Trieste | Italy | 12·14 September

PhotonMEADOW 2023

FEL Photon Diagnostics, Instrumentation, and Optics Workshop

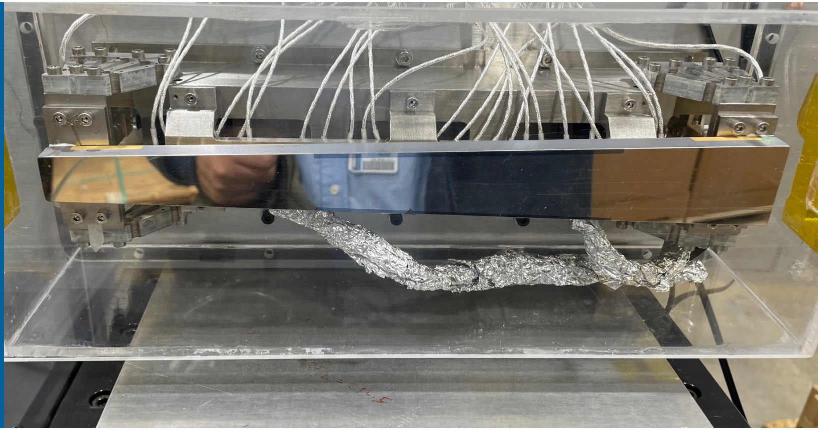
MEtrology, Astronomy, Diagnostics and Beamline Design Workshop

Elettra Sincrotrone Trieste

FELs OF EUROPE

Argonne NATIONAL LABORATORY

AI-DRIVEN REAL-TIME OPTICS CONTROL SYSTEM TO ACHIEVE ABERRATION-FREE COHERENT WAVEFRONTS AT 4TH-GENERATION SYNCHROTRON RADIATION AND FREE ELECTRON LASER BEAMLINES



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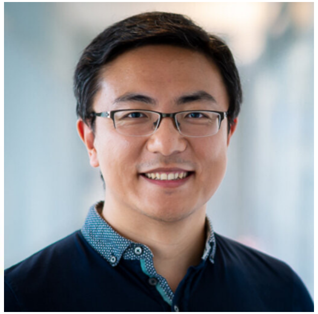
SUMMARY

- INTRODUCTION
- ML-DRIVEN CONTROL OF ADAPTIVE OPTICS (BIMORPH MIRROR)
- AI-DRIVEN AUTOFOCUSING SYSTEM FOR A NANOFOCUSING KB MIRROR
- TOWARDS APS-U: A PORTABLE, AI-DRIVEN OPTICS CONTROL SYSTEM

THE APS TEAM

Optics Group

L. Rebuffi



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INTRODUCTION

ML-DRIVEN CONTROL OF ADAPTIVE OPTICS (BIMORPH MIRROR)

AI-DRIVEN AUTOFOCUSING SYSTEM FOR A NANOFOCUSING KB MIRROR

TOWARDS APS-U: A PORTABLE, AI-DRIVEN OPTICS CONTROL SYSTEM

INTRODUCTION: NEW CHALLENGES

fast and comprehensive analyses of materials and devices in real-time scenarios

advancing speed and resolution in x-ray imaging and coherent techniques

4th Generation Synchrotron Radiation and FEL facilities

focused hard X-ray beams that exhibit minimal wavefront distortion, exceptional stability, and, in some cases, adjustable focal sizes

INTRODUCTION: NEW CHALLENGES

Coherent Surface Scattering Imaging

X-ray Photon Correlation Spectroscopy

Coherent X-ray Diffraction Imaging

Tomography

Preserving the wavefront and coherence of the beam

Wavefront distortions degrade the sample speckle contrast, which can hinder data interpretation

INTRODUCTION: OPTICAL ELEMENTS

Meticulously align optical components via high-precision actuators

Manufactured with a surface figure closely following an ideal mathematical shape

Stringent control over the vibrations and heat-induced deformations

Maintaining a coherent wavefront while suppressing undesired static distortions and dynamic disturbances

Repeatably align and focus the beam to match different sample and experiment requirements

Provide real-time correction in response to wavefront deformations

SOLUTIONS?

Adaptive Optics: Successful AO implementation requires high-precision components and sophisticated control systems (i.e. deformable mirrors, in-situ surface profilers, wavefront sensors, etc.), relies on the linearity, dynamics, and repeatability of the optics response to various actuator formats, including mechanical bending, piezoelectric bimorph. iterative control method based on linear response models could be slow to converge or inaccurate.

Automatic Alignment: Manual alignment and optimization of optical systems, even when limited to a few degrees of freedom, could fail to achieve an optimal configuration. On 4th generation optical systems, with numerous degree of freedom, manual approaches are considered inefficient and, in many cases, nearly impossible.

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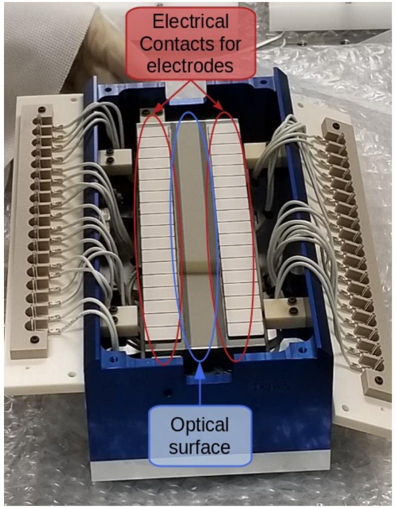
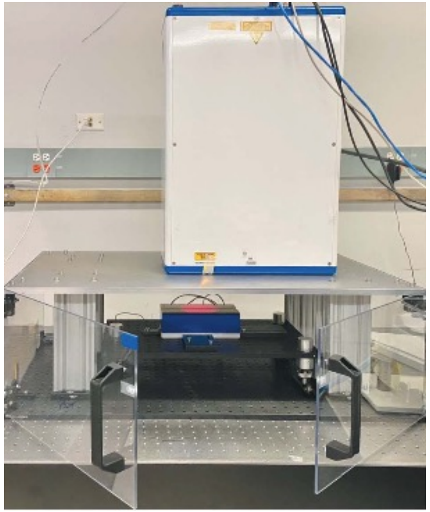
TOWARDS APS-U: A PORTABLE, AI-DRIVEN OPTICS CONTROL SYSTEM

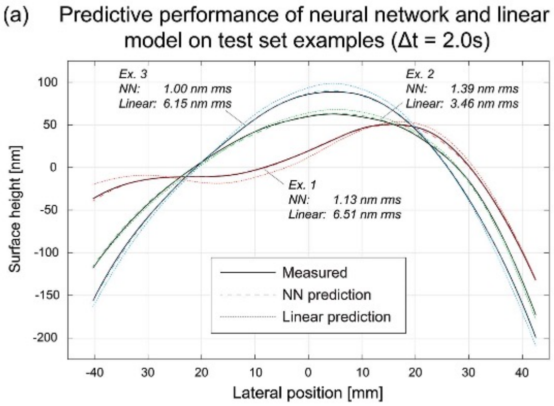
Gunjala et al., J. Synchrotron Rad. (30) (2023). DOI: 10.1107/S1600577522011080

PRELIMINARY STUDIES

Preliminary results: control of adaptive X-ray optics with piezo-bimorph actuators via a Neural Network-based, discrete-time model using random mirror shapes and interferometric measurements as training data





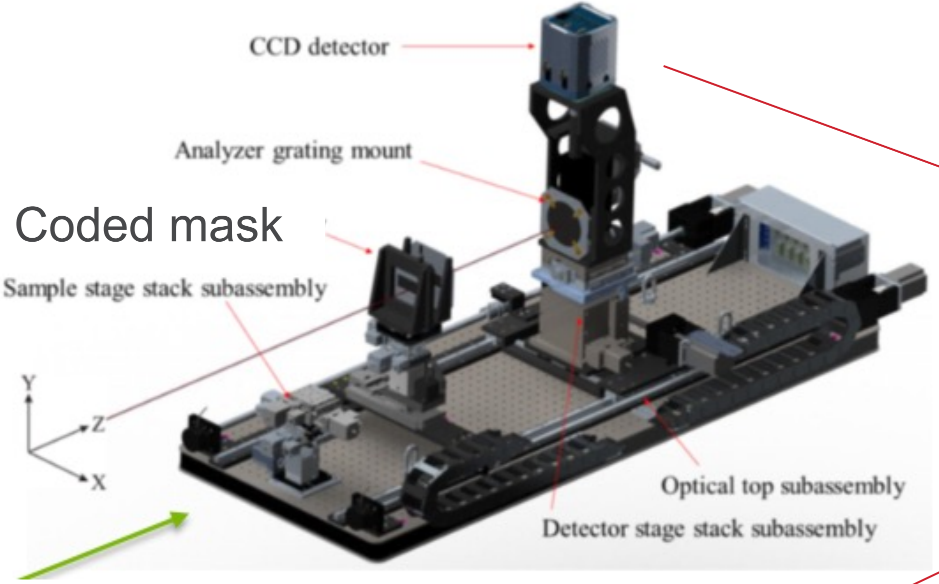


- **Can we extend this methodology from using surface shapes to X-Ray wavefronts?**
- **Can we efficiently collect and store a proper number of accurate wavefront data?**

WAVEFRONT SENSOR

X. Shi et al., *Synchrotron Radiat. News* **35**(2), 37-42 (2022).
Z. Qiao et al., *Appl. Phys. Lett.* **119**(1), 011105 (2021).
Z. Qiao et al., *Optica* **9**(4), 391-398 (2022).

