Online Models for X-ray Beamlines Using Sirepo-Bluesky

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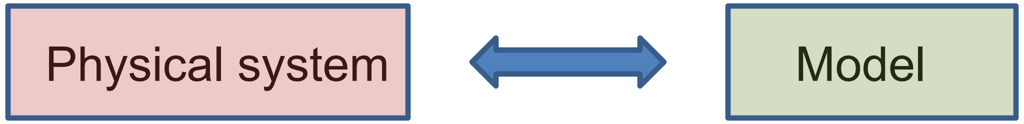
Outline

- Types of Online models
- Sirepo-Bluesky overview
- Models for x-ray optics
  - Reduced model and simulation codes
  - Partially coherent Gaussian optics with apertures
  - Linear canonical transforms
- Simulation codes from RadiaSoft
- Direct optimization: Bayesian optimization
- Conclusions and references

What is an Online Model



An **online model** is a model that runs in real time, in parallel with operations, that is updated based on diagnostics measurements.

A **reduced model** is a limited fidelity model with adequately fast computation speed.

Sirepo supported codes and apps

Command line & ML

jupyterhub

Activait

Neutron Transport

OpenMC

Plasmas

FLASH

Vacuum nanoelectronics

WARP

Accelerators

elegant

Synergia

MAD-X

WARP

OPAL

Zgoubi

Controls

EPICS

BLUESKY

X-ray optics

Shadow

SRW

Magnets

Radia

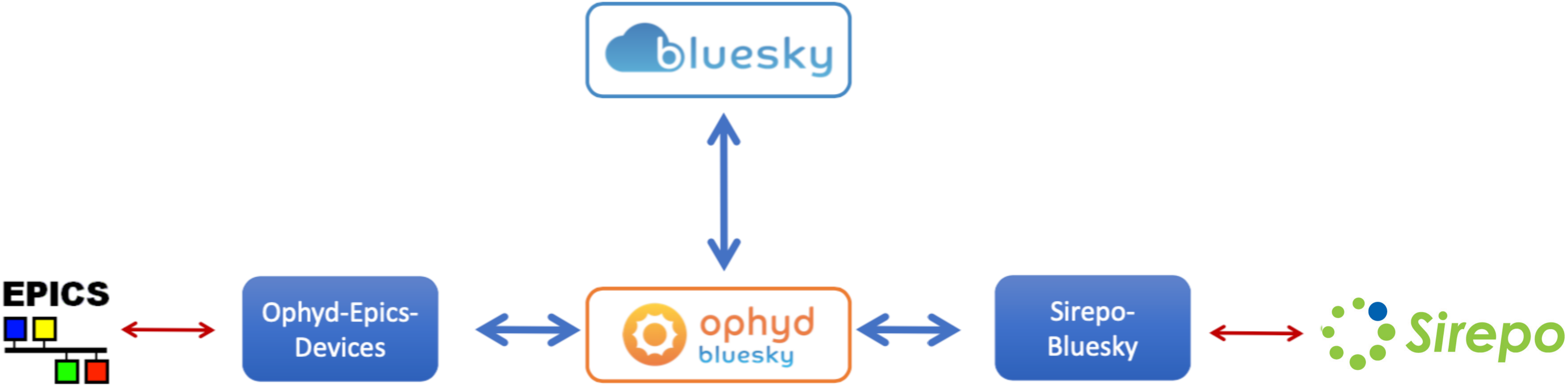
FELs

GENESIS

Cooling

JSPEC

Connecting Online Models to Experiments

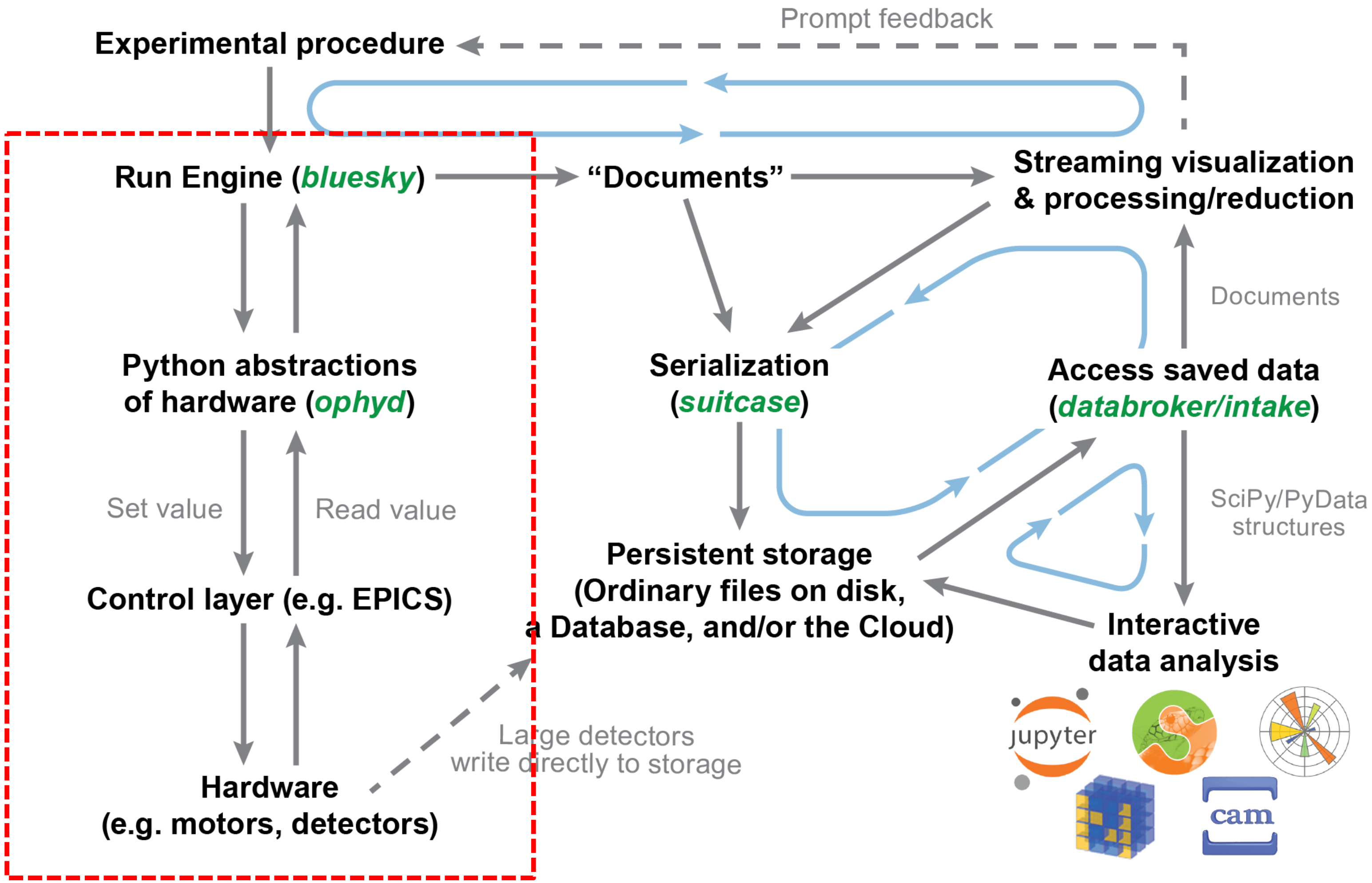


Operations
Experimentalists

SRW
SHADOW
MAD-X
Reduced models

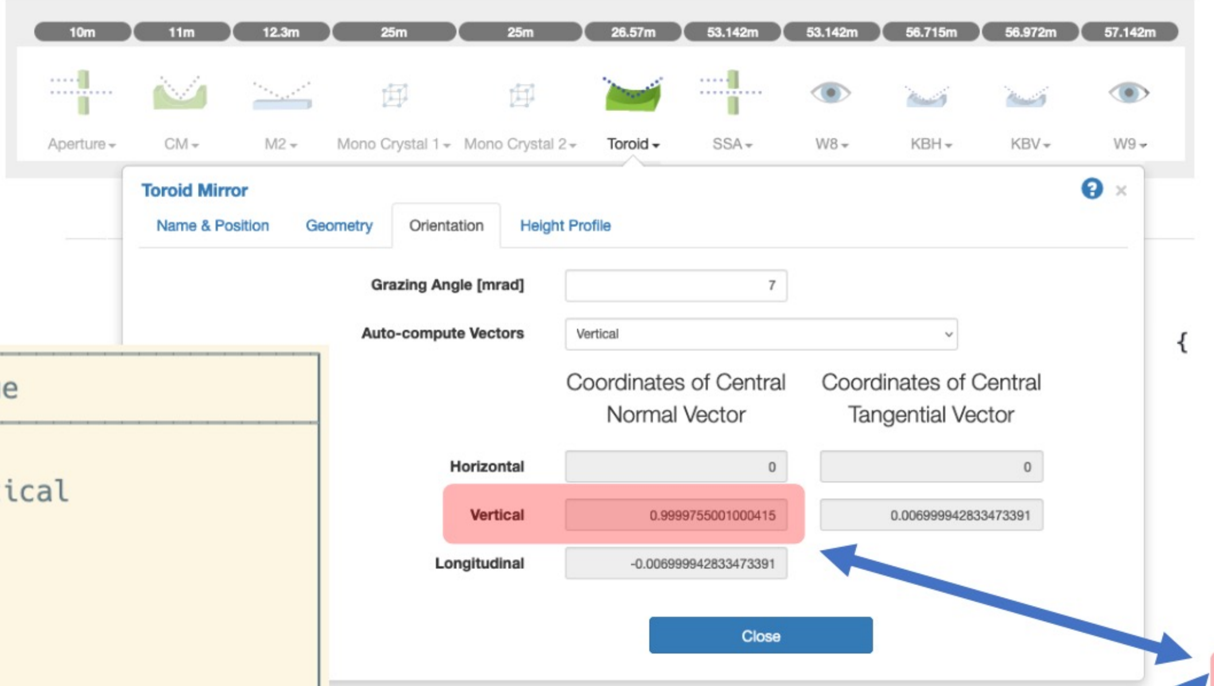
Model result can be used to make choices on the beamline!

Bluesky Data Collection Ecosystem



https://blueskyproject.io
https://doi.org/10.1080/08940886.2019.1608121

Sirepo-Bluesky: Linking Simulated Devices with Operations



Ophyd Device Representation

Ophyd object/component	Value
toroid_apertureShape	r
toroid_autocomputeVectors	vertical
toroid_grazingAngle	7
toroid_heightAmplification	1
toroid_heightProfileFile	
toroid_horizontalPosition	0
toroid_id	6
toroid_normalVectorX	0
toroid_normalVectorY	0.9999755001000415
toroid_normalVectorZ	-0.006999942833473391
toroid_orientation	y
toroid_sagittalRadius	0.186
toroid_sagittalSize	0.08
toroid_tangentialRadius	24500
toroid_tangentialSize	0.96
toroid_tangentialVectorX	0
toroid_tangentialVectorY	0.006999942833473391
toroid_title	Toroid
toroid_type	toroidalMirror
toroid_verticalPosition	0
toroid_element_position	26.57

Sirepo JSON

```
{
    "apertureShape": "r",
