Machine learning to enhance XFEL operation at LCLS-II

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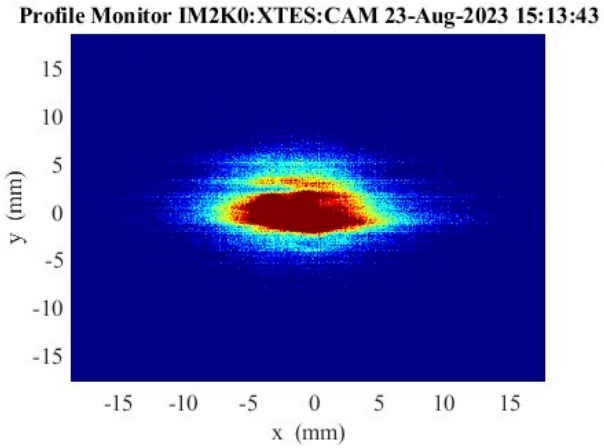
SLAC NATIONAL ACCELERATOR LABORATORY

Stanford University | U.S. DEPARTMENT OF ENERGY

LCLS-II: Brighter, Faster, Smaller

LCLS-II: at the forefront of X-ray science

- Increase the beam repetition up to 1 MHz
  - Advanced electron source
  - Superconducting accelerator
  - Novel beam/FEL configurations
- Provide unique capabilities for scientific exploration
  - Fully coherent and high-repetition-rate X-rays
  - Simultaneous generation of SXR and HXR



SXR Undulator lasing achieved on 8/23/2023

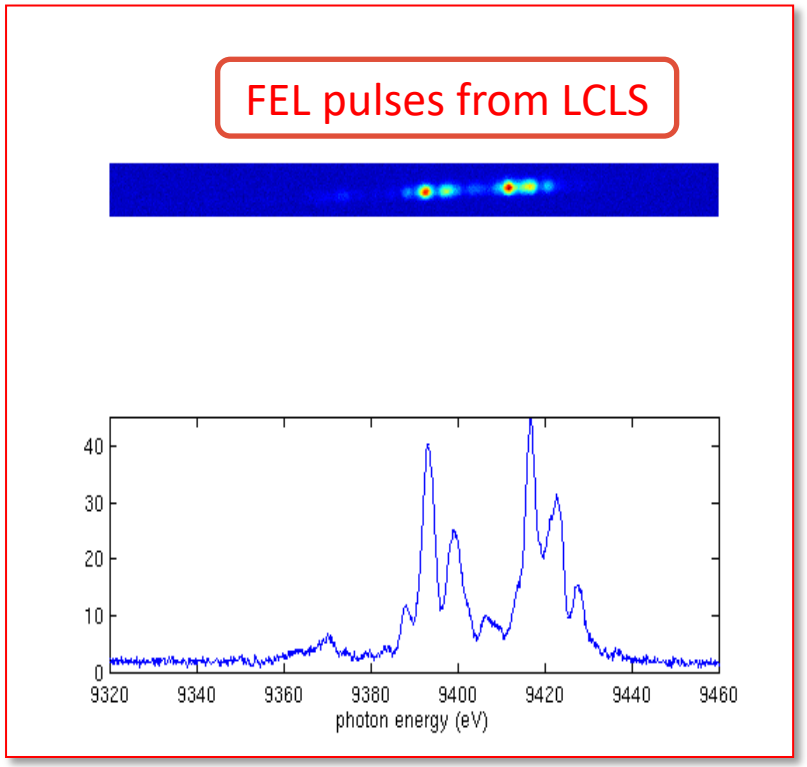
Challenges of daily operation in XFELs

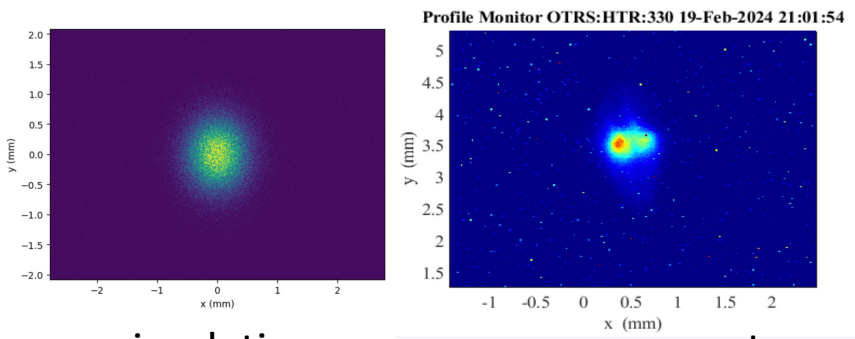
Online tuning in desired state:

- Beam properties customization
- **Fast switch** between different beam/undulator configurations
- **Stable performance** of FEL pulses for experiments

Challenges when tuning in control room:

- Beam behavior varies from simulated results
- Highly **non-linear** and **time-dynamics** system
- Output pulses suffer from **drift** and **jitter**
- Operation based on empirical tuning