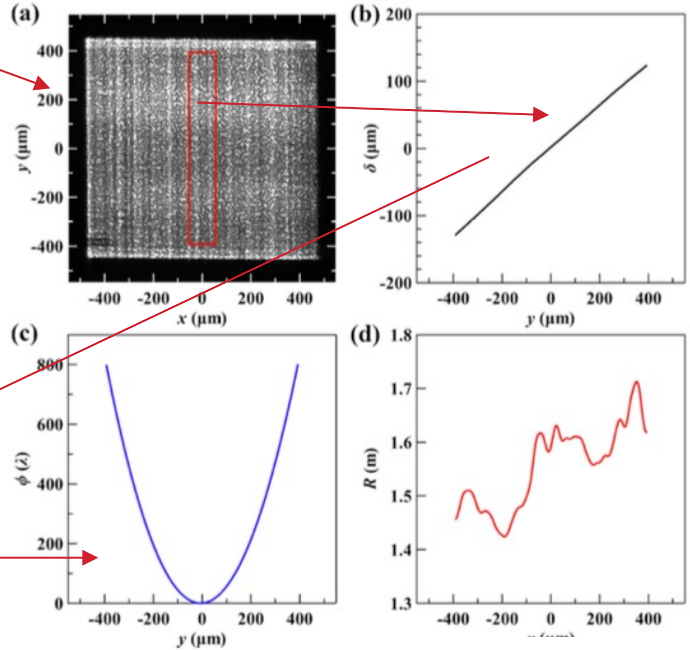
Coded mask



$$\Delta x_0 = \frac{\lambda a D}{2\pi}\Phi'_x, \quad \Delta y_0 = \frac{\lambda a D}{2\pi}\Phi'_y,$$

Speckle Pattern

Local displacement of speckle



Phase in unit of λ

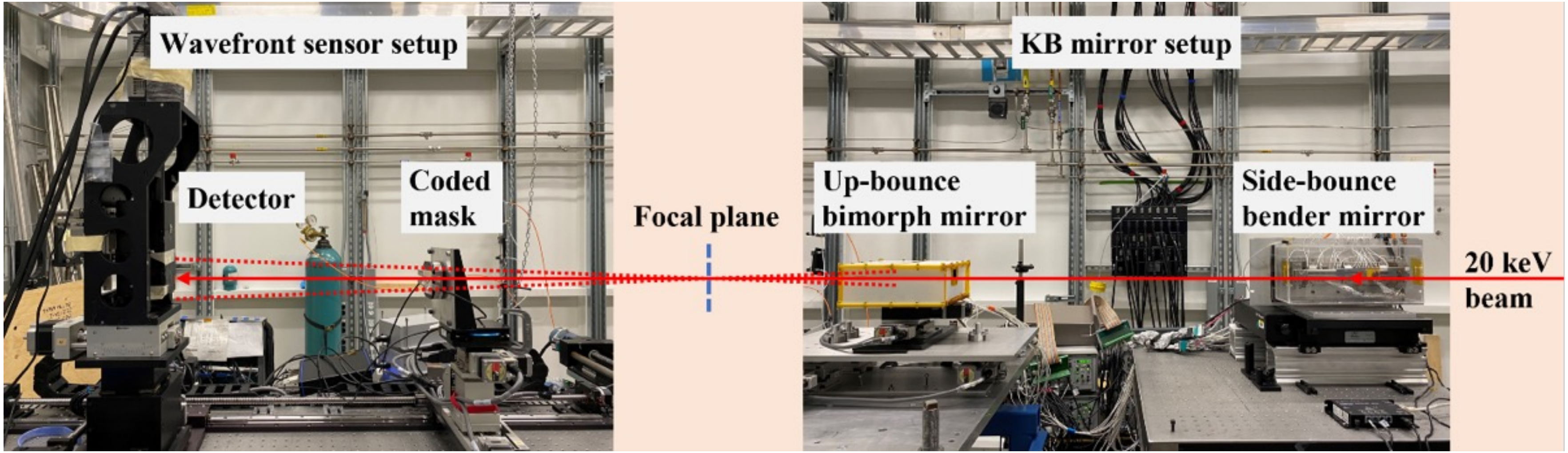
Local radius of curvature

ML-DRIVEN SYSTEM

NN-driven predictive model	NN-driven actuators controller
For any time t, the predicted wavefront property wp_{t+1}, at $t + \Delta t$, is expressed as a function of a history of n discrete-time set of voltages $v_{t-k} = \left[v_i^{actuator}\right]_{t-k}^{i=1\ldots N_a}$ applied to the chosen N_a actuators at time $t - k \cdot \Delta t$ and corresponding obtained wavefront property wp_{t-k+1} at time $t - (k-1) \cdot \Delta t$, with $k = 0,1 \ldots n$ (0 = current time), given by $$wp_{t+1} = f(wp_t, wp_{t-1}, \ldots, wp_{t-n+1}, v_t, v_{t-1}, \ldots, v_{t-n}).$$ The meaning of wp_{t+1} is that the model predicts the wavefront property spatial distribution one time step in the future given a finite history of wavefront property shapes and voltages, starting with its current shape, and applied set of voltages, going back to n time steps.	The controller provides the succession of m set of voltages to be applied to the actuators every Δt seconds, by directly minimizing the non-convex objective function using Adam. The cost function is given by $$\{v\}^* = \arg\min_{\{v\}} \sum_{t=1}^{m} c_t \cdot \lVert wp_t - wp^* \rVert_2^2,$$ with initial conditions $$wp_t = wp_0 \;\forall t \le t_0, v_t = v_{0-1} \;\forall t \le t_0$$ where wp^* is the desired wavefront property spatial distribution, and c_t coefficients are used to apply a weighted penalty to the prediction error at each time step.

ML-DRIVEN SYSTEM FOR BIMORPH MIRROR

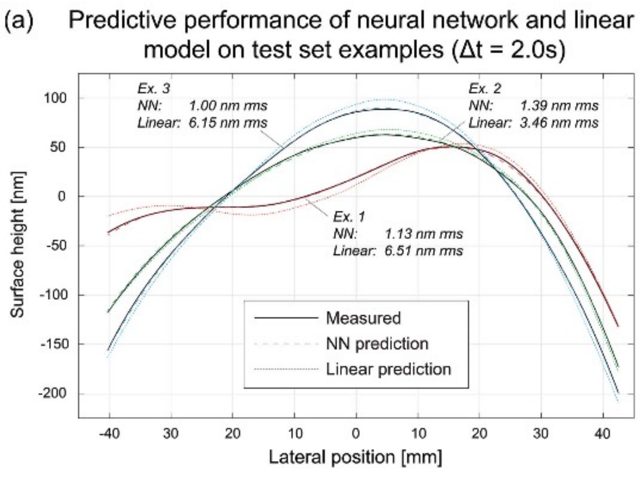
KB-mirror system at 28-ID-B IDEA beamline at the APS

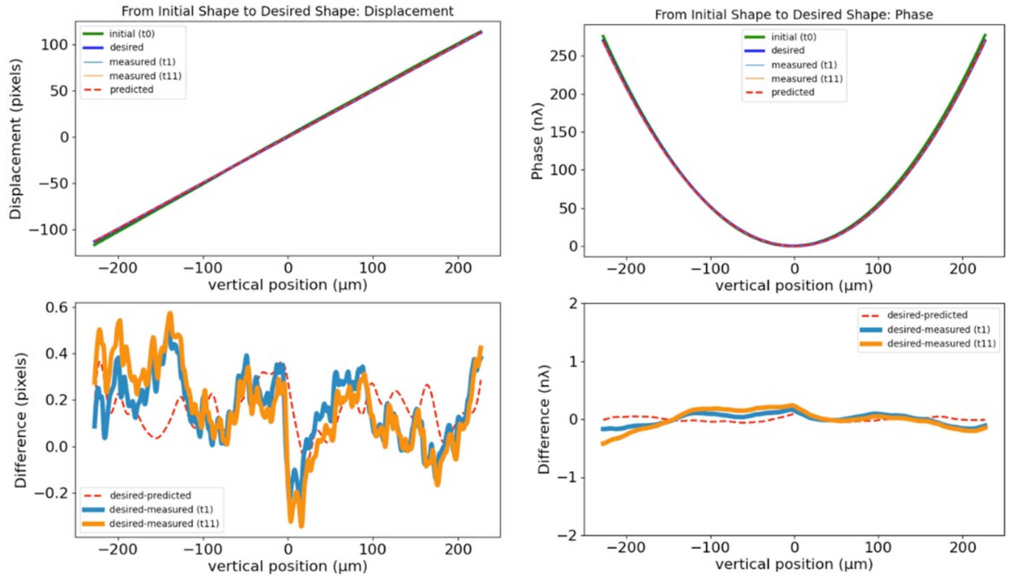


Fully automated software framework for data collection, image processing, neural network training, neural network-driven controller, experiments and data analysis:

https://github.com/APS-XSD-OPT-Group/Bimorph_Mirror

ML-DRIVEN SYSTEM FOR BIMORPH MIRROR





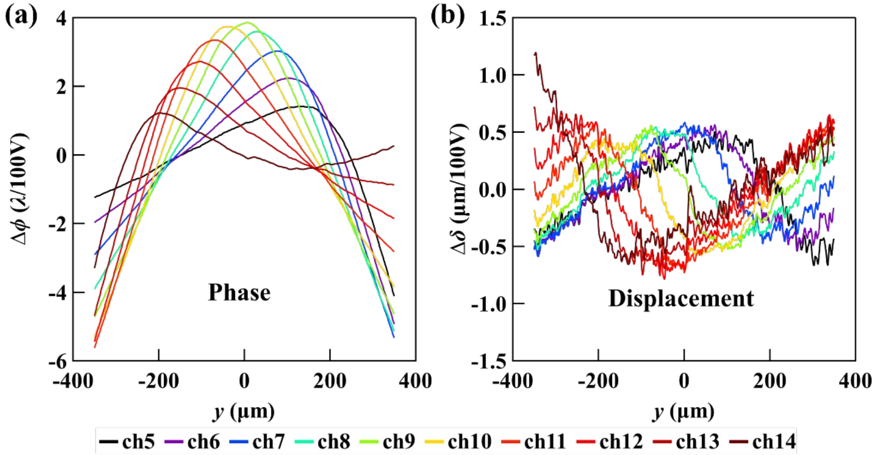
Preliminary study: Training and results in terms of resulting surface shape of the mirror vs applied voltages to the actuators

Operating conditions: Training on the wavefront speckle displacement and results in terms of absolute phase of the wavefront vs applied voltages to the actuators

ML-DRIVEN SYSTEM FOR BIMORPH MIRROR

Comparison with linear prediction model based on response functions

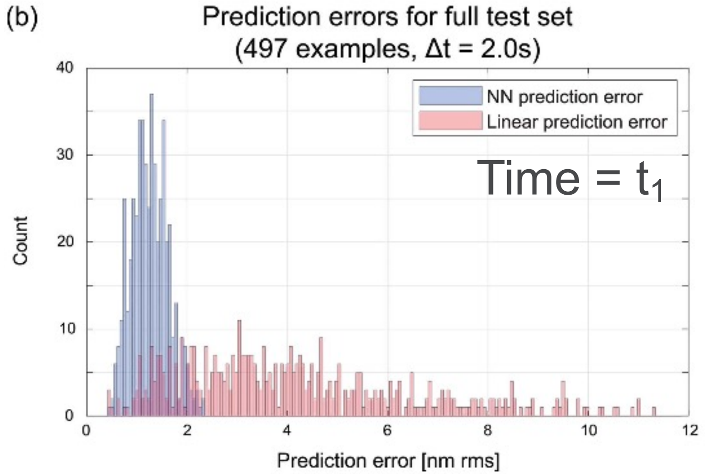
Preliminary Study: Measured response functions in terms of surface shape changes per 100 V changes on each piezo electrode.



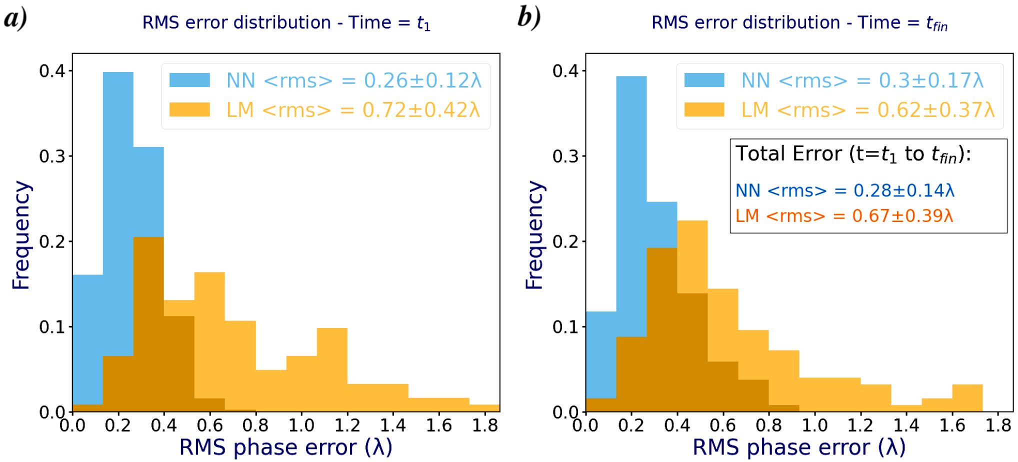
Operating Conditions: Measured response functions in terms of (a) wavefront phase and (b) speckle displacement changes per 100 V changes on each piezo electrode

L. Rebuffi et al., Opt. Express 31, 21264 (2023). DOI: 10.1364/OE.488189

ML-DRIVEN SYSTEM FOR BIMORPH MIRROR



Preliminary study: mean RMS errors between the measured and prescribed shapes are 1.44 nm after one step and 1.51 nm after 10 steps (20 seconds). The predictive performance (figure error rms) of the neural network is ~2.5 times better than the linear model across a full test dataset.

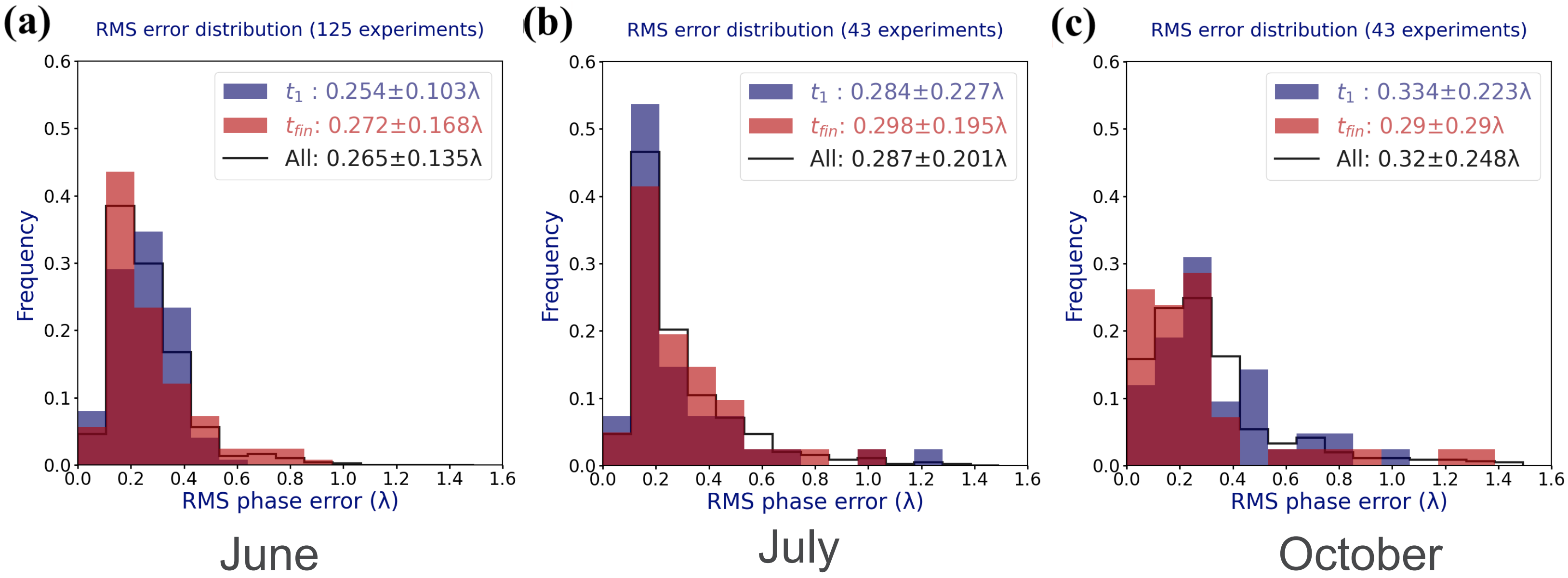


Operating Conditions: mean RMS errors between the measured and prescribed shapes in terms of phase error, projected on the surface of the mirror, corresponds to 1.8nm after one step, 2.0nm after 10 steps (20 seconds) and 2.1 nm after one minute.
The predictive performance (phase error rms) of the neural network is ~2.4 times better than the linear model across a full test dataset.

THE SAME CONCEPT WORKS WITH X-RAYS AND WAVEFRONT SENSING, IN REAL OPERATING CONDITIONS OF A SYNCHROTRON BEAMLINE.