    "autocomputeVectors": "vertical",
    "grazingAngle": 7,
    "heightAmplification": 1,
    "heightProfileFile": "",
    "horizontalPosition": 0,
    "id": 6,
    "normalVectorX": 0,
    "normalVectorY": 0.9999755001000415,
    "normalVectorZ": -0.006999942833473391,
    "orientation": "y",
    "position": 26.57,
    "sagittalRadius": 0.186,
    "sagittalSize": 0.08,
    "tangentialRadius": 24500,
    "tangentialSize": 0.96,
    "tangentialVectorX": 0,
    "tangentialVectorY": 0.006999942833473391,
    "title": "Toroid",
    "type": "toroidalMirror",
    "verticalPosition": 0
},
```

Applications

- Sirepo-bluesky supports three simulators: shadow, SRW, and MAD-X

- The Sirepo-Bluesky library is used in the following projects:

  - https://github.com/NSLS-II/bloptools: beamline optimization tools
  - https://github.com/BNL-ATF/profile_atf: BNL ATF facility uses it for MAD-X simulations
  - https://github.com/NSLS-II-ARI/profile_sirepo_ari: used to prototype data acquisition plans for the future NSLS-II ARI beamline (currently under construction)

Sirepo-Bluesky

https://github.com/NSLS-II/sirepo-bluesky
https://nsls-ii.github.io/sirepo-bluesky
https://doi.org/10.1117/12.2569000

DOI 10.5281/zenodo.8265981 | Tests passing | PyPI v0.7.2 | conda-forge v0.7.2

- Available on **conda-forge** and **PyPI**
- Support of the **SRW**, **Shadow3**, and **MAD-X** applications in Sirepo
- Simulations are performed on a Sirepo server (a VM, Docker container, or HPC resources)
- Communication is done over HTTP(s) with Sirepo REST API
- Watchpoints or other Sirepo “reports” are wrapped into dedicated “detector” Ophyd objects
- All other optical elements are wrapped into Ophyd’s **`Devices`** with **`Signals`** corresponding to individual parameters in Sirepo
- The exchange format is JSON
- List of predefined simulations in Sirepo: https://nsls-ii.github.io/sirepo-bluesky/simulations.html

List of predefined simulations in Sirepo

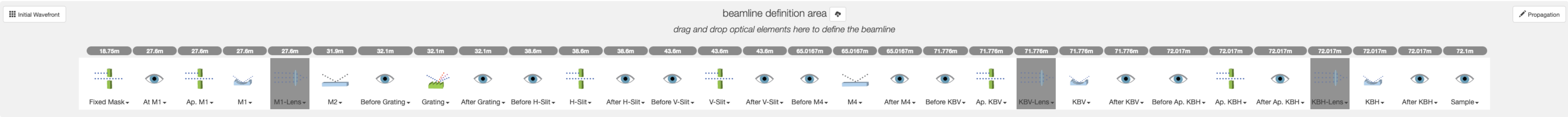
Below is a list of custom/predefined simulations available when one starts Sirepo following the Sirepo startup instructions, that are currently used for tests and demos.

