UED-117

SCHOOL OF ENGINEERING

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

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Brookhaven National Laboratory

Argonne NATIONAL LABORATORY

Los Alamos NATIONAL LABORATORY EST. 1943

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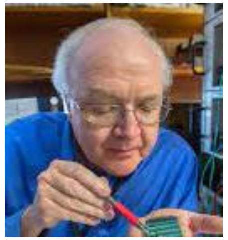
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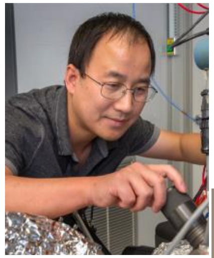
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Mikhail Fedurin


Kevin Brown

Overarching UNM research goals at ATF

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

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

- Control of accelerator and peripherals
  - This experiment (**UED117**), funded by DOE's EPSCoR.
  - Experiment by A. Aslam (-), Cornell Center for Bright Beams, funded by NSF.

- Material sciences
  - Experiment by M. Fazio (**UED110**), funded by DOE's EPSCoR.

Special Equipment Requirements and Hazards

- Experiment requires UED Beam.
- Special Equipment:
  - A dedicated computing node for UNM experiments
    - For logging of diagnostics data.
    - AI-controls implemented independently from operations controls.
- Special Requirements:
  - Data storage and data transmission to ALCF.
  - Autonomous control of the machine once the controllers are delivered (pending approval, UED117 is currently data-logging only).
- Hazards:
  - Those existing during accelerator operation: electrical, rf power, laser.

Experimental Time Request (CY2022)

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Experimental Time Request

CY2022 Time Request

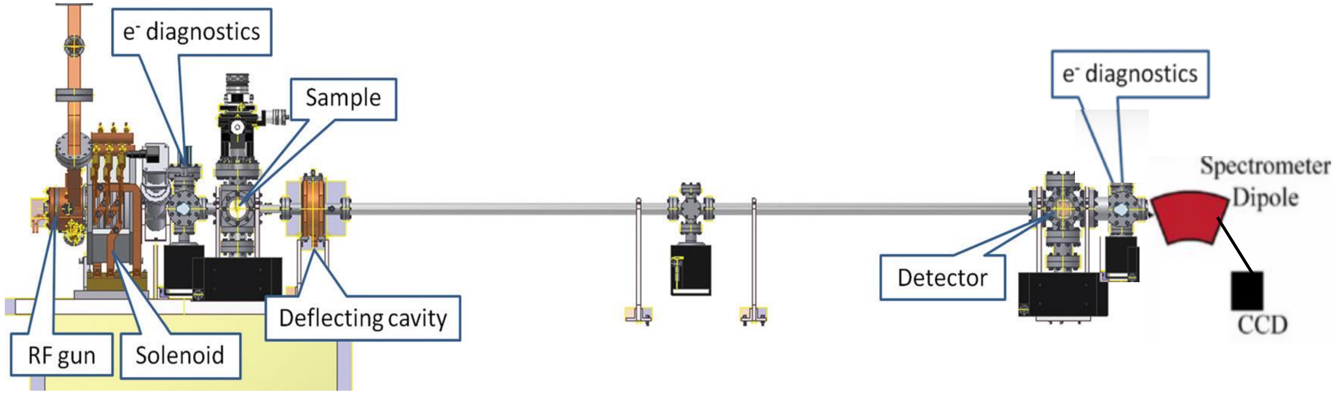
Capability	Setup Hours	Running Hours
UED Facility	150	150

Time Estimate for Remaining Years of Experiment (including CY2022)