L. Rebuffi et al., Opt. Express 31, 21264 (2023). DOI: 10.1364/OE.488189

ML-DRIVEN SYSTEM FOR BIMORPH MIRROR



Robustness: experiments repeated in two additional experimental sessions using the same model trained in the first session. In the two subsequent sessions, the entire optical system was rebuilt from scratch (same conditions for undulator source, white beam mirrors, slits, monochromator, KB mirrors, wavefront sensor, focal position)

INTRODUCTION

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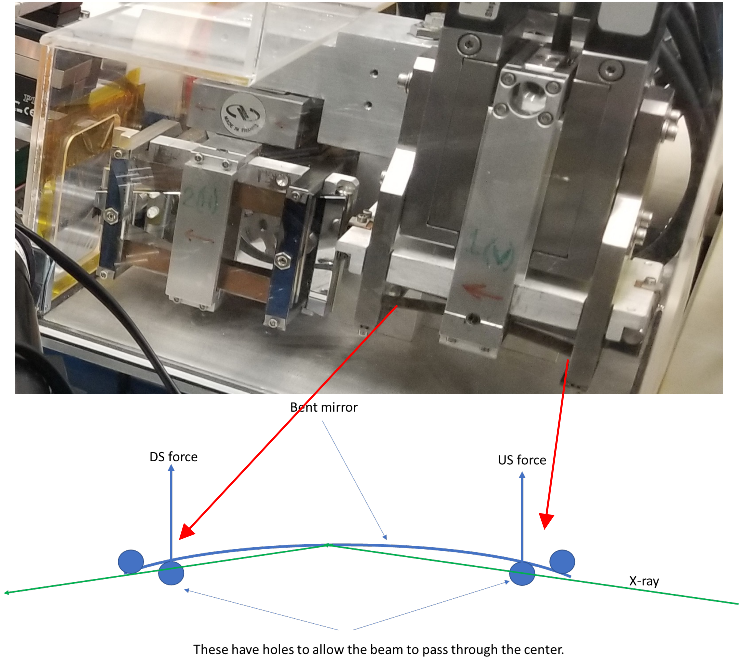
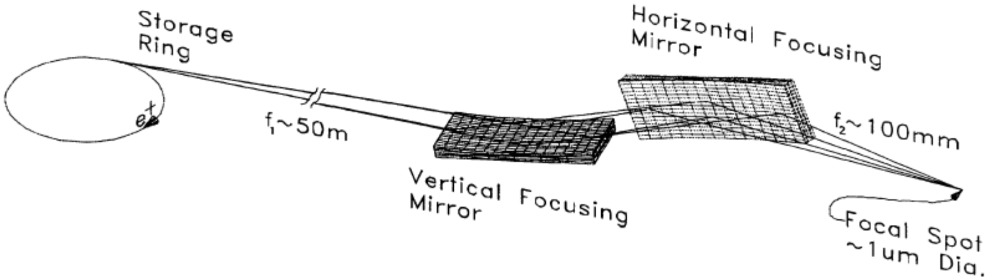
AI-DRIVEN AUTOFOCUSING SYSTEM FOR A NANOFOCUSING KB MIRROR

TOWARDS APS-U: A PORTABLE, AI-DRIVEN OPTICS CONTROL SYSTEM

AI-DRIVEN AUTOFOCUSING SYSTEM: 34-ID BEAMLINE



The 34-ID-C Nanofocusing KB-mirror is composed by two bendable mirrors, each equipped with 4 motors:



Motor	Experiment parameters
Motor 1	to adjust upstream bending force
Motor 2	to adjust downstream bending force
Motor 3	to adjust incident angle (pitch angle in API)
Motor 4	to adjust the position of the mirror in the direction of its surface normal

AI-DRIVEN AUTOFOCUSING SYSTEM: 34-ID DIGITAL TWIN

*L. Rebuffi and X. Shi, Proc. SPIE **11493**, 1149303 (2020). DOI: 10.1117/12.2567501*

OrAnge SYnchrotron Suite
OASYS
Powered by orange

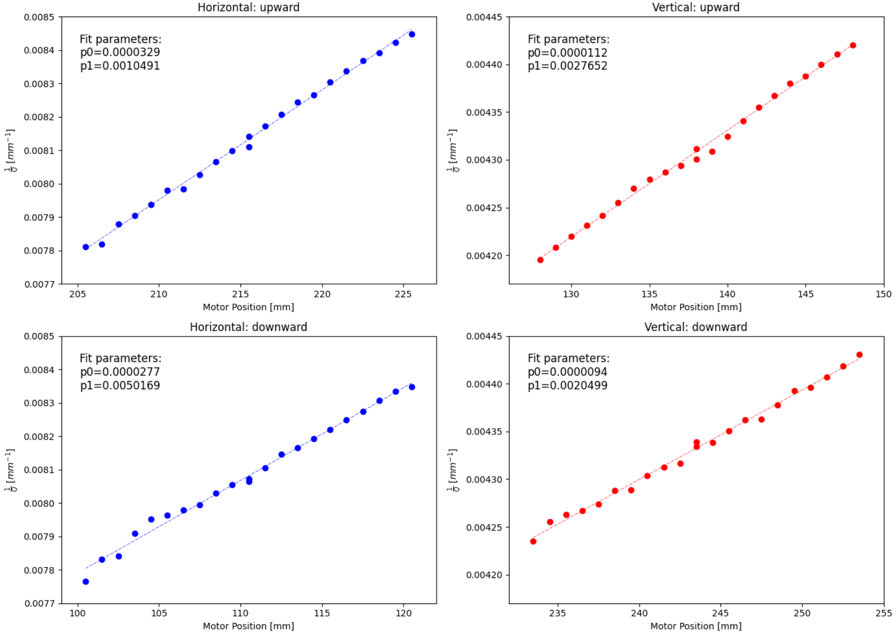
Shadow
Hybrid

SRW

DABAM

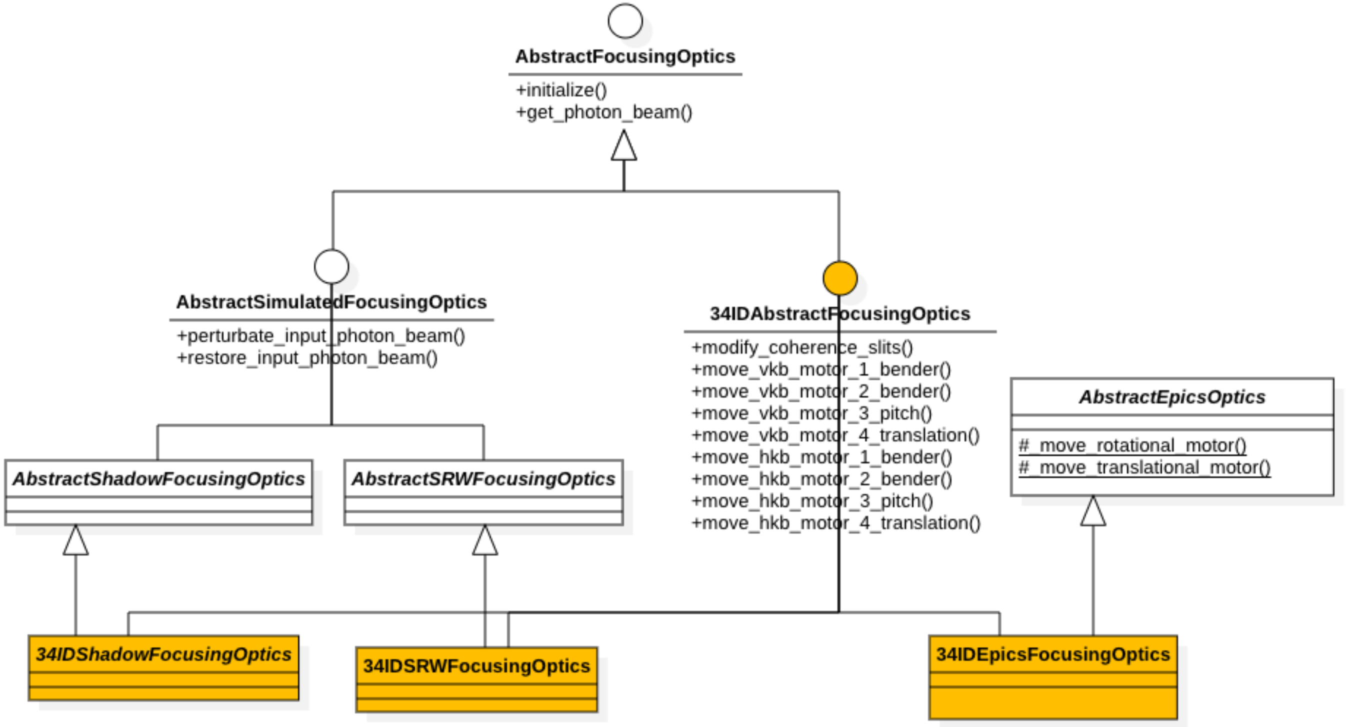
Calibration of bender motors:
q in function of real motor position

$$\frac{1}{q} = p_0 x + p_1$$



OASYS advanced tools: simulation of a a real bender with equations that correlate the desired focus position (q) to a surface profile of the deviation from an ideal profile.

