Machine development R&D: ePix detector, AI/ML and gun designs

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SLAC National Accelerator Laboratory

UED Advisory Board Meeting FY25 Q1
Nov 18th, 2024

Outlines

- UED R&D roadmaps and scientific needs
- ePix single electron detector developments
- High brightness electron source developments
- AI/ML for improving facility operations and assist in scientific discoveries
- Summary

R&D roadmap and scientific needs in critical areas

- ➢ KHz Repetition rate operation upgrade (Joel)
- ➢ THz Timing tool (TT) development (Joel)
- ➢ **ePix single electron detector**
- ➢ **UED gun developments**
- ➢ **AI/ML**

MeV-UED instrument development

Today: 360 Hz system, 150 fs resolution

Near (ongoing R&D): 1080 Hz + 1st gen time tool

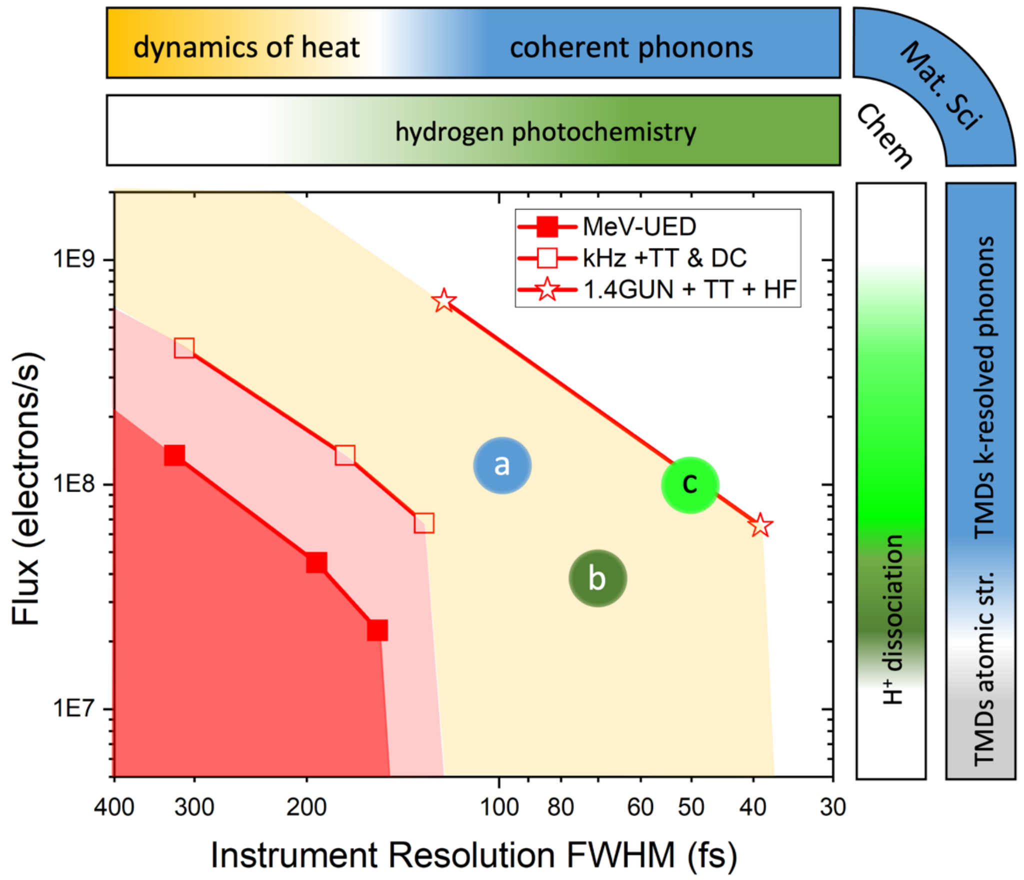
Medium (proposed): UED-optimized gun + shot-by-shot arrival monitor + hollow fiber pump compression

Enabled Science Cases

a. Momentum-resolved transient phonon populations in mono-layer WSe_2

b. Resolve structural and electronic dynamics during photodissociation of ammonia

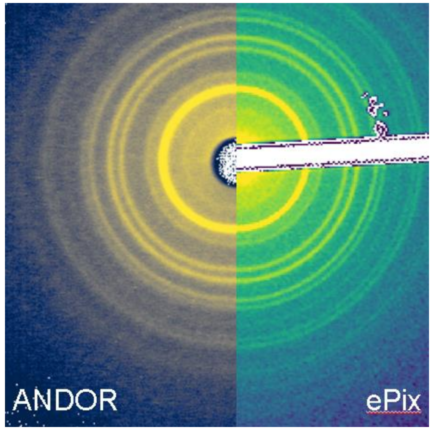
c. Measure intramolecular proton transfer in 2-nitrophenol



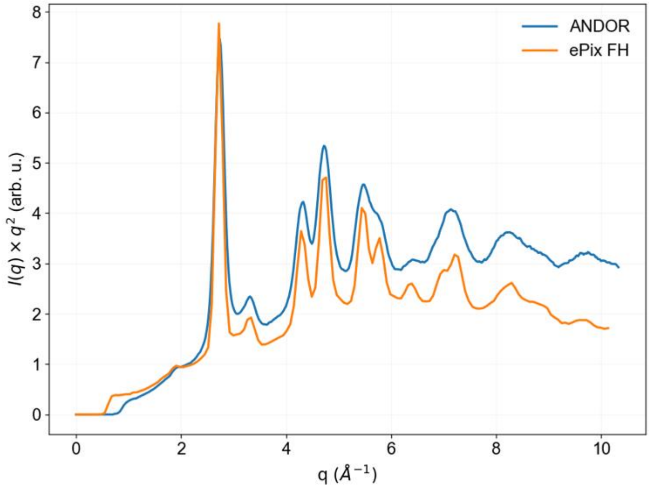
Y. Liu, X. Shen and A. Reid, **UED Instrument Retreat Report**, March 14, 2023

Direct electron detector (2022)

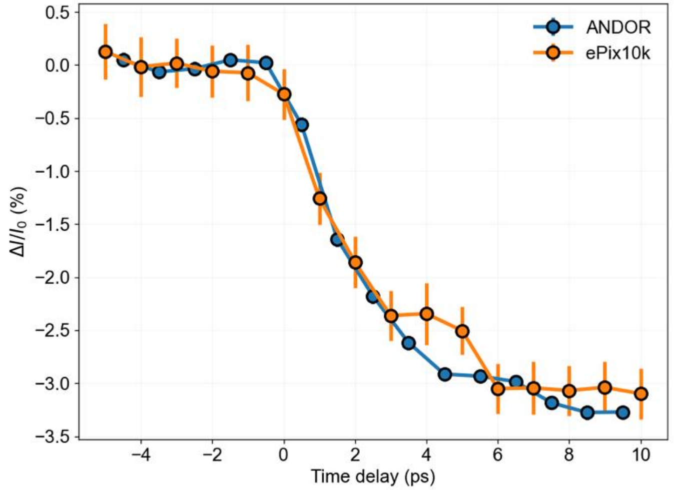
Polycrystalline Bismuth thin film sample



Diffraction pattern



Radial profile



Pump-probe signal

ePix10k detector
- Single electron detection
- 704 x 768 pixel sensor
- Flexible gain modes
- Pixel size: 100 um
- Readout rate 360 frame/s

- 1st round commissioning (2022) demonstrates frame-by-frame collection of single-pulse electron diffraction patterns at the MeV-UED instrument.
- Capable of performing single electron detection and eliminate cosmic-rays/stray light backgrounds and optical aberrations
- Generates 360 frame/s data flow, running single electron finding algorithms with > 300 CPUs on SLAC computation cluster S3DF