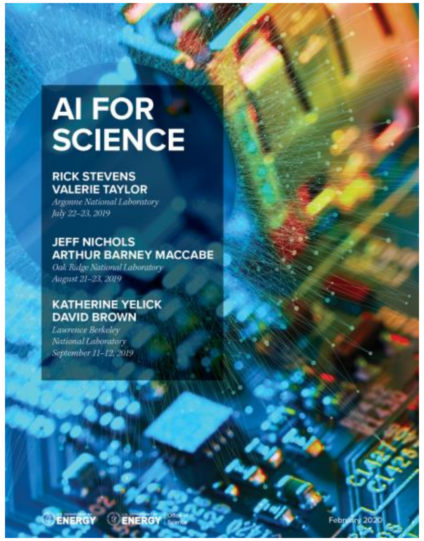
Capability	Setup Hours	Running Hours
UED Facility	150	150

Two DOE facilities are involved: ATF and ALCF

Accelerator Test Facility (MUED beamline)



Argonne Leadership Computing Facility (ALCF)

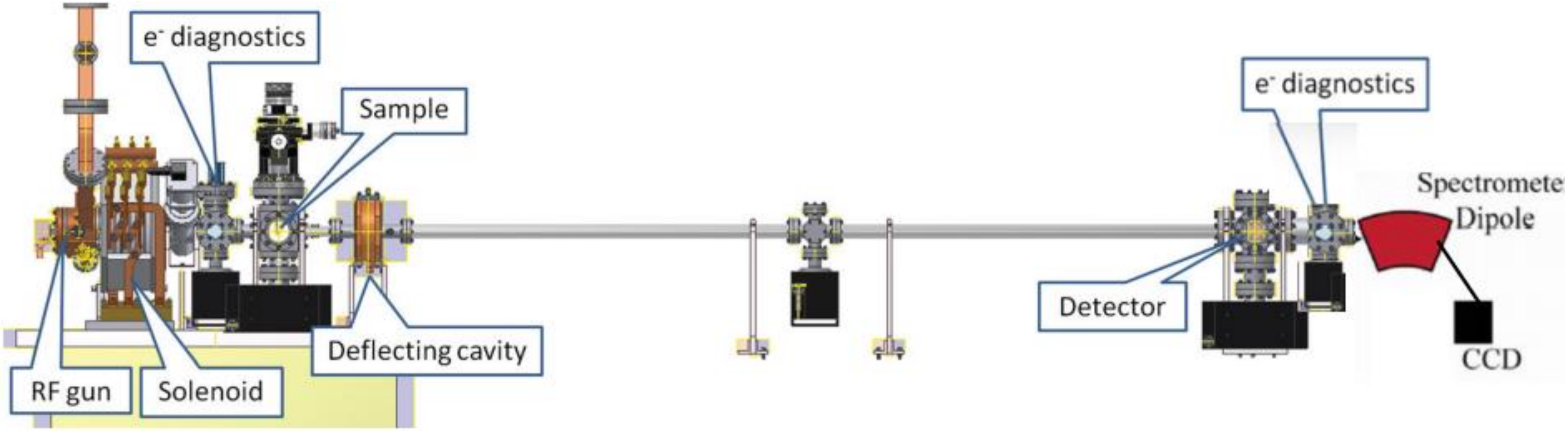


The combination of machine hardware, advanced computing for simulation, and data science for surrogate modelling, training of neural networks and data analysis is inspired by our past work and our participation on DOE meetings, workshops and reports such as AI for Science (*https://www.anl.gov/ai-for-science-report*).

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.
- MUED uses a high-gradient electron gun and small number of electrons (~$10^{4\text{-}6}$) 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.

THETA @ Argonne Leadership Computer Facility

- THETA is a 11.69 petaflops system based on the second-generation Intel® Xeon Phi™ processor, **281,088 cores.**

- General THETA architecture:
  - Theta has 4392 (KNL) nodes.
  - Each node has 64 physical cores.
  - Each core has 4 hardware threads.

- We currently use THETA for:
  - Electromagnetic simulations with VSim.
  - Optimization
  - AI, ML, DL, Surrogate models, etc.

