Advanced Modeling of Beam Physics and Performance Optimization for Nuclear Physics Colliders

Ji Qiang

Nuclear Physics Accelerator R&D, PI Exchange Meeting
Dec. 2, 2024

Project members:

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- LBNL: **Ji Qiang**, Xiaoye Li, Yang Liu, Yi-Kai Kan (postdoc)
- MSU: **Yue Hao**, William Fung (graduate student)

Outline:

1) Introduction

2) Current project status

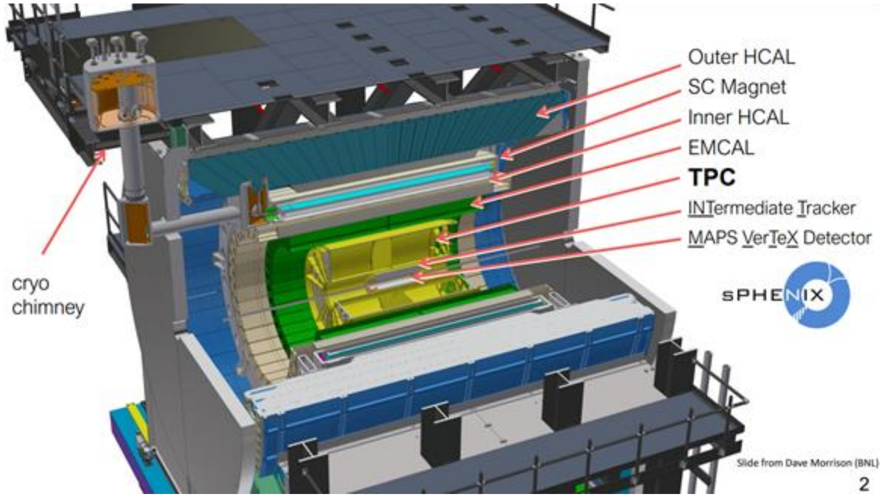
3) Future work

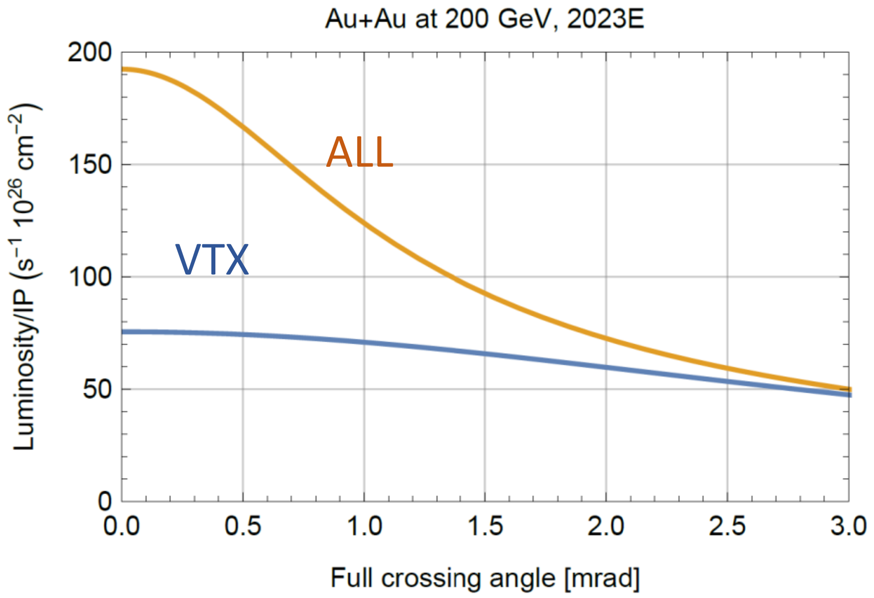
4) Summary of expenditures

Luminosity Optimization Needed at the New RHIC Jet Detector

- New jet detector sPHENIX was commissioned in 2024.
- Physics study needs higher luminosity.