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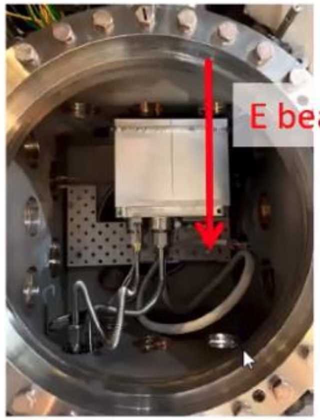
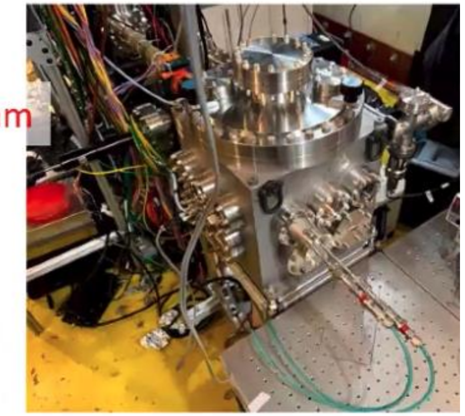
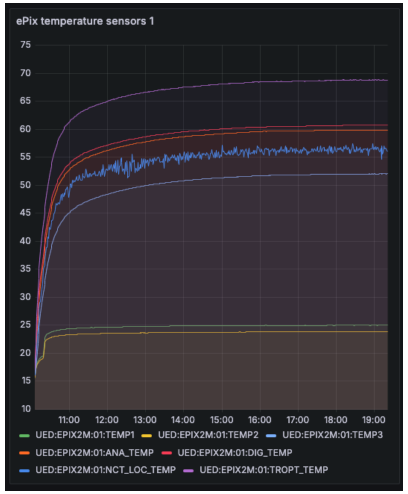
Direct electron detector (current)

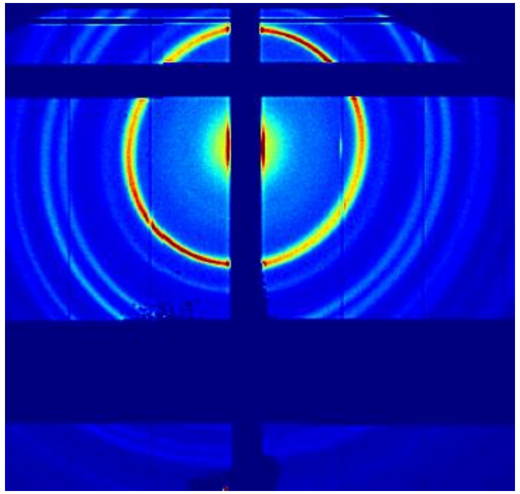




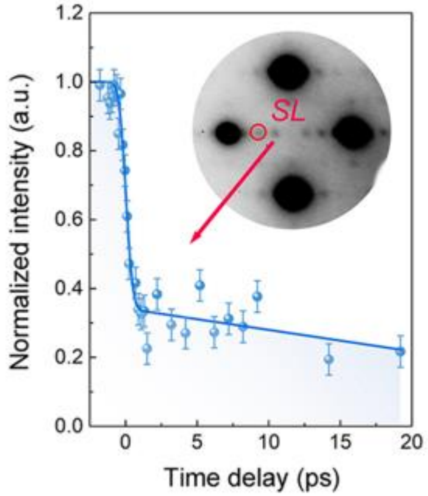
Temp sensor readouts



Data taken on Nov 12, 2024



CO quenching in Fe3O4

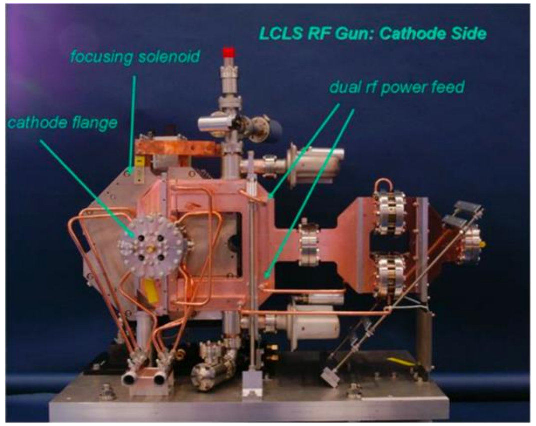


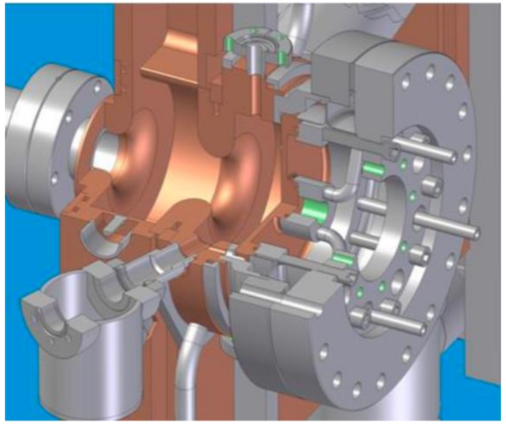
Physical review B 106, 195131(2022)

- Detector malfunctioning due to heating damage-> Adding temperature sensors to monitor detector status
- Repair and re-installation of ePix detector in Sept 2024
- **<u>Demonstrated 360 Hz data taking over 12 hours operation,</u>** commissioning experiment undergoing aims to run the ePix detector in a non-trivial solid-state experimental scenario over 24-hour shifts
- The result will allow user groups to make informed decisions about their run 5 experimental configurations and whether to use the ePix detector instead of the EMCCD platform

Ultra-high brightness electron source R&D

The SLAC/UCLA/BNL type 1.6 cell S-band RF gun





- ✓ Electron source for SLAC MeV-UED and LCLS-I
- ✓ 1.6 cell design, mature 2.86 GHz normal conducting technology
- ✓ Demonstrated stable operation for > 10 years
- ✓ High gradient operation, 90-120 MV/m cathode gradient
- ✓ Direct output MeV energy beams (3 – 4.2 MeV)

$$\mathcal{B}_{4\mathrm{D}} \propto \frac{E_z}{\mathrm{MTE}} \qquad A = \frac{\sigma_x m_e}{\sigma_t^2 E_z e}$$

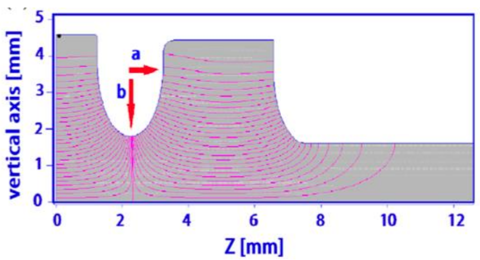
for pancake (A>>1) beam

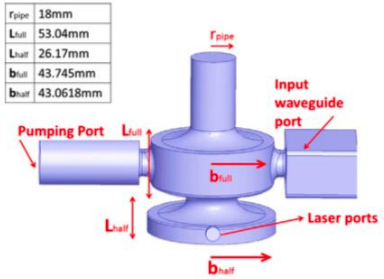
I. Bazarov, B. Dunham, and C. Sinclair, *PRL 102, 104801(2009)*

S-band 1.4 cell photoinjector design for high brightness beam generation

E. Pirez [a], P. Musumeci [a], J. Maxson [a], D. Alesini [b,*]

[a] *Department of Physics and Astronomy, UCLA, Los Angeles, CA 90095, USA*
[b] *INFN-Laboratori Nazionali di Frascati, Via Enrico Fermi 40, 00044 Frascati, Rome, Italy*





- For 1.6 cell gun, launching phase is ~37 degree -> 54 MV/m launch gradient
- Shorter cathode cell -> larger acc field at cathode

