PROPOSAL ID:UED-308096

SCHOOL OF ENGINEERING

ADVANCED CONTROL OF THE ATF MUED ELECTRON BEAM USING AUTOMATION, ARTIFICIAL INTELLIGENCE, AND HIGH-PERFORMANCE COMPUTING

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Funding source:

DOE's Established Program to Stimulate Competitive Research (EPSCoR). Status: Funded.

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Los Alamos NATIONAL LABORATORY EST.1943

Founding source: DOE's Established Program to Stimulate Competitive Research (**EPSCoR**).

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Funding secured through DOE EPSCoR program

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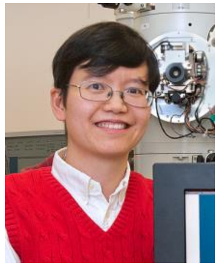

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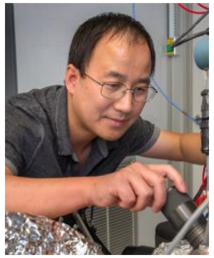

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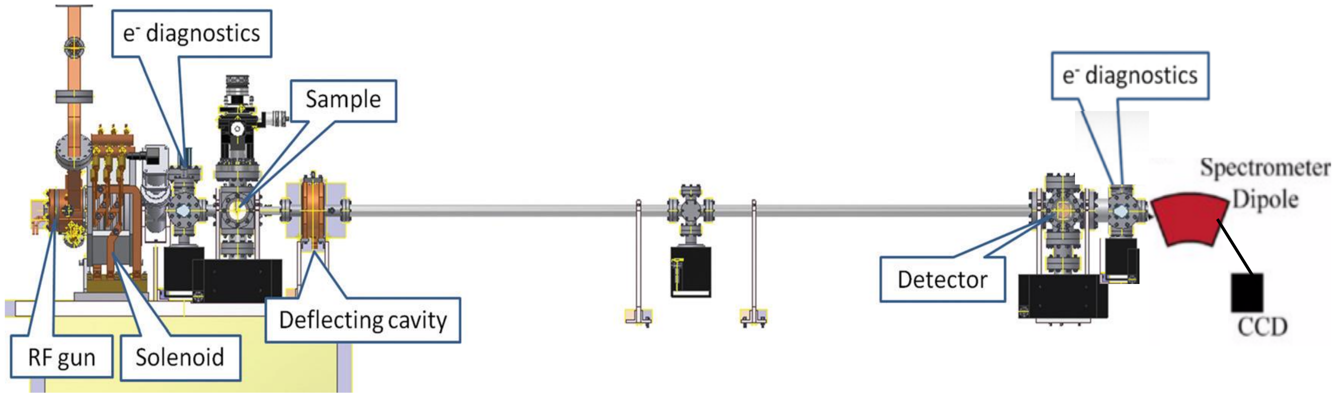
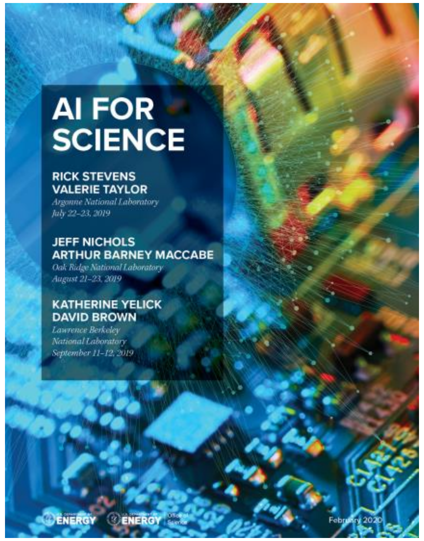
Two DOE facilities are involved: ATF and ALCF

Accelerator Test Facility (ATF)



Argonne Leadership Computing Facility (ALCF)



The combination of machine hardware, advanced computing for simulation, and data science for surrogate modelling, training of neural networks and data analysis is inspired by our past work and our participation on DOE meetings, workshops and reports such as AI for Science (*https://www.anl.gov/ai-for-science-report*).

Special Equipment Requirements and Hazards

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- Experiment requires UED Beam.
- Some simultaneous operation with a dedicated sample and pump laser would be optimal for complete data set collection.
- Special Equipment:
  - Additional data-loggers might be needed to record the MUED diagnostics data.
  - FPGA might be needed to integrate the ML-controllers into MUED.
- Special Requirements:
  - Data storage and data transmission infrastructures to external computing resources.
- Hazards:
  - Those existing during accelerator operation: electrical, rf power, laser.