1. VTX (+/-10 cm)
2. Crossing angle (2mrad)
3. S/N - Background





Courtesy of W. Fischer

Luminosity depends on:

- Global Parameters:
1. Orbit (Dipole)
2. Tune (Quadrupole),
3. Chromaticity (Sextuple)
4. Octupole
5. RF cavity

- Local (IR8) Parameters:
1. Beta*
2. S* (more sensitive than head on)
3. Bunch length

Project Goals:

- Develop an advanced modeling framework based on first-principle physical simulations, lattice models and the state-of-the-art machine learning methods.

- Apply this framework to the performance improvement of the RHIC experiments (sPHENIX).

- Train and educate early career researchers.

Major Deliverables and Schedule

Year 1:

Q1: Develop data manipulation package that can be used to extract and label data from RHIC measurements, and to interface with the simulation packages; Build an analytical luminosity model from integration, including the hourglass effect, crossing angle and IP optics.

Q2: Modify the existing beam-beam simulation code to include the requirements of sPHENIX; Interlink the analytical model with RHIC optics model and the GPTune framework.

Q3: Connect the GPTune to the simulation tools; Test the beam in RHIC for luminosity optimization using GPTune (without sPHINEX detector knobs).

Q4: Analyze the initial experimental data and benchmark the analytical model; Build models and control knobs to maximize the performance of RHIC, especially the sPHENIX experiment**;** Explore new prior functions and kernel functions in the GPTune based on the physics knowledge.

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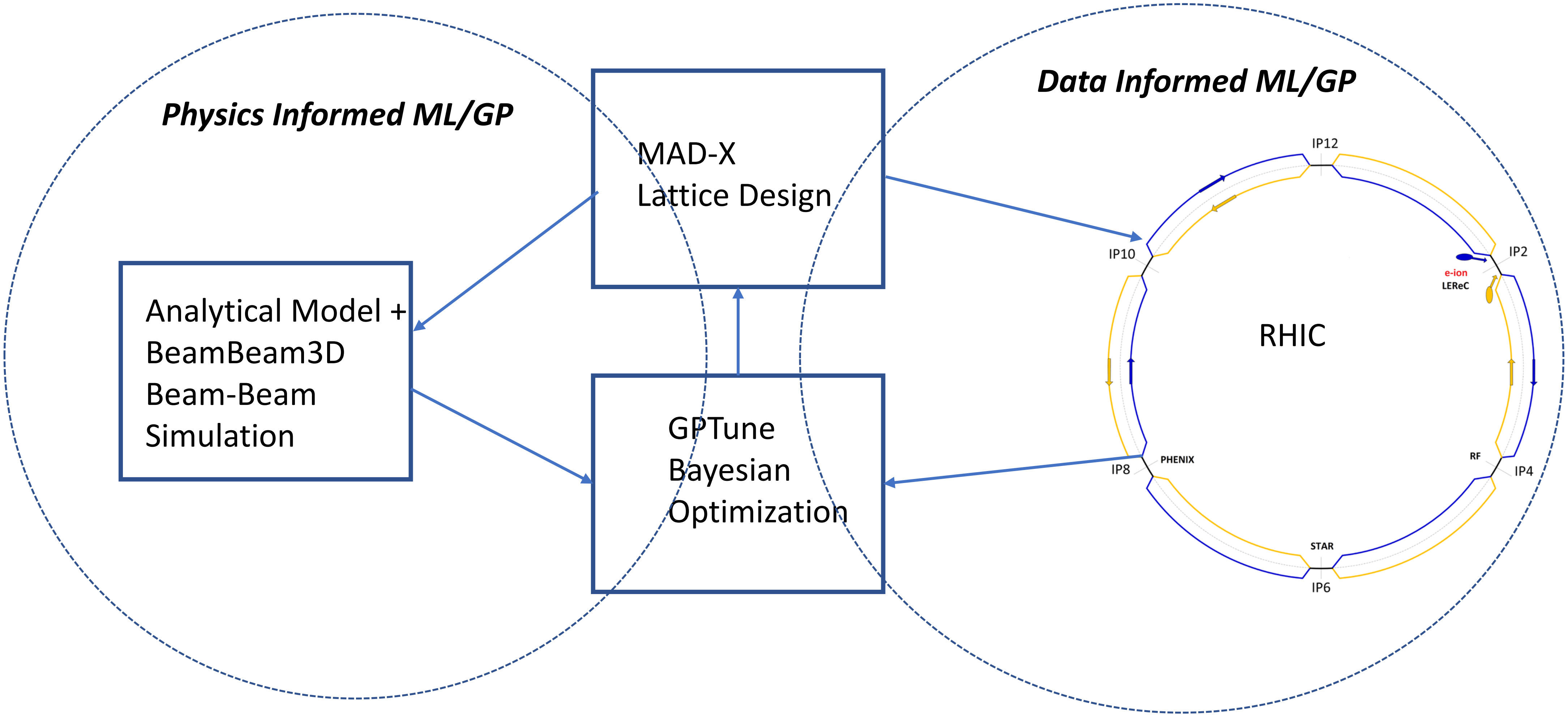
Q1: Extend the GPTune Bayesian optimization framework's capability to include the general experimental control knobs; Add the sPHINEX related control and analytical model in the optimization routine using GPTune.

