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U.S. DEPARTMENT OF ENERGY

Simulation-aided Instrument Optimization using Artificial Intelligence and Machine Learning Methods

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Automated alignment of beams

- Automated alignment has several benefits, e.g.:
  1. Better optima for better experiments.
  2. Quicker optima for faster commissioning.
  3. Fully autonomous experiments.
- Automated alignment is a noisy, high-dimensional, expensive-to-sample optimization problem.
- By far the best algorithm for these kinds of problems is Bayesian optimization.

Bayesian optimization

The BO algorithm iterates over these steps:

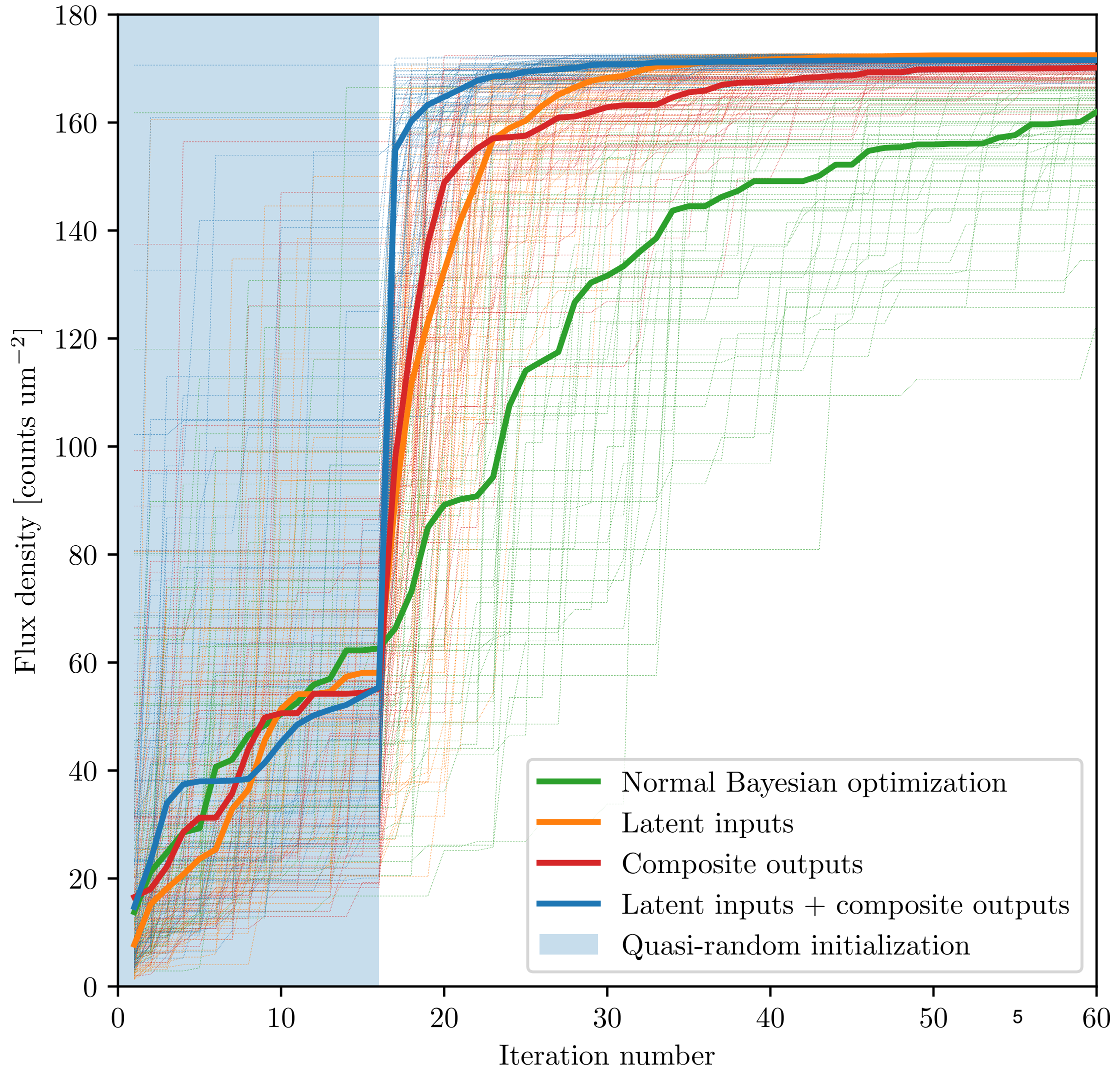
1. Given an existing set of data {x, y}, construct a prior about the function f, usually with a GP.
2. Use the data to construct a posterior $p(x)$ about f (i.e. constraining f such that $f(x) = y$). Very efficient to do with a GP.
3. Find the point(s) x^* that gives the best posterior (e.g. the largest expected improvement).
4. Sample that point.