Experimental Time Request (CY2021)

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Experimental Time Request

CY2021 Time Request

Capability	Setup Hours	Running Hours
UED Facility	150	150

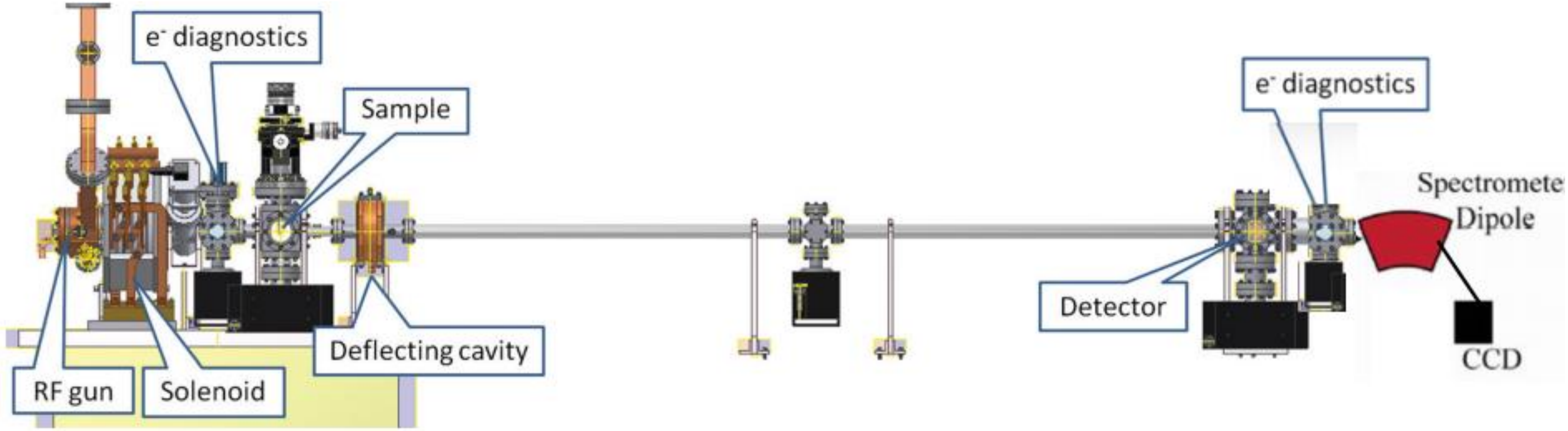
Time Estimate for Remaining Years of Experiment (including CY2021)

Capability	Setup Hours	Running Hours
UED Facility	150	150

MeV-Ultrafast Electron Diffraction System

MUED is a well-established technique to study the crystal structure of solids

- Brookhaven National Laboratory (BNL) developed a femtosecond time-resolved MeV-class electron diffraction instrument.
- Use a high-gradient electron gun and small number of electrons (~10^{4-6}) emitted in a short time period.
- Overcomes space-charge effects dominant in electrostatic electron diffraction systems: (TEM/SEM/STEM) .



M.A. Palmer, M. Babzien, M. Fedurin, C.M. Folz, M. Fulkerson, K. Kusche, J. Li, R. Malone, T. Shaftan, J. Skaritka, L. Snydstrup, C. Swinson, F.J. Willeke, "Installation and Commissioning of an Ultrafast Electron Diffraction Facility as part of the ATF-II Upgrade," Proceedings of NAPAC2016, Chicago, IL, USA, 742-744.

Overarching research goals (3 years)

Automation, optimization, AI in support of ATF/MUED operations:

- Control of accelerator and peripherals (1 year).
  - This proposal (**308096)**, funded by DOE's EPSCoR.
  - Proposal by A. Aslam (**308095)**, Cornell Center for Bright Beams, funded by NSF.
- Material sciences (3 years).
  - Proposal by M. Fazio (**308073)**, funded by DOE's EPSCoR.

Research motivations

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- To reduce the time to *materials discovery* by increasing sample and user throughput with enhanced MUED operation.

- To provide stable, robust control and rapid *in-situ* data analysis via AI/ML and high-performance computing (HPC) resources.

- To promote synergistic relationships between DOE user facilities and universities (ATF-BNL, ALCF-ANL, LANL, UNM).

Argonne Leadership Computer Facility

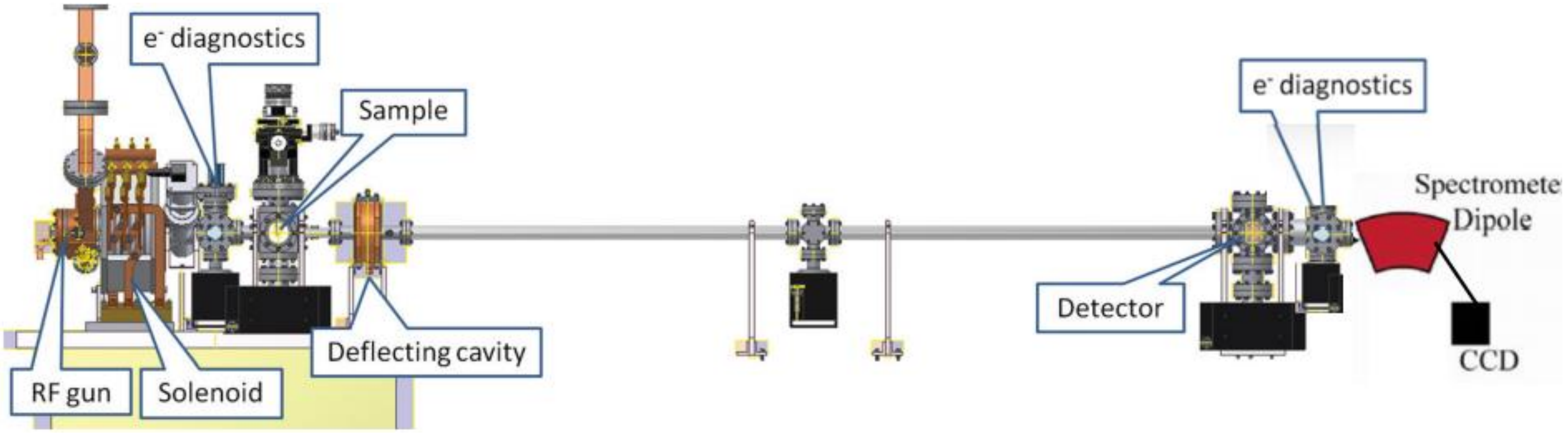
- Our AI for accelerators projects have allocations at the ALCF’s THETA supercomputer.