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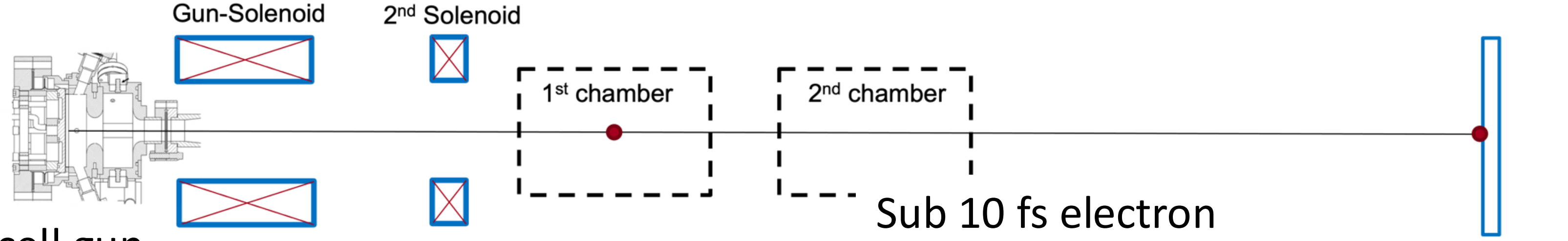
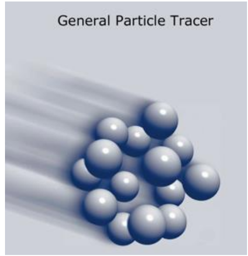
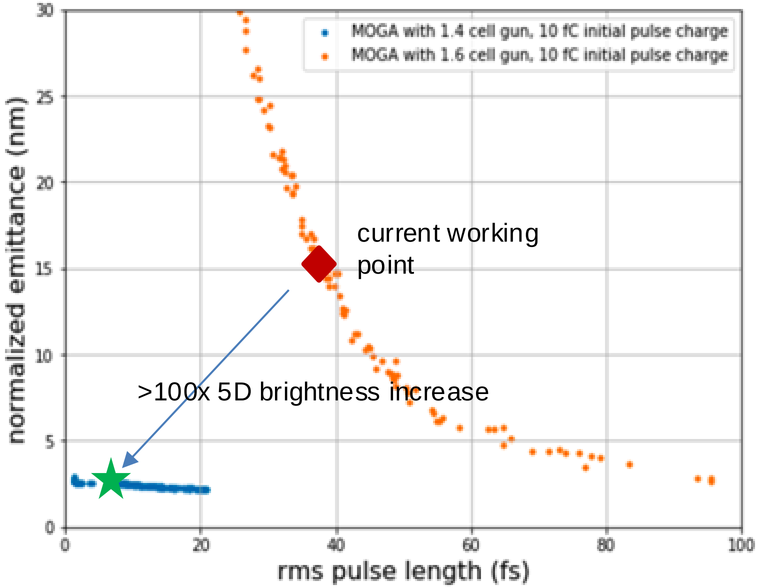
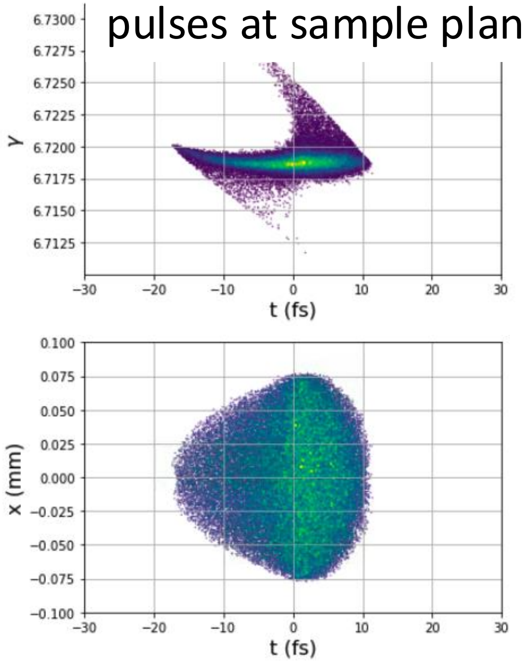
Ultra-high brightness electron source R&D

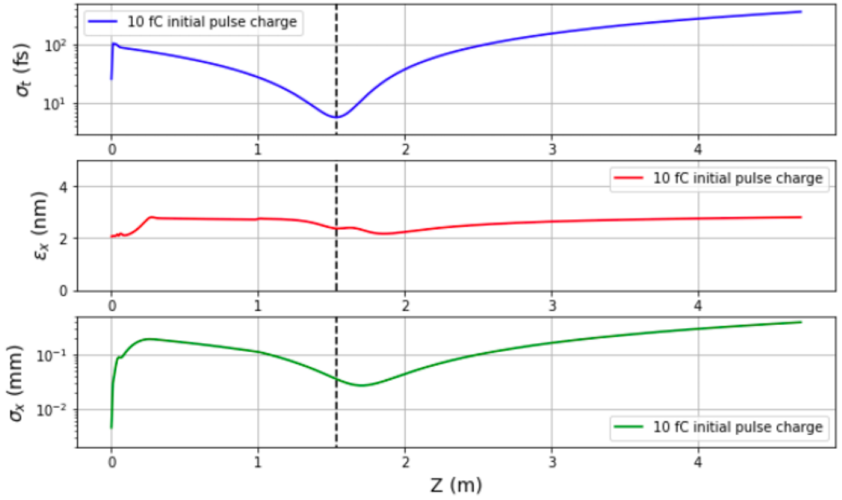






Sub 10 fs electron pulses at sample plane

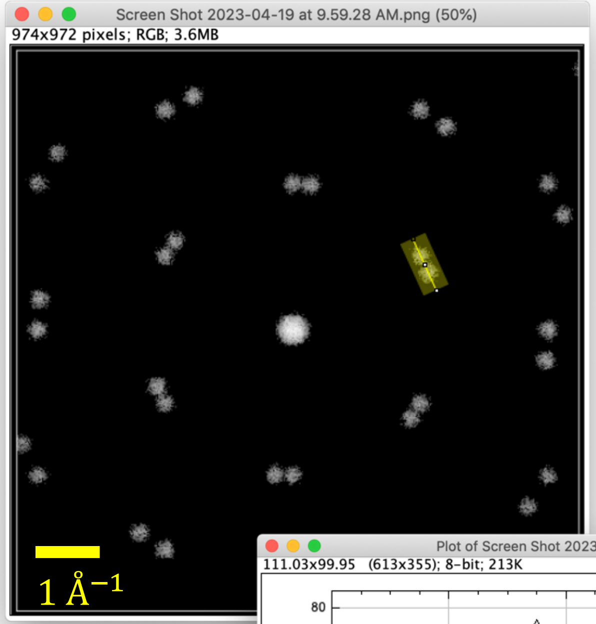


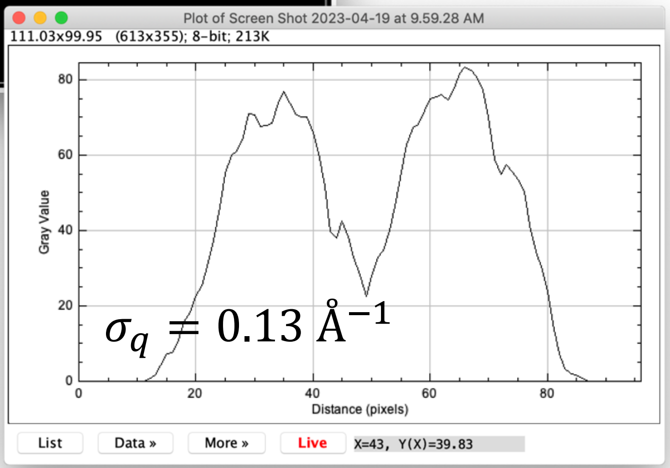


- Multi-objective genetic optimizations using the proposed 1.4 cell gun and the UED beamline configurations
- Simulations show that a by tuning the gun phase, a strong bunching configuration can be achieved
- Beam parameters at sample plane: rms pulse length = 5.02 fs, normalized emittance = 2.36 nm

Ultra-high brightness electron source R&D

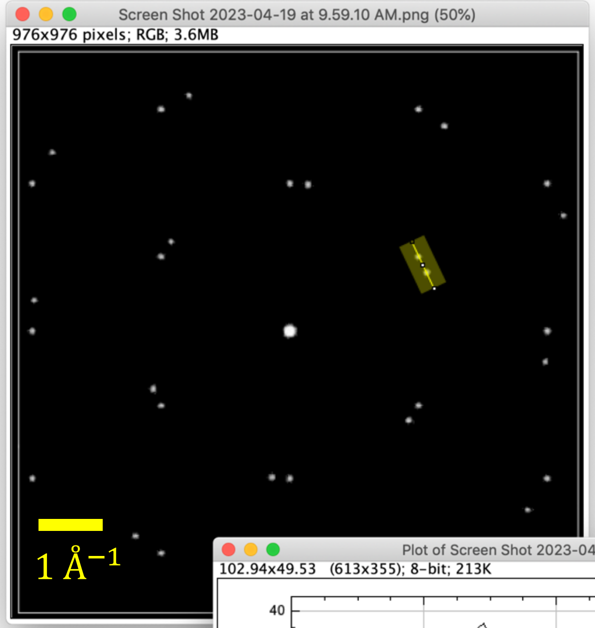
Current ASTA 1.6 cell gun → Alternative 1.4 cell gun