THETA is the current ALCF flagship supercomputer.
https://www.alcf.anl.gov/theta

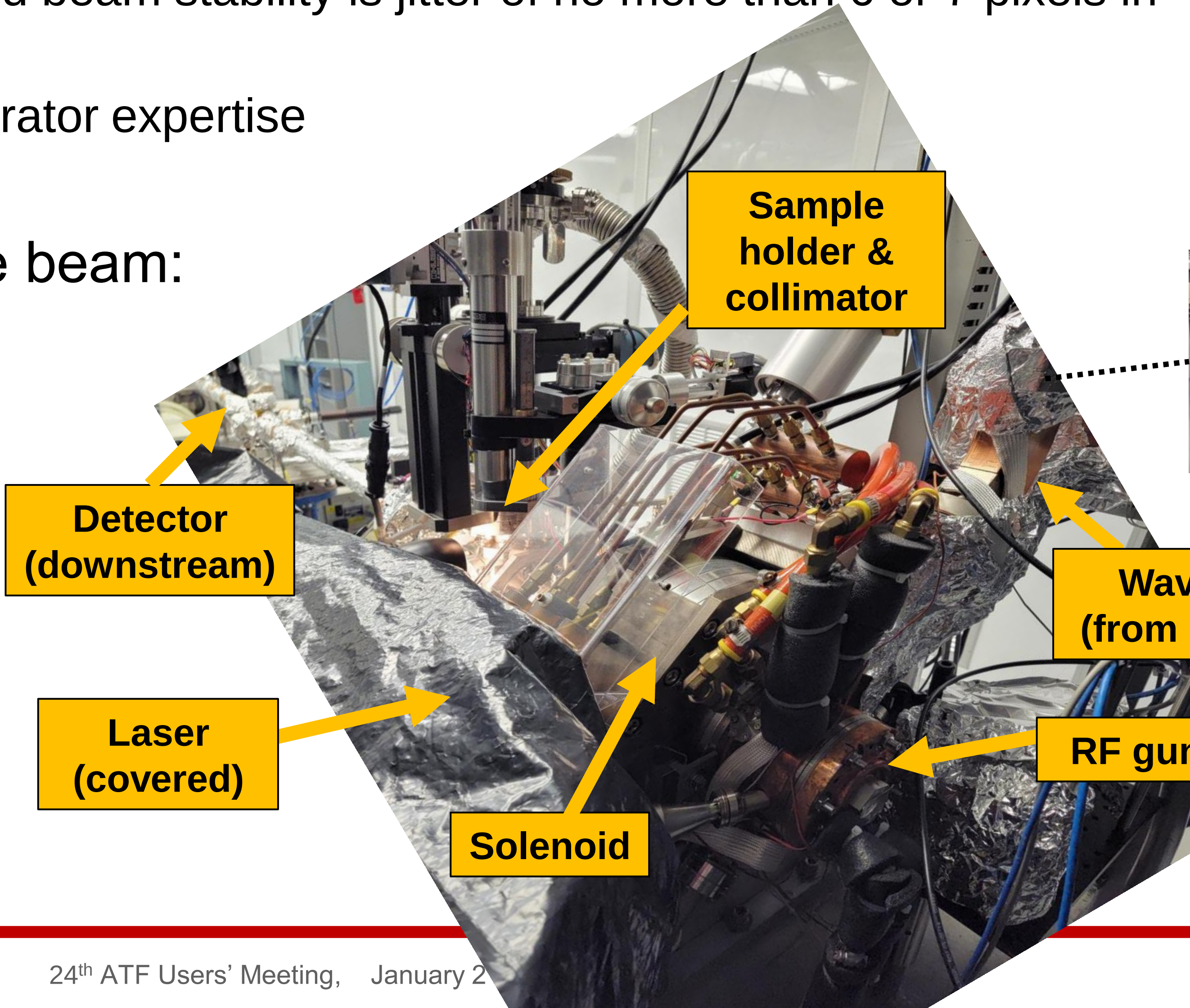
Vision for advanced MUED controllers

The goal would be electron **beam stability** for improved quality of data

- From experienced operator, good beam stability is jitter of no more than 6 or 7 pixels in the horizontal plane of detector
- Beam optimization relies on operator expertise