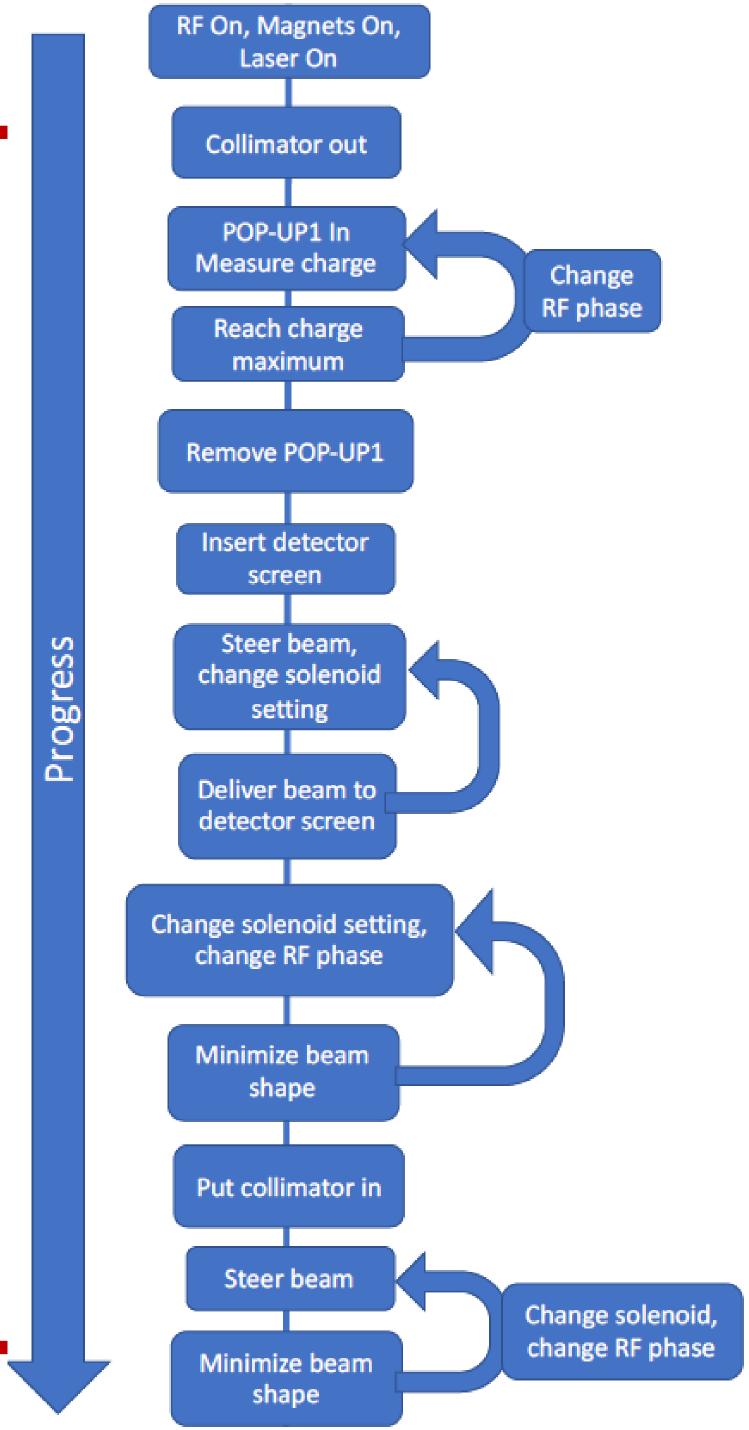
- We currently use THETA for:
  - Electromagnetic and PIC simulations using VSim.
  - Deep learning and optimization.
  - Surrogate models
  - Training of AI-based controllers.

- Multiple computation resources and experimental user facilities are available at DOE labs like ORNL, LANL, SLAC, etc.

THETA is a 11.69 petaflops system based on the second-generation Intel® Xeon Phi™ processor, **281,088 cores.**
For more information: https://www.alcf.anl.gov/theta

Automation of accelerator control tasks





Automated initialization

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- Input from accelerator operators.
  - Need to know existing procedures for initialization, and different settling times.
  - Identify steps and time intervals that can be conducted automatically.
  - Need to have **complete diagnostics** to check the system evolution.

- An automated initialization manager would bring the system to a "ready-for-users" configuration in as short as time as possible

- Dedicated electron beam runs would be needed to test that the system is in fact being initialized as expected.