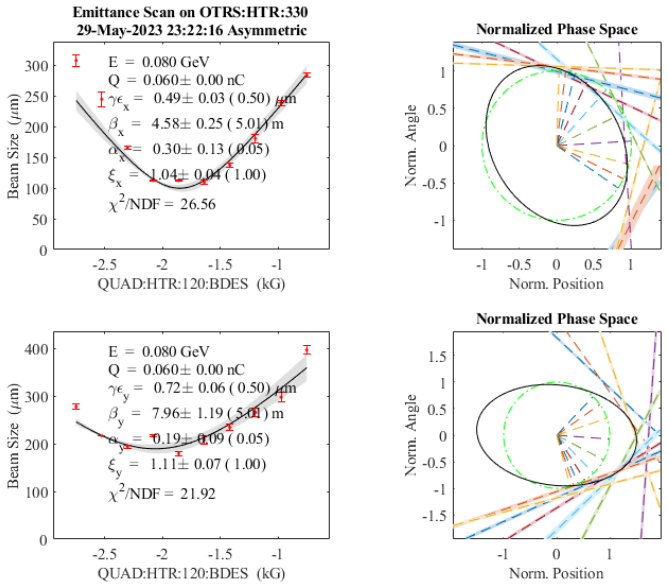


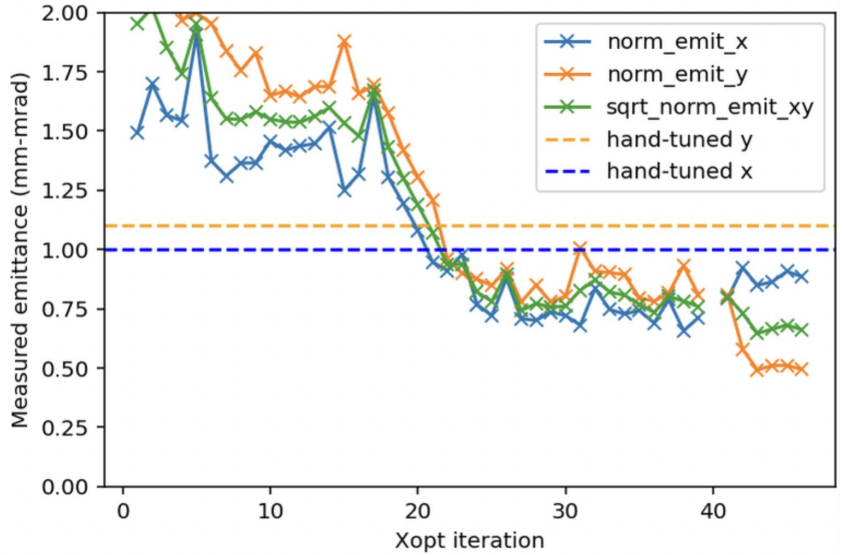
simulation measurement

Online optimization during LCLS-II commissioning

https://christopherm ayes.github.io/Xopt/

Xopt with Bayesian optimization

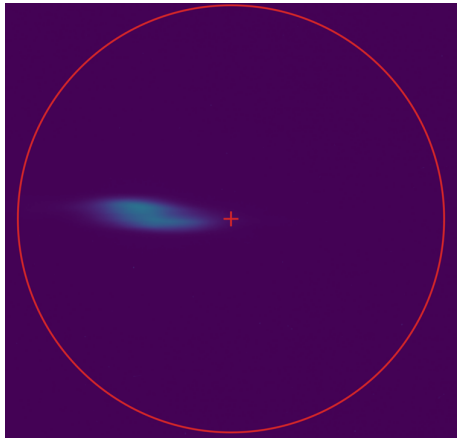


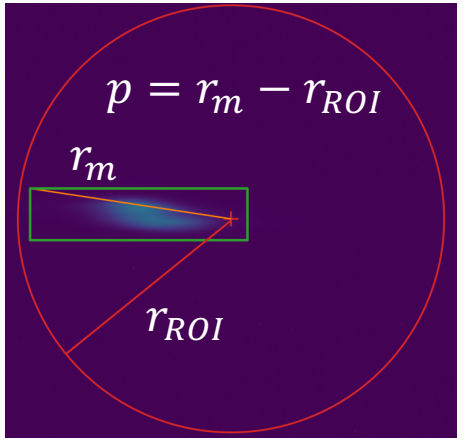


Define a **smoothly varying** penalty function to act as a constraint

Define a circular ROI

Measure maximum distance from the ROI center to bounding box corners.





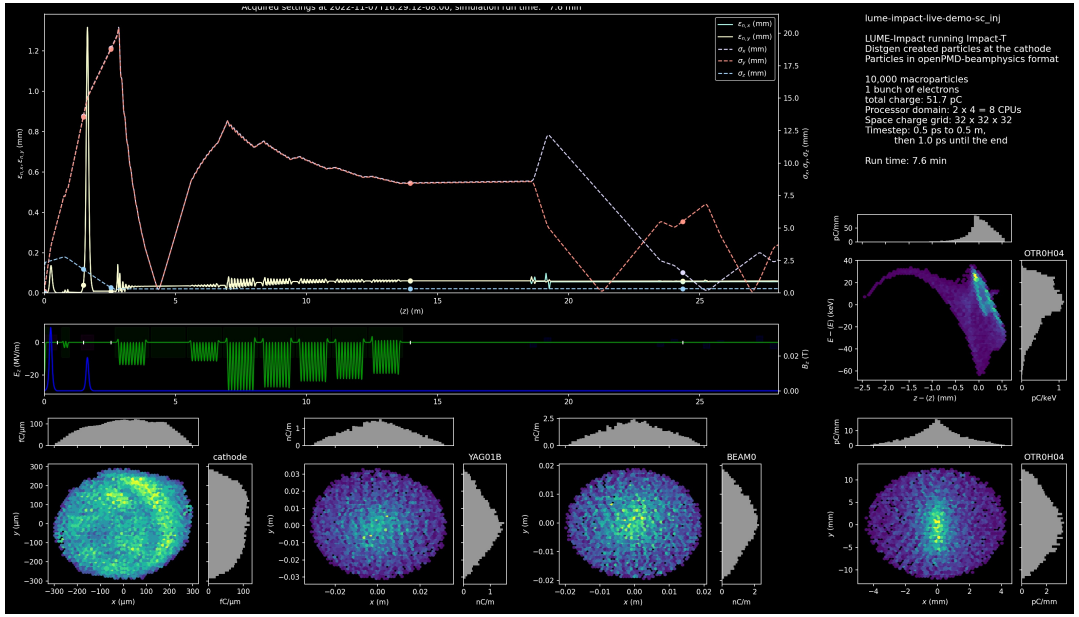
Injector emittance tuning with 6 variables:
SOL1, SOL2, SQ1, CQ1, SQ2, CQ2

Avoid dark current and beam loss simultaneously

Combination of live models and online optimization

Real-time physical simulation and Bayesian optimization to aid injector commissioning