Relevant "knobs" that control the beam:

1. RF Gun phase
2. Solenoid
3. Collimator
    - Three different apertures
    - Two axis control degree
4. Steering magnets



Vision for advanced MUED controllers

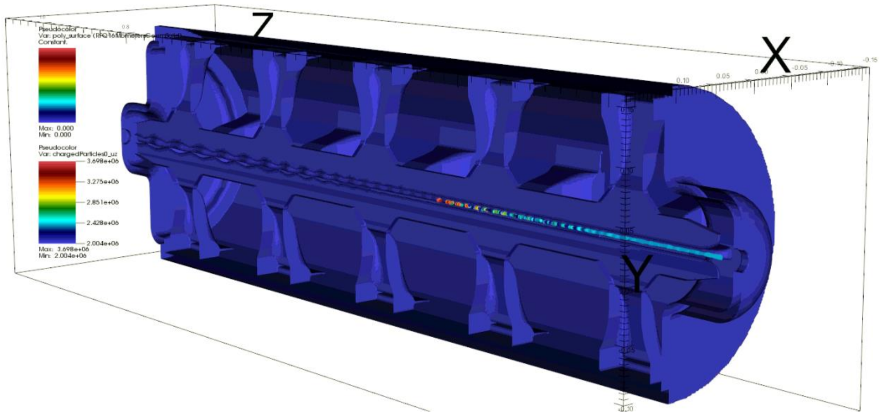
- Automation and task managers reduces operator input in recurrent, time-consuming tasks.
  - Initialization
  - Long term stability
- Automation and optimization produce more consistent beam states, even under different starting conditions.

- Test a surrogate model for experimental runs:
  - Long term stability

AI-Controls: Surrogate model of MUED

- We are exploring the use of surrogate models for controls of particle accelerators.
  - Different ML algorithms can be applied.

- The surrogate model aims at coding the VSim simulation of the RFQ into a quick “look up” table-NN that can be used quickly in support of control tasks.



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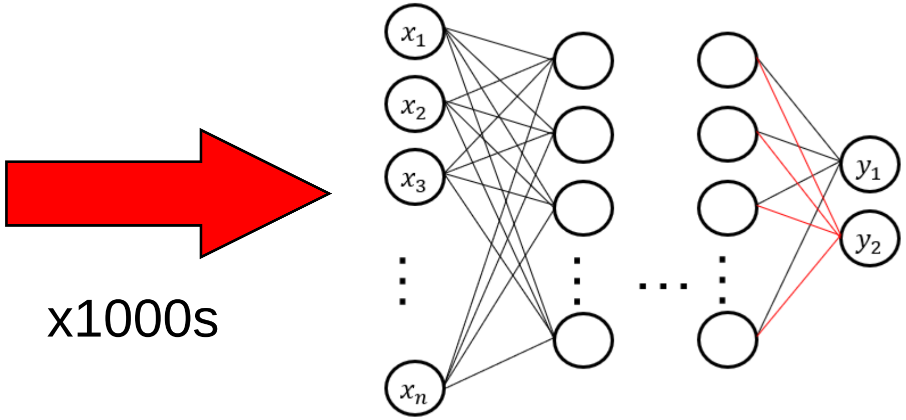

EM simulation (VSim)

- Physics detailed
- Computationally intensive
- Not ideal for real-time controls

Surrogate model

- Trained NN produces real-time results
- Training is done offline
- Training is computationally intensive
- Training data set requires multiple full VSim simulations (use of HPC is a must).