Q2: Apply the enhanced GPTune optimizer to RHIC measurement data to test the model and the control knobs using RHIC 's accelerator physics experiment (APEX) time; Test beam with luminosity optimization including sPHINEX requirements (maximize the vertex luminosity while minimize the background).

Q3: Update the optics tuning model with the experimental data, improve the tuning strategy; Apply to RHIC measurement data to test the model using RHIC's accelerator physics experiment (APEX) time.

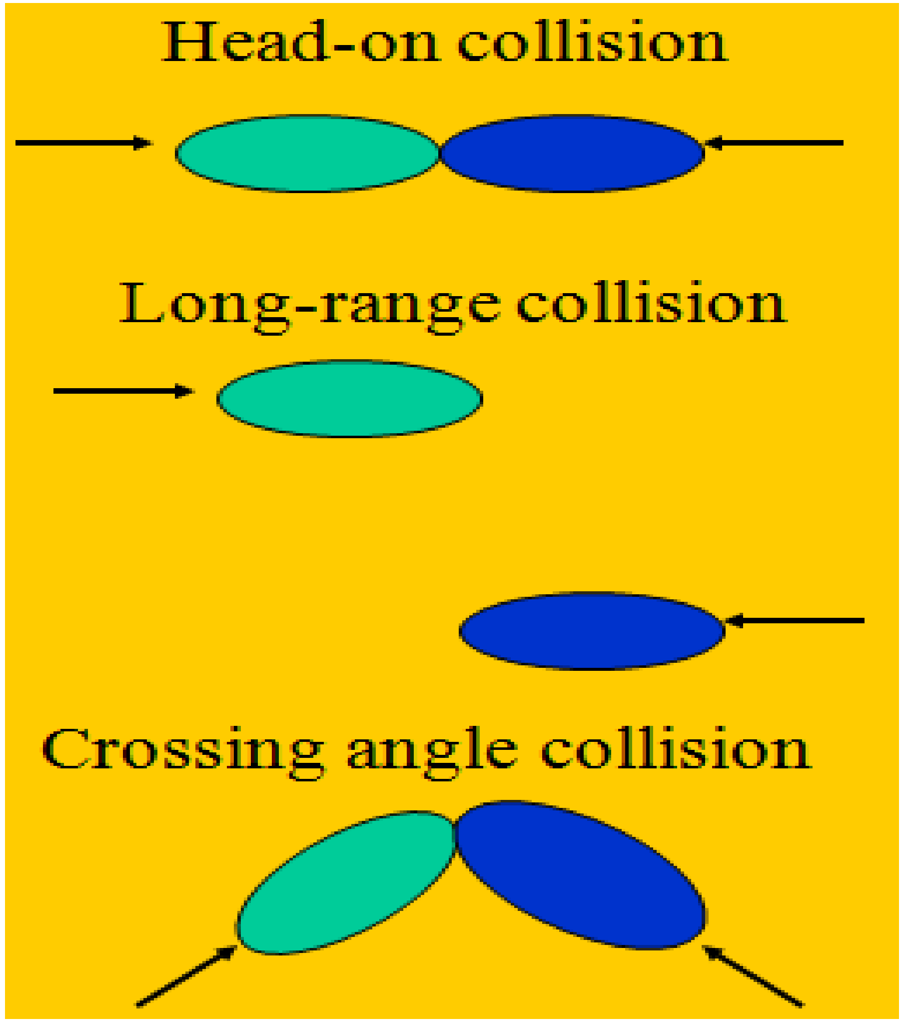
Q4: Continue to apply optimization to the RHIC measurement control knobs using RHIC 's accelerator physics experiment (APEX) time; Test beam with updated optimization strategy and further improve sPHINEX performance.

