Updates on the surrogate model design for MUED

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Abstract

The MeV Ultrafast Electron Diffraction (MUED) system at Brookhaven National Laboratory presents a unique capability for material science. As part of the plan to make this a true user facility, we are exploring machine development approaches based on tools like Machine Learning, we are designing a surrogate model of the MUED beamline to support control tasks of the instrument. We use VSim to model the beam dynamics of the rf gun and elegant to transport the beam through the rest of the beamline. We use High Performance Computing to generate the data for the surrogate modeling based on the original simulation as well as training of the model.

The MeV Ultrafast Electron Diffraction beam-line at BNL

- The MUED system at Brookhaven National Laboratory uses ultra-short pulses of MeV electrons to produce high resolution diffraction images of materials.
- MUED is composed by a radiofrequency gun and optical elements to help direct the beam into the sample and into the detector.

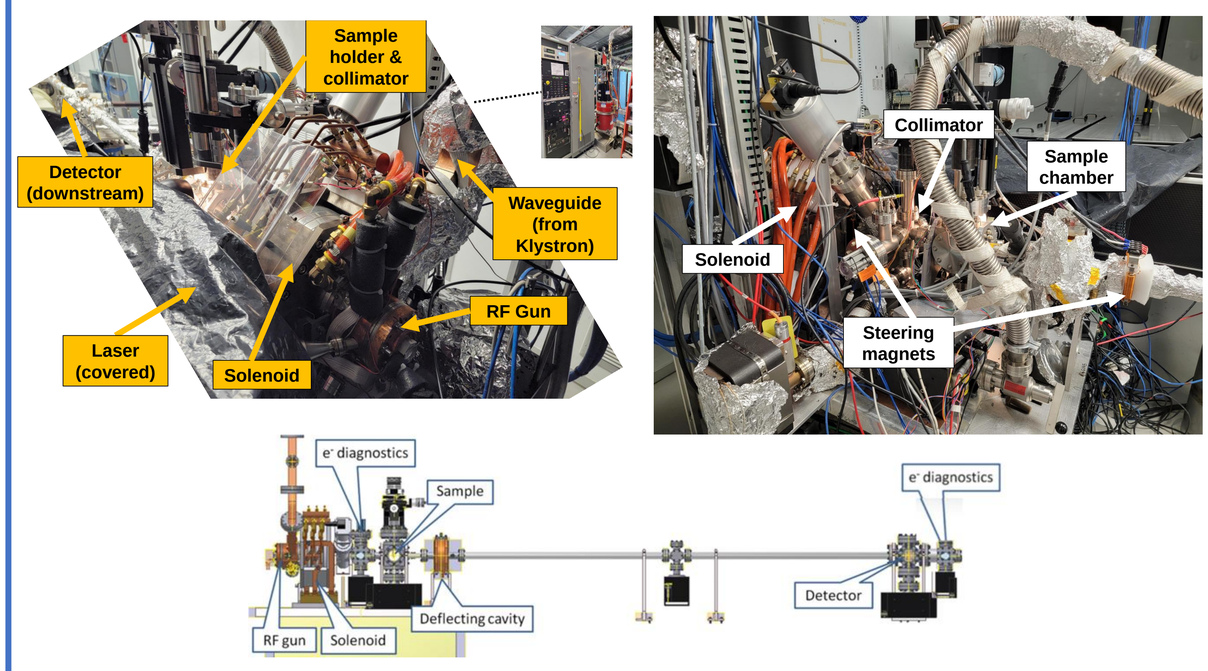


Figure. The radiofrequency gun and beam control elements of MUED.

- The 2856 MHz normal conducting radiofrequency gun.
- A solenoid helps focus the beam after the gun.
- Horizontal and vertical corrector magnets help direct the beam towards the sample and into the detector downstream.
- Collimator and sample holder.
- The detector sits at the end of the beamline and is imaged by an *Andor* camera.

- Our interest in MUED is two-fold, to maximize the throughput of experimental data by integrating ML algorithms into the data analysis and processing, and to minimize instrumentation downtime by means of intelligent controls.

Summary and future work

- We are using VSim (rf gun) and elegant (optical elements) to simulate the beam dynamics of the MUED instrument at BNL.
- This model will be used to train a surrogate model of MUED, suitable for controls and operations.
  - A surrogate model harness the accuracy of physics-intensive simulations, while capable of producing a result close to real-time.
- We are coupling our simulation capabilities with the HPC resources at the Argonne Leadership Computing Facility.
  - Including real-time data transfer, analysis and processing between ATF-BNL and ALCF through a Globus Point.
- We are scheduled for beam-time later this Summer. We'll benchmark our model against experimental data and produce data for training.