SRW

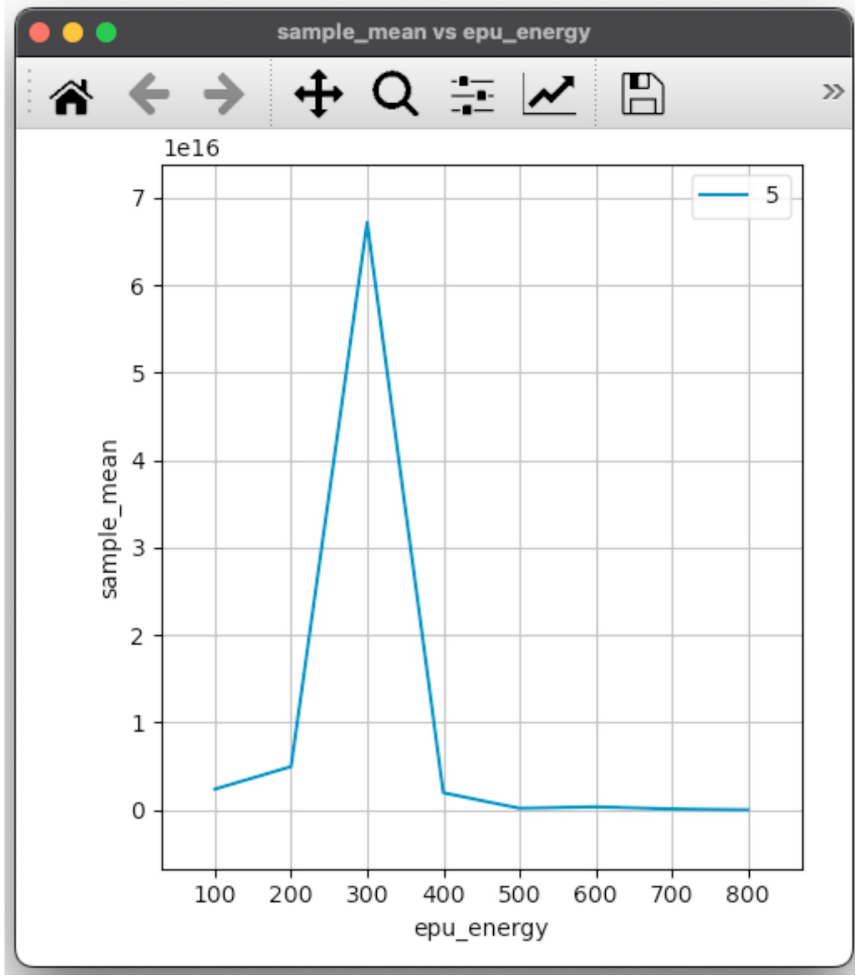
SRW simulations used for testing

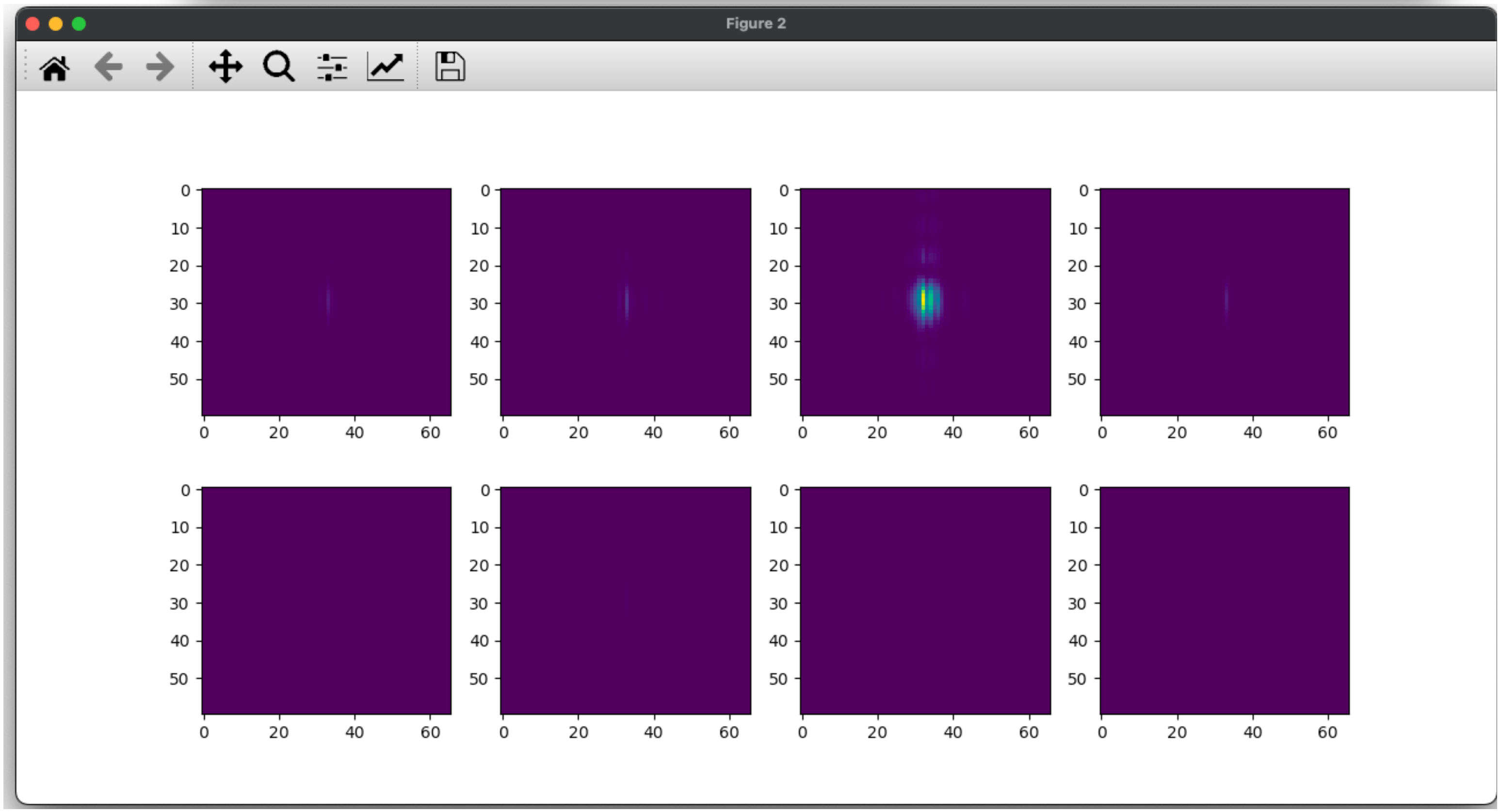
Simulation ID	Description
`00000000`	Young’s Double Slit Experiment
`00000001`	basic
`00000002`	TES
`00000003`	PD ARI-RIXS 250eV_JulyReviewVersion oc
`00000004`	PD ARI-RIXS 400eV (tuned) oc
`00000005`	PD ARI-ARPES 150eV JulyReviewVersion oc
`00000006`	PD ARI-ARPES 250eV JulyReviewVersion oc
`00000007`	SXN_PD_lowE_250eV
`00000008`	SXN_PD_medE_1000eV
`00000009`	SXN_PD_highE_2000eV