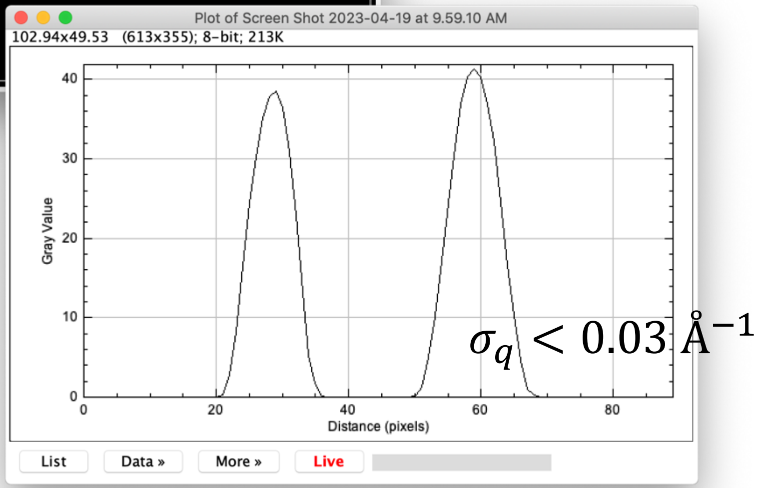




Simulated q-resolution enhancement with new high brightness gun design

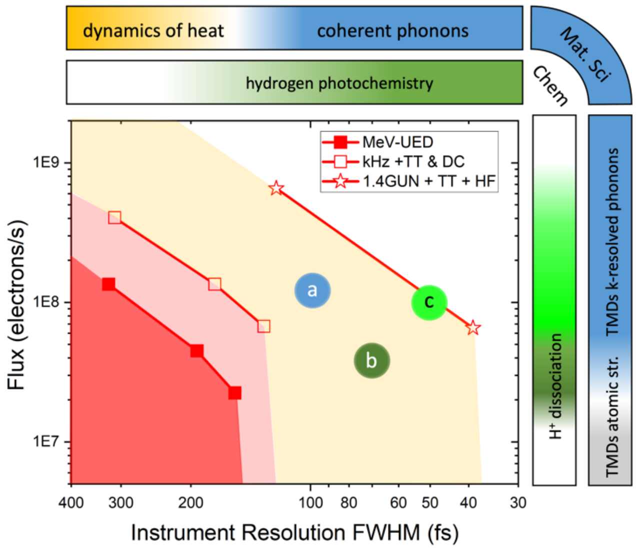
- 10 fC pulse charge (nominal condition for MeV-UED operation)
- GPT simulation of 7 deg rotated WS_2 bilayer
- Results can be further improved with collimation



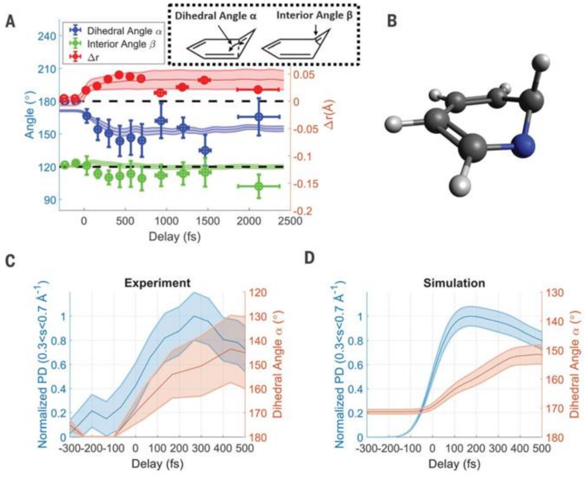


AI/ML for improving MeV-UED operations

- How to optimize the facilities and instruments for achieving physics limited performance to enable the discovery of new sciences? -> <u>AI/ML based methods</u>
- The requirements for electron beam properties are multi-dimensional
  - Gas/liquid phase: temporal length, pulse charge
  - Solid state: temporal length, probe size, momentum space resolution
- Electron beam property optimization often relies on time-taking hand tuning by human operators. Algorithm based tuning strategies are highly desired

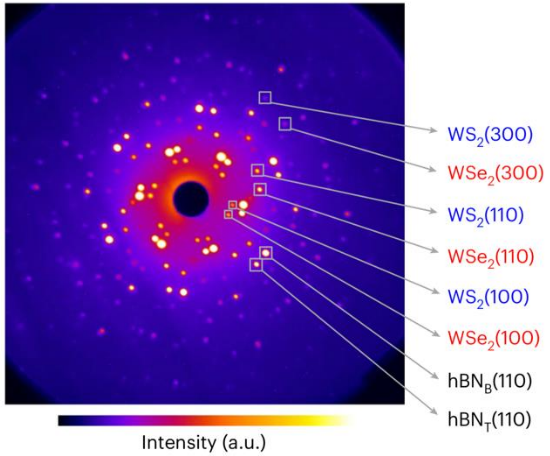


Fast process



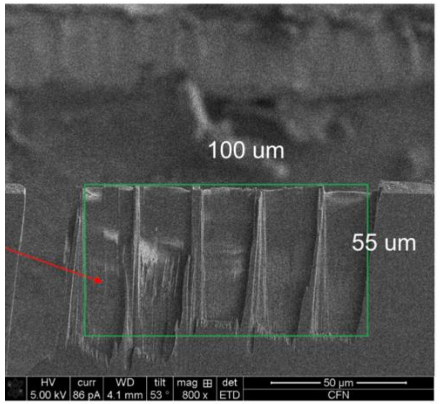
Science 368, 885-889 (2020)

Complex features in momentum space



Nature Nanotechnology 18, 29–35 (2023)

small sample



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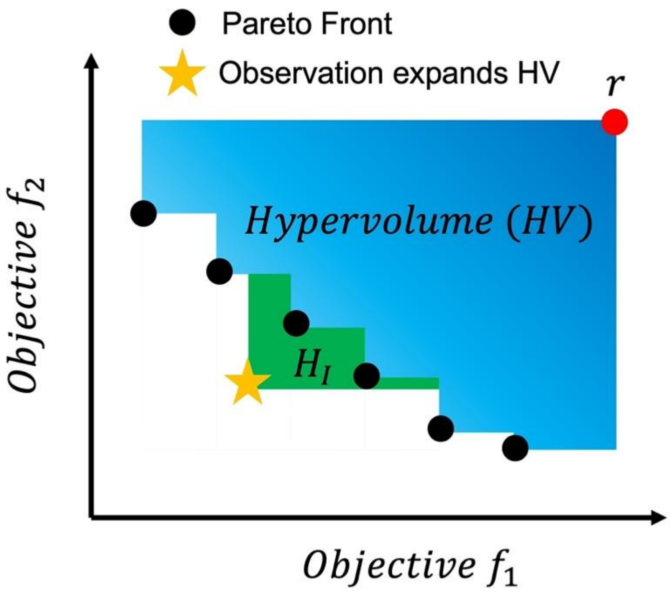
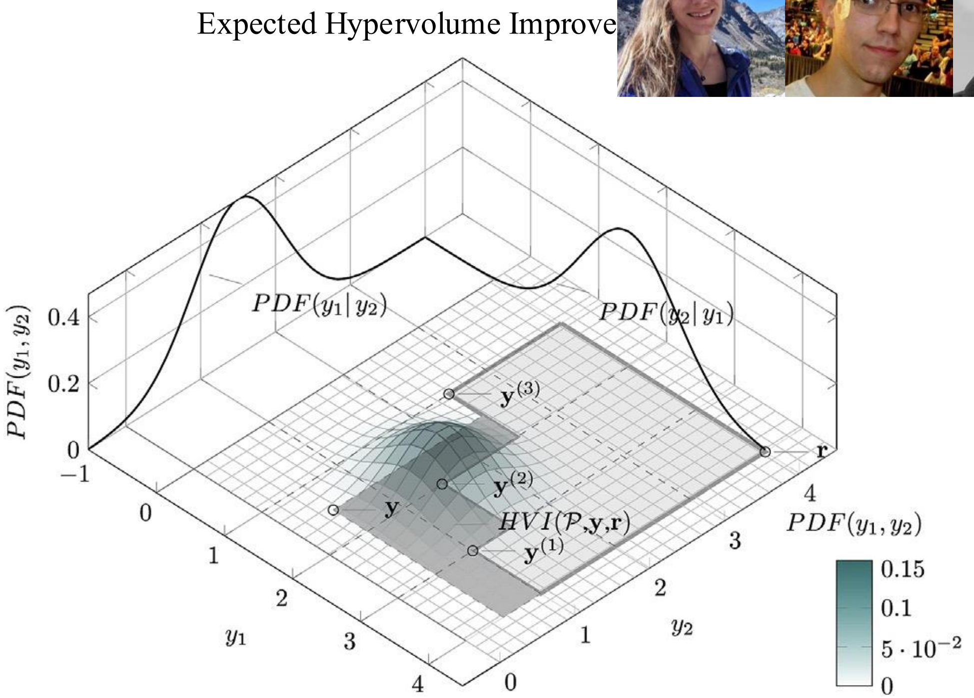
Multi-objective Bayesian optimization (MOBO)