Automation of accelerator control tasks

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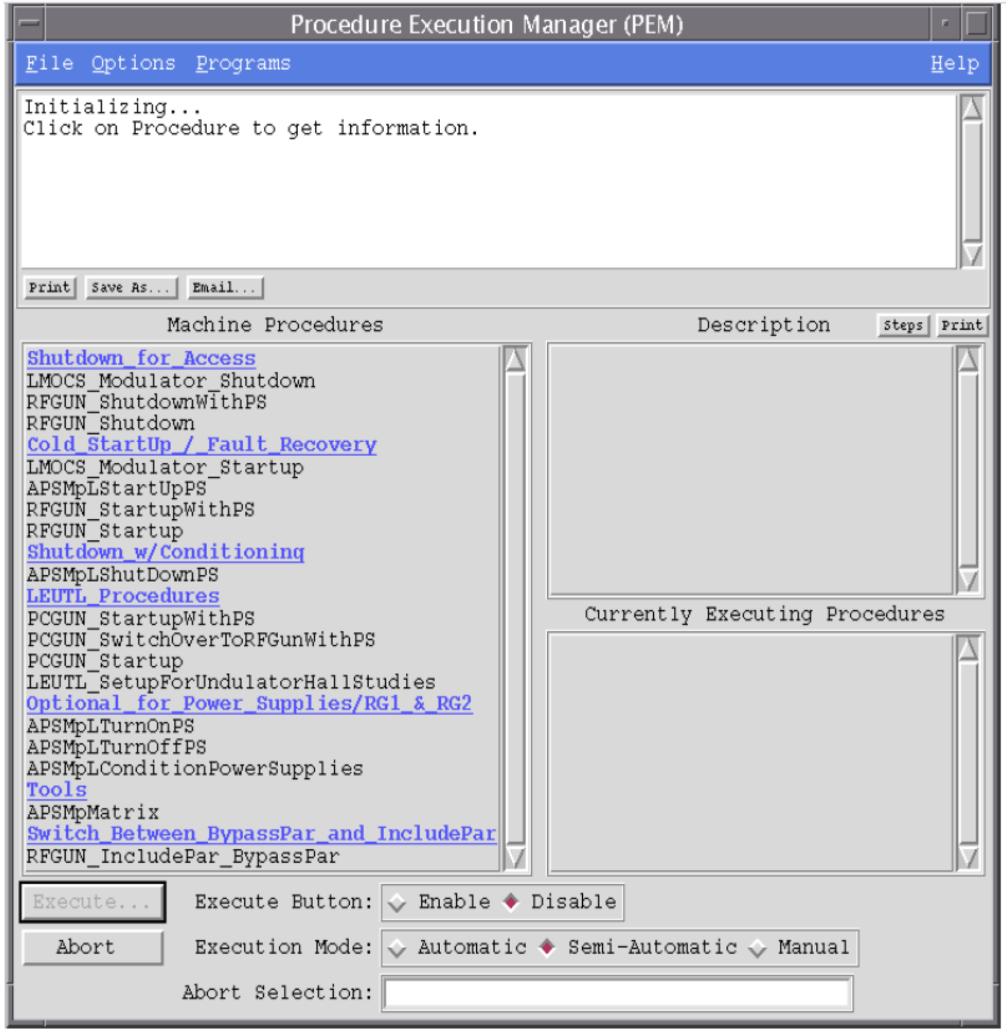
- Automation and task managers reduce operator intervention in recurrent, time-consuming tasks:
  - Initialization
  - Long term stability
- Our group collaborators have experience in automating tasks of accelerators control.
  - Procedure Execution Manager for the Advanced Photon Source Linac
- Two-step automation and control framework:
  - Automation using standard control methods and managers.
  - Incorporate intelligent tools like optimization and AI.