NSLS-II ARI virtual beamline

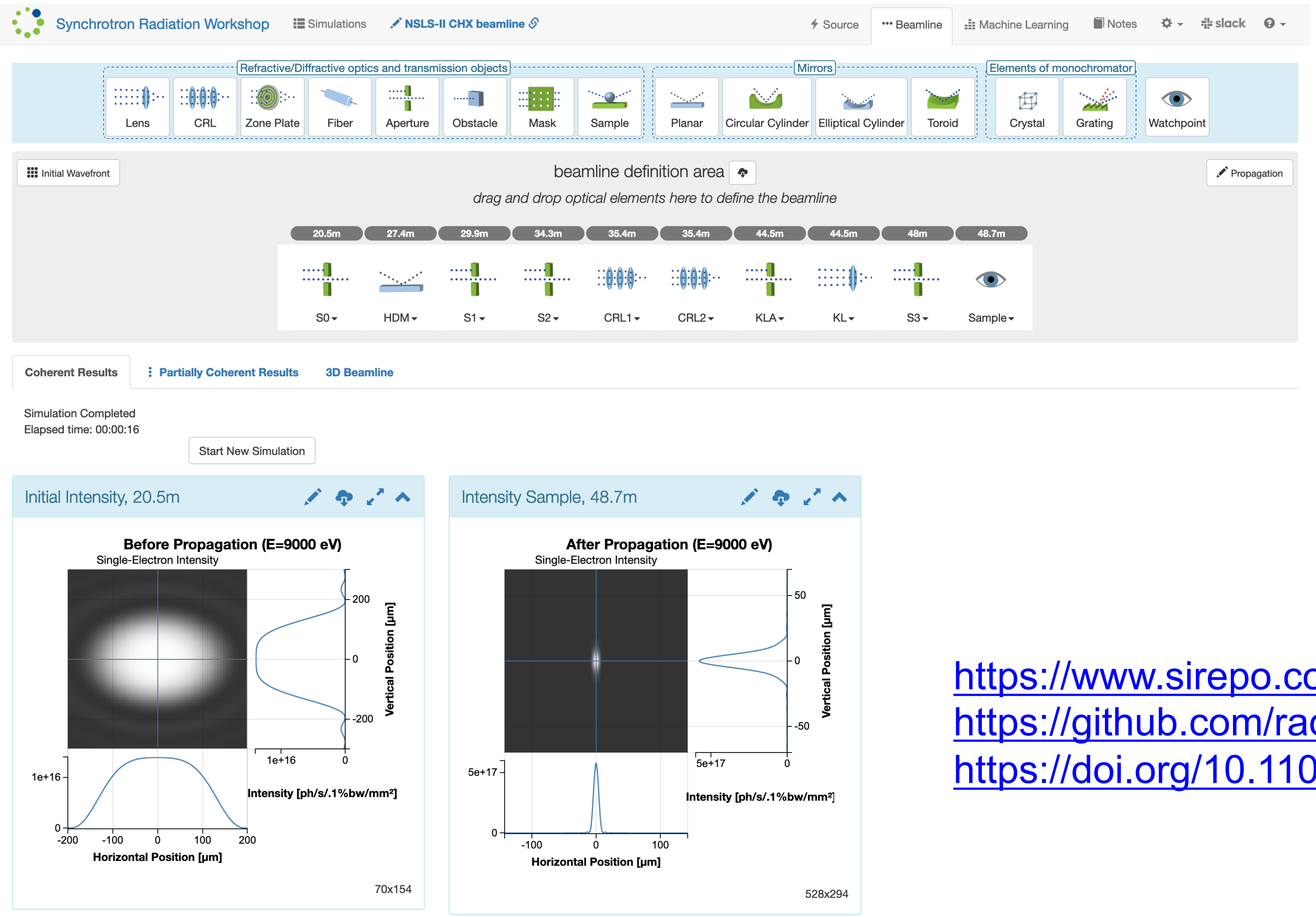


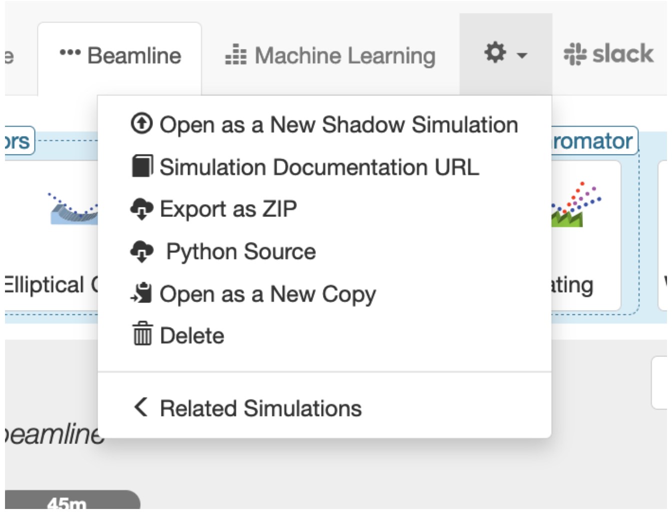

```
RE(bp.scan([sample], epu.energy, 100, 800, 8))
```





Sirepo SRW application





SRW to SHADOW

https://www.sirepo.com
https://github.com/radiasoft/sirepo
https://doi.org/10.1107/S1600577518010986