SLAC AD Machine Learning group

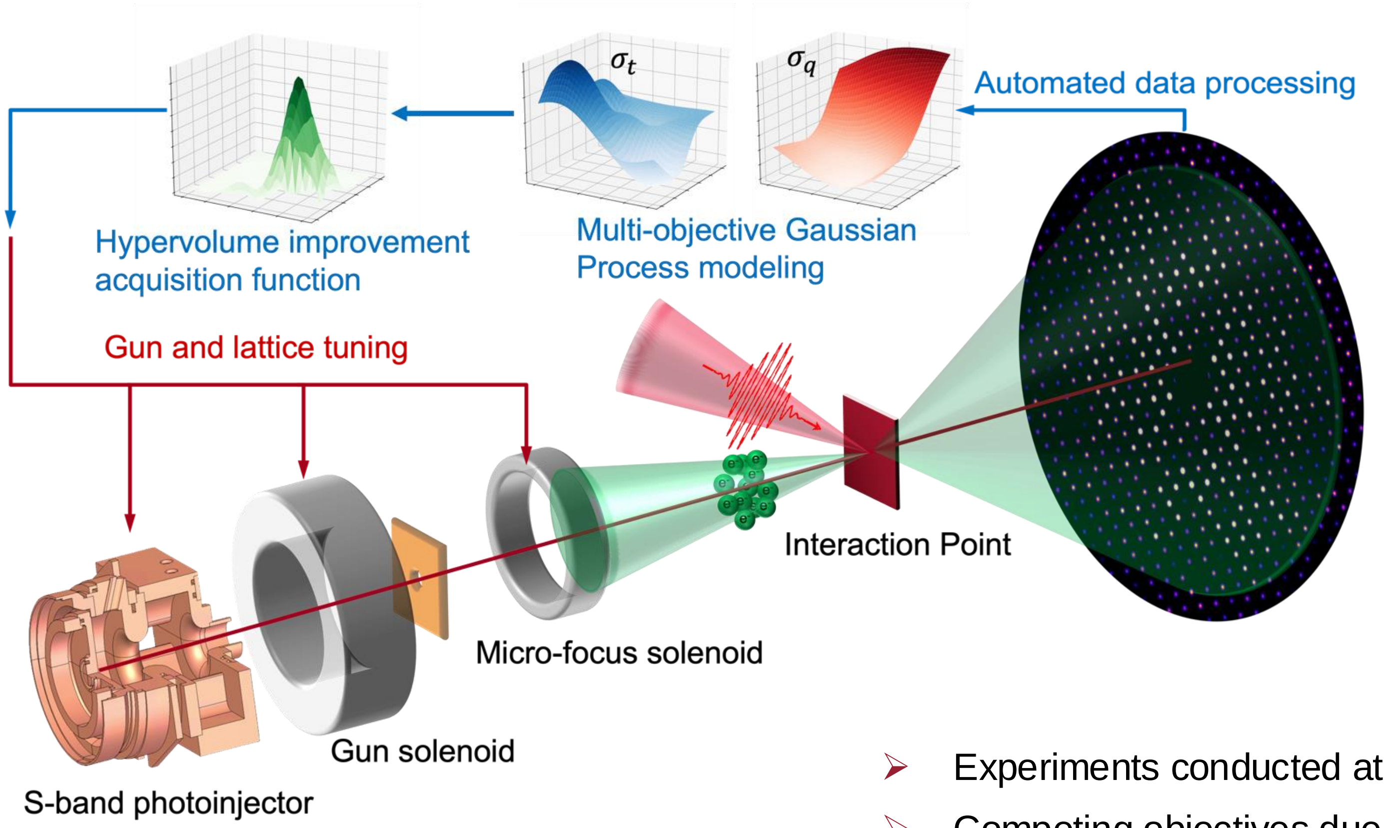




Swarm and Evolutionary Computation 44 (2019) 945–956

- The goal is to determine the Pareto Front giving the best achievable trade-offs between objectives
- Deployed cutting-edge AI algorithm(MOBO) at MeV-UED
- 10 times more efficient than evolutionary algorithms
- A critical step toward online multi-objective optimization on real accelerator systems

Multi-objective Bayesian active learning for MeV-UED



F. Ji, *et al.*, *Nat. Commun. 15, 4726 (2024)*

Input: Given a set of observations $\mathcal{D}_N = \{(\boldsymbol{x}_1, \boldsymbol{y}_1), (\boldsymbol{x}_2, \boldsymbol{y}_2), \ldots, (\boldsymbol{x}_N, \boldsymbol{y}_N)\}$

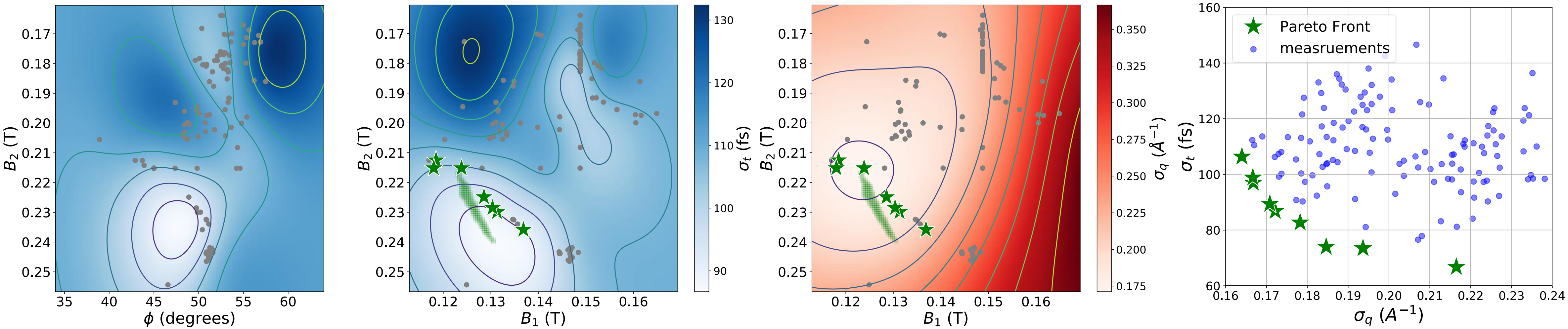
for i in range(number of measurements):

1. Each objective modeled as an independent GP model:
   $$y_m \sim GP_m[\mu_m(\boldsymbol{x}), k_m(\boldsymbol{x}, \boldsymbol{x}')]$$
2. Calculate the EHVI acquisition function
   $$\alpha_{EHVI}(\mu, \sigma, \mathcal{P}, \boldsymbol{r}) = \int_{\mathbb{R}^M} H_I(\mathcal{P}, \boldsymbol{y}, \boldsymbol{r}) \cdot \mathcal{N}_{\mu,\sigma}(\boldsymbol{y})\, d\boldsymbol{y}$$
3. Determining next observation point
   $$\boldsymbol{x}_{next} = argmax(\alpha_{EHVI})$$
4. Do observation
   $$\boldsymbol{y}_{next} = f(\boldsymbol{x}_{next})$$
5. Update $\mathcal{D}_N$

end for

- Experiments conducted at SLAC-MeV UED facility
- Competing objectives due to space charge forces: electron pulse length (σ_t), spot size at sample (σ_x) and momentum space resolution (σ_q)
- Explore the responses of $[\sigma_t, \sigma_x, \sigma_q]$ to gun phase (ϕ), gun solenoid strength (B_1) and micro-focus solenoid strength (B_2) and obtain Pareto Fronts giving trade-offs between them