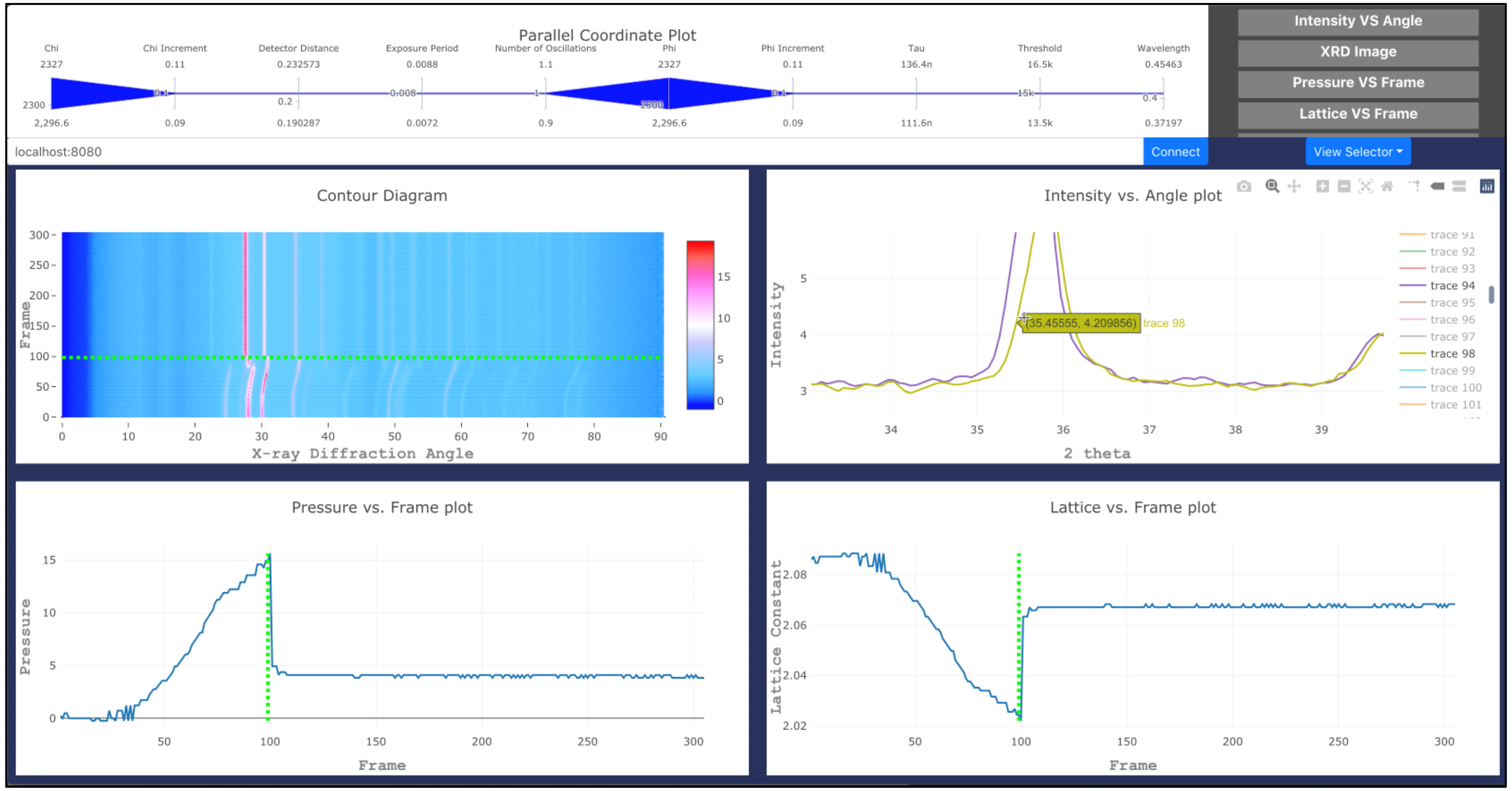


Automated operation of APS Linac using Procedure Execution Manager.

R. Soliday, S. Pasky, M. Borland, "Automated Operation of the APS Linac Using The Procedure Execution Manager," In: arXiv:physics/0008093, Argonne, IL, USA, Aug. 2000.

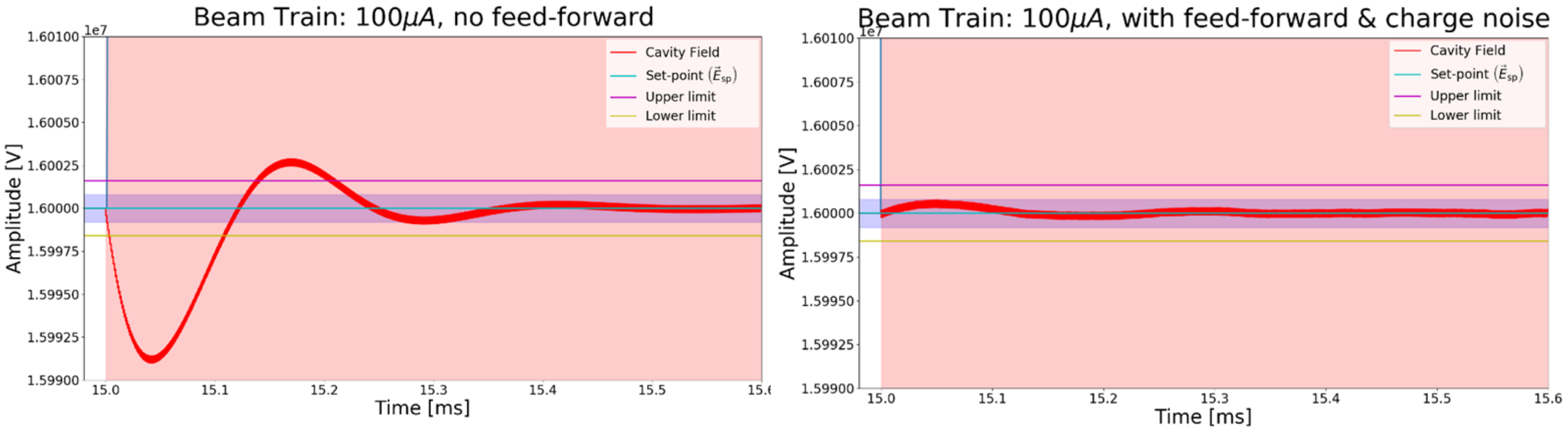
Data visualization tools

We can incorporate the use of data visualization tools such as *Cinema:bandit* (C. Sweeney, LANL) in support of automated tasks.