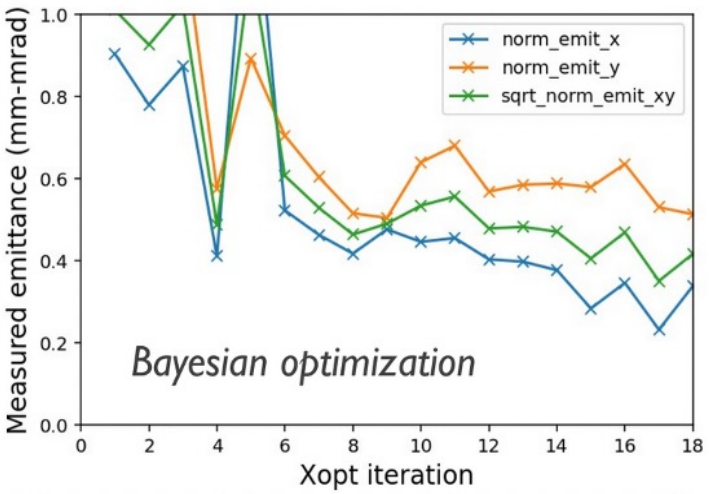
Readings from machine via EPICS

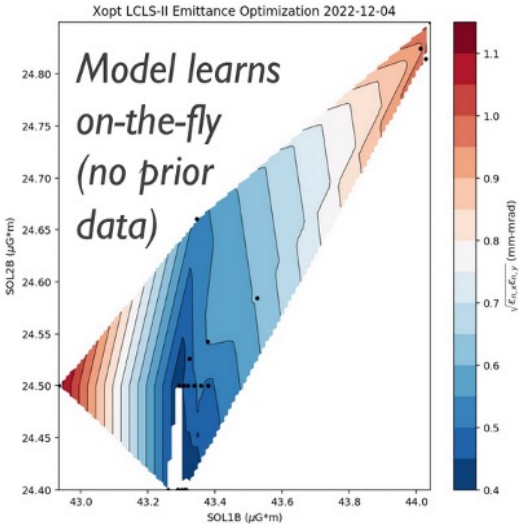


LUME-IMPACT live model simulates on HPC and display in control room

Adjust machine parameters with insight from prediction

Hand over to BO for subsequent fine tuning



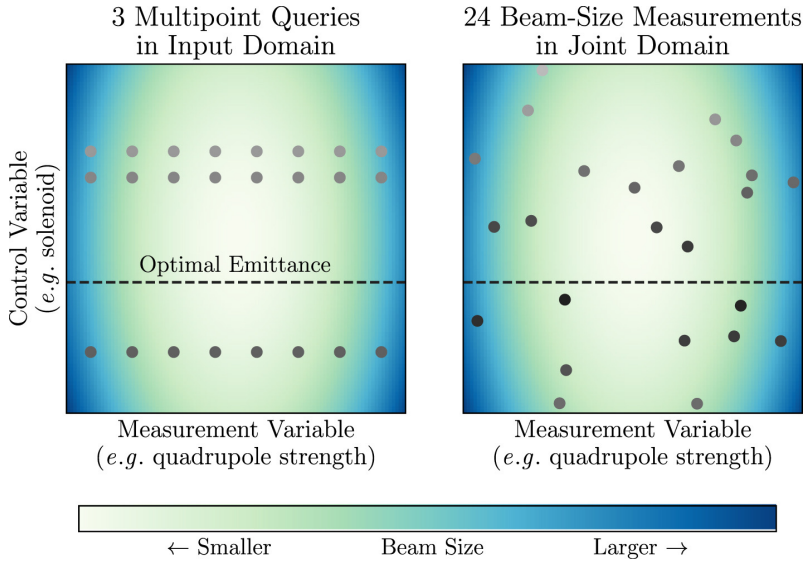


Best emittance yet obtained during LCLS-II injector commissioning

Information-based Bayesian Algorithm Execution (BAX)

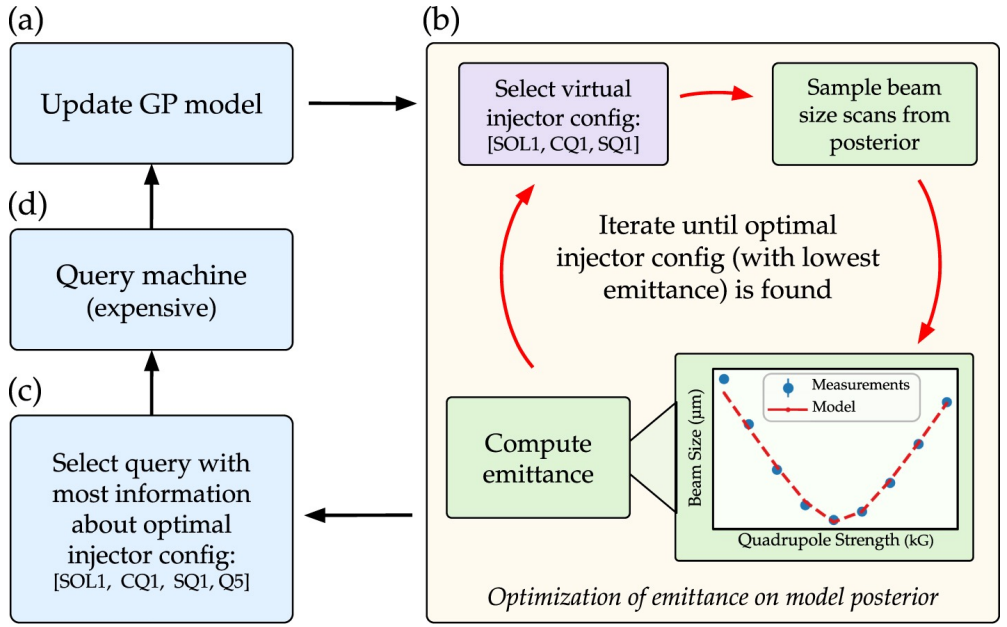
Motivation: Emittance measurement is time-consuming

- Calculation is based on scanning a focusing magnet's strength while observing the change in beam size on the downstream screen
  - Requires a "secondary scan" along the quad domain
  - Lose the information from the individual quad scan



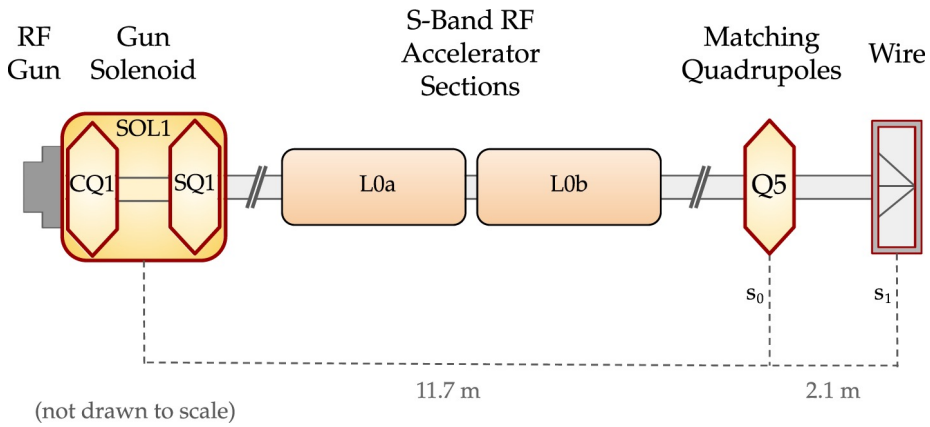
Miskovich, et al., doi:10.1088/2632-2153/ad169f.

- Build a model of the beam size as a function of quad strength during optimization
  - Model developed based on direct observables
  - Emittance prediction based on surrogate



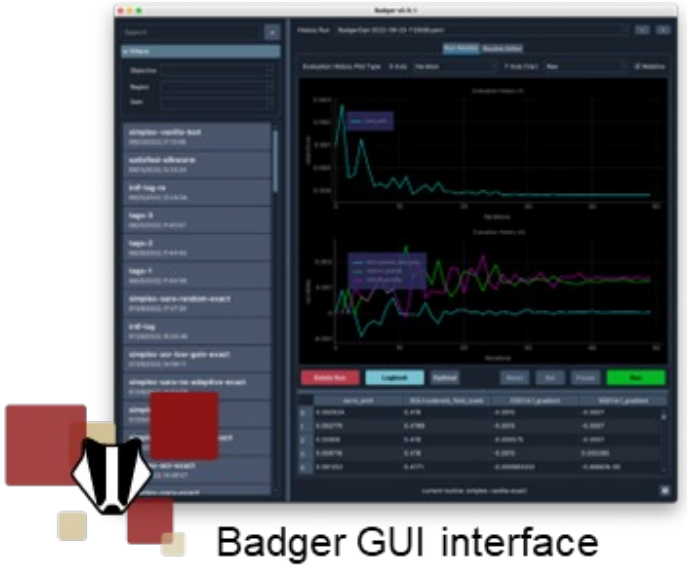
Information-based BAX for emittance optimization