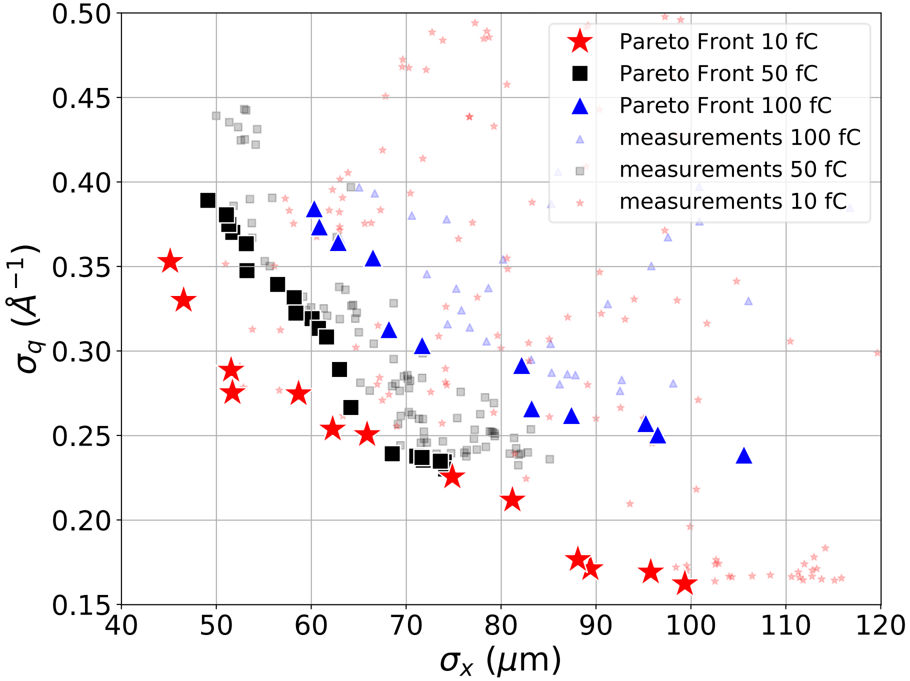
Multi-objective Bayesian active learning for MeV-UED

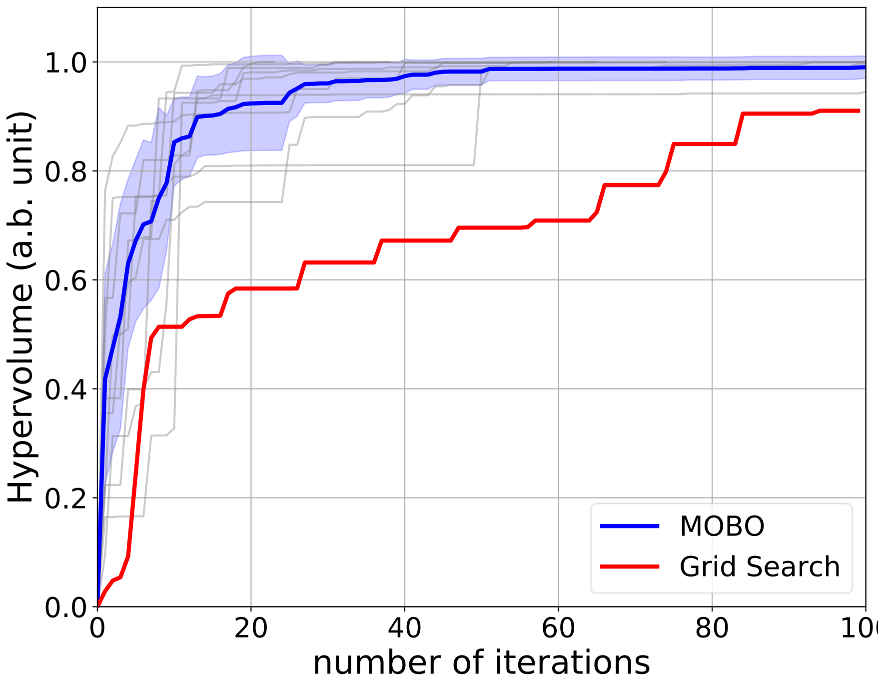


F. Ji, *et al., Nat. Commun. 15, 4726 (2024)*

- Measurements of σ_t, σ_q projected to the $\phi - B_1$ and $B_1 - B_2$ subspace, along with posterior mean predicted by the GP
- MOBO strategically proposes the next observation point, and is more data efficient than a broad, undirected search for the PF
- The Learned PF provide an unprecedented overview of system behavior and can assist human scientist in rapid decision making during very limited beamtime
- Marks the first instance where MOBO has been applied to actively learn and navigate through the trade-offs of key beam properties that have a direct and substantial impact on the outcome of scientific user experiments

Multi-objective Bayesian active learning for MeV-UED





F. Ji, *et al.*, *Nat. Commun. 15, 4726 (2024)*

- Spot size vs q-resolution optimizations under different initial pulse charges
- Convergence plot shows hypervolume achieves 95% of it's maximum within 30 measurements in average
- The hypervolume obtained using a grid search(GS) was 62% of that obtained using MOBO after 30 measurements.
- The comparison between MOBO and GS shows clear advantage of MOBO to improve both optimization efficiency and maximum achievable hypervolume

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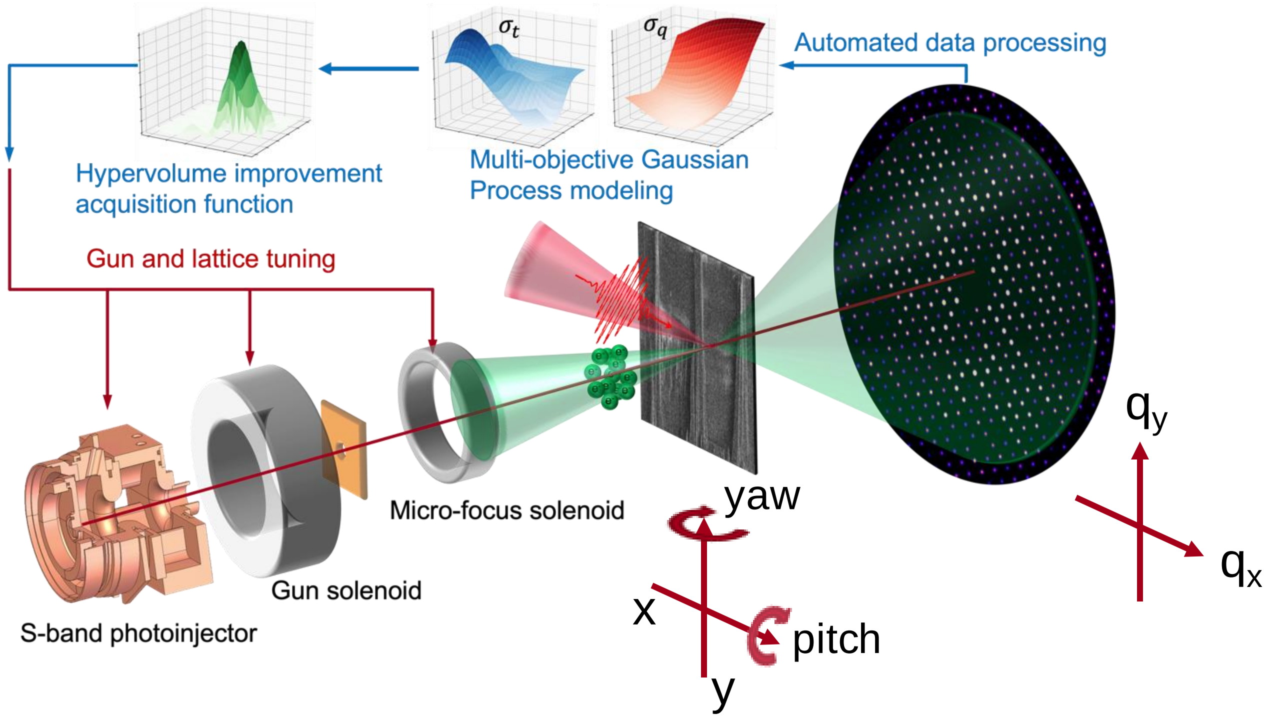
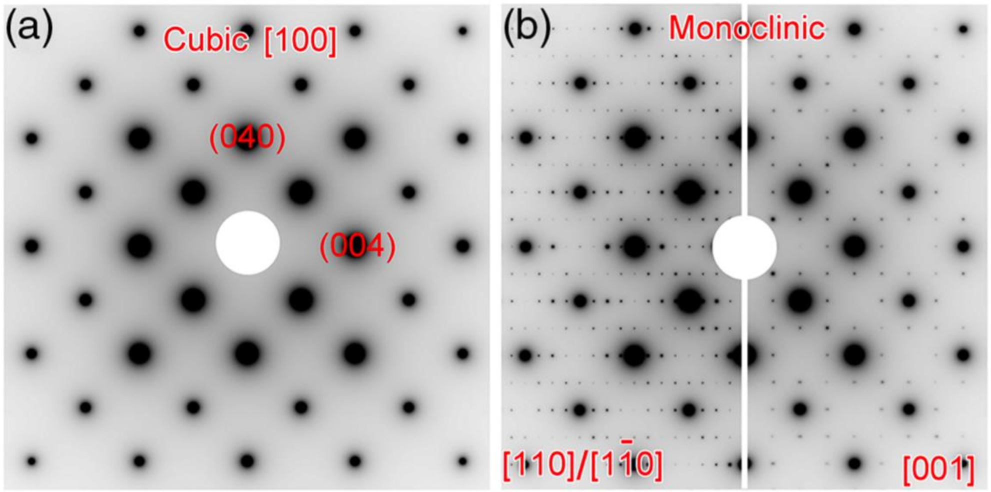
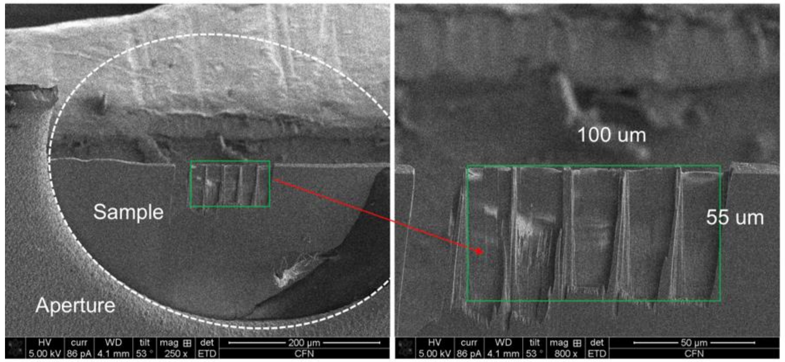
AI/ML to assist in accelerating scientific discoveries