AI-Controls: Surrogate model of MUED

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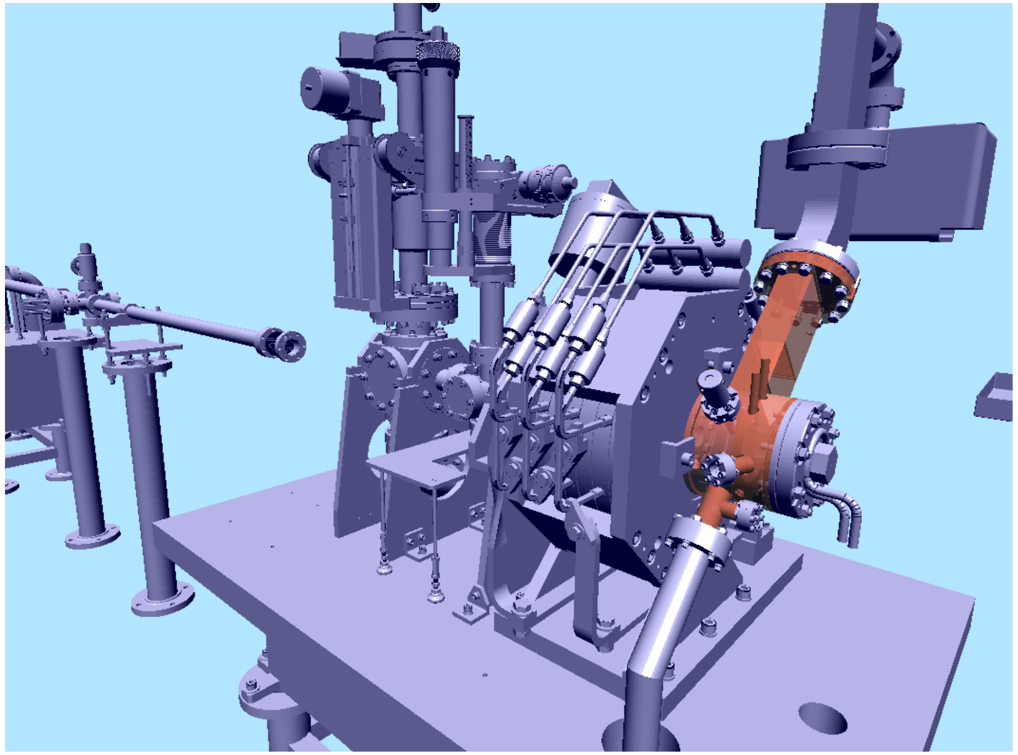
VSim

- Use of VSim and Elegant for a complete model of the MUED beamline.
- VSim for modeling the dynamics in the RF gun.
- Elegant for modeling the rest of the beamline:
  - Solenoid
  - Drifts
  - Collimator
- A surrogate model can be created for fast simulations and online operations.



