it is not possible to reproduce or rerun these successful procedures with high reliability. This is because many of the conditions devised for the manual or semi-manual synthesis are not uniformly recorded. The situation is even worse when the literature is investigated. For example, our preliminary studies reveal that >80% of all the published procedures fail to replicate without the help of an expert.

In this talk I will outline how we have solved this problem by devising a universal approach to chemical synthesis that allows us to translate all procedures, manual or automatic, to a new interchange format, XDL, that allows chemistry to be universally communicated. Furthermore, this new approach maps into a universal programming language for chemistry that is accessible to ALL synthetic chemists and will work on ALL robotic systems (subject to suitable specification). We demonstrate that the process is universal, and by analogy with computation, we call systems capable of universally turning code into reliable chemistry and materials processes *Chemputation*, see Figure.

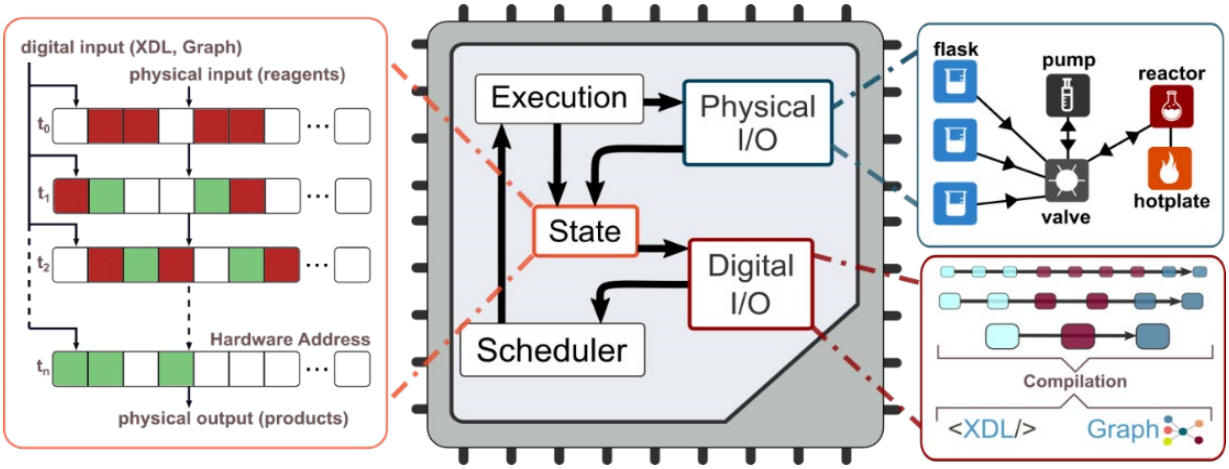

Figure: Depiction of a chemical state machine (CSM) for synthesis that is capable of Chemputation. The input is a combination of reagents, process information and hardware addresses. The CSM organizes the reagents and the processes by using a scheduler that then gets executed in the hardware as a function of the available state until the product is formed.

I will also explain why our Chemical Synthesis Machine is really a Chemical State* Machine (CSM) and why you should care. This because our CSM can be used with AI and machine learning to search for new reactivity, reactions, materials, and molecules – that once discovered, can be reproduced using the CSM. This allows us to build the ultimate system that can both reproduce, search, discover, and update chemical knowledge autonomously in real time. I will show this working with real world examples from energy materials to small molecule drug candidates.

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Time-Frequency Analysis and Multimodal Imaging of Energy Materials Using Scanning Probe Microscopy

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The combination of functional scanning probe microscopy with data science techniques has led to new discoveries on a wide range of materials. In this presentation I will discuss our work using data-driven scanning probe methods and analysis techniques as applied to functional imaging of energy materials. These projects include multimodal correlations of optical and SPM data as well as measurements of sub-microsecond dynamics using time-resolved electrostatic force microscopy (trEFM) on halide perovskite photovoltaics. I will discuss how we use newer advances in time-frequency analysis, thereby demonstrating some of the advantages of employing ideas from the broader signal processing literature in SPM techniques. Lastly, I will show how we can utilize neural networks to analyze instantaneous frequency behavior in AFM. Together, these projects represent different methods for analyzing SPM data in new ways.