Phys. Rev. B.106.195131 (2022)



Courtesy of BNL TEM group

- <u>Solid state UED</u>
  - Sample tuning: 4 degrees of freedom: x, y, pitch and yaw
  - 2D slices of the reciprocal space on detector
  - Other variables: temperature, pump wavelength/energy, pump-probe delays
- <u>Bayesian algorithms to assist in the search of charge orders in strong correlated materials</u>

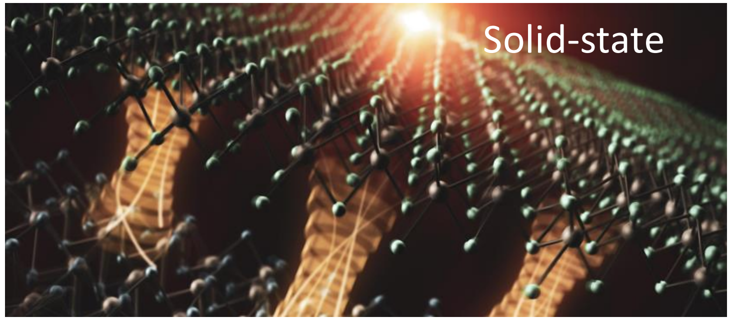
Summary

- Critical needs have been identified from UED strategic planning efforts and user feedback
- Intense R&D efforts undergoing aiming at improving flux and resolutions of the MeV-UED instrument
  - ePix detector capable of performing shot-by-shot single electron detection and achieving ultrahigh SNR, ready for production for UED run5
  - 1.4 cell gun optimization studies showing that ultrahigh brightness beams with < 10 fs pulse length, < 2 nm normalized emittance could be achieved
- Cutting edge AI algorithm applied for online optimizations of key beam properties
- AI/ML techniques holds the potential of improving facility operations and accelerating scientific discovery

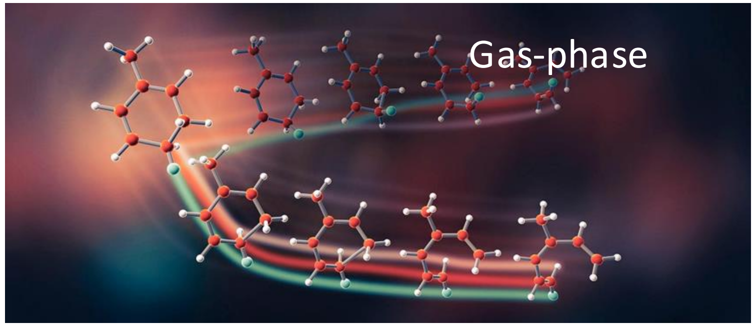
Acknowledgements

Thank you!

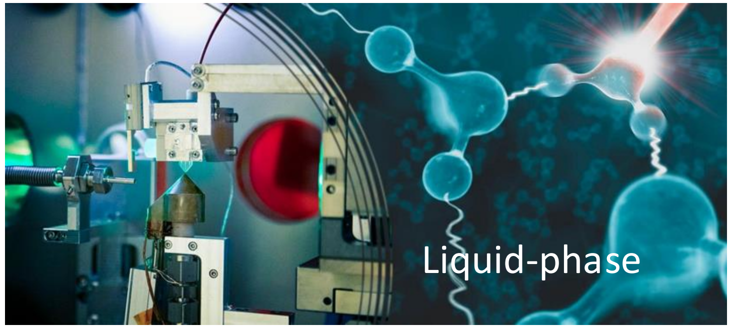
MeV-UED: Capabilities and Science enabled



Rapid energy transfer between two-dimensional hetero-structures (**Nature Nanotechnology** 18, 29-35 (2023))



Conformer-specific photochemistry imaged in real space and time (**Science** 374, 178-182 (2021))



Ultrafast hydrogen bond strengthening in liquid water (**Nature** 596, 531-535 (2021))

Ultrafast phase dynamics switches in a quantum electronic device (**Science** 373, 352-355 (2021))

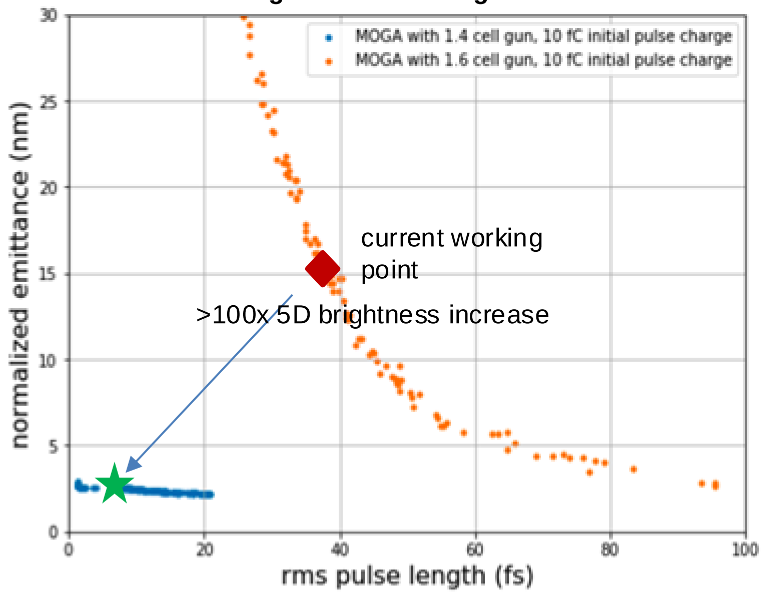
- Probe structural and electronic dynamics in solid, gas and liquid systems under optical pumps and operando excitations
- Science opportunities in the key areas:
  - Resolve *structural and electronic dynamics* during photodissociation events
  - intramolecular *Proton transfer & migration dynamics*
  - Momentum-resolved transient *phonon populations* in thin mono-layer materials
  - Exploring *energy pathways and structure-function relationships* in hetero-structure based low dimensional systems