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

VSim model of the MUED gun

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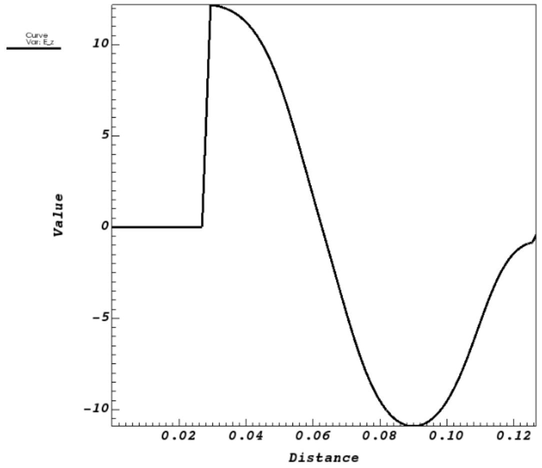
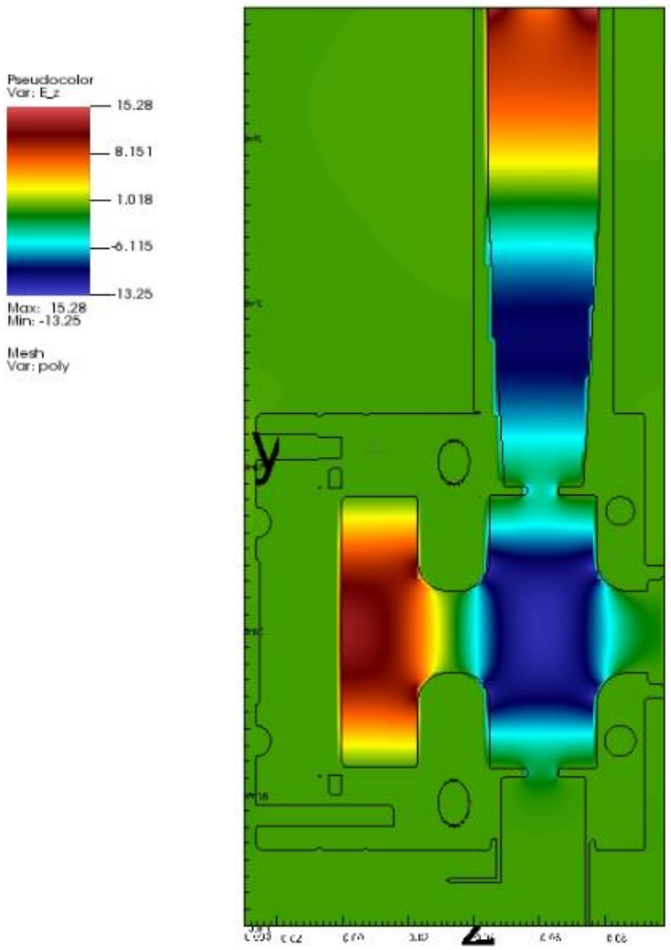
- The MUED gun fundamental EM mode is TM_{010} (π-mode)
  - Includes a section of the waveguide.
- Corresponding frequency (VSim) close to 2856 MHz.
  - No tuners modeled yet.
- Expected field pattern.
- Beam (PIC) simulations now underway



Longitudinal electric field amplitude along the gun axis.



Longitudinal electric field in the MUED rf gun.

Simulations anchored to experimental data

- Benchmark the simulation to typical un-diffracted beam data.
  - W/o collimator, beam is ~50 pixels
  - Dimension is 80 μm p/pixel