Demonstration on emittance tuning for LCLS injector



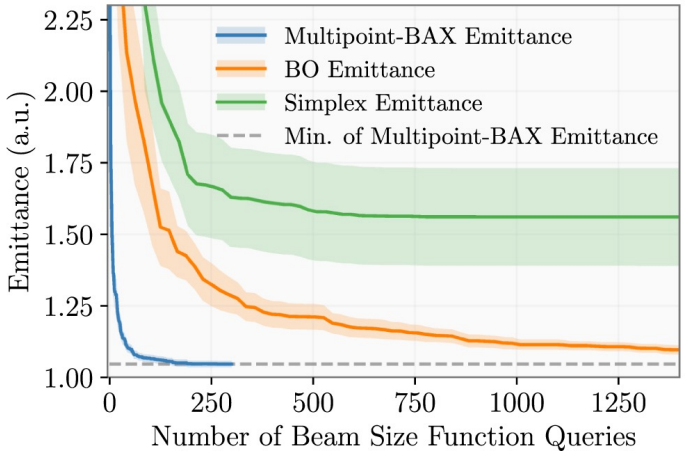
Xopt

https://christophermayes.github.io/Xopt/

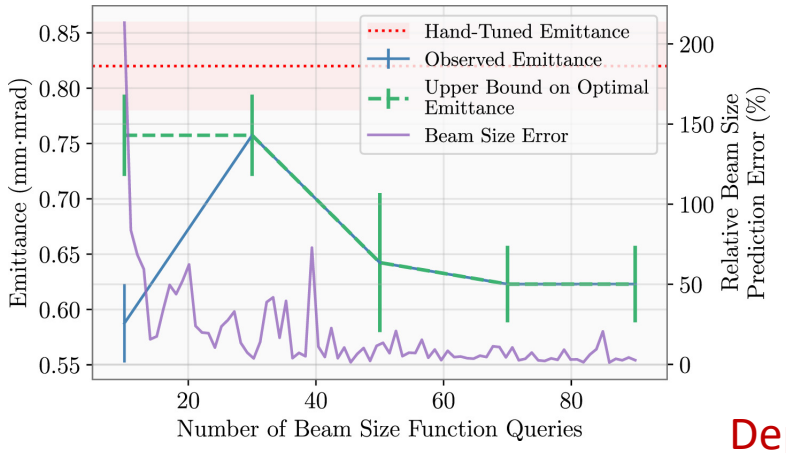


https://slaclab.github.io/Badger/

Simulation



Experiment



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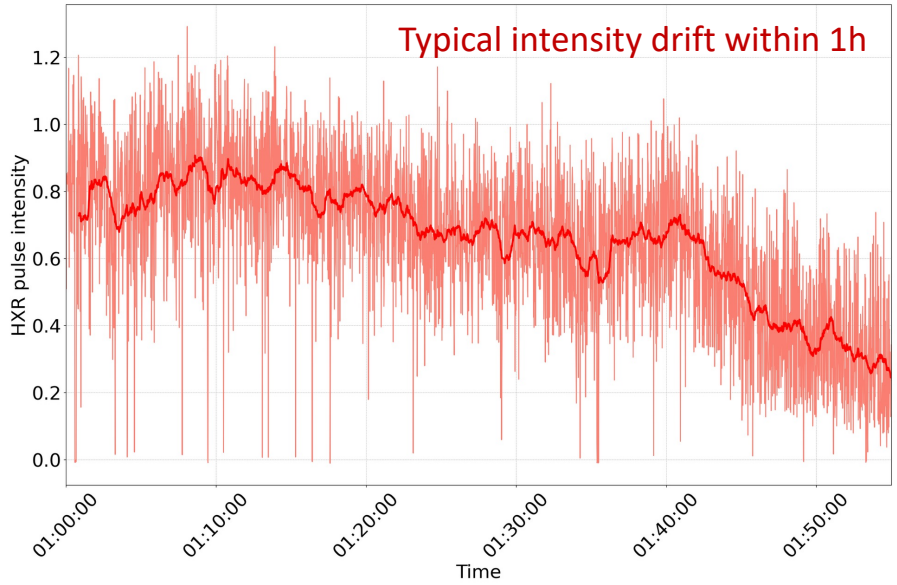
Deployment in progress at LCSL-II injector

FEL robust modeling at LCLS/LCLS-II

Challenges in modeling FEL pulse intensity

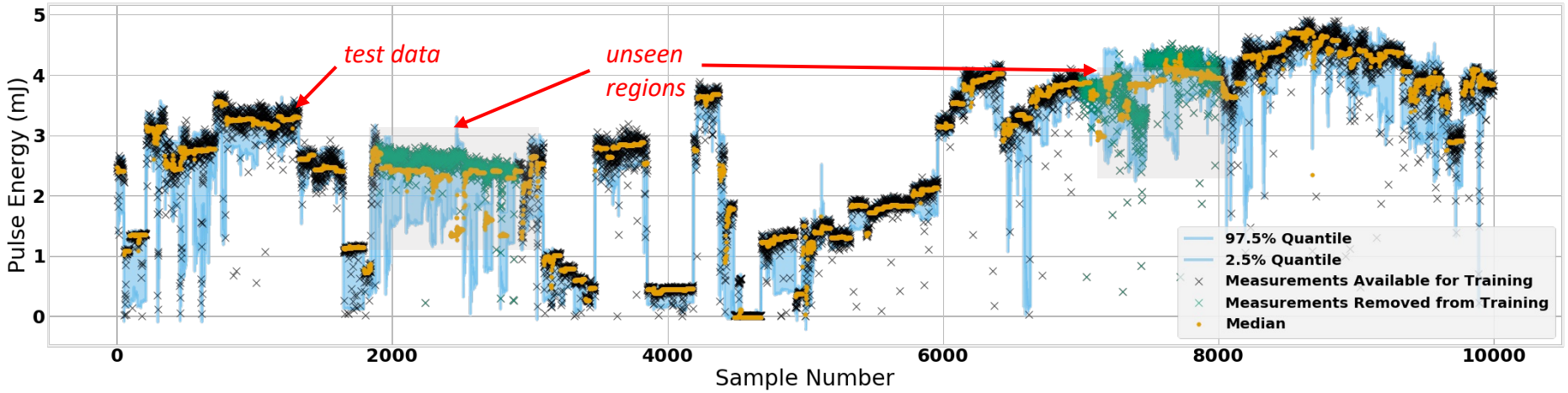
- Intensity signal is inherently noise-dominated
- Output drifts over time
- abnormal subsystem condition / hidden anomalous behavior



Current approaches:

- Ensembles
- Gaussian Processes
- Bayesian NNs
- Quantile Regression

Previous work from Lipi Gupta



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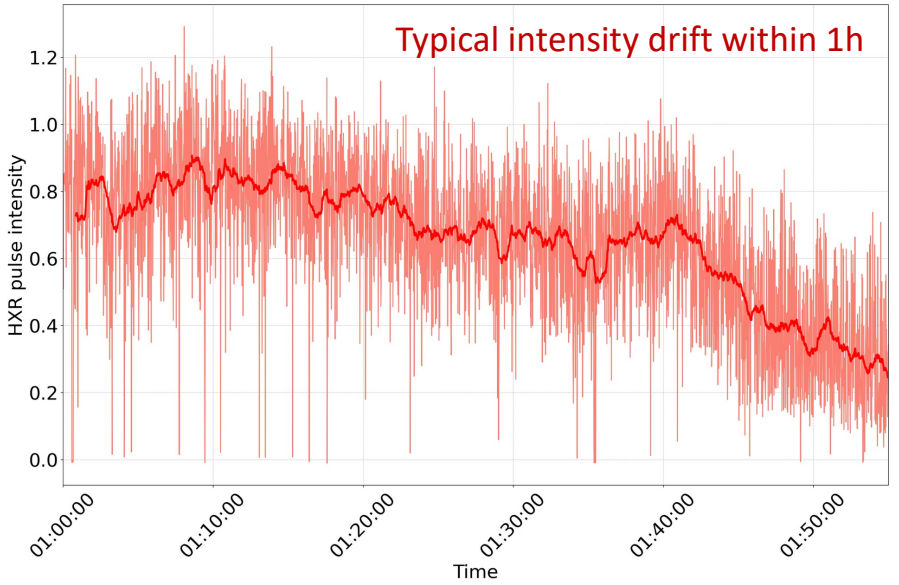
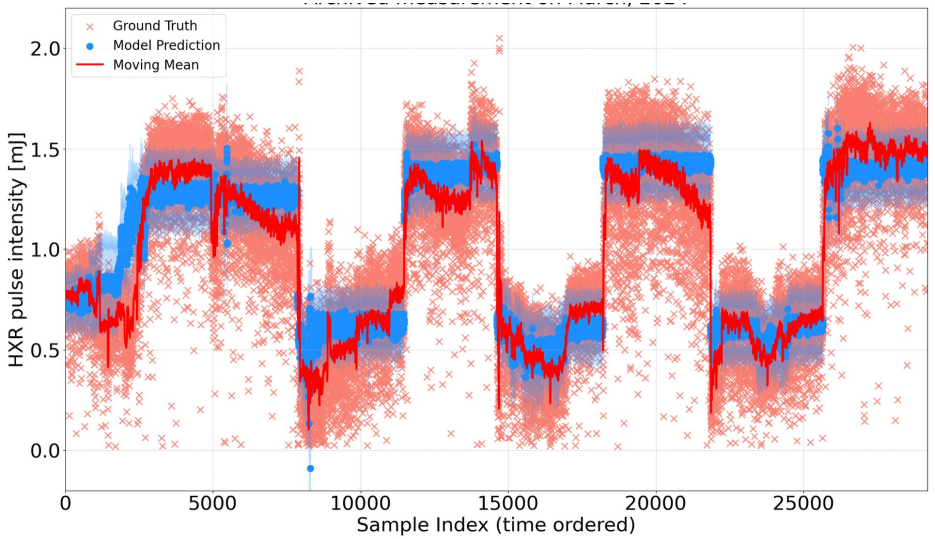


Quantify uncertainties in NN with model ensembles

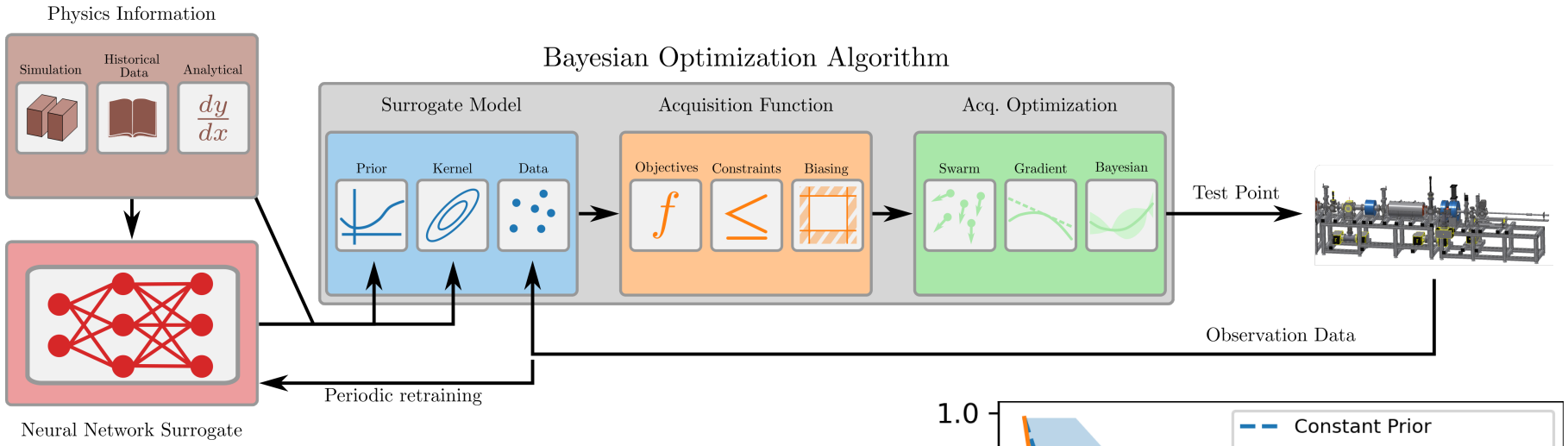
- Dig data through the archive
- Input features include quad strengths, beam energy, charge, bunch length readback at different location
- Model ensembling with bootstrap aggregation
- More ML approaches to be tested

Work in progress



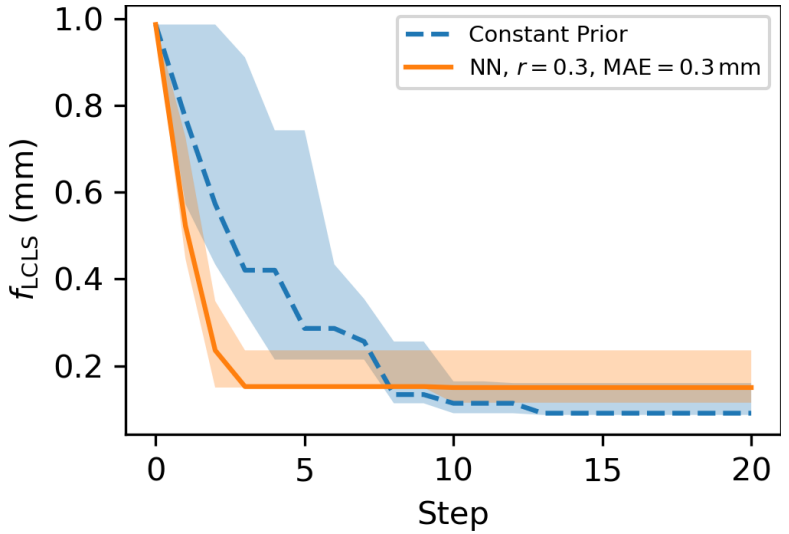
Future Directions

Neural net acts as prior for online BO



Demonstration at LCLS injector

- Incorporate NN prior based on simulations
- Minimize the beam size while keeping it round
- Use combination of correlation and MAE