Machine Learning for Sparse Nonlinear Modeling and Control

Steven Brunton – University of Washington

Abstract: This work describes how machine learning may be used to develop accurate and efficient nonlinear dynamical systems models for complex natural and engineered systems. We explore the sparse identification of nonlinear dynamics (SINDy) algorithm, which identifies a minimal dynamical system model that balances model complexity with accuracy, avoiding overfitting. This approach tends to promote models that are interpretable and generalizable, capturing the essential "physics" of the system. We also discuss the importance of learning effective coordinate systems in which the dynamics may be expected to be sparse. This sparse modeling approach will be demonstrated on a range of challenging modeling problems in fluid dynamics, and we will discuss how to incorporate these models into existing model-based control efforts.

Enabling autonomous scanning probe microscopy imaging of single molecules with deep learning

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Abstract

Scanning probe microscopies allow characterizing surfaces with high resolution in real space. However, these microscopies are not widely used considering their potential. The need of experienced users, the interpretation of data and the time-consuming experiments that require continuous user supervision are among the limitations that prevent a wider use. In this presentation, I will go through some previous works on AFM automation, with a focus on those using Machine Learning techniques. I will then present an algorithm that we recently developed for controlling the operation of an Atomic Force Microscope for the specific purpose of acquiring high-resolution images of single molecules. The algorithm made use of two deep learning techniques. One of them was an object detector, YOLOv3, whose function is to locate the molecules in the acquired images. The other one was a Siamese network, capable of identifying whether the molecules detected by the object detector in different scans corresponded to the same molecule. This allowed e.g., zooming on the same molecule while decreasing the scanned area, as well as keeping track of molecules already imaged at high resolution, thus, avoiding loops where the same molecule would be imaged an unlimited number of times.

Random and sparse mixed-scale convolutional neural networks with pyMSDtorch

Eric Roberts, Peter Zwart
Center for Advanced Mathematics for Energy Research Applications (CAMERA) at Lawrence Berkeley National Laboratory

Abstract: We introduce a new python software library, pyMSDtorch, which provides easy access to a number of segmentation and denoising methods using convolution neural networks in PyTorch. PyMSDtorch focuses on two network paradigms, both of which surpass popular U-Net architectures when labeled training data is low, namely:

1) mixed-scale *dense* network (MSDNet), a relatively simple architecture which relies on dense interconnectivity of *all* intermediate feature maps and dilated convolutions to capture features at different scales, and

2) *sparsely*-connected mixed-scale networks, a lean, lower-parameter MSDNet variant based on stochastically-generated graph networks with user-configurable complexity.

With microscopy and synchrotron-imaging/scattering data in mind, this talk will present the motivation and results for both dense and sparse networks paradigms, including comparisons with established U-Nets and aggregations of multiple lower-parameter sparse networks. Overall, this talk aims to showcase the ease-of-use and flexibility of the pyMSDtorch library.

Fast Label-Free Nanoscale Composition Mapping of Eukaryotic Cells Via Scanning Dielectric Force Volume Microscopy and Machine Learning

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Mapping the biochemical composition of eukaryotic cells without the use of exogenous labels is a long-sought objective in cell biology. Recently, it has been shown that composition maps on dry single bacterial cells with nanoscale spatial resolution can be inferred from quantitative nanoscale dielectric constant maps obtained with the scanning dielectric microscope [1]. In this presentation, I will show that this approach can also be applied to the much more challenging case of fixed and dry eukaryotic cells [2], which are highly heterogeneous and show micrometric topographic variations. More importantly, it is demonstrated that the main bottleneck of the technique (the long computation times required to extract the nanoscale dielectric constant maps) can be shortcut by using supervised neural networks, decreasing them from weeks to seconds in a workstation computer. This easy-to-use data-driven approach opens the door for in situ and on-the-fly label free nanoscale composition mapping of eukaryotic cells with scanning dielectric microscopy.

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Tutorial – Variational Autoencoders: applications and physical invariances

We will explore how variational autoencoders can be used for finding main factors of variation from high-dimensional datasets and show how the addition of rotational, translational, and scale invariances to variational autoencoders allows for better disentanglement of these (latent) factors.

Tutorial – Mapping structure-property relationships with the encoder-decoder architectures

We will explore how to use neural networks with the encoder-decoder type of architecture for predicting property (spectra) from structure (images) and for getting insights into the structure-property relationship via the analysis of the model's latent space.

Rapid Unsupervised Fitting using Physics Constrained Neural Network Approximates

Scientific experiments can generate tremendous volumes of scientific data. Conventionally, this data has been processed by fitting data to empirical expressions. This imposes challenges for high-throughput applications, noisy data, and automated control systems. Neural networks have been used a data driven surrogates to extract information from scientific data. Most of these approaches lack physical constraints making it difficult to interpret the results. Furthermore, because of the underlying mathematics these models lack parsimony. In this tutorial we combine neural network approximates constrained with empirical expressions to conduct rapid fitting of spectroscopic data. This general approach can be applied to real-time fitting of spectroscopic data broadly.

