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DESIGN OF A SURROGATE MODEL FOR MUED AT BNL USING VSim, elegant AND HPC

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Abstract

The MeV Ultrafast Electron Diffraction (MUED) instrument at Brookhaven National Laboratory is a unique capability for material science. As part of a plan to make MUED a high-throughput user facility, we are exploring instrumentation developments based on Machine Learning (ML). We are developing a surrogate model of MUED that can be used to support control tasks. The surrogate model will be based on beam simulations that are benchmarked to experimental observations. We use VSim to model the beam dynamics of the radio-frequency gun and Elegant to transport the beam through the rest of the beam-line. We also use High Performance Computing resources from Argonne Leadership Computing Facility to generate the data for the surrogate model based on the original simulation as well as training the ML model.

INTRODUCTION

The MeV Ultra-fast Electron Diffraction (MUED) system at Brookhaven National Laboratory (BNL) is a unique research tool that enables the study of the crystalline structure of materials using electron diffraction [1]. At the center of the MUED operation is the radio-frequency gun, which provides an energy gain of 3 MeV to the electron beam [2]. The high accelerating gradient helps reduce the space charge effect in the beam, which is significantly reduced with increasing energy. The electron gun is a normal conducting radio-frequency cavity, composed of 1.6 cells and designed to operate at 2856 MHz in the TM_{010}, π-mode [2]. The electron beam is produced via photo-electric effect on a Cu cathode using a frequency-tripled Ti:Sapphire laser. The Cu cathode doubles as the wall of the half-cell of the rf gun. A solenoid magnet sits immediately after the rf gun, and it helps focusing the beam. A pair of horizontal and vertical corrector magnets are also used to control the beam towards the collimator, the sample holder and the detector, which sits 4 m downstream. Figure 1 shows a photograph of the beam optics elements of MUED. After the material sample, the beam drifts for a long stretch, which improves the resolution on the diffraction pattern. The MUED detector is a Phosphor screen and is imaged with a cryogen-cooled Andor CCD camera.

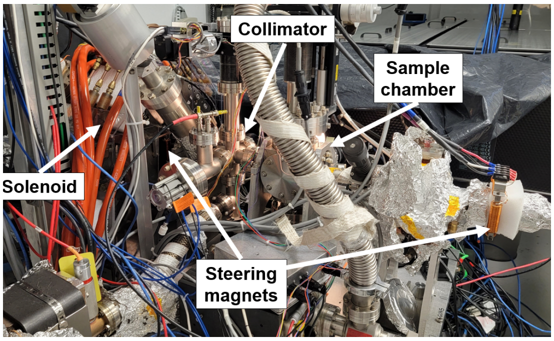

Figure 1: The MUED focusing magnets and sample holder.

MUED also has the capability of laser-pumping the material sample. The Ti:Sapphire laser can be used to photo-excite the material sample, this can drive phase transitions in the material, and can be analyzed by looking at the evolution of the diffraction patterns before and after a time-zero T_0 when the laser pulse arrives at the sample.

With these capabilities on-hand, there is interest in developing the instrumentation of MUED to maximize the throughput of science and users, and to minimize the facility experimental down-time. As MUED users, we are exploring the use of ML and optimization tools to support MUED operations. After our first dedicated beam-time at BNL, we learned that an important concern for experimental data-runs is the energy jitter of the electron beam. Energy variations arise from variations in the rf phase of the gun. Variations in beam energy directly translate into the aperture angle of the diffraction patterns, making the laser-pump measurements particularly noisy. We believe ML and optimization tools can be deployed at MUED to help with the beam stability. In particular, we envision a surrogate model capable of taking the detector images as inputs and producing the required instrument control settings that optimize the beam [3–5].

SURROGATE MODEL FOR MUED

Computer simulations are generally used as a way to understand the dynamics of a system, whether on the developing phase or when trying new system configurations. Simulations can provide accurate results, but more often than not, the computing time required to produce a solution is not suitable for real-time operations.

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We are creating an end-to-end simulation of MUED that accurately replicates the experimental observations. This simulation can then be used to calculate the expected output beam phase space given a set of input parameters. By running the simulation for thousands different sets of input parameters, we can produce data to train our ML model, effectively coding the accuracy of the computer simulation into a ML model capable of producing an output fast enough that it can be used for real-time control [3]. We are basing our simulation on the nominal values of the instrument [2] and will introduce random variations of these parameters and in different combinations. A surrogate model can also be used to help diagnose the system by acting as virtual diagnostics where instrumentation is not physically available, or the impact to operations is considerable, e.g. when using destructive diagnostics.

In its current state, most of the MUED health checks rely on the camera detector. Because of this, we envision a ML model that takes the image from the Andor camera as an input, and outputs the required instrumentation settings that optimize the beam given some constraints. For MUED in particular, the energy stability of the electron beam translates into high-resolution diffraction patterns. Figure 2 shows an example of the un-diffracted data we collected during our last dedicated user beam-time.