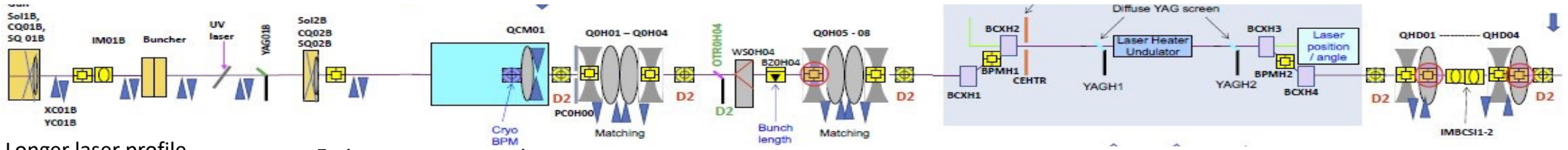
More details in Tobias Boltz's talk

Injector system modeling at LCLS-II

More complicated beam dynamics

Lower gun gradient

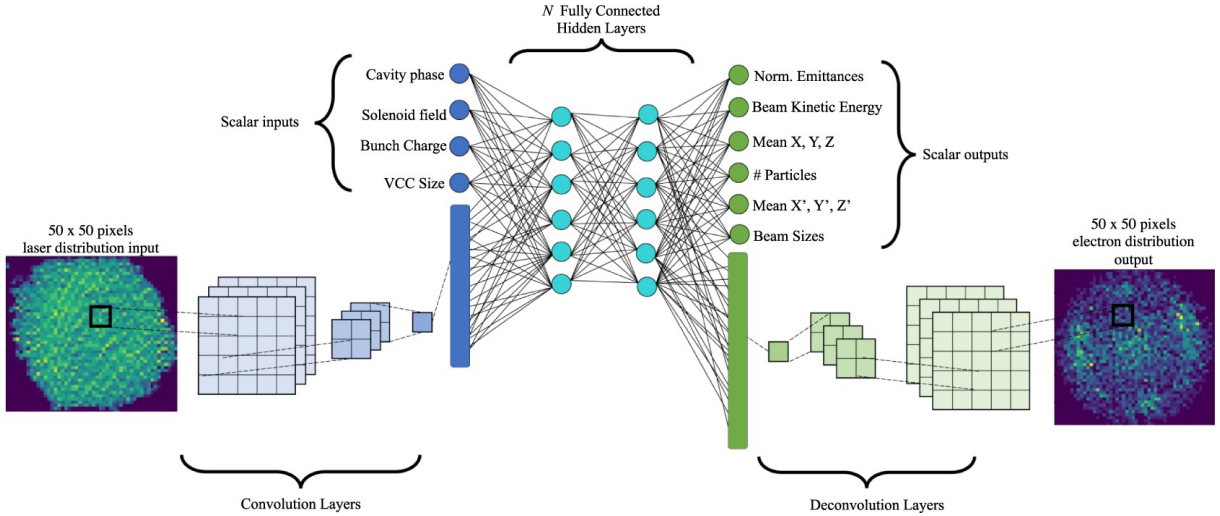
Velocity bunching

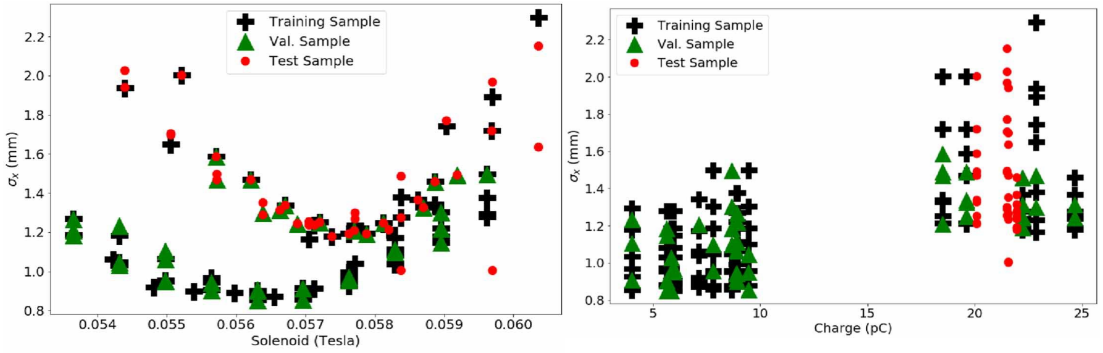


Longer laser profile

Emittance compensation

A fast and reliable simulator is on demand during machine operation



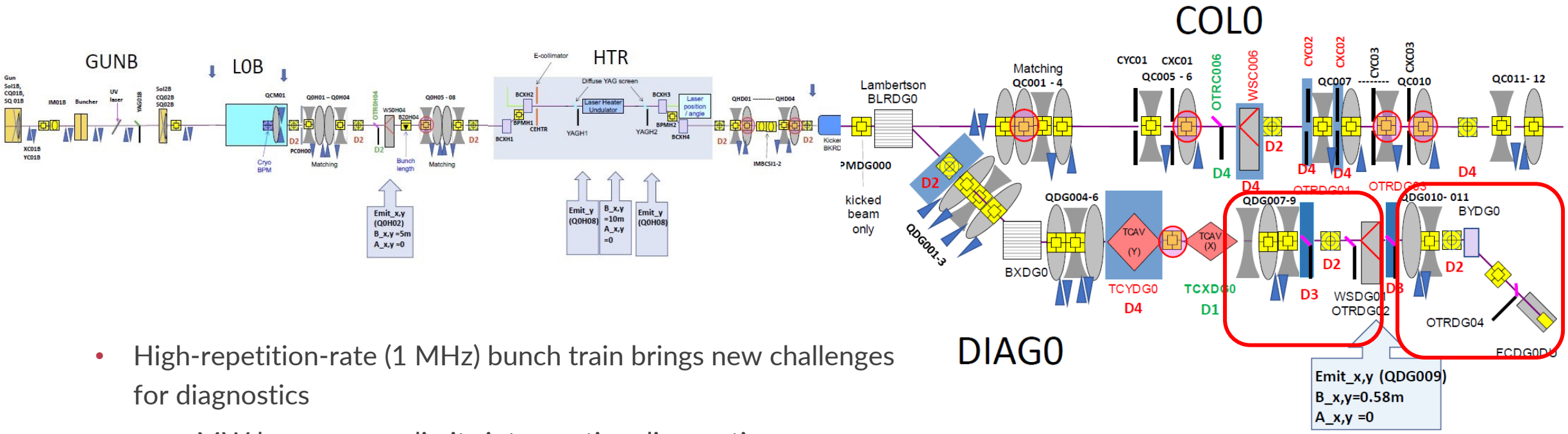


Lipi Gupta *et al* 2021 *Mach. Learn.: Sci. Technol.* **2** 045025

Work in progress

Autonomous LCLS-II Beam Measurement

DIAG0: Diagnostic line at the injector end without interfering beam delivery



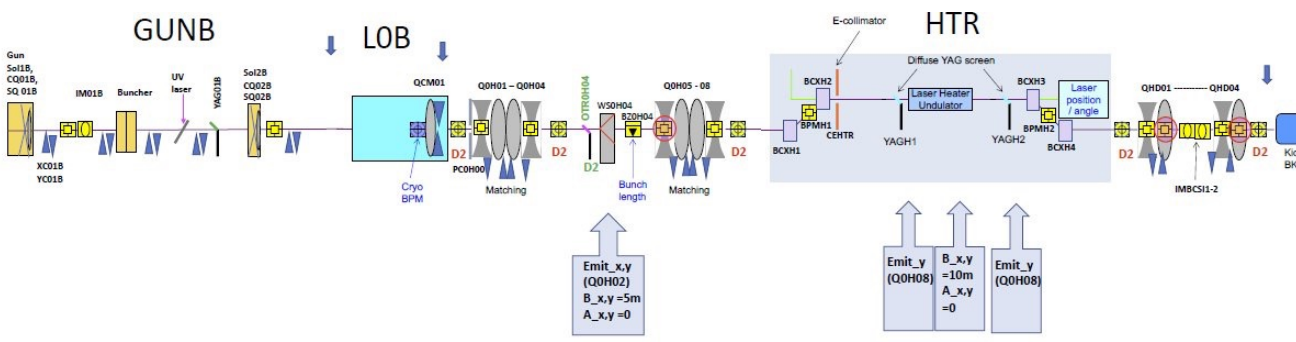
- High-repetition-rate (1 MHz) bunch train brings new challenges for diagnostics
  - MW beam power limits intercepting diagnostics usage
- DIAG0: A low rate (120 Hz) diagnostic line at the injector end
  - Fast kicker to extract beam within bunch train to DIAG0
  - Constantly run in background without interfering beam delivery and human monitoring