Bayesian Optimization for beamlines

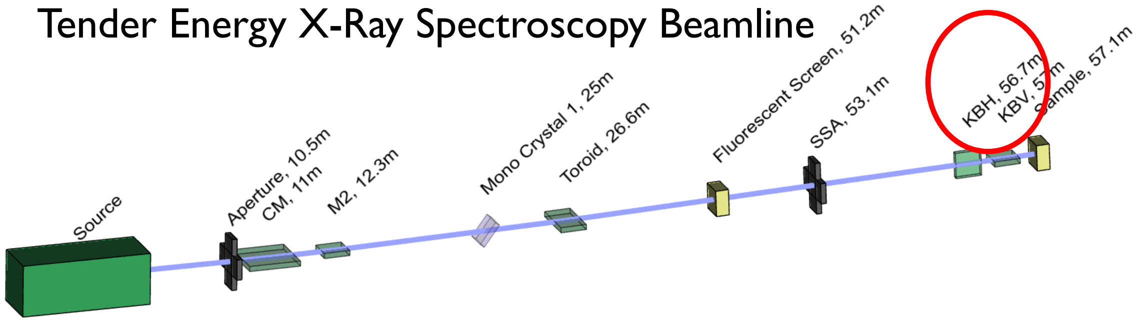
- This approach is used in the bloptools package
  - Establishes an interface between Bluesky and BoTorch GPyTorch
  - The same code works for beamlines and their digital twins
  - Tested at NSLS-II (TES, ISS) and ALS (5.3.1) beamline
  - Forthcoming: more beamlines, BNL's Accelerator Test Facility

- For more information see https://github.com/NSLS-II/bloptools

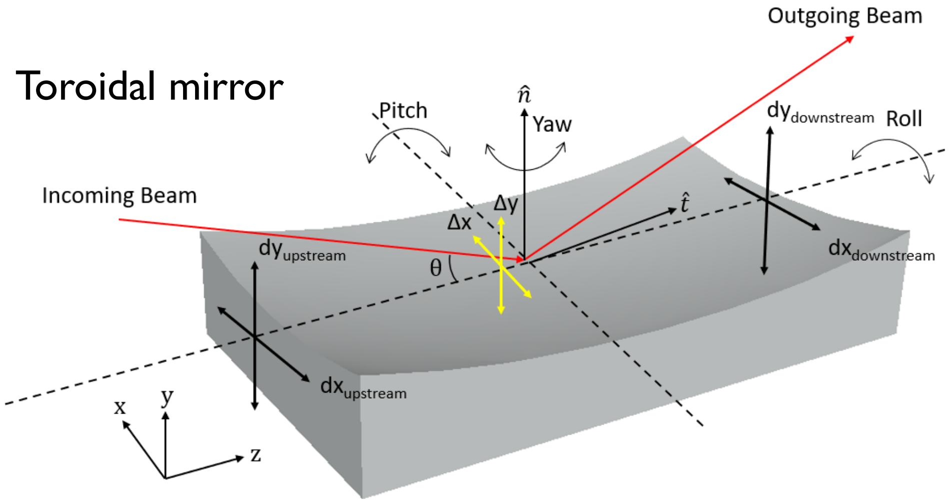
Bloptools developed by T. Morris

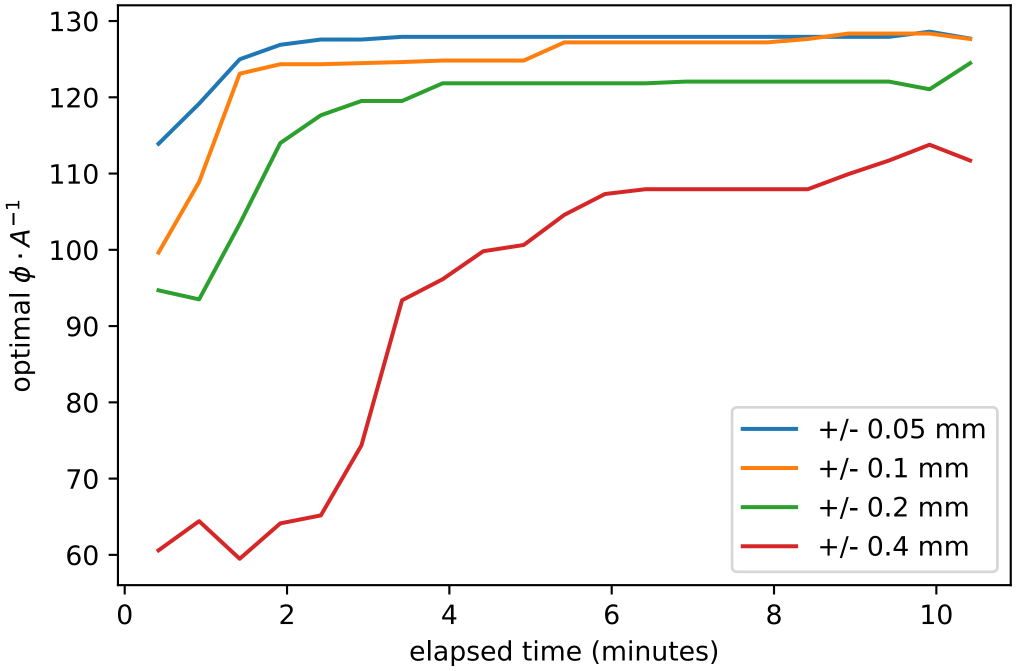
Automatic alignment via Bayesian Optimization

Tender Energy X-Ray Spectroscopy Beamline



Toroidal mirror





Increasing range of parameter variation

Varying 4 alignment motors of KB mirror to optimize flux/(beam area)