AI-DRIVEN AUTOFOCUSING SYSTEM: 34-ID DIGITAL TWIN



We developed an Object-Oriented framework to build the ultra-realistic simulation of the beamline, providing a software interface emulating the real controller of the beamline.

https://github.com/AI-ML-at-APS/AI-ML_Control_System

AI-DRIVEN AUTOFOCUSING SYSTEM: 34-ID DIGITAL TWIN

```
if self._simulation_mode:
    factory_parameters, init_parameters = self._initialize_simulation_parameters(save_images,
                                                                              every_n_images,
                                                                              use_denoised,
                                                                              add_noise,
                                                                              noise,
                                                                              percentage_fluctutation,
                                                                              calculate_over_noise,
                                                                              noise_threshold,
                                                                              layout)
else:
    factory_parameters, init_parameters = self._initialize_hardware_parameters(save_images,
                                                                            every_n_images,
                                                                            use_denoised,
                                                                            calculate_over_noise,
                                                                            noise_threshold,
                                                                            **kwargs)

self._focusing_system = focusing_optics_factory_method(execution_mode=self._parameters.params.execution_mode,
                                                       implementor=self._parameters.params.implementor,
                                                       **factory_parameters)
self._focusing_system.initialize(**init_parameters)
```

hardware controller and corresponding digital twin of the focusing system using the same software interface

Completely transparent to AI agents

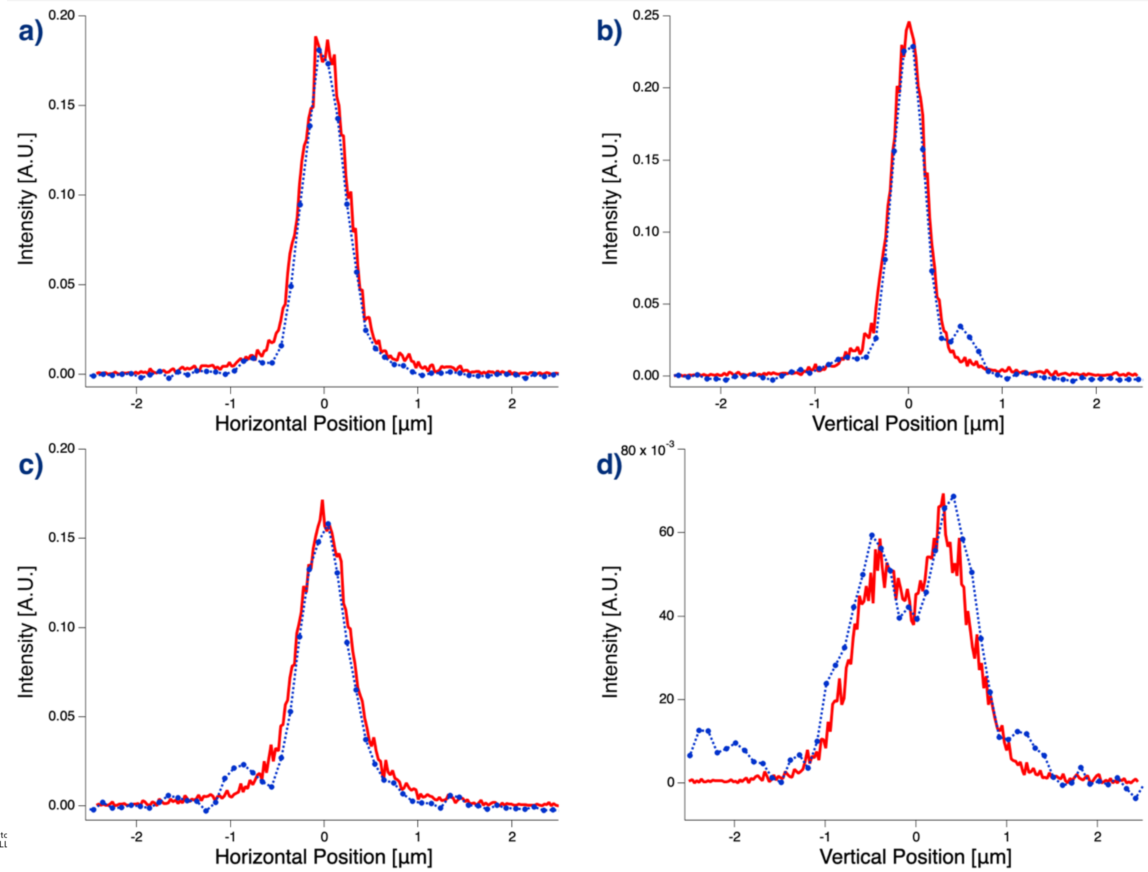
AI-DRIVEN AUTOFOCUSING SYSTEM: 34-ID DIGITAL TWIN

Horizontal Direction | Vertical Direction

At Focus

Off Focus

bender motors position +5 μm



Real Data

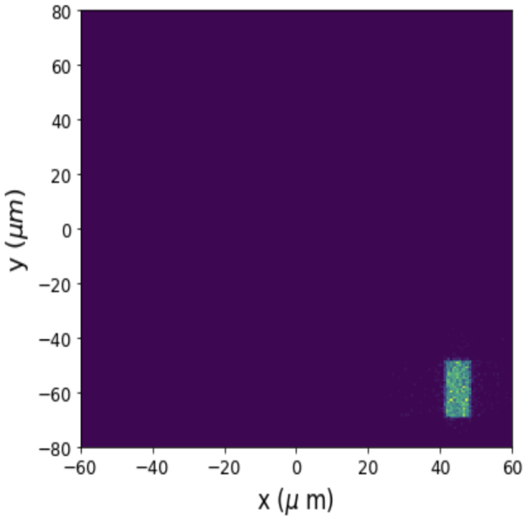
Simulation

AI-DRIVEN AUTOFOCUSING SYSTEM: 34-ID DIGITAL TWIN

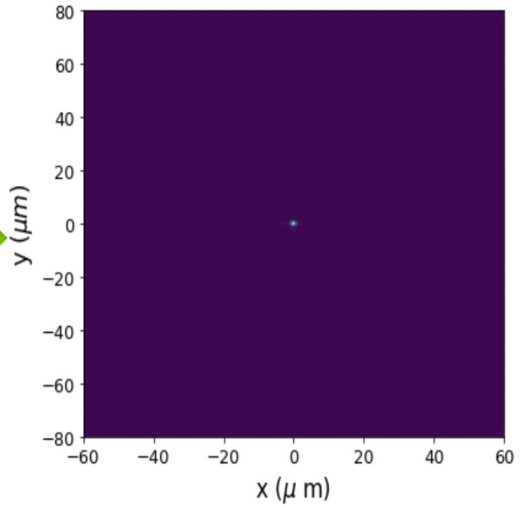
Multi-Objective Bayesian optimization using Gaussian Processes provided the most promising results, in treating the the autofocusing problem as a is a “black-box” or “derivative-free” optimization problem, where we want to minimize a “loss function”, in terms of a set of desired beam characteristics.

- Start with a focused beam
- Perturb the 8 motors randomly
- Feed the perturbed structure to the solver.
- Solver uses the digital twin to iteratively modify the motor value and access the generated beam profile.
- Use the centroid + FWHM as the loss (objective) function.

Initial Beam



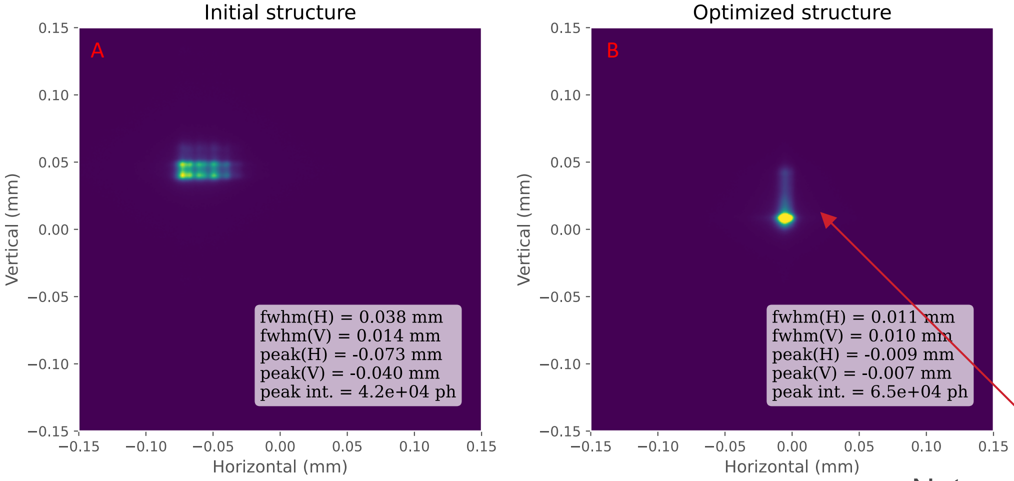
Optimized Beam

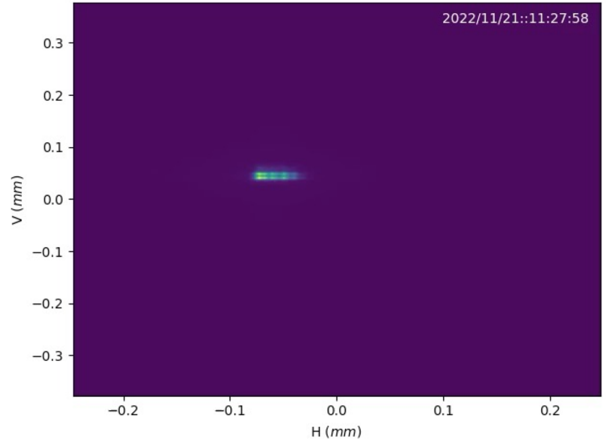


L. Rebuffi et al., Optica Open (preprint). DOI: 10.1364/opticaopen.23934903

AI-DRIVEN AUTOFOCUSING SYSTEM: 28-ID BEAMLINE

- We tested the autofocusing system by reproducing the 34-ID-C focusing system at the beamline 28-ID-B.
- The optimizer has been tested with several loss function combinations in terms of peak position, fwhm (minimum or target one) and peak intensity.
- Autofocusing was achieved in less than 100 iterations (potentially ~5-10 minutes, but depending on the motor drivers)





Note: coma aberration from vertical mirror

CHALLENGES AND CONSIDERATION

- If the overall goal of the experiment is to maintain a stable optical system through multiple runs of the autofocusing routine, then reusing the information acquired in one auto-alignment run could accelerate future auto-alignments on the same optical system

- In a more sophisticated approach, we could exploit the idea of multi-fidelity optimization to create and dynamically update a complex GP-based (or NN-based) model of the optical system, then exploit this extra surrogate for accelerated optimization.