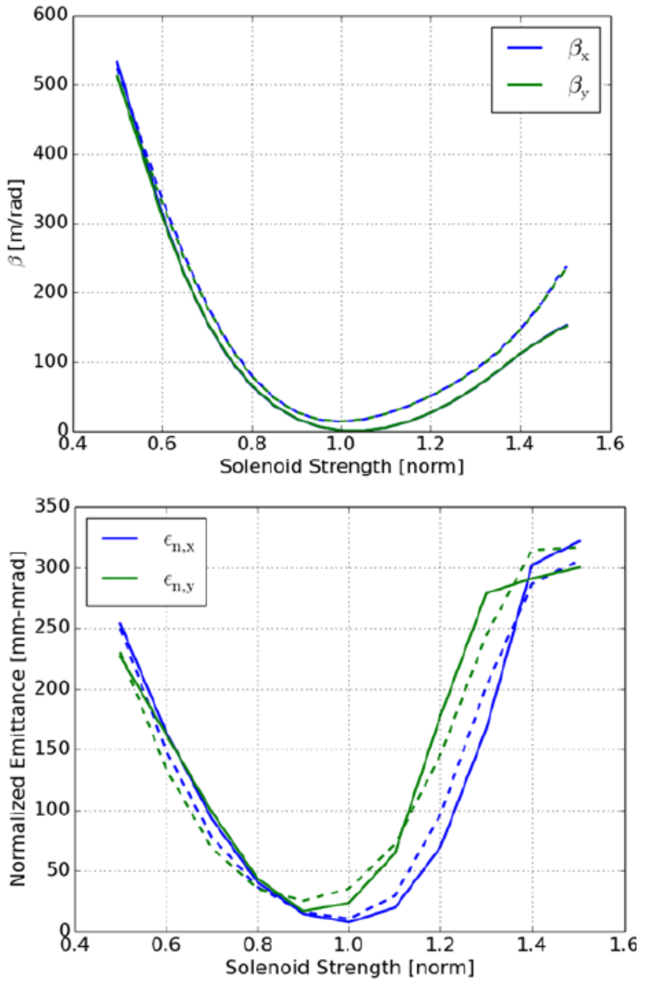


Intelligent controls: Previous experience

- AI-enabled control techniques reduce machine down time and operator intervention
  - ML-controller ensures beam stability during experiments



Amplitude control for the LCLS-II LLRF.



Dashed lines are NN predictions of downstream beam parameters.

J.A. Diaz Cruz, R. Pirayesh, S.G. Biedron, M. Martinez-Ramon, S.I. Sosa, 2019, "Studies in Applying Machine Learning to Resonance Control in Superconducting Cavities," Proc. of NAPAC, WEPLM01.

A.L. Edelen, S.G. Biedron, S.V. Milton, J.P. Edelen, 2017, "First Steps Toward Incorporating Image Based Diagnostics into Particle Accelerator Control Systems Using Convolutional Neural Networks," In: Proc. NAPAC.

AI-Controls: Overview

- Data logging under different MUED operation scenarios.
  - Test/monitor open loop, no operator intervention, see whether there are stability issues.
- AI-model: Neural networks (NN) for scalar data, Convolutional NN for image processing:
  - Inputs are diagnostic readouts: bpm, detector, spectrometer, etc.
  - Outputs are instrument setpoints: llrf, power supplies, etc.
- Training data:
  - Experimental data from parameter scans.
  - Data generated with a virtual model of the system.
  - Can be combined into hybrid operational data set.
- Incorporate optimization algorithms, e.g. Bayesian.
- Integrate controllers (FPGA)
- Test virtually and experimentally.

AI-Controls: Data logging

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- **Data logging and diagnostics implementation**
  - We want to characterize the complete state of the system at any given time.
  - Data needs to be correlated.
- **Parameter space scan**
  - EM field of rf gun, strength of solenoid and correctors, any other ‘knobs’ represent a parameter space.
  - Can use these to control the phase space and properties of electron beam, which can later be optimized (low emittance, high current).

- **Initial step, discuss whether any additional diagnostics, data-logging is required?**
- **Data repository and online interfacing to ALCF and other computing resources.**