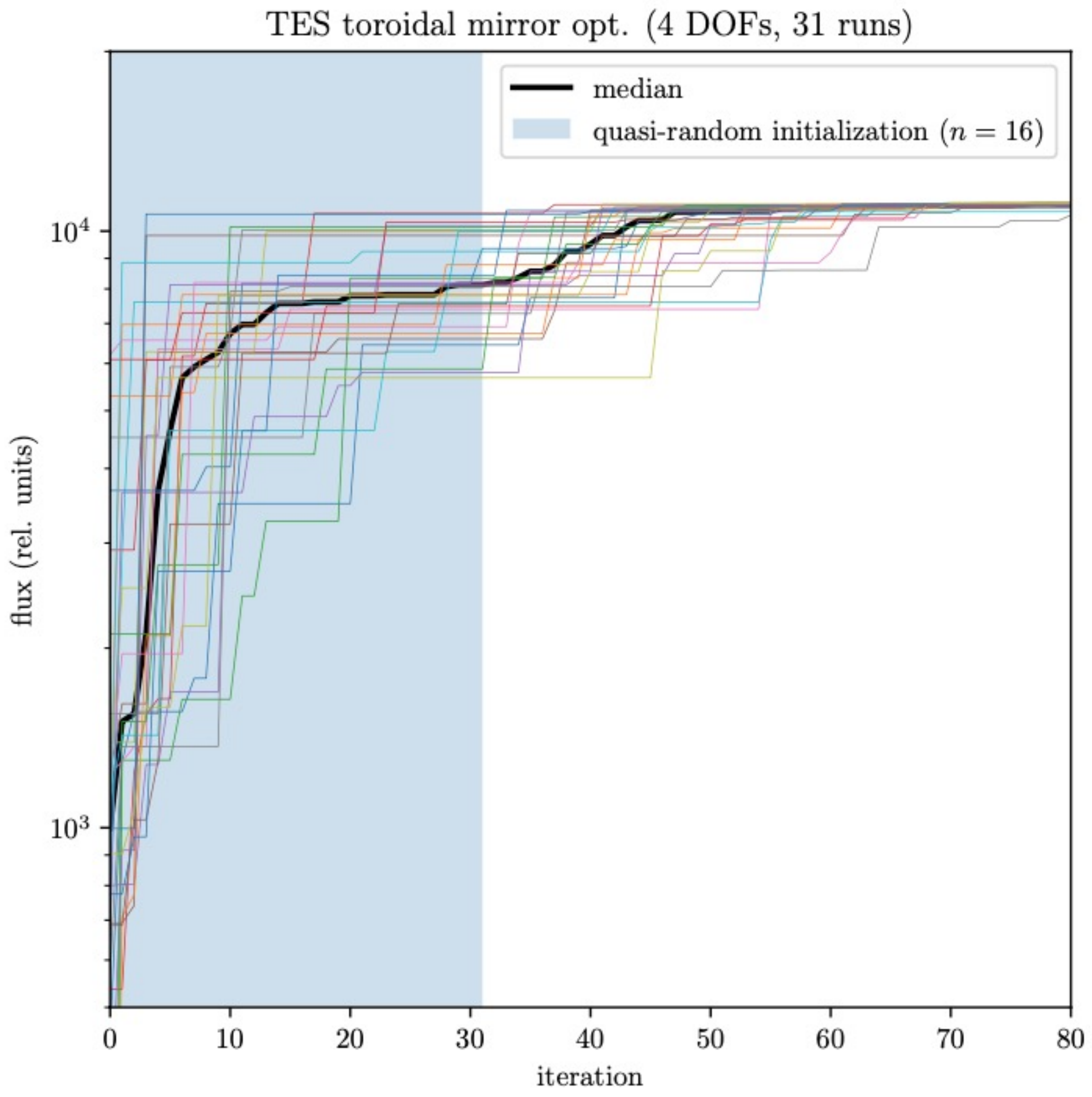
By hand, this process can take > 1 hour.
Via GPyTorch based optimizer, it takes < 10 min.

The code is a submodule of https://github.com/NSLS-II/bloptools

The optimization tool was tested and implemented in the Sirepo-Bluesky framework

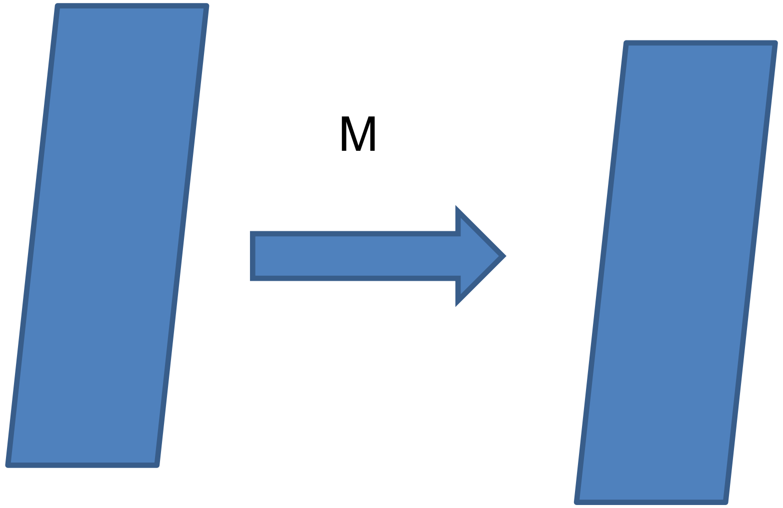
We've also tested this at ALS to optimize the toroidal mirror on Beamline 5.3.1.

Using BO on the TES beamline with Sirepo-Bluesky and SHADOW



T. Morris

Linear Canonical Transforms



final wavefront

(e.g. passing across KB mirror system)

Linear Canonical Transform (LCT)

$$\mathcal{L}_M[f](\vec{u}) = \frac{1}{\sqrt{\det iB}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp\left[i\pi p(\vec{u}, \vec{v})\right] f(\vec{v})\, d^2\vec{v}$$

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

$$p(\vec{u}, \vec{v}) = \vec{u}^{\,\mathrm{tr}} D B^{-1} \vec{u} - 2\vec{v}^{\,\mathrm{tr}} B^{-1} \vec{u} + \vec{v}^{\,\mathrm{tr}} B^{-1} A \vec{v}$$

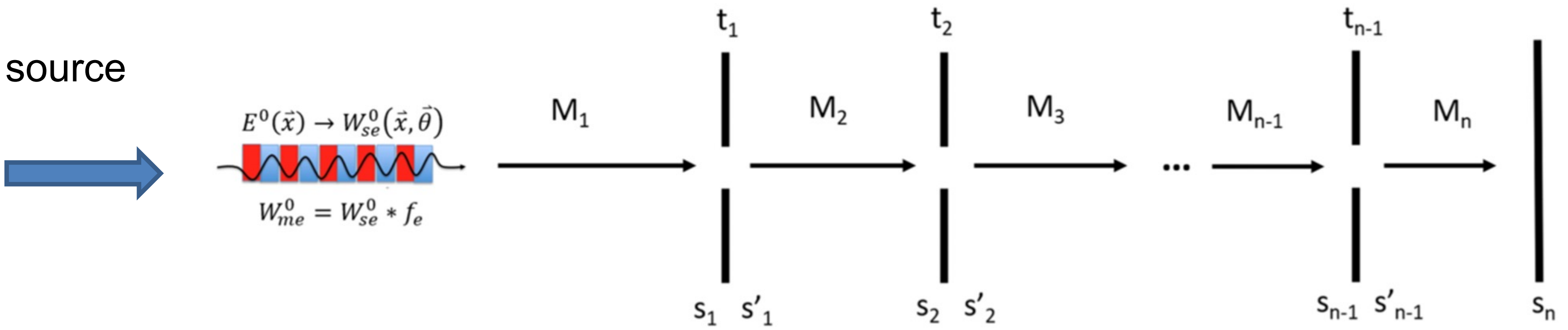
Generalization of Fresnel transform, Fourier transform, etc.

https://github.com/radiasoft/rsmath/blob/master/rsmath/lct.py ← Library is available here

https://accelconf.web.cern.ch/ipac2022/doi/JACoW-IPAC2022-THPOPT068.html ← reference

Simplified reduced models: matrix aperture beamline

Synchrotron radiation source
- Bending magnet
- undulator



Corresponding hierarchy of reduced models:

$\vec{z}_i$	M_1	t_1		M_2	t_2		M_3	$\vec{z}_f$
Σ_i	$\mathcal{S}_{M_1}$	Σ_1	Σ'_1	$\mathcal{S}_{M_2}$	Σ_2	Σ'_2	$\mathcal{S}_{M_3}$	Σ_f
$\vec{E}_i$	$\mathcal{L}_{M_1}$	$\vec{E}_1$	$\vec{E}'_1$	$\mathcal{L}_{M_2}$	$\vec{E}_2$	$\vec{E}'_2$	$\mathcal{L}_{M_3}$	$\vec{E}_f$
W_i	$\mathcal{T}_{M_1}$	W_1	W'_1	$\mathcal{T}_{M_2}$	W_2	W'_2	$\mathcal{T}_{M_3}$	W_f