- It could be beneficial to add some known physical behavior (analytical formulas) to pre-initialize the system before optimization.

- Directly measuring a submicron focal spot with a 2D detector is exceptionally challenging or even impossible: **our single-shot wavefront sensing technique should also provide all the needed information in term of position, size and shape of the focal spot.**

FUTURE WORK

- Study different libraries (Optuna vs Ax) of the Multi-Objective Bayesian Optimization

- Study the effect of parallel separate optimization of vertical and horizontal directions

- Study other AI technologies (limitations and benefits):

    - NN-driven approach? Digital training data?
    - Reinforcement learning?

- Develop a full back-propagation routine for wavefront data analysis, to determine additional wavefront information (i.e.: 3D focus position, spot size at focus) and be completely independent by the beamline detectors.

INTRODUCTION

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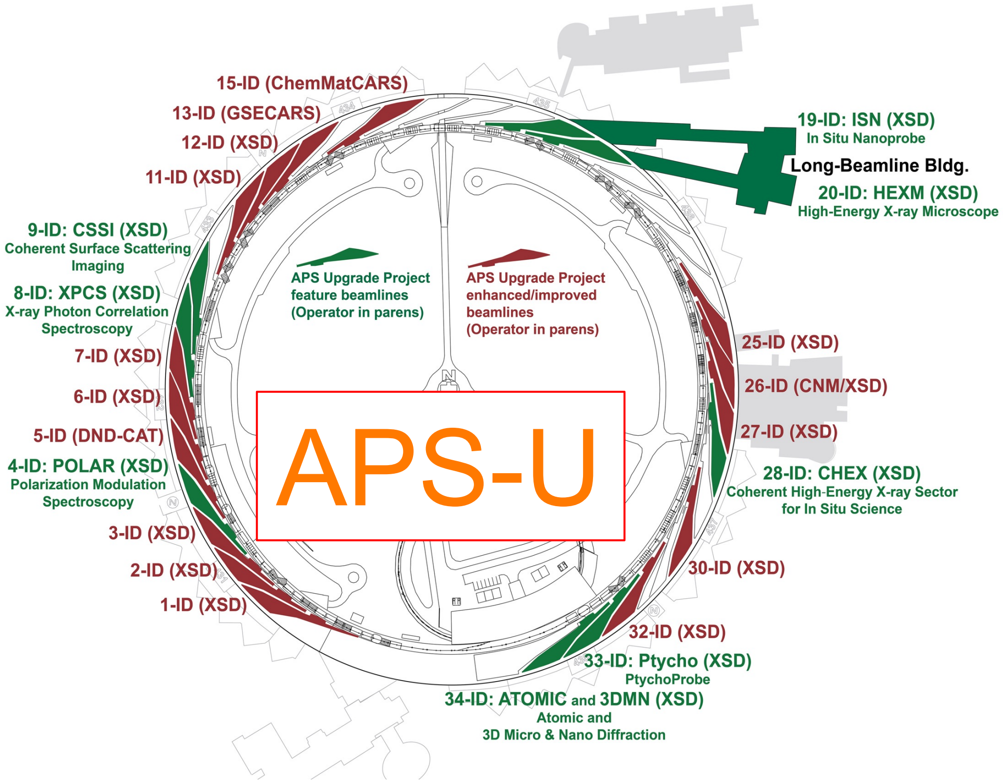
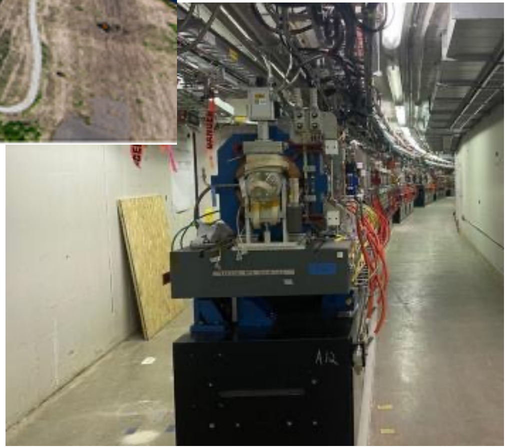
AI-DRIVEN AUTOFOCUSING SYSTEM FOR A NANOFOCUSING KB MIRROR

TOWARDS APS-U: A PORTABLE, AI-DRIVEN OPTICS CONTROL SYSTEM

TOWARDS APS-U





TOWARDS APS-U

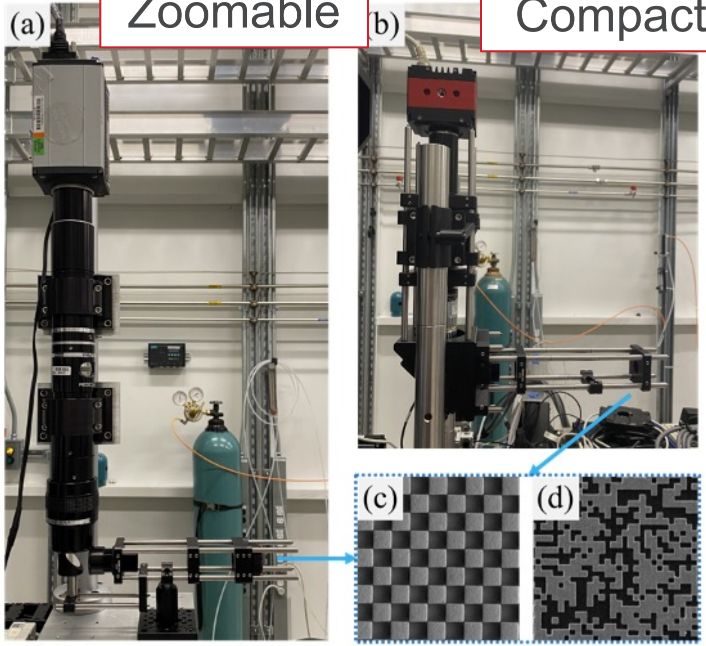
We require a common paradigm for all the beamlines where an optical setup capable of steadily maintaining the coherence properties of the radiation is enabling fast, accurate and new in-situ and in-operando studies.

A portable AI-driven optics control system, combining wavefront sensing, artificial intelligence and adaptive optics, capable of optimizing **AND** controlling the wavefront on coherent beamlines.

A PORTABLE, AI-DRIVEN OPTICS CONTROL SYSTEM

28-ID-B Beamline

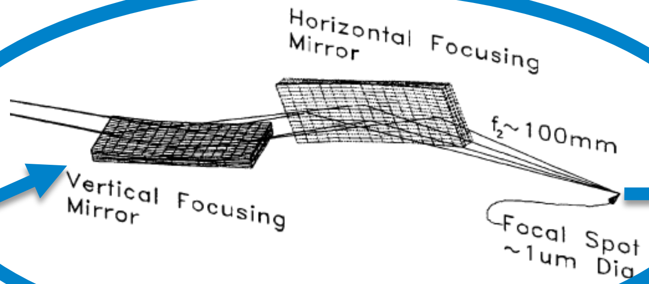
WE NEED MORE PORTABLE WAVEFRONT SENSORS!