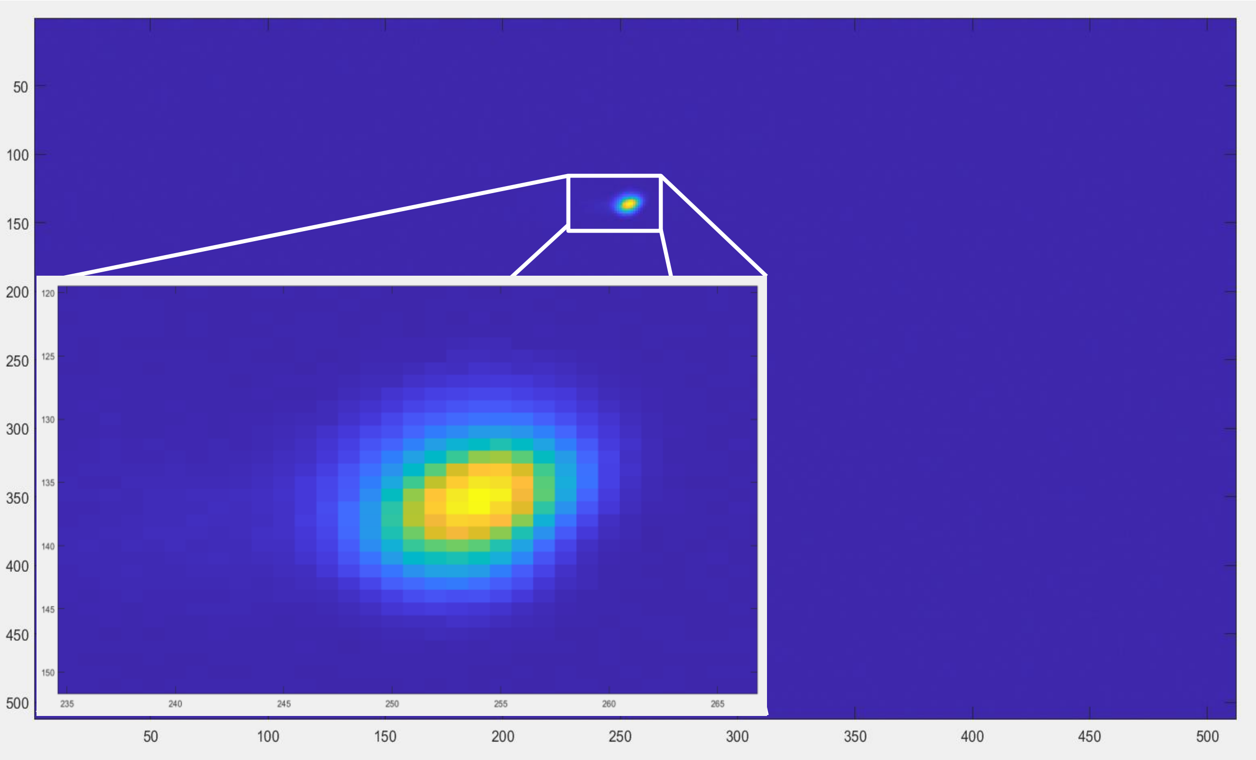


Fig. MUED detector is a 512 x 512 CCD at end of beamline.