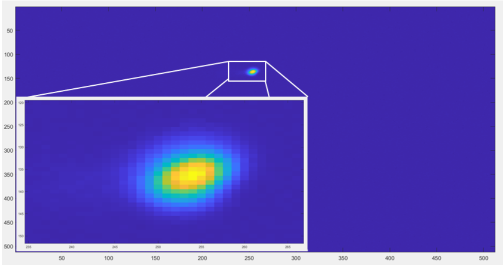

Figure 2: Un-diffracted electron beam as imaged at the MUED detector.

Computer Model of MUED

The reality of ML models is that they are only as good as the data used for training. In designing a reliable surrogate model of MUED, we want our simulation to capture as much detail from the system as possible, and to produce accurate results. We differentiate two main regions of the MUED beam-line: the radio-frequency gun and the beam optics elements. This distinction is because of the nature of the electromagnetic fields present, where the electron gun operates in radiofrequency, but the beam optics elements are DC. We are particularly interested in an accurate model of the rf gun and variations of the rf phase. For this reason, we use VSim [6, 7] to model the electromagnetic active region of MUED and Elegant [8] to propagate the beam through the rest of the beamline. Figure 3 shows a cross-section view of the rf gun in VSim. VSim uses finite-difference time-domain methods to resolve the electrodynamics inside the simulation region. The rf gun is driven by a rectangular waveguide and the model includes tuners, as well as laser and vacuum ports. Elegant takes the beam produced by VSim as an input, and propagates the beam phase space along the rest of the beam-line.

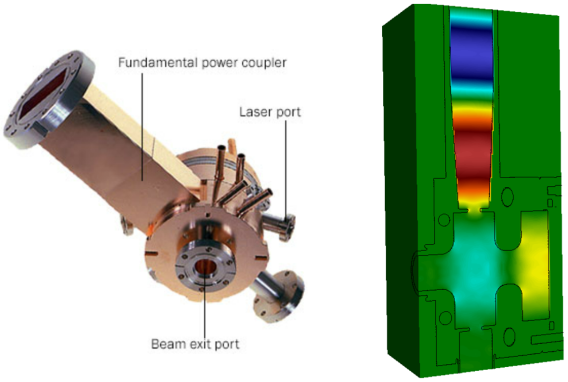

Figure 3: The 1.6 cell radio-frequency gun at BNL (left). A VSim simulation showing the longitudinal electric field inside the electron gun (right).

The available input parameter space that we are able to model with our simulation is summarized in Table 1. The output of the combined simulation is the beam phase space at the detector. The effects of misalignments can also be included in the parameter space.

Table 1: Input Parameter Space of the MUED Simulation

Parameter	Code
RF freq.	VSim
RF phase	VSim
Input power	VSim
Phase space (IN).	VSim
Sol. field strength	Elegant
Correctors (H/V)	Elegant
Collimator pos.	Elegant

High Performance Computing

In order to be able to produce thousands of data-points using our VSim simulation, we rely on the use of HPC to expedite the computation time. We have deployed VSim in the THETA supercomputer at the Argonne Leadership Computer Facility and optimized the hardware affinity for VSim PIC simulations. Figure 4 shows the optimal use of parallel processes is 1024.

COMMENTS

This is an on-going effort. Here we describe the MUED instrument at BNL and discuss a plan for creating a surrogate model using computer simulations. We are using VSim and Elegant to simulate the beam dynamics from the cathode to the detector. VSim is used to model the rf gun, including the waveguide, ports and tuners. Elegant is used to simulate

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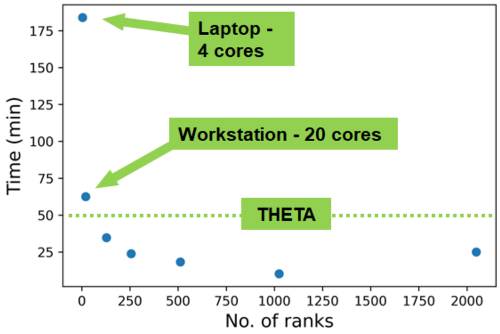

Figure 4: Optimization of parallel processes on a VSim PIC simulation at THETA.

the beam along the beam optics DC elements. Using this model, we are now benchmarking our simulation to existing un-diffracted beam date recorded during experimental runs. To create a surrogate model of MUED, we need to run multiple simulations with different initial conditions that can serve as training data for our ML model. We use the THETA supercomputer at ALCF to optimize the individual simulation run time.

Future Work

In the near term, our group is scheduled for beam-time in the Summer of 2022, we are planning to integrate our codes with the control interface of MUED and start collecting instrumentation data to evaluate the accuracy of our model. We are also submitting simulation jobs to THETA to produce training data for our ML model and to use THETA for training of the ML model. We are planning to test multiple ML algorithms and to optimize the hyper-parameters using the resources available at ALCF.

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