RadiaSoft scientists are developing these reduced models:

- Beam moments
- Coherent Wavefront, LCT
- Partially coherent Wigner functions

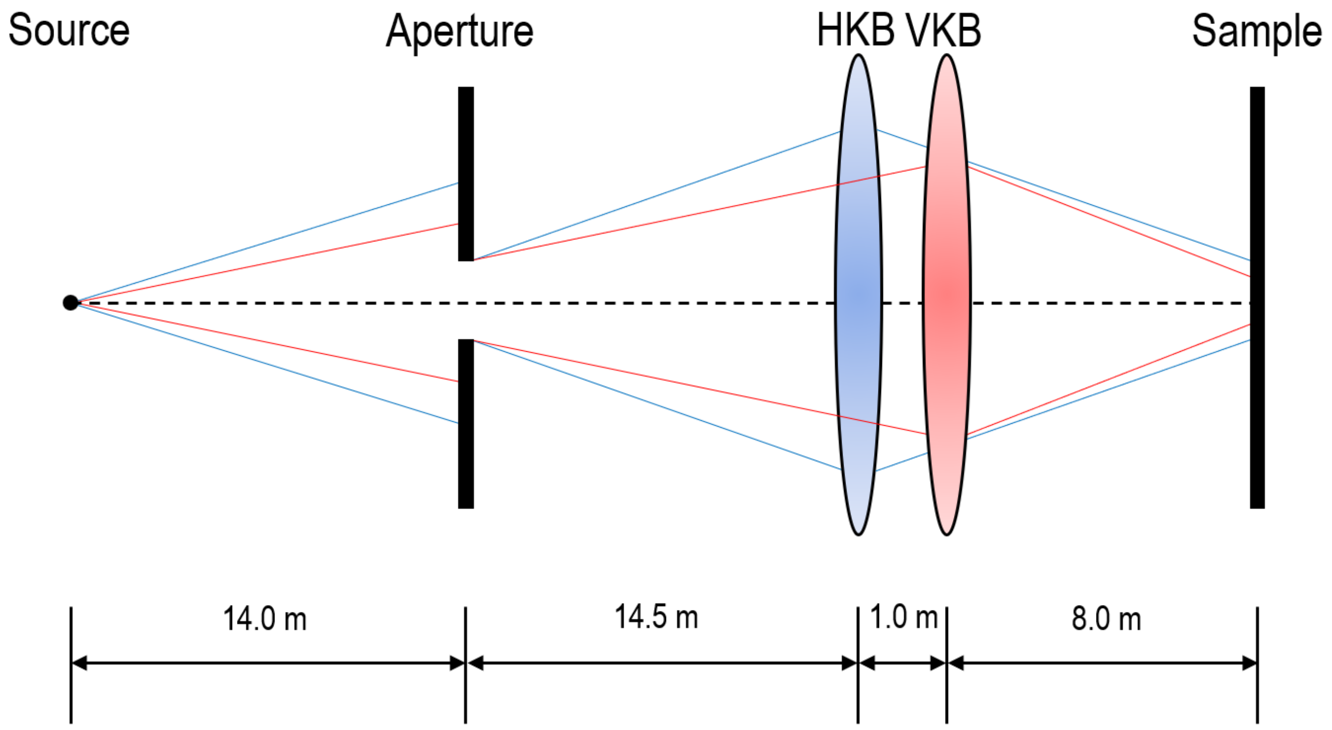
Fully developed beamline simulation codes