Machine Learning for Microscopy: from Imaging to Autonomous Experiments

Sergei V. Kalinin

The Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831

Machine learning and artificial intelligence (ML/AI) are rapidly becoming an indispensable part of physics research, with domain applications ranging from theory and materials prediction to high-throughput data analysis. However, the constantly emerging question is how to match the shallow correlative nature of classical ML with deep hypothesis-driven causal nature of physical sciences. In parallel, the recent successes in applying ML/AI methods for autonomous systems from robotics through self-driving cars to organic and inorganic synthesis are generating enthusiasm for the potential of these techniques to enable automated and autonomous experiment (AE) in imaging.

In this presentation, I will discuss recent progress in automated experiment in electron and scanning probe microscopy, ranging from feature to physics discovery via active learning. The applications of classical deep learning methods in streaming image analysis are strongly affected by the out of distribution drift effects, and the approaches to minimize though are discussed. We further present invariant variational autoencoders as a method to disentangle affine distortions and rotational degrees of freedom from other latent variables in imaging and spectral data. The analysis of the latent space of autoencoders further allows establishing physically relevant transformation mechanisms. Extension of encoder approach towards establishing structure-property relationships will be illustrated on the example of plasmonic structures. I will briefly discuss the transition from correlative ML to physics discovery, incorporating prior knowledge and yielding generative physical models of observed phenomena. Finally, I illustrate transition from post-experiment data analysis to active learning process. Here, the strategies based on simple Gaussian Processes often tend to produce sub-optimal results due to the lack of prior knowledge and very simplified (via learned kernel function) representation of spatial complexity of the system. Comparatively, deep kernel learning (DKL) methods allow to realize both the exploration of complex systems towards the discovery of structure-property relationship, and enable automated experiment targeting physics (rather than simple spatial feature) discovery. The latter is illustrated via experimental discovery of the edge plasmons in STEM/EELS in MnPS3, the lesser-known 2D material, and hysteresis loop measurements in PFM.

Reinforcement learning: Improving behavior through evaluative feedback

Michael Littman – Brown University

The field of reinforcement learning is experiencing a bit of a renaissance. In this talk, I will survey some of the background and foundations of this subarea and its relation to other forms of machine learning. I will also describe some recent high-profile successes of reinforcement-learning techniques including smart thermostats, automatic content filtering, and mastery of games via self play ranging from 80s-era video games to the ancient board game Go. Time permitting, I will also plug some of my own research in the area.

Michael L. Littman's research in machine learning examines algorithms for decision making under uncertainty. He has earned multiple awards for teaching and his research has been recognized with three best-paper awards and two influential paper awards. Littman has served on the editorial boards for the Journal of Machine Learning Research and the Journal of Artificial Intelligence Research. He was general chair of International Conference on Machine Learning 2013 and program chair of the Association for the Advancement of Artificial Intelligence (AAAI) Conference 2013. He is also a AAAI Fellow and an ACM Fellow.

"Intelligent" and Practical Machine Learning in Scanning Probe Microscopy

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Machine learning has become an essential analysis tool in materials science. Open-source packages (e.g., TensorFlow and PyTorch) have democratized state-of-the-art machine learning methods making them easy to adapt to materials science problems. This accessibility, however, is a double-edged sword. The easiness to deploy these powerful and adaptive models can give the perception of success, even passing conventional validation and benchmarks, without genuinely achieving a robust and physically meaningful understanding of the problem. Here, we discuss three exemplars in materials science where traditional machine learning provides unsatisfactory results. We demonstrate intelligent corrections that enable these methods to achieve practical value in accelerating scientific discovery. First, we discuss ways to extract similarity projections from a collection of >25,000 images. We show that through symmetry-aware featurization and recursive interactive projections that we can discover essential correlations in unstructured materials microscopy. Second, we demonstrate the ability of convolutional neural networks (CNNs) to give a false perception of learning 2D-wallpaper group symmetry on a dataset of more than 2 million images. We demonstrate how custom kernels can improve robustness enabling learning a general concept of 2D-wallpaper group symmetry. Finally, we show how to create ultra-compact unsupervised neural networks for real-time physics-constrained fitting of band-excitation piezoresponse force microscopy to simple-harmonic oscillator models. Our method enables fitting at >5000 fits/second on a single GPU-accelerated workstation. This provides real-time insight to guide subsequent scientific experimentations. We will conclude with a perspective on emerging opportunities for fast (sub-ms) machine learning approximates for materials characterization and control on the edge.

