Toward Autonomous Beam Tuning for MeV-Ultrafast Electron Diffraction with Constrained Multi-Objective Bayesian Optimization

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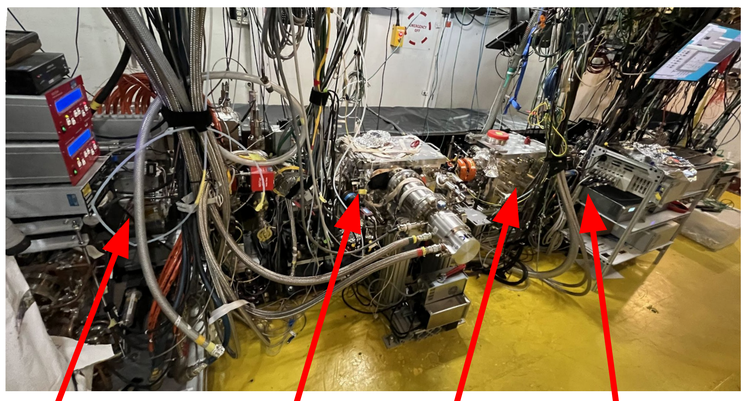
BACKGROUND

- Automation of MeV-UED e-beam tuning could substantially improve performance and efficiency
- MOBO algorithm recently demonstrated at MeV-UED, achieving performance comparable to that obtained by experienced human operators
- Constrained two-stage MOBO could dramatically improve the valid data efficiency by learning the feasible region

MeV-Ultrafast Electron Diffraction (MeV-UED)

- Pump-probe scattering technique using MeV electrons to study time-resolved, ultrafast dynamics in various solid, liquid and gas systems
- Recently deployed THz timing tool (Othman et al., 2022) enables online shot-by-shot measurements of electron pulse duration and time-of-arrival



Tuning Parameters	Objectives
RF gun phase Gun solenoid strength 2nd solenoid strength Steering magnet XC00 Steering magnet YC00 Steering magnet XC01 Steering magnet YC01 Steering magnet XC02	Spot size (Minimize) q-resolution (Minimize)
Constraints	
Transmission through collimator and THz timing structure (Q >= 0.3 fC)	

Constrained Multiobjective Bayesian Optimization (MOBO)

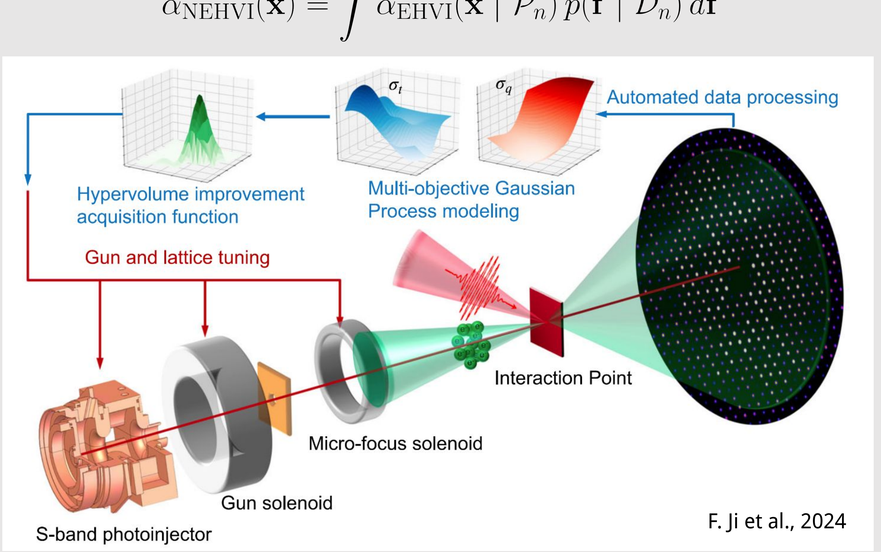
- Nondominated points in the objective space form the Pareto Frontier, which represents crucial trade-offs
- Acquisition function determines optimal next sampling points from a Gaussian Process surrogate model

Constrained Expected Hypervolume Improvement (EHVI) acquisition function: (F. Ji 2025)

$$\alpha_{\mathrm{cEHVI}}(\mathbf{x}) = \int_{\mathbb{R}^M} H_I(\mathcal{P}, \mathbf{y}, \mathbf{r}) \mathcal{N}_{\mu(\mathbf{x}),\Sigma(\mathbf{x})}(\mathbf{y})\, d\mathbf{y} \times \prod_{i=1}^{m} \Phi\left(\frac{\mu_{c_i}(\mathbf{x}) - Q_i}{\sigma_{c_i}(\mathbf{x})}\right)$$

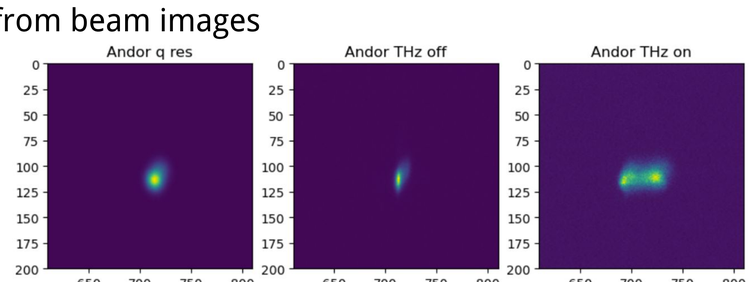
Noisy EHVI: (S. Daulton 2021)

$$\alpha_{\mathrm{NEHVI}}(\mathbf{x}) = \int \alpha_{\mathrm{EHVI}}(\mathbf{x} \mid \mathcal{P}_n)\, p(\mathbf{f} \mid \mathcal{D}_n)\, d\mathbf{f}$$