AI-Controls: Neural network model

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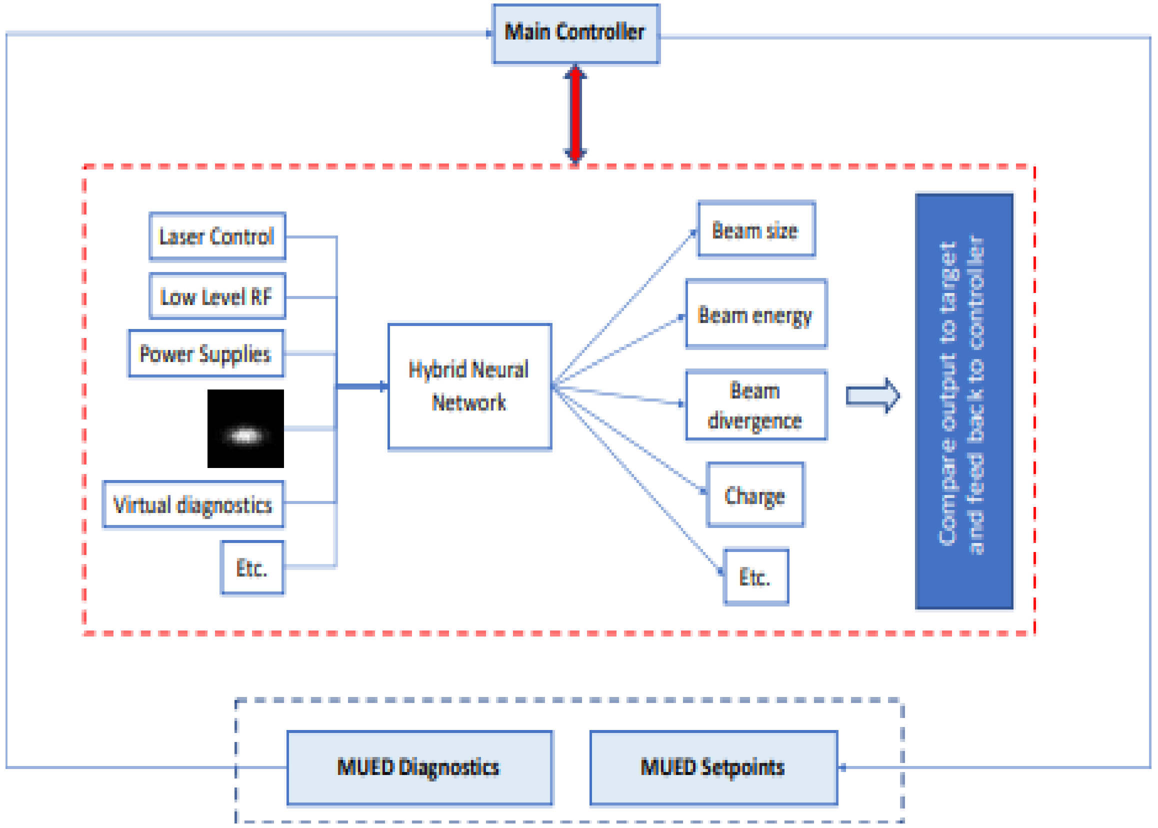
Operational data will enable us to train any ML model in support of MUED operation

- This model should accurately predict the correct setpoints (LLRF, power supplies, etc.) that produce/maintain desired beam parameters
- The strength of a supervised algorithm relies on selecting the best possible setpoints based on previous data for good machine states
- Can use data logged from the machine itself or from an accurate computer simulation of the system



AI-Controls: Simulated model of MUED

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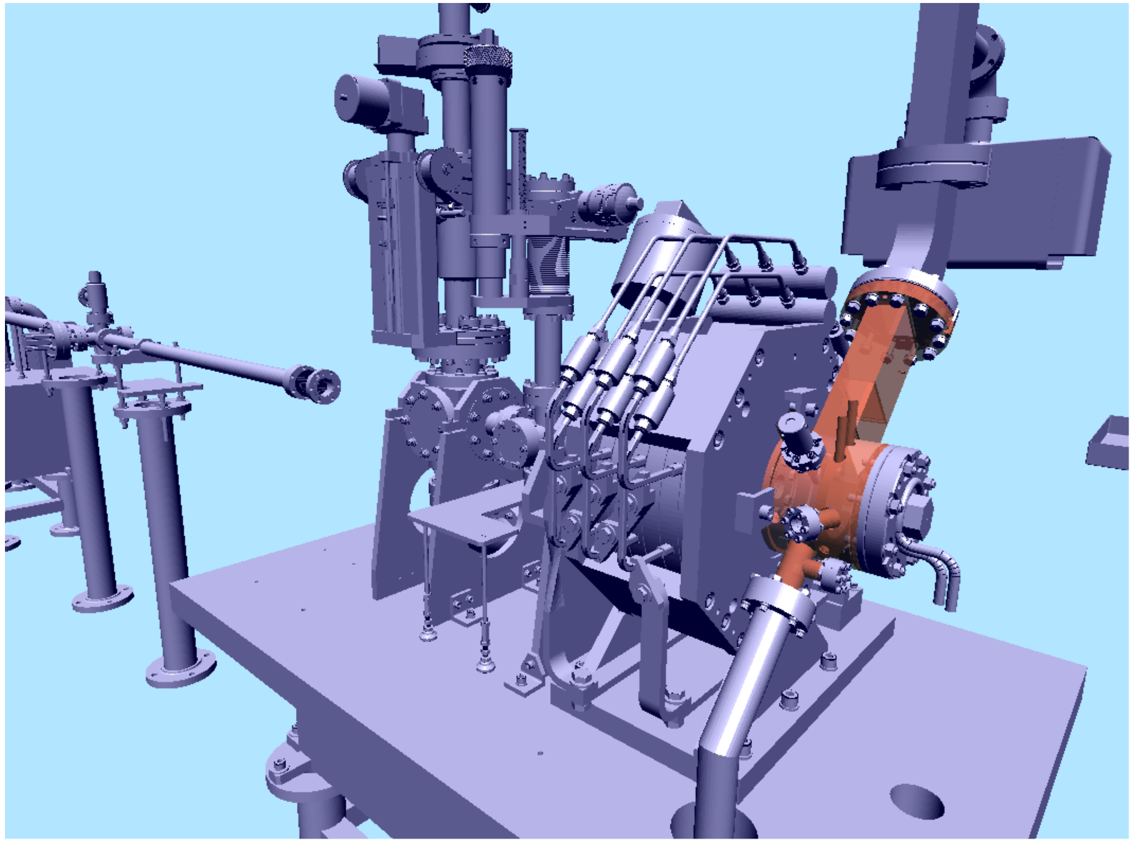
VSim