Automated experimentation in piezoresponse force microscopy

Kyle P. Kelley,[1] Maxim Ziatdinov,[1] Rama K. Vasudevan,[1] and Sergei V. Kalinin[1]

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Domain structures and topological defects in ferroelectric materials underpin a broad range of applications ranging from materials with giant electromechanical responses to domain wall electronics and logic devices. Correspondingly, exploring the functionalities of domain walls and controlled modifications of the domain structures is of interest for a broad spectrum of applications. However, the dynamic nature of these objects severely constrains the experimental approaches to explore their functionality. Here, we introduce fundamentally new approaches for the control and modification of domain structures within an automated piezoresponse force microscopy framework. First, we utilize real space image-based feedback to control the atomic force microscope tip bias during ferroelectric switching allowing for modification routes triggered by domain states under the tip. Specifically, by applying voltage pulses at domain walls in $PbTiO_3$ thin films in an automated fashion, we are able to create metastable phases with enhanced electromechanical response and explore domain wall dynamics. Additionally, we are able to separate reversible and irreversible domain wall motion providing fundamental insight into domain wall propagation. Secondly, we deploy a computer-vision based algorithm to identify locations of interest and track domain wall motion under an applied electric field. These studies highlight a new pathway toward discovery and control of metastable states in ferroelectrics, and more generally paves way for automated systems for controlled modification of domain walls and defects to improve material properties.

Hystorian: A Processing Tool for Scanning Probe Microscopy and Other n-Dimensional Datasets

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Research in materials science relies increasingly on the correlation of information in ever larger datasets. With this data processing becoming an increasingly important and unavoidable aspect of scientific work, modern researchers are faced with various challenges. The acquired data must first be extracted from (usually) proprietary data formats and transformed into a shape more suitable for further analysis — whereby useful physical metadata, such as the physical scale of an image, may be lost. Analysis is further complicated by the use of datasets from disparate sources, especially when quantitative comparison is required, as is increasingly becoming the norm in large scale collaborations between groups with complementary areas of expertise. This all leads to a need for processing tools that can operate on these distinct datasets, while also ensuring that both raw and processed data is stored, accessible, and verifiable.

A cross-platform Python library, *Hystorian*, has been developed to seamlessly load, merge, and operate on arbitrarily-sourced datasets [1], with a focus towards improving the traceability, reproducibility, and archival ability of scientific data processing. This is performed by converting proprietary data formats into open hierarchal data format (HDF5) files, with both datasets and the outputs of subsequent workflows automatically stored in a single location to allow easy management of the multiple data types. Wrapper functions also allow existing processing functions to apply over both raw datasets and subsequent process outputs, as well as additional metadata that is produced during data collection. *Hystorian* also contains
various in-built functions to streamline particularly materials-science data processing, including drift correction within series of (scanning probe) microscopy images, or binarization of piezoresponse force microscopy phase channels to identify the local polarization.

This presentation will begin by discussing the structure of the HDF5 files created by *Hystorian*, focusing on the benefits and ease of use brought by the file conversion process and use of wrapper functions. We then illustrate some distinct, practical applications of *Hystorian*: the integration and correlation of piezoresponse force microscopy images with second harmonic data in ferroelectric thin films to highlight the non-Ising, chiral behavior of ferroelectric domain walls; the identification and tracking of 180° domain walls in a sample cross-hatched with 90° domain walls; the interpolated positions of iced regions on a sample surface in

humid environments; and the application of unsupervised machine learning algorithms to elucidate hidden characteristics of ferroelectric domain walls.

