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SURROGATE MODELING FOR MUED WITH NEURAL NETWORKS

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Abstract

Electron diffraction is among the most complex and influential inventions of the last century and contributes to research in many areas of physics and engineering. Not only does it aid in problems like materials and plasma research, electron diffraction systems like the MeV ultrafast electron diffraction (MUED) instrument at the Brookhaven National Lab also present opportunities to explore and implement surrogate modeling methods using artificial intelligence/machine learning/deep learning algorithms. Running the MUED system requires extended periods of uninterrupted runtime, skilled operators, and many varying parameters that depend on the desired output. These problems lend themselves to techniques based on neural networks(NNs), which are suited to modeling, system controls, and analysis of time-varying/multi-parameter systems. NNs can be deployed in model-based control areas and can be used simulate control designs, planned experiments, and to simulate employment of new components. Surrogate models based on NNs provide fast and accurate results, ideal for real-time control systems during continuous operation and may be used to identify irregular beam behavior as they develop.

INTRODUCTION

MeV Ultrafast Electron Diffraction (MUED) [1, 2] is a class of high-energy electron diffraction instrument employed for novel materials characterization. The MUED system leverages the large interaction cross-section between electrons and matter to yield diffraction patterns of high spatial resolution that can resolve fine structural details. However, as with all complex instruments, MUED systems require downtime between experiments for beam alignment, operator input, data processing, diagnostics, and other typical procedural delays.

Surrogate modeling can be used to cut down some of these delays. Whenever a diagnostic would be inconvenient or destructive, having a similar or nearly equivalent system to apply it to instead can save a lot of time. Similar sentiments towards beamline stabilization can also be made. Machine learning (ML) offers a variety of models in this vein, including deep neural networks (DNNs). DNNs are already capable of acting as learning surrogate models [3] and show promise towards solving a wide array of inverse problems. Because DNNs are already employed to make accurate predictions toward electromagnetic and optical problems [4], this also makes them good candidates for choosing good beam parameters for a desired output in real time.

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SIMULATIONS

One of our interests is to build a surrogate model of MUED that supports control tasks and optimization of the beam, which should result in increased resolution of the experiment. A surrogate model can be used effectively during online operation because it has been pre-trained with previous available experimental data and with data from simulations. We need to get sufficient data in order to train an accurate model. Experimental dedicated runs for data production may be scarce, or impact the user's schedule, and are in general expensive. This is our motivation to look into detailed computer models of MUED as a way to populate the training data set that will lead to the surrogate model.

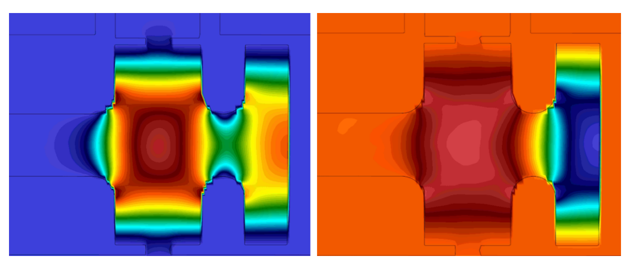

Figure 1: Pass-band modes of the 1.6 cell RF gun of MUED. Left is the 0-mode and right is the π mode.

We are using `VSim` [5], an electromagnetic and Particle-in-Cell software developed by Tech-X, to create an accurate model of the electrodynamically active regions of MUED, like the radio-frequency gun and the compensating solenoid, and all the way to the sample location. For example, Fig. 1 shows the longitudinal electric field corresponding to the two pass-band modes of the MUED RF gun as modeled in `VSim`: in the 0-mode, the two cavities are on phase while on π-mode, which is the mode of operation, the cells are off phase. Note the fractional cell is required so that the electric field is maximized at the location of the photo-cathode, ensuring the efficient extraction of electrons.

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VSim scales really well into High Performance Computing in similar beam simulations [6], which will be very important when we get to the data production phase for the surrogate model, since using our allocation at the Argonne Leadership Computing Facility will enable us to create a big ensemble of MUED simulations with different operating conditions in a short amount of time.

EXPERIMENTAL

The Accelerator Test Facility at Brookhaven National Lab houses the MUED instrument, which has the system parameters shown in Table 1. Its 1.6-cell RF gun operates at a resonance frequency of 2.856 GHz with a maximum repetition rate of 48 Hz to produce 2-5 MeV electrons. To generate these electrons, a frequency-tripled Ti:Sapphire drive laser producing near-infrared pulses is directed towards a copper cathode, which emits femtosecond electron pulses by way of the photoelectric effect. This is followed by the sample chamber, an RF deflecting cavity, and then a high efficiency detector four meters down the line whereupon the diffraction pattern is imaged with a phosphor screen.

Table 1: MUED Source Paramaters for Typical Operation

Beam energy:	3 MeV
Number of electrons per pulse:	1.25×10^6
Temporal resolution:	180 fs
Beam diameter:	100 - 300 µm
Repetition rate:	5 - 48 Hz
Number of electrons per sec per μm^2:	88 - 880

DISCUSSION

The COVID-19 pandemic has delayed experiments on the MUED instrument. However, because a model of it is being developed in VSim, we may still be able to move forward with the DNN-based surrogate model. While the VSim model is currently mostly used to characterize the electromagnetic modes of the RF gun's accelerating cavity, we will also be able to use it to generate simulated data in order to pre-train the DNN-based surrogate. Once experiments on the MUED instrument begin again, we would then be able to just refine our DNN with real data from only a few experiments [7], but it may require significantly more; in this case, data gathered from normal operation of the instrument by other users can be used to supplement the surrogate's training data. This DNN-based surrogate model will serve as a testbed for total ML-based controls of the MUED instrument, enabling start-up, initialization, and operations with minimial operator intervention and in situ corrections and analysis in order to increase experimental throughput and the rate of novel materials discovery.

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