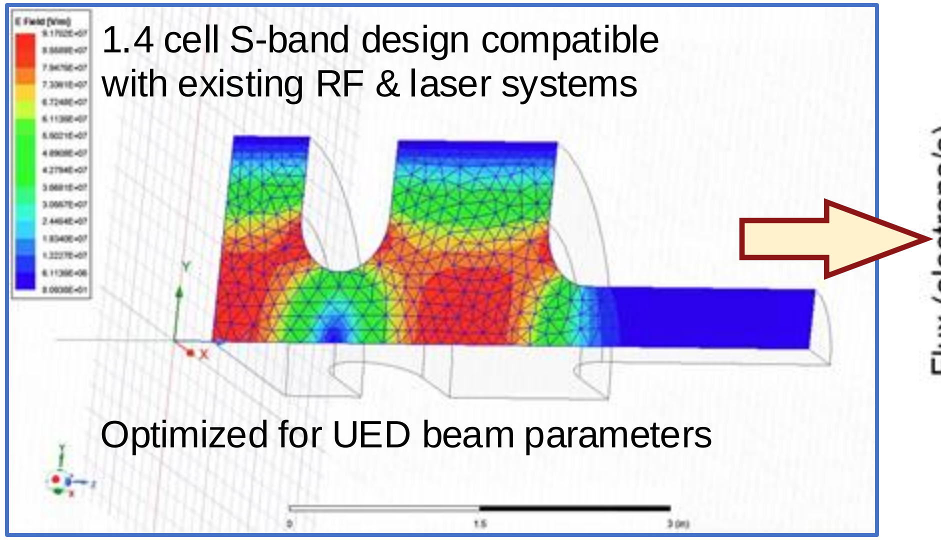
Ultra-high brightness electron source R&D

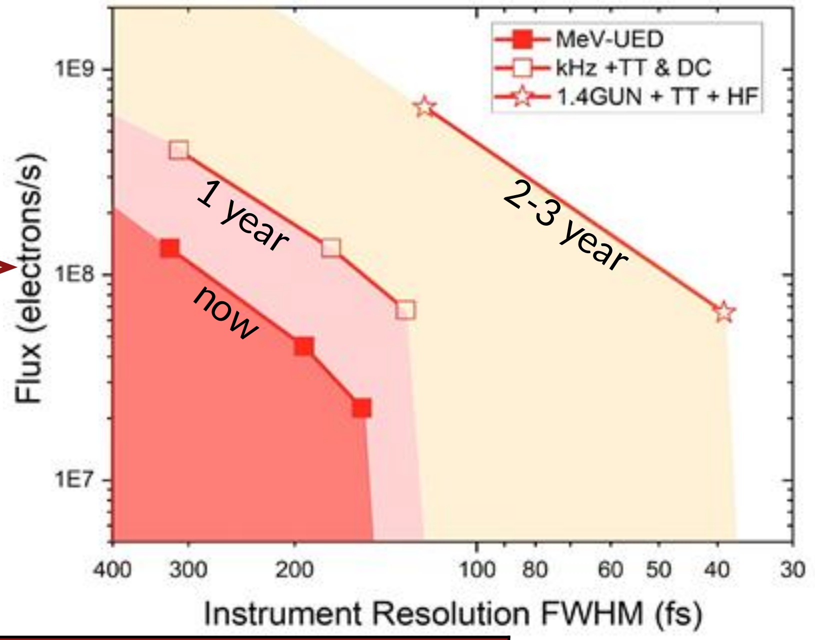
- Improve instrument time resolution towards 50 fs
- Increase electron flux to > 1e8 electrons/sec
- Improve transverse emittance to reach Δq = 0.01 Å^{-1}

To meet future user requirements on electron flux, spot size, and time resolution, a new higher brightness, lower emittance electron source is needed

Current ASTA gun vs new design







Mid-Term (1-2 Year) Goals / Milestones	Key Personnel/Responsibilities
Prototype of 1.4-cell S-band gun design	UED AD with Test Fac and TID RFAR support
Dedicated online (shot-to-shot) THz time-tool	UED AD & LCLS team with Laser & Nanni Groups
Upgrade of the ePix detector to kHz rep rate	UED AD & LCLS team with TID Sensor Group
Laser DFG + HCF wavelength extension for UV pump	UED LCLS with Laser group support

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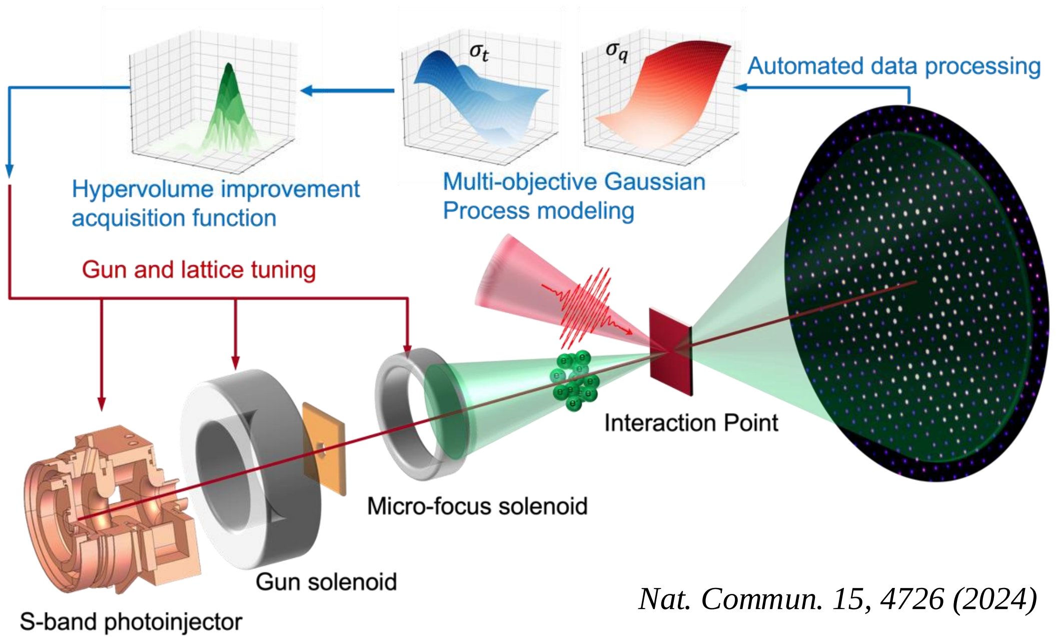
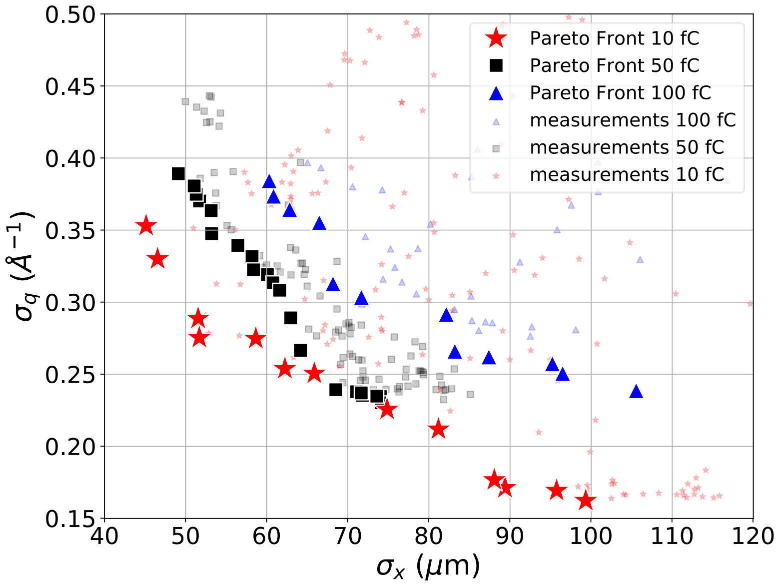
Multi-objective Bayesian active learning for MeV-UED



Nat. Commun. 15, 4726 (2024)



- The MOBO algorithm was used for sampling the parameter space efficiently with little prior knowledge
- The achieved performance was comparable with that obtained by experienced human operators and takes significantly fewer measurements
- Marks the first instance where MOBO has been applied to actively learn and navigate through the trade-offs of key beam properties that have a direct and substantial impact on the outcome of scientific user experiments
- This method is is flexible, efficient and can be used in other experimental scenarios

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Acknowledgements

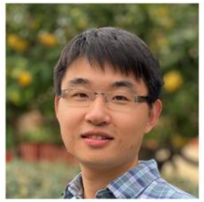
SLAC MeV-UED team

Alex Reid

Mike Minitti

Joel England

Xiaozhe Shen



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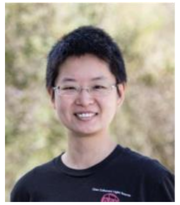

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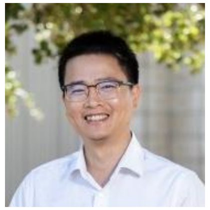

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Tianzhe Xu

Sharon Philip

Matthias Hoffmann

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