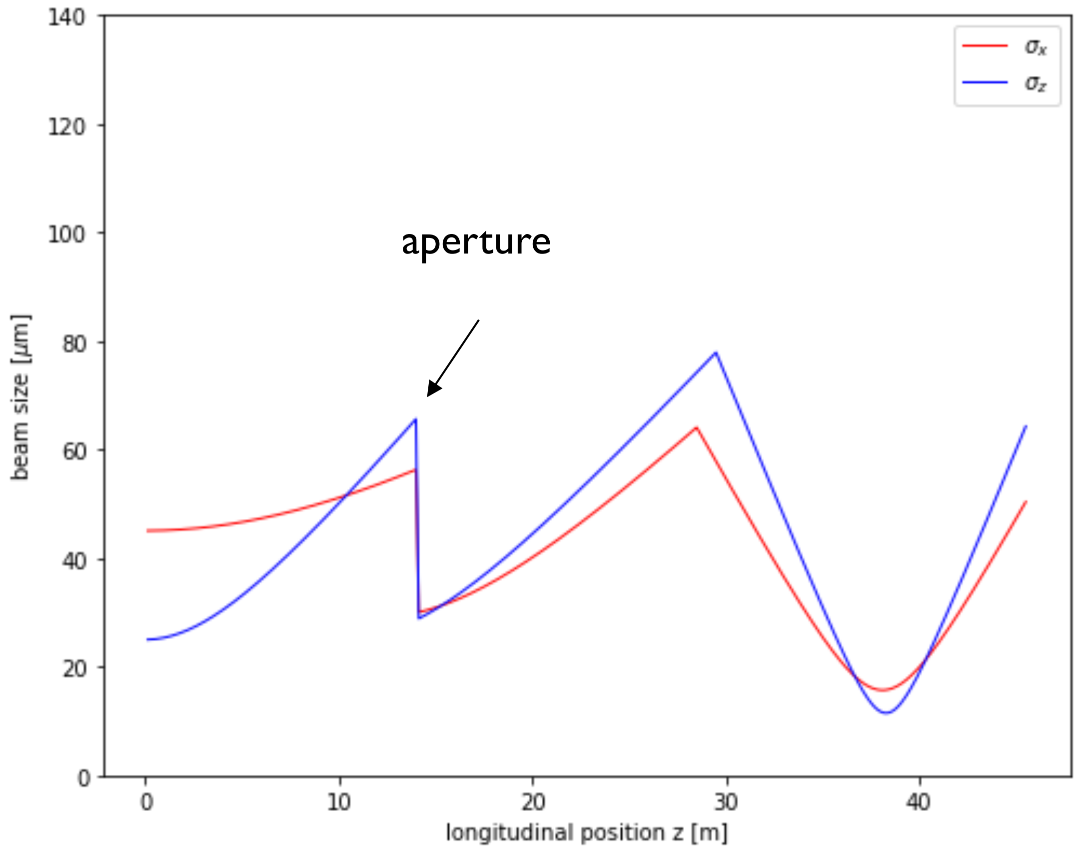
Ray Tracing:
- SHADOW
- XRT

Wavefront propagation:
- Synchrotron Radiation Workshop (SRW)
- XRT

Sirepo Interfaces to these codes

Example: KB beamline

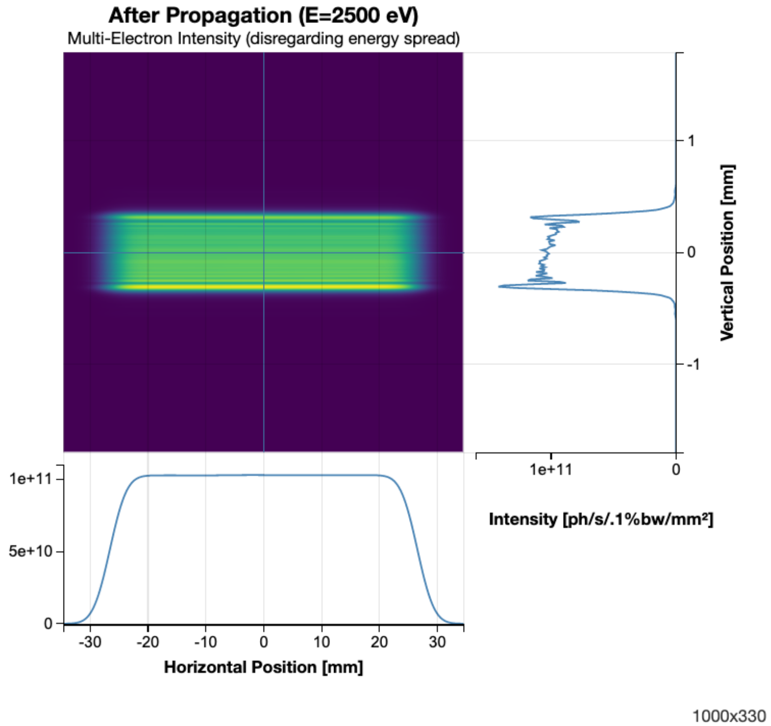




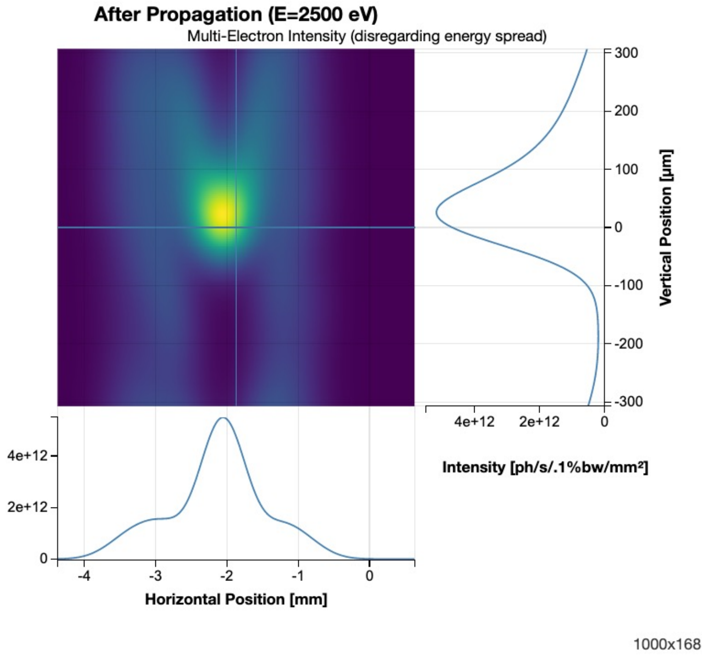
Pogorelov, Ilya V., Boaz Nash, Dan T. Abell, Paul Moeller "Propagation of a Gaussian Wigner Function Through a Matrix-Aperture Beamline." arXiv, 20 Sept. 2023, doi:10.48550/arXiv.2309.11008. (to be submitted to PRAB)

Gaussian Wigner function in Sirepo SHADOW

SRW in Sirepo interface:

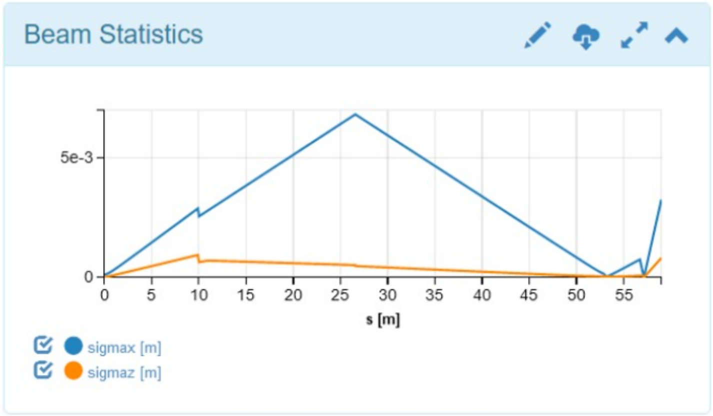


Intensity pre-Toroid, 26.57m

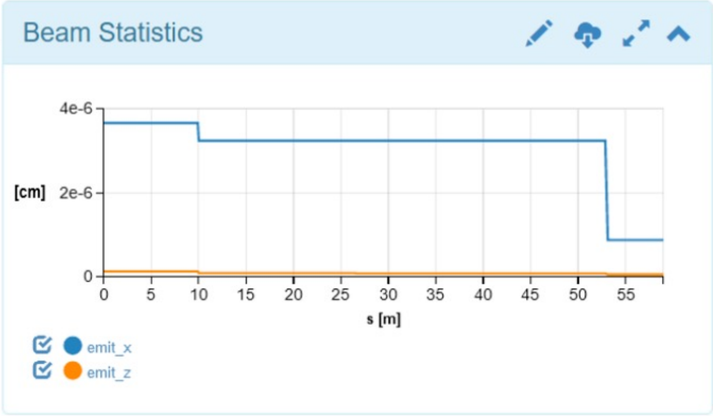


Intensity FS, 51.242m

a.



b.



Gaussian Wigner function through TES

Conclusions

- Online models are commonly used in particle accelerators
- Developing this technology for x-ray beamlines requires both reduced models and integration with diagnostics
- We have developed a reduced Gaussian model for partially coherent radiation and a LCT library for coherent propagation
- Bluesky is a growing framework for running experiments at synchrotron light sources
- The Sirepo-Bluesky library allows access to Sirepo simulations of x-ray beamlines from Bluesky experimental sessions.
- Sirepo-Bluesky allows for beamline algorithm development with a virtual beamline
- We have used Sirepo-Bluesky to help develop our Bayesian optimization routines that have been used on the TES beamline at NSLS-II
- We look forward to working with more beamlines at multiple facilities to bring online models into the x-ray domain

References

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[2] Nash, Boaz, et al. Linear Canonical Transform Library for Fast Coherent X-Ray Wavefront Propagation. JACOW Publishing, Geneva, Switzerland, 2022, doi:10.18429/JACoW-IPAC2022-THPOPT068.

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Thanks for your attention!

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