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The applications of novel machine-learning approaches to the laser-selective integrated additive/subtractive manufacturing of ceramics

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We report the application of novel laser processing techniques such as picosecond (PS) laser micromachining and CO_2 laser ultra–fast sintering of direct ink written (DIW) alumina paste, and a machine learning approach to predict the microstructure of the laser-sintered alumina. The bulk ceramic green body of complex geometries was fabricated using the DIW method. Using CO_2 laser irradiation, we found that the extruded alumina powder can be sintered close to full density within a few tens of seconds. Since the microstructure of laser-sintered alumina is significantly different from the furnace-sintered ones, to predict alumina's microstructure under laser sintering, we developed an elegant machine learning (ML) algorithm to predict the microstructure under arbitrary laser power. We name this algorithm, regression-based conditional generative adversarial networks (GANs) with Wasserstein loss function and gradient penalty (RCWGAN-GP). After training, the RCWGAN-GP realistically regenerates the SEM micrographs under the trained laser powers, in terms of the grain size, porosity and microstructure morphologies. It also accurately predicts the alumina's microstructure under unexplored laser power. We further establish a ML-based monitoring method allowing *in situ* monitoring of microstructure during laser sintering of ceramics. We used a camera to record the brightness of the laser spot. After training using the laser spot brightness and corresponding SEM micrographs, the RCWGAN-GP can accurately predict the microstructure from the laser spot brightness. Due to the fast result-generation rate of the ML model, we are able to integrate the ML model to the laser-based manufacturing platform for the in-situ monitoring of microstructure.

Tutorial – Gaussian Processes and Bayesian Optimization

Rama Vasudevan

In this tutorial, we will explore the concept of Gaussian Process Modeling as a nonparametric Bayesian machine learning method that is useful in a host of tasks where we need flexible function approximation along with uncertainty quantification. We will observe how different kernels and different kernel hyperparameters affect the functions drawn from the process, and then utilize our knowledge to perform simple regression on some textbook examples.

Next, we will introduce the concept of Bayesian Optimization that will show how model predictions with uncertainty can be leveraged to determine the next point to sample, via incorporation of suitable acquisition functions.

Workshop Tutorial – Physics Driven Multi-objective Bayesian Optimization

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Abstract

Optimization of materials performance for specific applications often requires balancing multiple aspects of materials functionality. Even for the cases where generative physical model of material behavior is known and reliable, this often requires search over multidimensional function space to identify low-dimensional manifold corresponding to required Pareto front. In this workshop, we introduce the multi-objective Bayesian Optimization (MOBO) workflow for the ferroelectric/anti-ferroelectric performance optimization for memory and energy storage applications based on the numerical solution of the Ginzburg-Landau equation with electrochemical or semiconducting boundary conditions. MOBO is a low computational cost optimization tool for expensive multi-objective functions, where we update posterior surrogate Gaussian process models from prior evaluations, and then select future evaluations from maximizing an acquisition function. Using the parameters for a prototype bulk antiferroelectric (PbZrO3), we first develop a physics-driven decision tree of target functions from the loop structures. Then, a physics-driven MOBO architecture is developed to build and explore Pareto-frontiers by maximizing multiple target functions jointly - e.g. energy storage and loss. This approach allows for rapid initial materials and device parameter selection for a given application and can be further expanded towards the active experiment setting. The tutorial starts with theoretical concepts on traditional MOBO with illustration to a simple benchmark problem, and then extends to notebook walkthrough of the physics-driven MOBO architecture and its implementation.

Tutorial – Adding Physics into Bayesian Optimization

We will explore a hybrid optimization/exploration algorithm created by augmenting the standard GP with a structured probabilistic model of the expected system's behavior. This approach balances the flexibility of the non-parametric GP approach with a rigid structure of physical knowledge encoded into the parametric model.

Variational Autoencoders for Physics Extraction: Latent View of Complex Processes

In this talk, I will discuss applications of the invariant variational autoencoders (VAEs) to analyze imaging and spectroscopic data with problems ranging from discovering chemical reaction pathways from atom-resolved movies to disentangling domain wall geometries and switching pathways in ferroelectric materials. The connection of the learned latent representations to the system's physical complexity and the fundamental length scale of the relevant physical mechanisms will be discussed. Finally, I will discuss applying variational encoder-decoder models to the analysis of the structure-property relationships in classical and quantum systems and the prediction of functional responses from structural observations alone, and how these can be utilized for autonomous experimentation.

Reinforcement learning for sequential decision tasks: A novel approach for microscopy optimization and design?

Matthew Taylor – University of Alberta

Reinforcement learning (RL) is a type of machine learning that has recently gained significant visibility. These autonomous agents have learned to beat world-class Go champions, play video games by only observing pixels, and optimize real-world systems like ride-sharing platforms and wastewater treatment. Because microscopes are able to manipulate atoms and molecules, they can likewise be considered an agent that could be optimized. This talk will provide a brief introduction to RL and suggest how it could be used to 1) learn more efficient manipulation techniques for microscopy and 2) allow microscopes to learn to autonomously construct new artefacts.