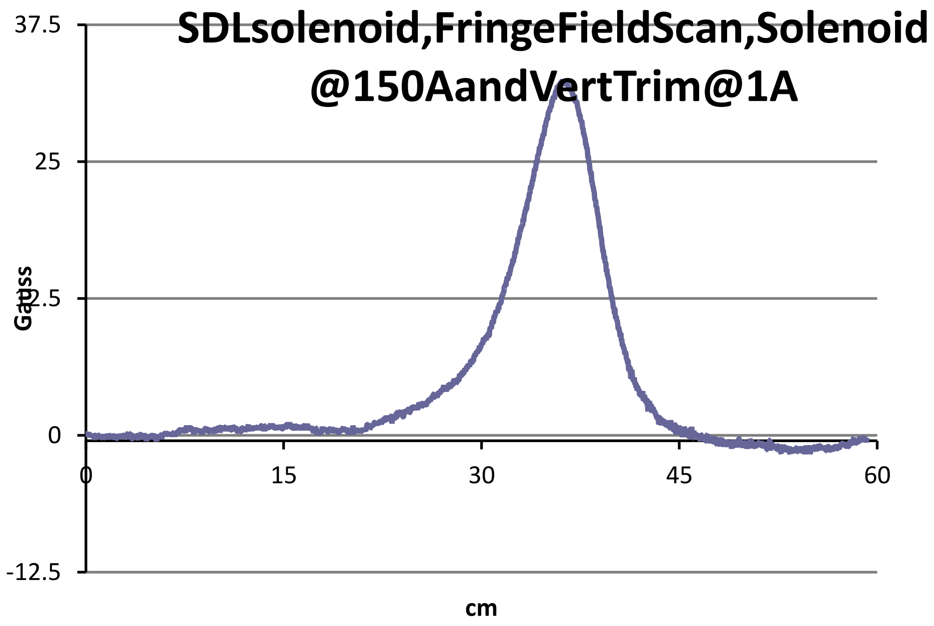


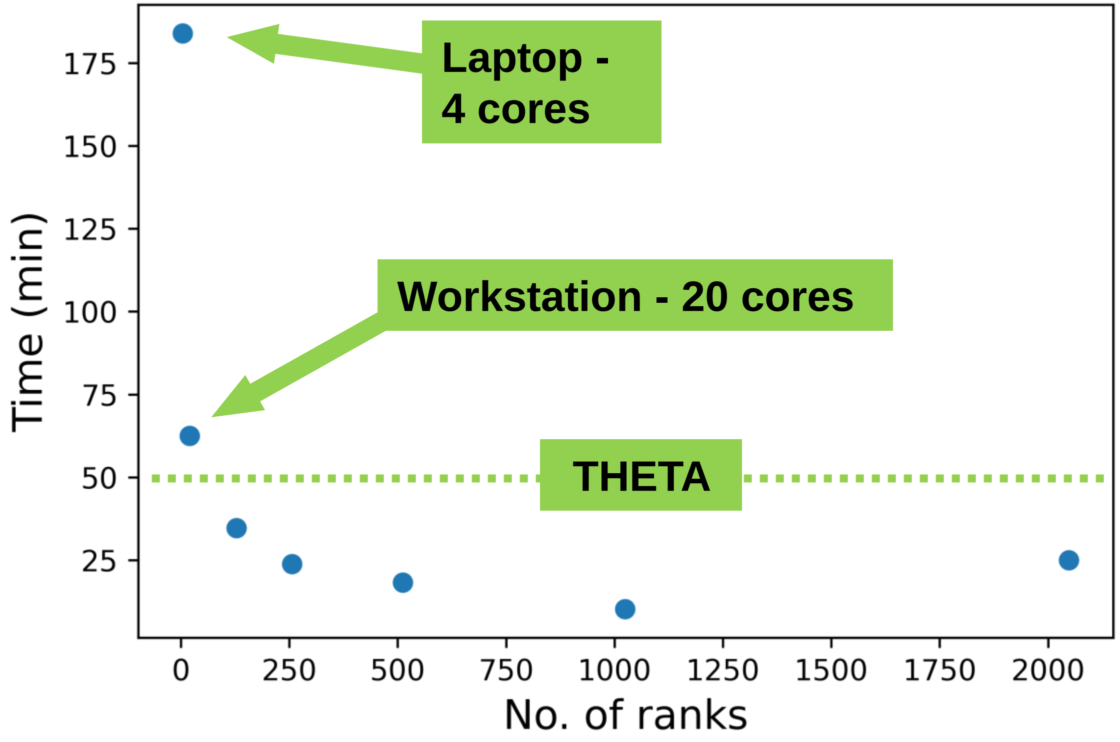
Fig. Example of solenoid field map measurement.

Simulation optimization on THETA

- General parallelization concept:
  - Problem is divided into discretized regions
  - Each of this regions is then assigned to a *processing rank* and run in parallel.

- Hardware resources need to be optimized for a specific problem.
  - Optimization tools available at THETA.

- Efficient use of resources becomes paramount for data production towards Machine Learning.



Computing time as a function of the number of processes when assigning a single process per core.

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 dedicated control node for tests without interfering with operations setup.

- 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

Summary of research tasks

- Setup of a computer node for UNM controls experiments (Thanks to B. Malone)
  - Logging capability of MUED diagnostic data to capture the system state at a given time and set-up an operational data repository that can later be used by the ATF community.
- Interfacing MUED to ALCF. (Thanks to T. Uram and B. Malone)
- Logging, automating, and testing of MUED initialization procedures.
- Data collection and parameter scan of the machine to record as many possible normal operational states that can later be used for simulation benchmarking and surrogate models.
- End-to-end electromagnetic simulations of the MUED system using VSim and particle tracker *elegant* on ALCF's THETA. (on-going)
- Integration of ML-models and Bayesian optimization models into the test controller node.
  - Testing of beam stability with virtual model
  - Test for beam stability with dedicated beam time.

Thank you for your attention!

And to the ATF/MUED staff for their support during our beamtime.