Challenges for optimizing beams

1. Highly coupled inputs
   - Solution: custom kernels to fit a latent orthogonal basis
2. Invalid beamline data (e.g. the beam goes off the screen, glitches, etc.)
   - Solution: A classifier for each model to constrain invalid points.
3. Many beam qualities with weird trade-offs
   - Solution: Model beam qualities compositely
4. Sampling is not expensive, but moving inputs is
   - Solution: Optimize the acquisition function in parallel with Monte Carlo sampling, and find an efficient route between them.

The effect of coupled inputs and composite outputs

- *Right:* optimizing the TES beamline at NSLS-II in 4 dimensions.
- An analogous principle is true at ATF, where allowing for coupled inputs and independent outputs is important.



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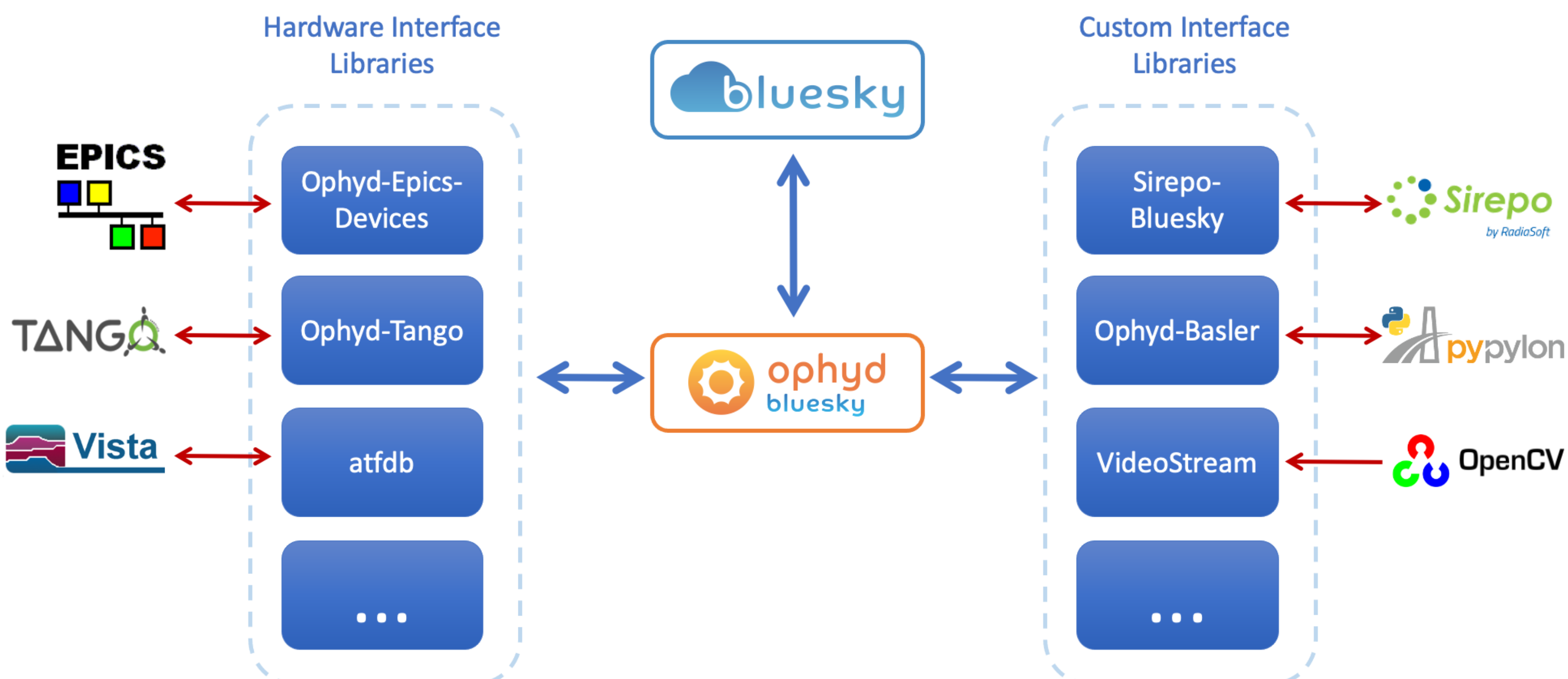
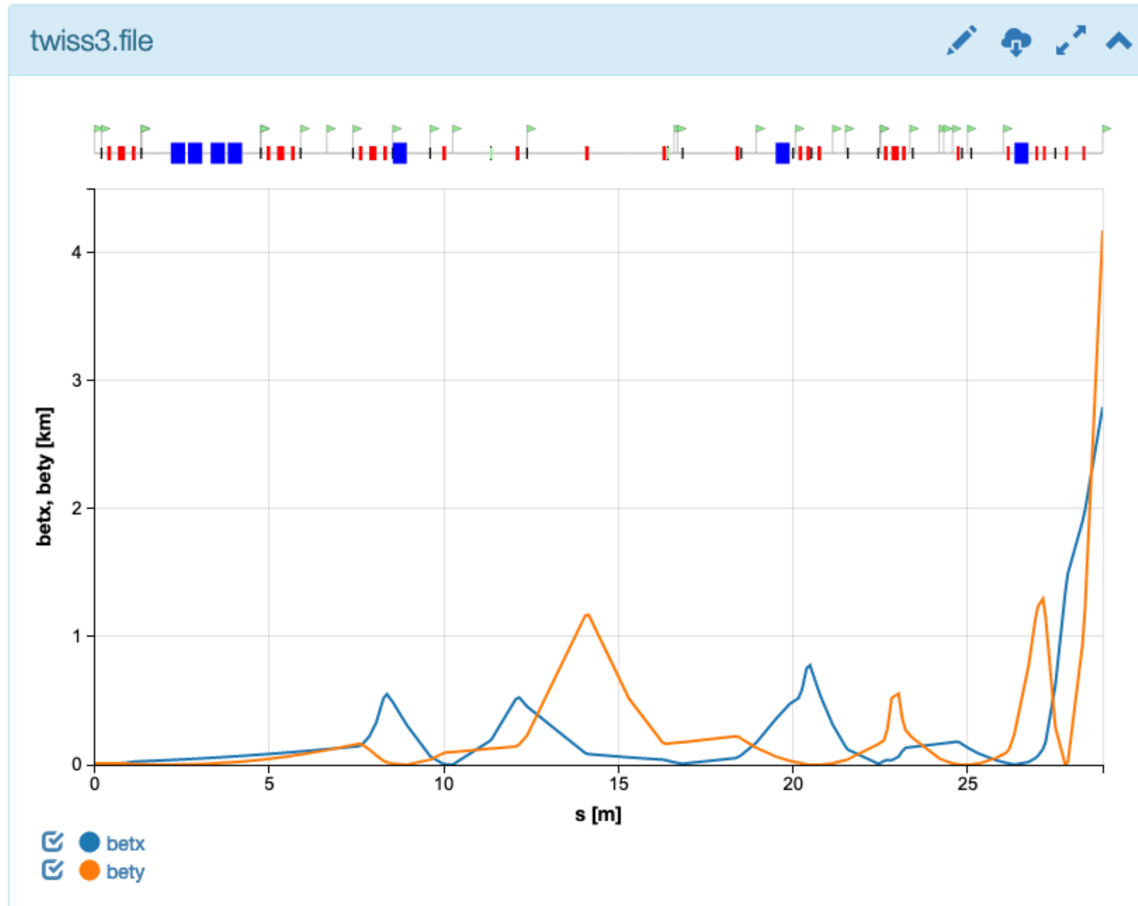
Custom code for ATF controls

- Interfacing with ophyd allows us to use the tools developed at NSLS-II, namely Bluesky and blop.



Testing optimization with simulations

- We can create a digital twin of ATF using Sirepo-Bluesky to interface with MAD-X, which lets us test different optimization strategies.