Sifting Self-Organisation: Automated Classification of Far-From-Equilibrium Nanostructures

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Nanoparticle-solvent films deposited on solid substrates are associated with a rich dynamic behaviour that gives rise to a wide variety of striking self-organized patterns. In the far-from-equilibrium regime (i.e. where solvent evaporation is rapid), a remarkably broad array of intricate, spatially correlated patterns form including "foam-like" cellular networks, labyrinthine structures similar to those formed in spinodal decomposition of binary fluids, and fractal morphologies [1-4]. In many ways the system is a playground for self-organisation driven far from equilibrium (and, coincidentally, has many parallels with the physics of coffee stains). Its ability to generate a panoply of patterns across a wide range of length-scales provides a stringent test of the ability of machine learning algorithms to sift and classify self-organised and self-assembled structures.

We have used a combination of Monte Carlo simulations, traditional statistical approaches, and machine learning to automatically distinguish a variety of spatially correlated patterns in a broad data set of experimental AFM images of self-organized nanoparticle patterns [5]. We do this regardless of feature-scale and without the need for manually-labelled training data. I will discuss the efficacy of the machine learning approach versus more traditional statistical image analysis techniques. Although convolutional neural nets are a powerful tool, we need always be wary of Maslow's aphorism: "If all you have is a hammer, everything looks like a nail."

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Machine-Driven Characterization and Classification over Au and WS2

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Point defect identification in two-dimensional materials enables an understanding of the local environment within a given system, where scanning probe microscopy that takes advantage of hyperspectral tunneling bias spectroscopy acquisition can both image and identify the atomic and electronic landscape. Transition metal dichalcogenides (TMDs) have gained substantial interest for a variety of unique properties in its monolayer form such as serving as a host substrate for photo- and spin- active functionalization and showing promise in tunable band gap control. Here dense spectroscopic volume is collected autonomously via Gaussian process regression (gpCAM), where convolutional neural networks are used in tandem for defect identification and subsequent feedback. Monolayer semiconductor is explored on sulfur vacancies within tungsten disulfide (WS2), to provide the first hyperspectral insight into available sulfur-substitution sites within a TMD, combined with spectral confirmation on the Auf111g herringbone reconstruction for both tip state verification and local fingerprinting, where face-centered cubic (fcc) and hexagonal-closed packed (hcp) regions are detected by machine learning methods.

Acquired data enable image segmentation across the above mentioned defect modes.

Characterizing possible failure modes in physics-informed neural networks

Aditi Krishnapriyan – University of California Berkeley

Directly incorporating fundamental physical laws into the machine learning process has numerous benefits, including better generalization and more efficient learning. As such, recent work in scientific machine learning has developed so-called physics-informed neural network (PINN) models. The typical approach is to incorporate physical domain knowledge as soft constraints on an empirical loss function and use existing machine learning methodologies to train the model. Here, we characterize different challenges associated with incorporating physical laws into the learning process. We demonstrate that, while existing PINN methodologies can learn good models for relatively trivial problems, they can easily fail to learn relevant physical phenomena even for simple PDEs. In particular, we analyze several distinct situations of widespread physical interest, including learning differential equations with convection, reaction, and diffusion operators. We provide evidence that the soft regularization in PINNs, which involves differential operators, can introduce a number of subtle problems. Importantly, we show that these possible failure modes are not due to the lack of expressivity in the NN architecture, but that the PINN's setup makes the loss landscape very hard to optimize. We then describe two promising solutions to address these failure modes. The first approach is to use curriculum regularization, where the PINN's loss term starts from a simple PDE regularization, and becomes progressively more complex as the NN gets trained. The second approach is to pose the problem as a sequence-to-sequence learning task, rather than learning to predict the entire space-time at once. We can achieve up to 1-2 orders of magnitude lower error with these methods as compared to regular PINN training.

Tutorial – Deep Kernel Learning

We will explore a machine learning framework that actively discovers correlative relationships between structural data and functionalities encoded in spectroscopic measurements and uses this knowledge to guide the experiment.

Tutorial - Reinforcement Learning

Rama Vasudevan

In this final tutorial, we will explore the concepts of reinforcement learning (RL) from a practical perspective. We will begin with a short discussion of two types of algorithms: Q learning, and the actor-critic algorithm, for discrete and continuous action tasks, respectively. We will explore how to implement these within Colab notebooks for some simple examples within the OpenAI Gym environments. We will discuss potential applications of RL within microscopy and the steps needed to turn these simple examples to real, tangible RL policies for microscope control.