Advanced Modeling Framework for RHIC Lum. Optimization



- Transfer learning improves the BO performance in RHIC luminosity optimization by using the GP model trained by the physics simulation.

BeamBeam3D: A Parallel Self-Consistent Colliding Beam Simulation Code



Some key features of the BeamBeam3D

- Multiple-slice model for finite bunch length
- New algorithm -- shifted Green function -- efficiently models long-range collisions
- Parallel particle-field based decomposition to achieve perfect load balance
- Lorentz boost to handle crossing angle
- Arbitrary closed-orbit separation
- Multiple bunches, multiple collision points
- Linear transfer matrix + one turn chromaticity
- Conducting wire, crab cavity, e-lens, crab waist compensation model
- Feedback model
- Wakefield model

https://github.com/beam-beam/BeamBeam3D

Bayesian Optimization: A Model Based Black-Box Method

- Problem: $\min_{x} y(x)$, x : parameter configuration
- Bayesian statistical inference is an iterative model-based approach
  - versatile framework for black-box derivative-free global optimization

Sampling: $y_1 \dots y_{n_0}$

Prior distribution

Surrogate Model $f(x)$

$\min f \approx \min y$

Update Posterior Distribution

Search Next:

$x_{n+1} \rightarrow y_{n+1}$

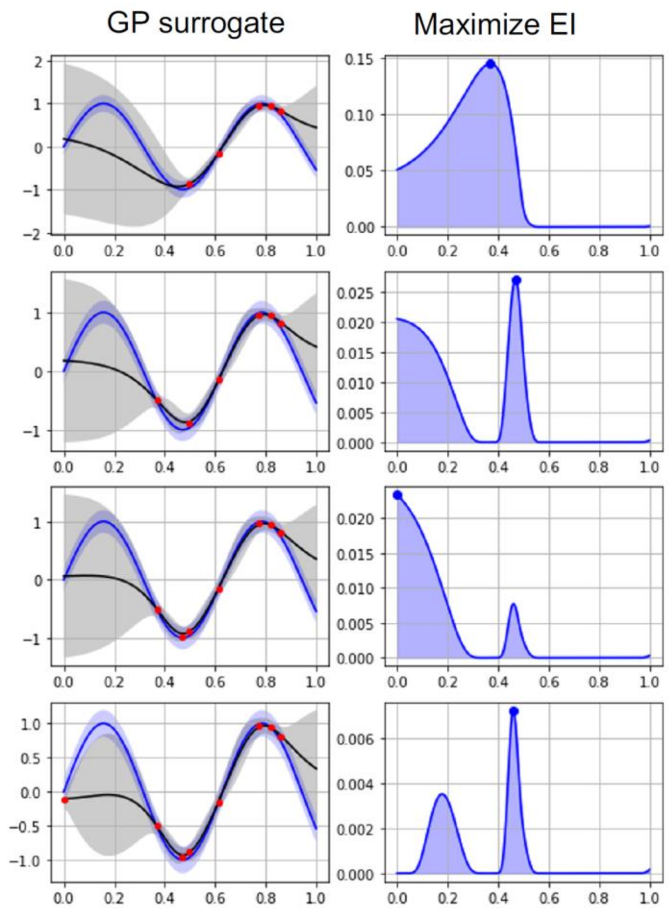
To optimize Acquisition Function

$p(y) = \mathcal{N}(\mu_0, \Sigma_0)$

Multivariate normal dist.