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Optimizing the e-beam at ATF

- We use the existing diagnostic (consisting of a frame-grabbing camera), which returns the beam flux, weight, and height.
- We use $f(x) = \text{flux}(x)/(\text{width}(x)^2 + \text{height}(x)^2)^{1/2}$ as a fitness function in order to enforce beam roundness.
- We model the fitness function of inputs $f(x)$ with a kernel $\left\langle f(x_i) f(x_j) \right\rangle = f\left(\left| D \exp S\left(x_i - x_j\right) \right| \right)$, which learns coupling between different quadrupole inputs.
- We use a Bayesian classifier model to exclude invalid beams (i.e. ones that go off the screen).

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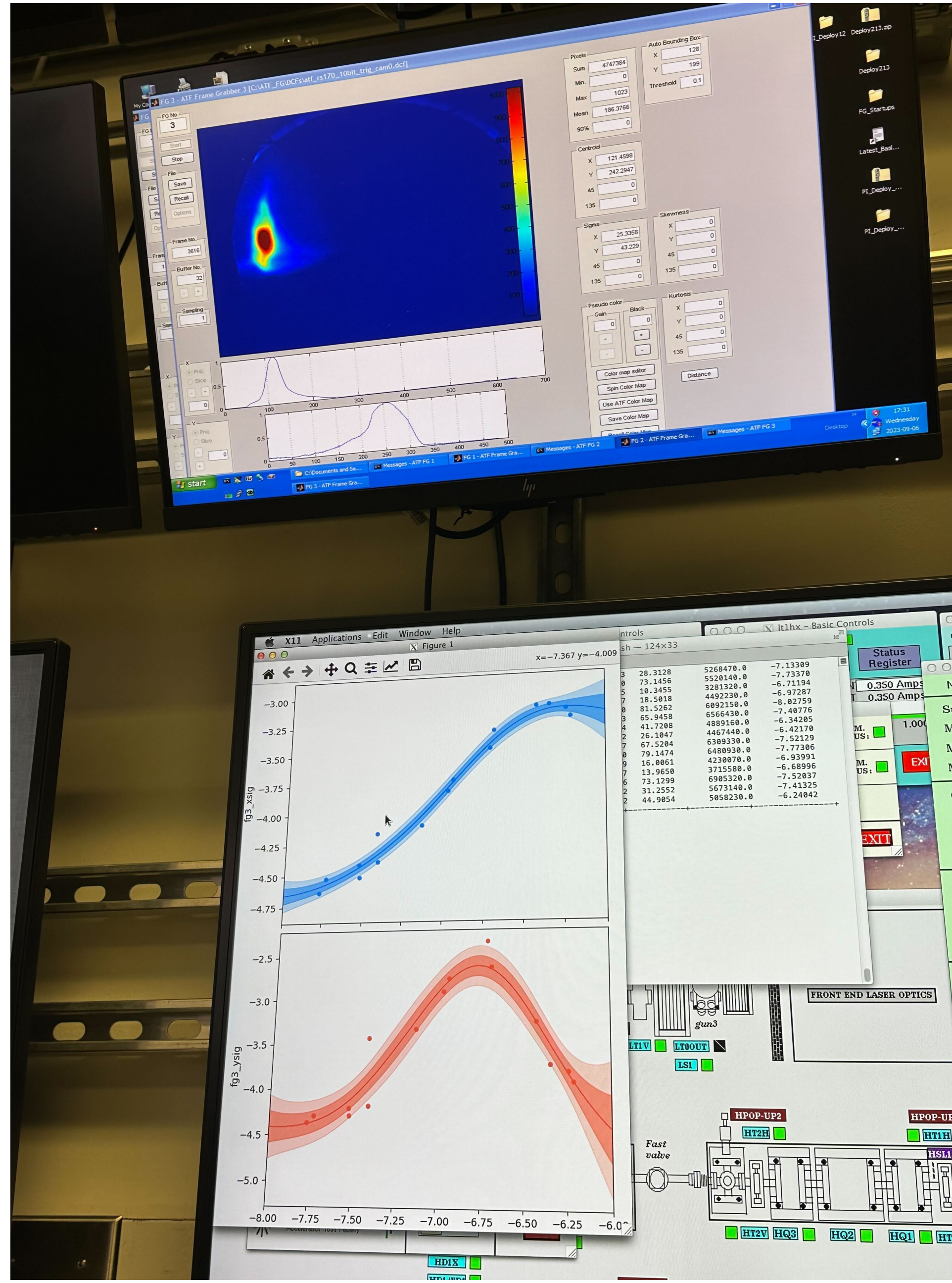
1D Bayesian optimization

- *Right:* we optimize over one quadrupole current.
- The diagnostics at ATF have a substantial amount of noise, so Bayesian optimization is ideal.