- Use of electromagnetic and particle tracking codes *VSim* and *Elegant* to create a virtual model of the MUED beamline.
- *VSim* model already exists for MUED instrument
  - Can use to model rf gun, solenoid magnet, and ports of the MUED system
  - Integrates well *Elegant* to model electron beam along drift sections.
- A surrogate model can be created for fast simulations and online operations.
- We have already deployed *VSim* at ALCF's THETA for other research projects.



First section of the MUED instrument as visualized with VSim. RF gun highlighted.

AI-Controls: Integration and tests

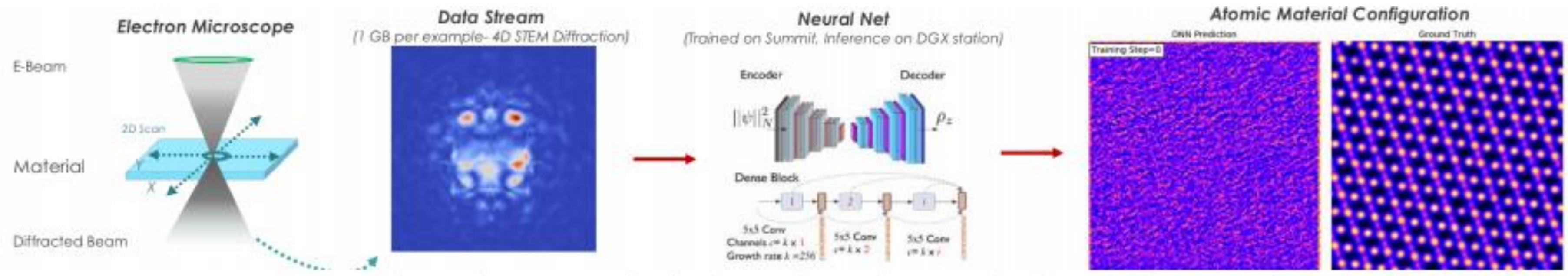
- Test the trained model on the virtual MUED model (*VSim+Elegant*).
  - Determine if the ML model needs to be tuned by using varied conditions, introducing errors and evaluating the model response.

- Integrate controller to the real system.
  - Use of FPGA or similar.

- Test the controller with dedicated beam time.
  - Conduct the same procedures as on the simulated beamline as a final check for safe and correct operations

AI-Controls: Intersection with proposal UED-308073

- Using diffraction patterns as they are produced, a deep learning algorithm will allow us to immediately adjust the system to correct virtual spot size and charge on the virtual cathode to enhance the diffraction pattern.
- Deep Artificial Neural Networks (DANNs) can be used to perform near real-time analysis of our diffraction patterns



Reconstruction of 3-D octahedral rotations from a single 2-D image with DANNs

- Diffraction patterns could be included to the AI-model with an extended hybrid networks that takes input in multiple data formats.

Summary of research tasks

- **Online** – Fitting the MUED beamline with additional data-logging capabilities that capture the system state at a given time and set-up an operational data repository that can later be used by the ATF community. **Est. time:** 2 weeks
- **Online** – Logging, automating, and testing of MUED initialization procedures. **Est. time:** 3 weeks
- **Online** – Data collection and parameter scan of the machine to record as many possible normal operational states that can later be used for training of ML and surrogate models. **Est. time:** 3 weeks
- **Offline** – End-to-end electromagnetic simulations of the MUED system using VSim and particle tracker *elegant* on ALCF's THETA. **Est. time:** No machine time
- **Offline** – Fusing of experimental and simulation data to train a ML or surrogate model that is physics-informed. **Est. time:** No machine time
- **Online** – Integration of ML-models and Bayesian optimization models into the main MUED controller scheme. **Est. time:** 3 weeks
- **Online** – Testing of the controllers with dedicated beam time. **Est. time:** 3 weeks
- **Online** – Interfacing with HPC at ALCF throughout the project. **Est. time:** Open

Thank you for your attention

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We appreciate all the support from our team members on the development of this proposal.

We also want to acknowledge our colleagues Dr. Christian Lavoie (*IBM Research*), Dr. Nouamane Laanait, Dr. Alan Tennant (*Oak Ridge National Laboratory*), Dr. Marek Osinski (*Center for High Technology Materials, UNM*), Dr. Timothy J. Bunning (*Air Force Research Laboratory*), Dr. Kevin Jensen (*Naval Research Laboratory*), Dr. Jeffrey Nelson (*Center for Integrated Nanotechnologies, Sandia and Los Alamos National Laboratory*) and Dr. Malachi Schram (*Pacific Northwest National Laboratory*).