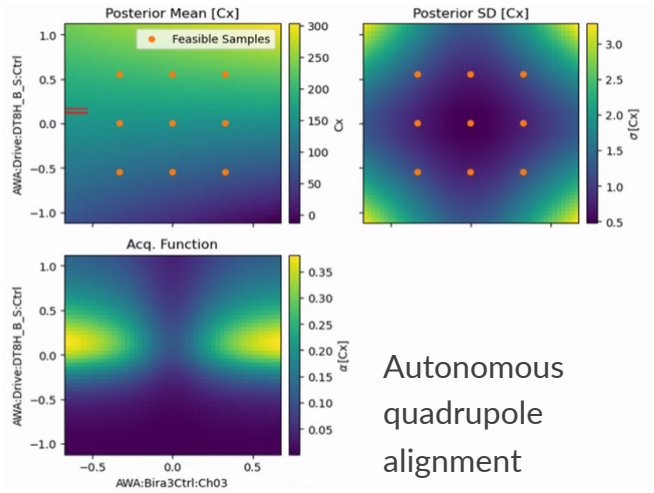
Emittance measurement

Energy spread measurement

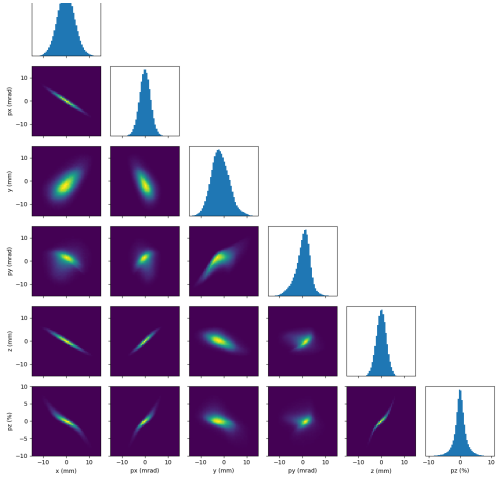
Autonomous LCLS-II Beam Measurement

DIAG0: Diagnostic line at the injector end without interfering beam delivery



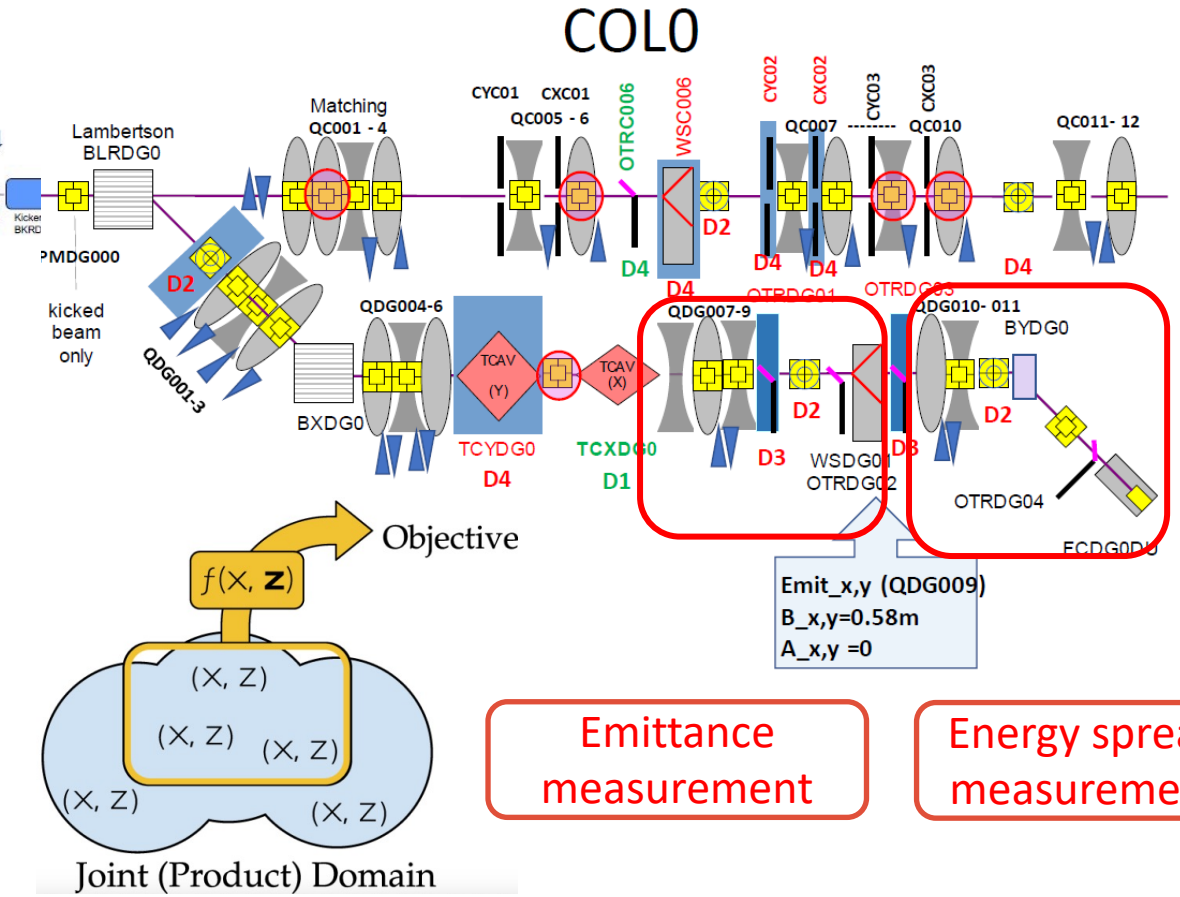


Autonomous quadrupole alignment



6-D phase space reconstruction

More detail in Ryan Roussel's talk tomorrow



BAX for emittance optimization

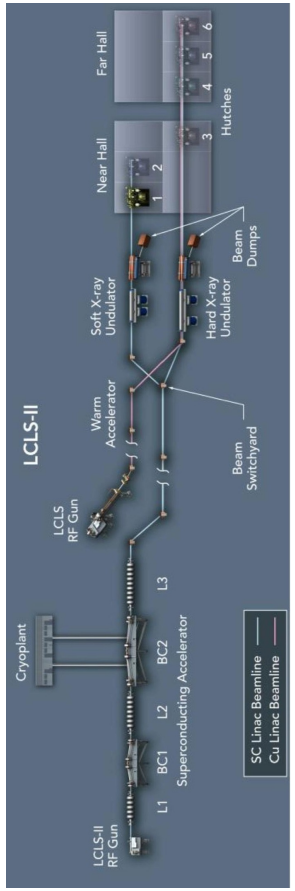
Emittance measurement

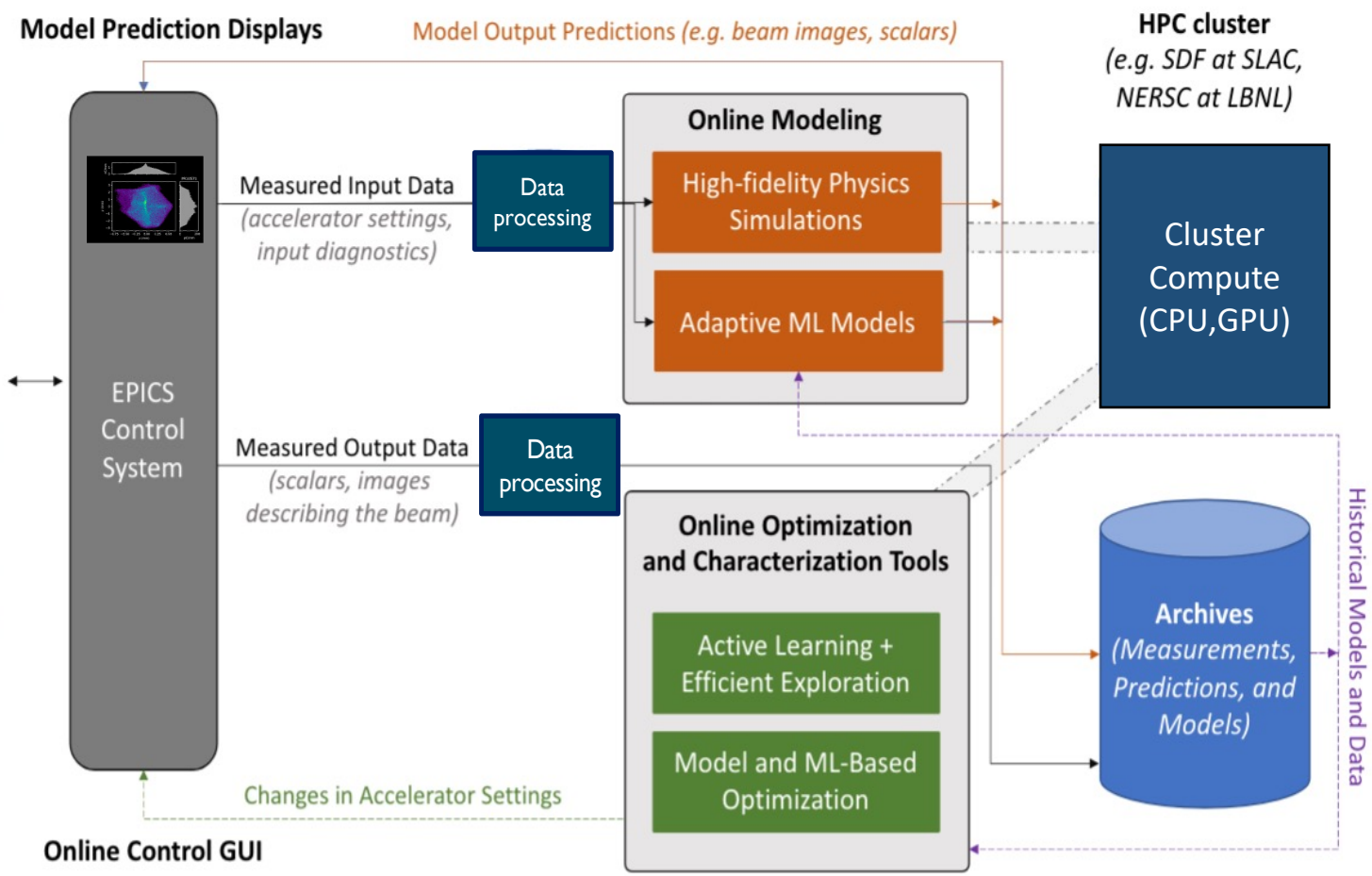
Energy spread measurement

Ecosystem development for physical simulations, AI/ML driven online optimization

LCLS-II fires up to a million beam/photon pulses per second

Goal: Integration of online system modeling, AI/ML driven optimization and simulations to aid operations





Summary

- We are working on integrating a variety of online modeling and tuning tools into regular operation at LCLS-II
  - Automatic alignment and characterization including 6-D phase space reconstruction
  - Live model run in parallel with machine operation
  - Sample-efficient emittance optimization with Information-based BAX
- Future work
  - Online modeling to beam/FEL pulses through linac to FEL
  - Using the historical data to capture the behavior and dynamics of accelerator system
  - HPC cluster at SLAC (S3DF) for real-time data processing and model updating

Comprehensive holistic view of the electron beam behavior to aid tuning, and extend downstream through the entire accelerator

Thank you!