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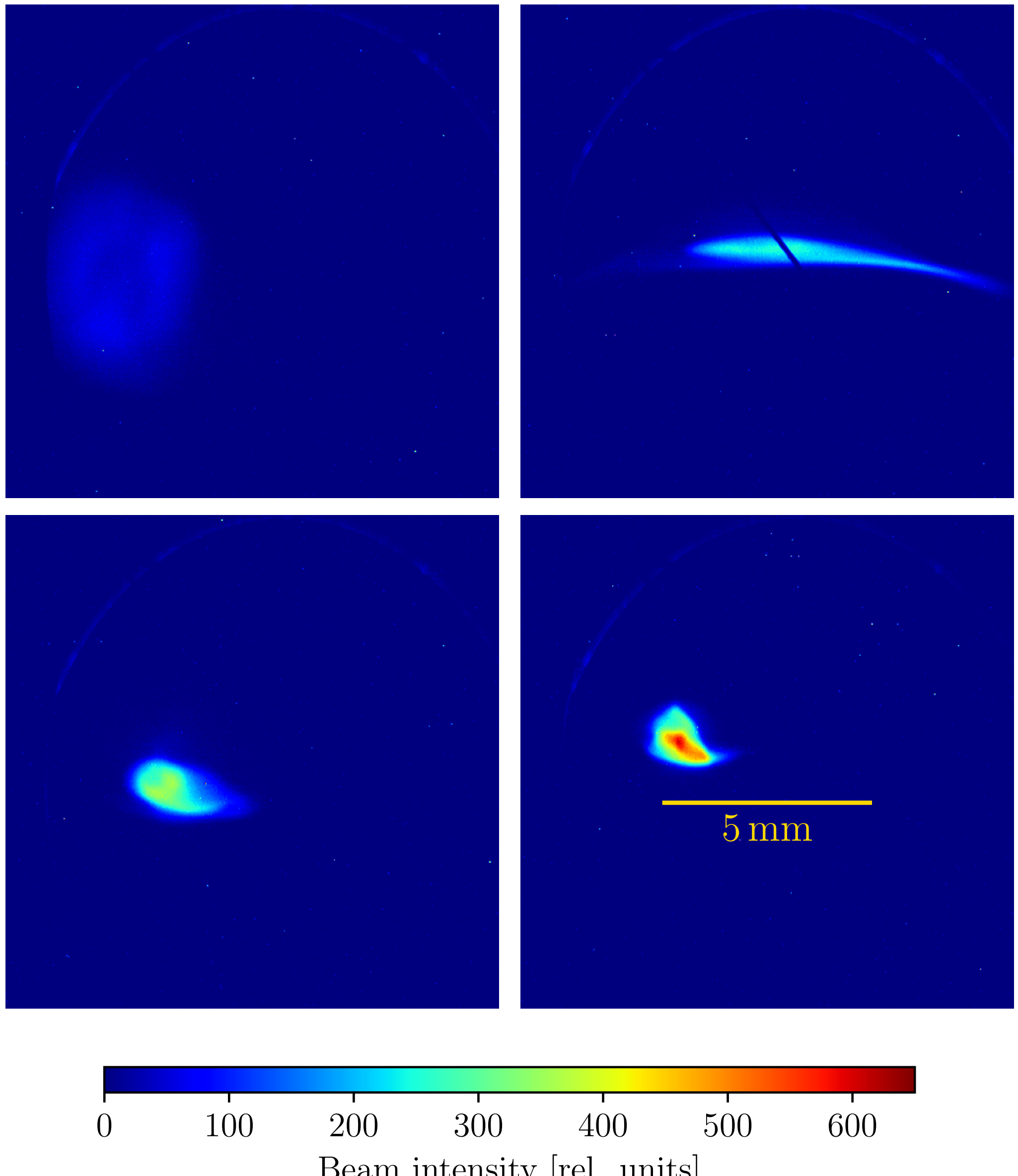
4D Bayesian optimization

- *Right:* we optimize over four currents.
- The beam converges to an optimum in only a few minutes.



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Further steps

- Higher dimension optimization of quadrupoles (up to 20 dimensions).
- Integrating Basler cameras to optimize different diagnostics
- Application of the same tools at LCLS and XFEL

Thank you!

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