A PORTABLE AI-DRIVEN SYSTEM: AUTOALIGNMENT

Compact Wavefront Sensor

Common User-Friendly Configurable



BO-driven Autoalignment

Software Library

Real-time Feedback Data

Autoalignment on Digital Twin

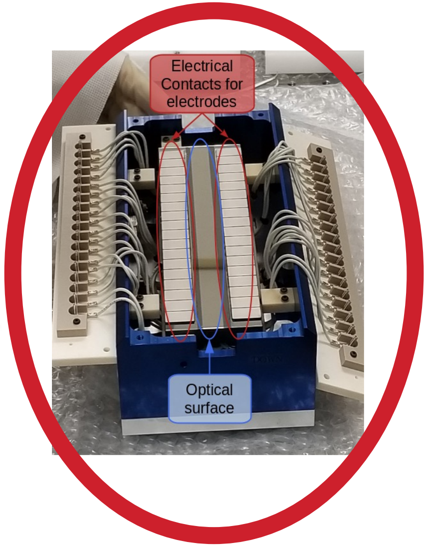
OASYS

A PORTABLE ML-DRIVEN SYSTEM: WAVEFRONT CONTROL

Compact Wavefront Sensor

Common User-Friendly Configurable

ML-driven Wavefront Correction



Software Library

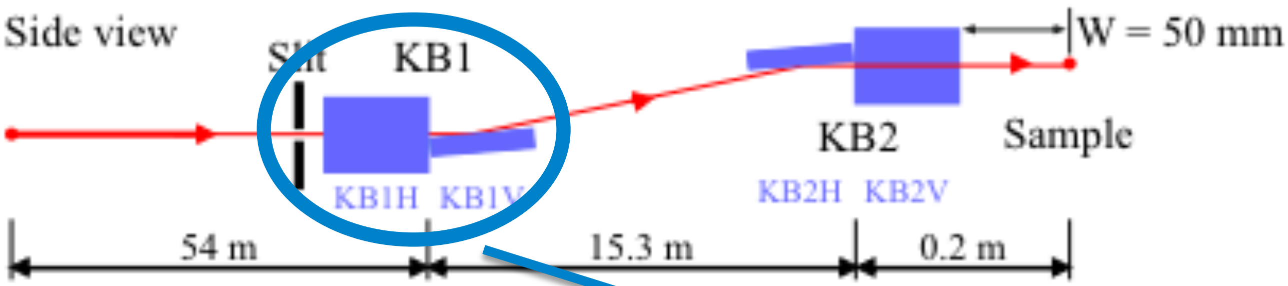
ML Training Data

ML Training Data

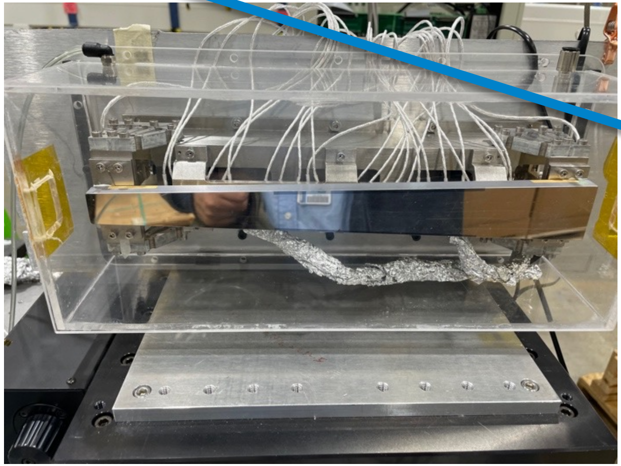
Wavefront Properties DB

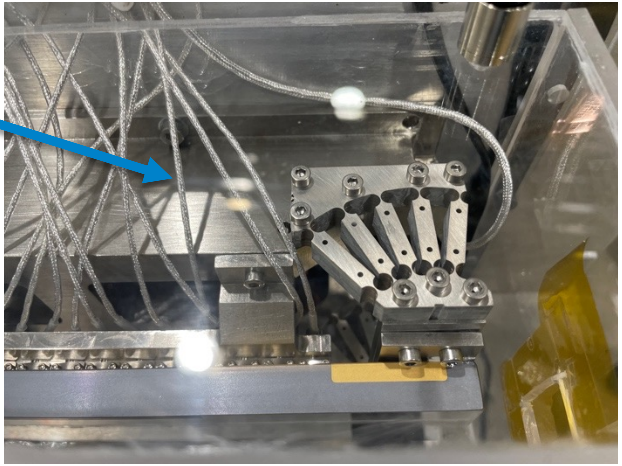
D. Shu et al., Proc. SPIE 11112, 111120N (2019). DOI: 10.1117/12.2529384

TOWARDS APS-U: THE ZOOM OPTICS FOR ATOMIC BEAMLINE

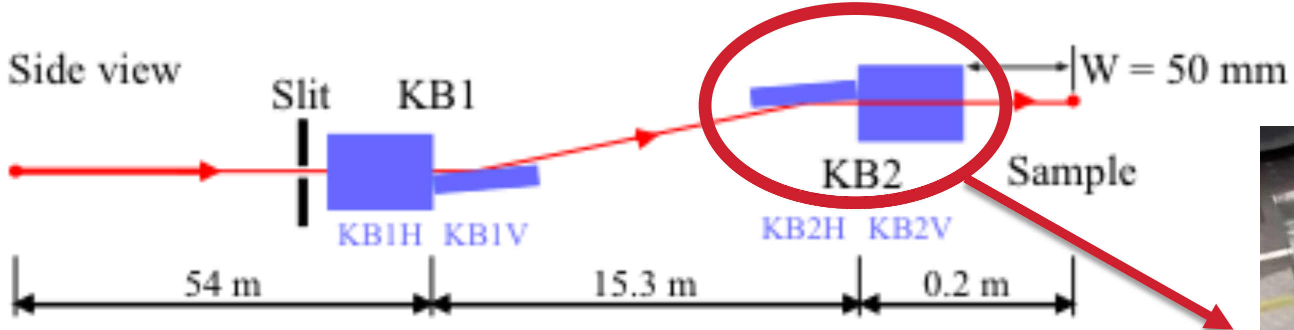


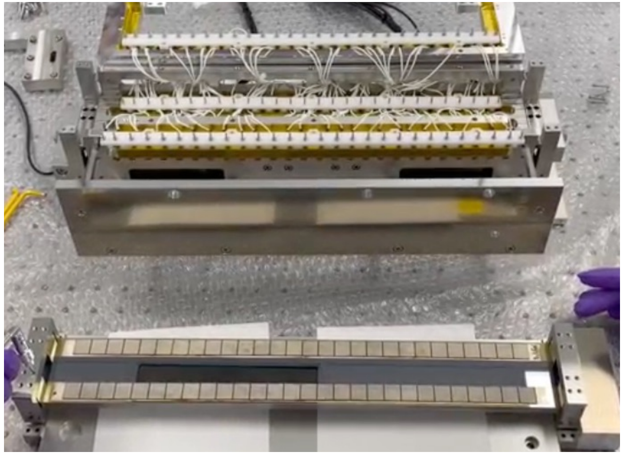
High-Quality bendable mirrors, using flexural nanopositioning stage system