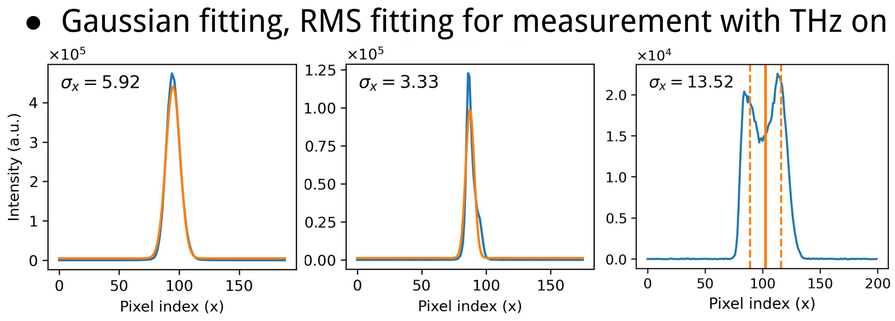


DATA ANALYSIS

- Spot size and THz streaking arrival time measurements from beam images



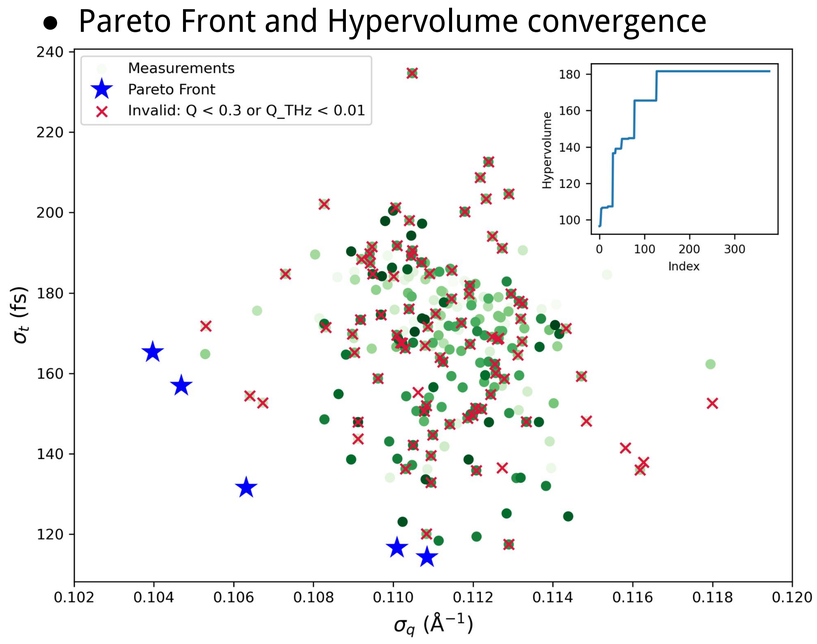
- Gaussian fitting, RMS fitting for measurement with THz on



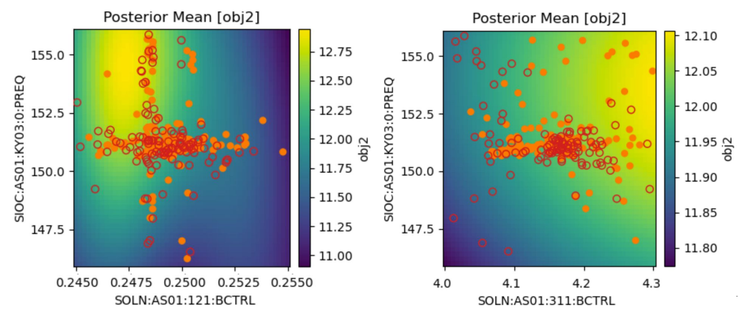
- Dataset cleaning/validation, background removal

RESULTS

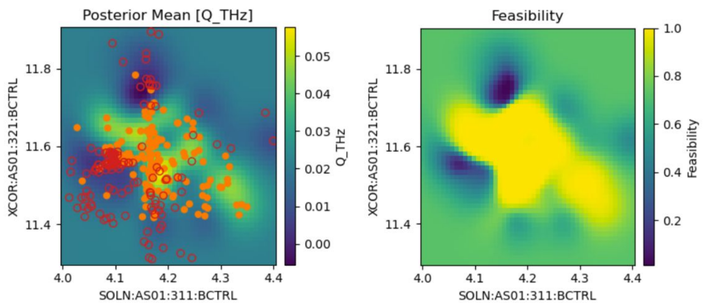
- Pareto Front and Hypervolume convergence



- Visualizations of Gaussian Process models
- Pulse length objective with respect to gun phase and solenoids 1 and 2



- Charge constraint behavior with respect to solenoid 2 and XC02 steering magnet



CONCLUSIONS AND FUTURE DIRECTIONS

- MOBO obtained a feasible region that informed decisions and improved sampling efficiency
- Successful application of two-stage constrained MOBO to a challenging practical tuning task
- Potential for broader application to other constrained tuning problems at SLAC

Learn more about MeV-UED!

ACKNOWLEDGEMENTS

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