End-to-end simulation of MUED

- We use VSim and elegant to model the beam dynamics of MUED.
  - VSim is used to model the rf gun in full detail, including waveguide, ports and tuners.
  - Elegant tracks the beam through the rest of the beamline.
- We use THETA supercomputer @ ALCF to expedite the VSim simulations.
  - Also, for ML data production and training.

https://txcorp.com/vsim/

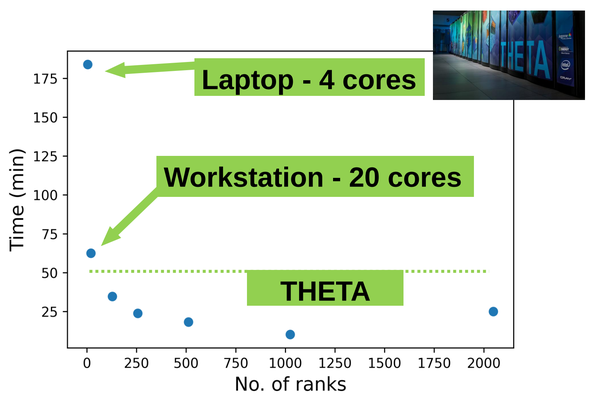


Figure. PIC code parallel optimization.

- Benchmarking simulation to experimental data (Summer 2022).

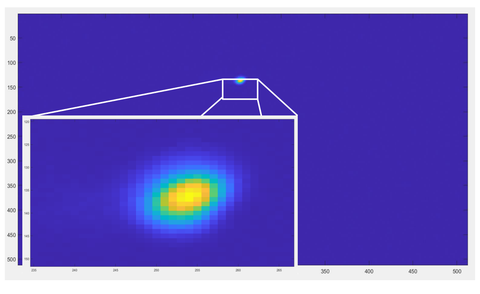


Figure. Benchmarking. Example of un-diffracted electron beam at the detector.

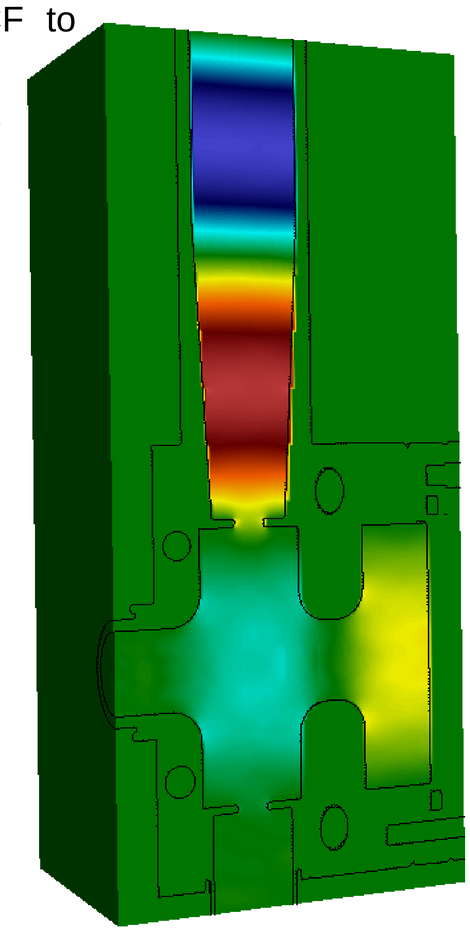
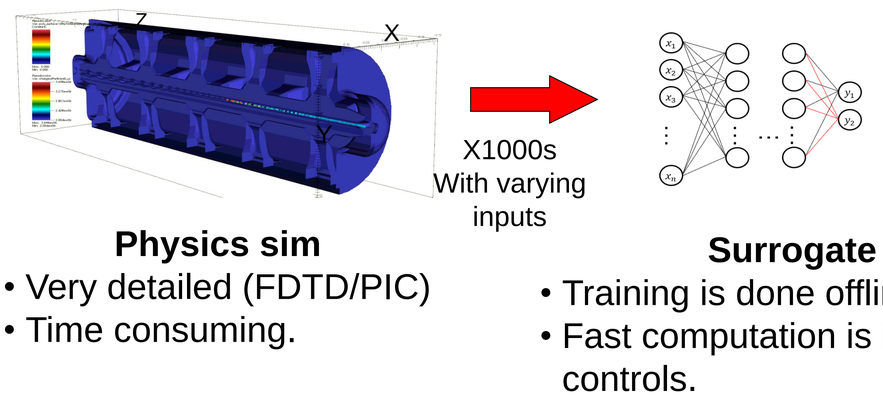


Figure. The longitudinal electric field on the MUED rf gun (VSim).

Surrogate model plan for MUED

- We are investigating surrogate models to support MUED operations.
- Physics simulations can produce accurate results but are also time and computationally intensive.



Physics sim
- Very detailed (FDTD/PIC)
- Time consuming.

Surrogate model
- Training is done offline.
- Fast computation is better suited for controls.

- Training data-set requires thousands of VSim-Elegant simulations with varying inputs.
  - Use of HPC and automation is required.

References

[1] X. J. Wang, X. Qiu and I. Ben-Zvi, "Experimental observation of high-brightness microbunching in a photocathode rf electron gun," in *Phys. Rev. E 54.R3121, 1996.*

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