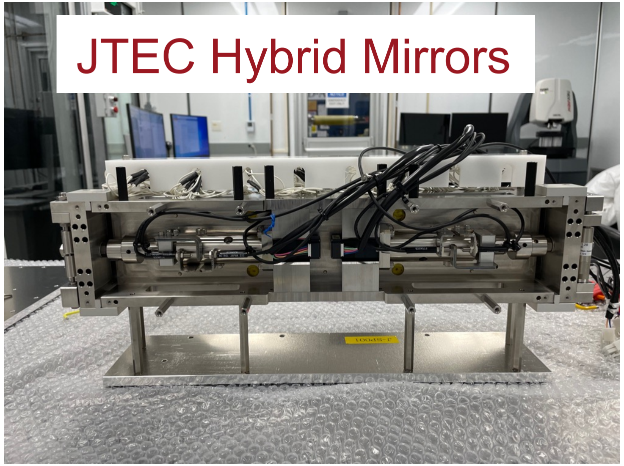


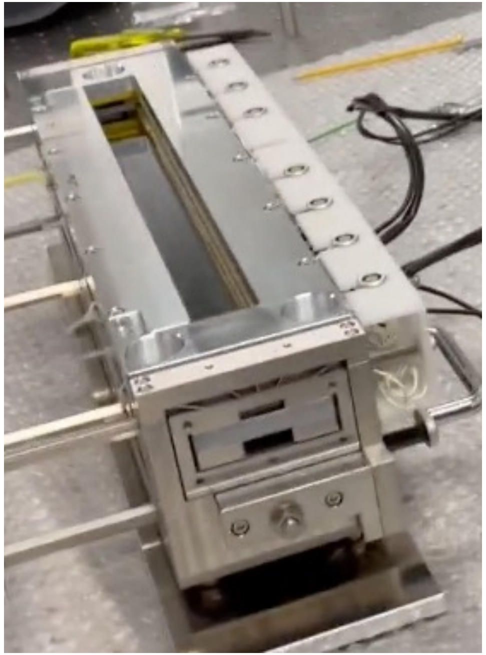


TOWARDS APS-U:
THE ZOOM OPTICS FOR ATOMIC BEAMLINE

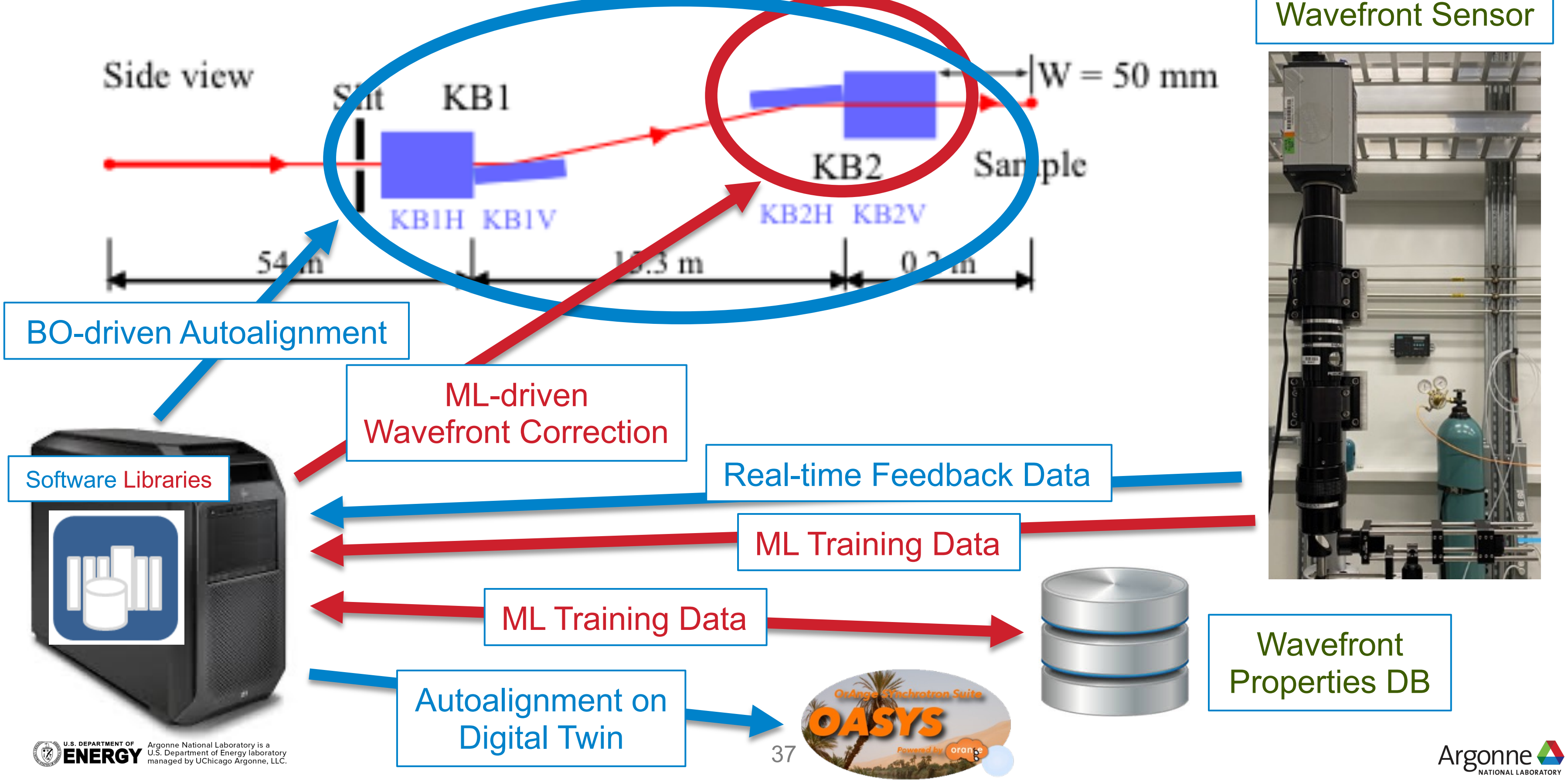








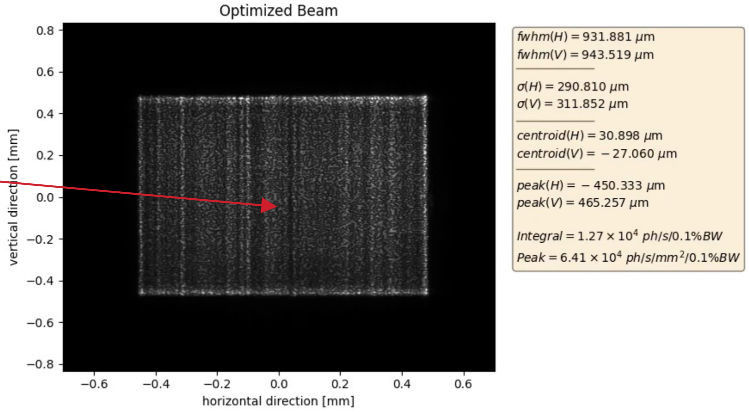
A PORTABLE AI-DRIVEN SYSTEM FOR THE ZOOM OPTICS



A PORTABLE AI-DRIVEN SYSTEM FOR THE ZOOM OPTICS

- Any data-driven ML system needs consistency between the conditions when training data have been collected and when the predictions of the model are applied. In the case of a synchrotron beamline this translates into **stability of the beam and the optical setup**.
- The AI-driven optimizer, coupled and running in parallel with the ML-driven controller(s) of the adaptive optics, can also maintain the beam characteristics all along the ML life cycle (data collection, training, prediction)

At 28-ID we tested the AI-driven optimizer on keeping stable **the position of the off-focus wavefront sensor image**, for a **time span of 4 days**.



FULLY AUTOMATED AI-DRIVEN ZOOM OPTICS: PERSPECTIVES

PORTABLE AI-DRIVEN ZOOM OPTICS CONTROL

BO-DRIVEN AUTOFOCUSING

ML-DRIVEN WAVEFRONT CONTROL

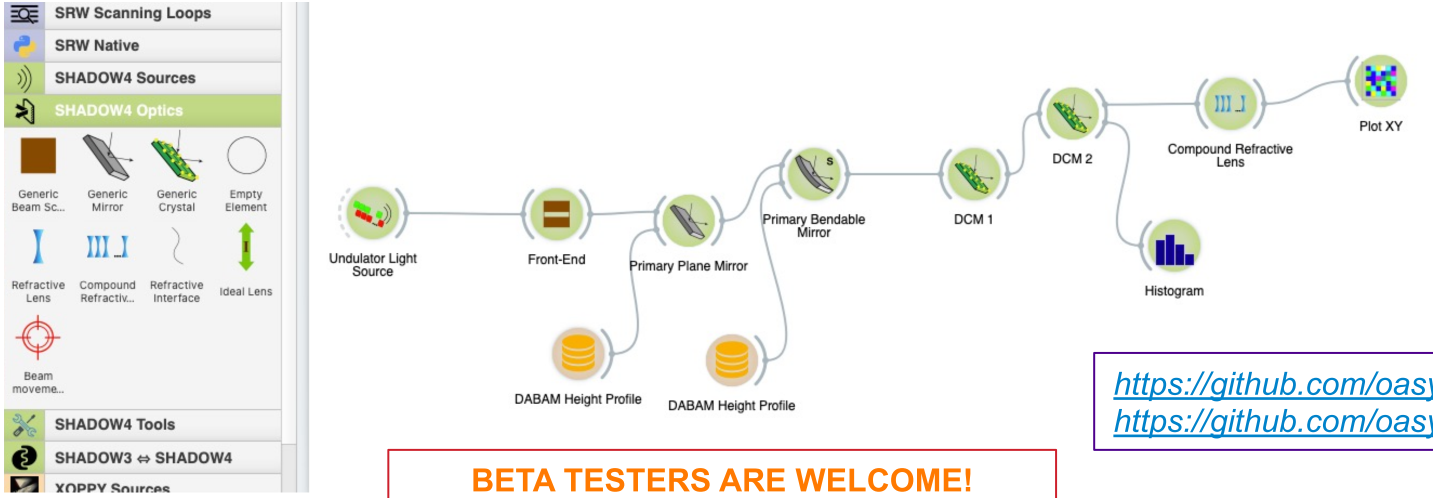
3D-ultra-high-resolution Bragg CDI studies of nanoscale in-situ electrochemical grain growth and dissolution, important across electrocatalysis, synthesis, and corrosion. In-situ experiments of dissolution and growth require a coherent, focused variable-spot beam to follow the size of the sample, changing on the scale of minutes, that the beamline optical system need to match.

TOWARDS OASYS1.4: SHADOW 4

a revised and optimized new version of *Shadow*, fully implemented in python

We are including all the lesson learned in developing the digital twins for the autofocusing system, while implementing SHADOW4 and its OASYS GUI, in collaboration with Manuel Sanchez del Rio at ESRF (FRA).

By using the powerful Object-Oriented framework for optical simulation and automatization tools of OASYS, we are closing the loop towards a fully **VISUAL** and **AUTOMATIC** creation of **DIGITAL TWINS** to be used for AI/ML studies/applications and FAST pre-configuration and test of our portable system.



https://github.com/oasys-kit/shadow4
https://github.com/oasys-kit/OASYS1-SHADOW4

BETA TESTERS ARE WELCOME!

CONCLUSIONS

- We successfully demonstrated the feasibility of a portable AI-driven optics control system, combining wavefront sensing, AI/ML and adaptive optics, capable of optimizing and controlling the beam shape and the wavefront on coherent beamlines

- We are now directed to deeply study the AI/ML technologies to improve and engineer our device to support APS-U beamline commissioning

- We are improving our wavefront sensing techniques to provide all the necessary beam properties to the optimization.

- We are also upgrading OASYS to automatically generate digital twins from the visual simulations

THANK YOU!