Bayes Rule

Update model with new data



- GP regression
  - LCM (multitask learning)
  - cGP
- Deep GP
- Other models …

- Expected Improvement (EI)
  - Maximize EI: GE, PSO, CMA-ES, …
- Other acquisition functions …

Gaussian Process: A Surrogate Model with Uncertainties

- GP defines a distribution over functions, and inference takes place in the space of functions
  - Every finite subset of variables follows multivariate normal distribution
- GP is specified by the mean function and covariance function $k(x, x')$ (kernel)

$$f(x) \sim GP\big(\mu(x), k(x, x')\big)$$
$$\mu(x) = \mathbb{E}[f(x)]$$
$$k(x, x') = \mathbb{E}[(f(x) - \mu(x))(f(x') - \mu(x'))]$$

- Gaussian kernel: These are the parameters need to be trained in the GP model

$$k(x, x') = \sigma^2 \exp\left(-\sum_{i=1}^{D} \frac{(x_i - x_i')^2}{l_i}\right)$$

covariance is large if two points are close

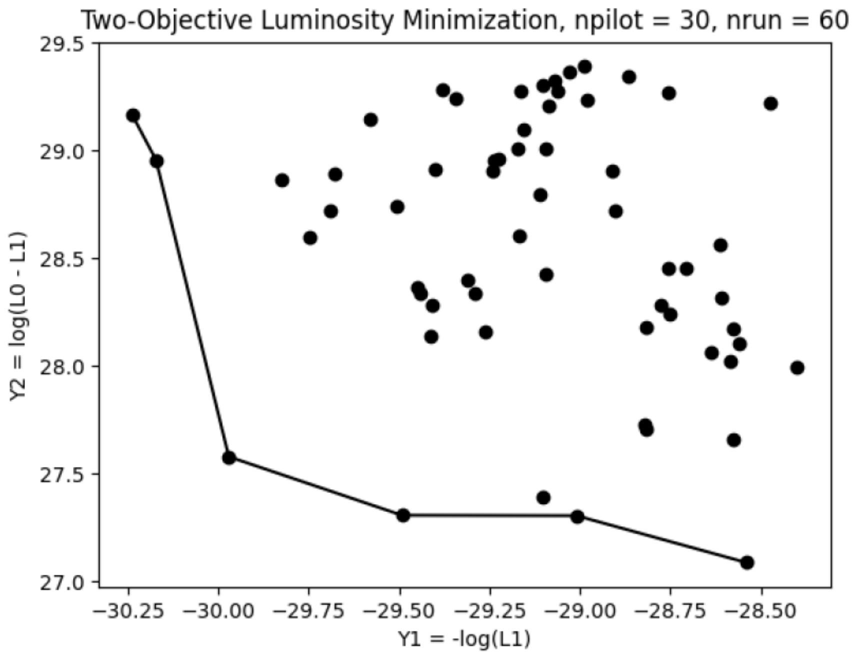
(Can use other kernels …) Matérn: $K_{\text{Matern}}(x, x') = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu}|d|}{\ell} \right)^{\nu} K_{\nu} \left(\frac{\sqrt{2\nu}|d|}{\ell} \right)$

Bayesian Optimization Software Package: GPTune

Some key features of GPTune include:

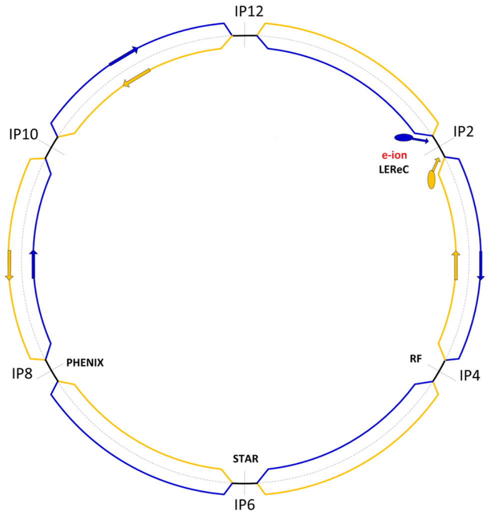
(1) relies on dynamic process management for running applications with varying core counts and GPUs
(2) can incorporate coarse performance models to improve the surrogate model
(3) allows multi-objective tuning such as tuning a hybrid of objectives
(4) allows multi-fidelity tuning to better utilize the limited resource budget
(5) supports checkpoints and reuse of historical performance database.

background



vertex signal

- on-line accelerator optimization must be constrained



https://gptune.lbl.gov

Bayesian Optimization with Black Box Constraints Needed for Safe On-Line Optimization

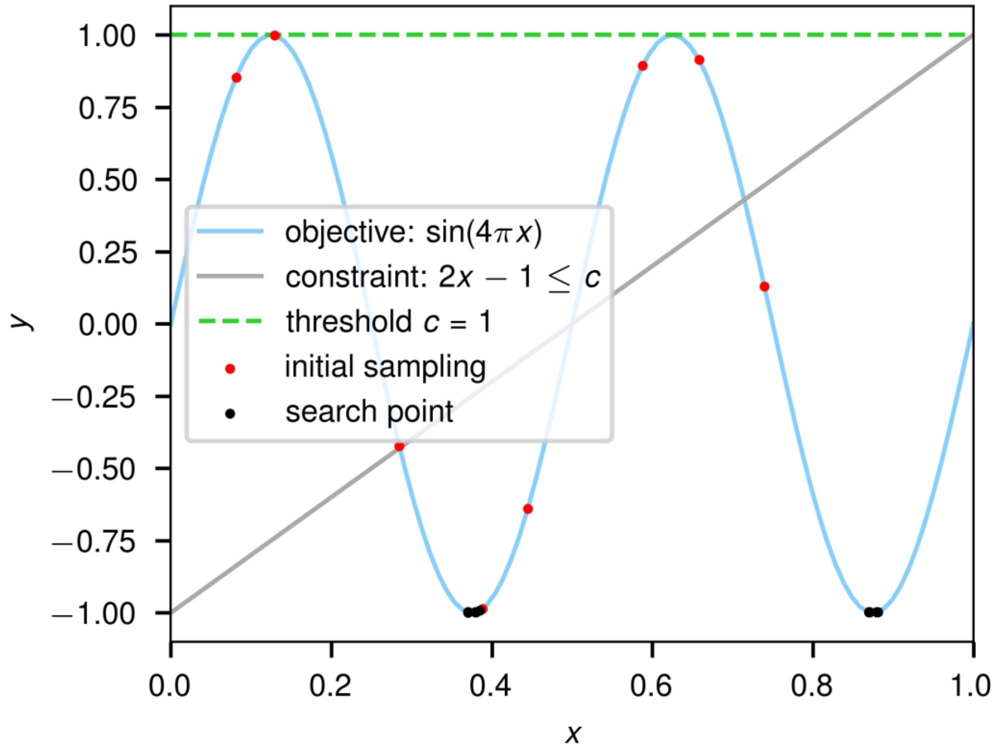
Optimization Problem:

$$\min \begin{cases} f_1(\vec{x}) \\ \cdots \\ f_n(\vec{x}). \end{cases} \text{subject to } g_i(\vec{x}) \leq 0, h_i(\vec{x}) = 0$$

- The Objective function *f* (e.g. luminosity) is approximated with a Gaussian process (GP).
- The constraint functions *g* and *h* (e.g. beam losses) are approximated with another Gaussian process.
- During the optimization process, both GPs are updated with the available data points.
- The constraint GP will be used in the BO to guide the prediction of next search point.

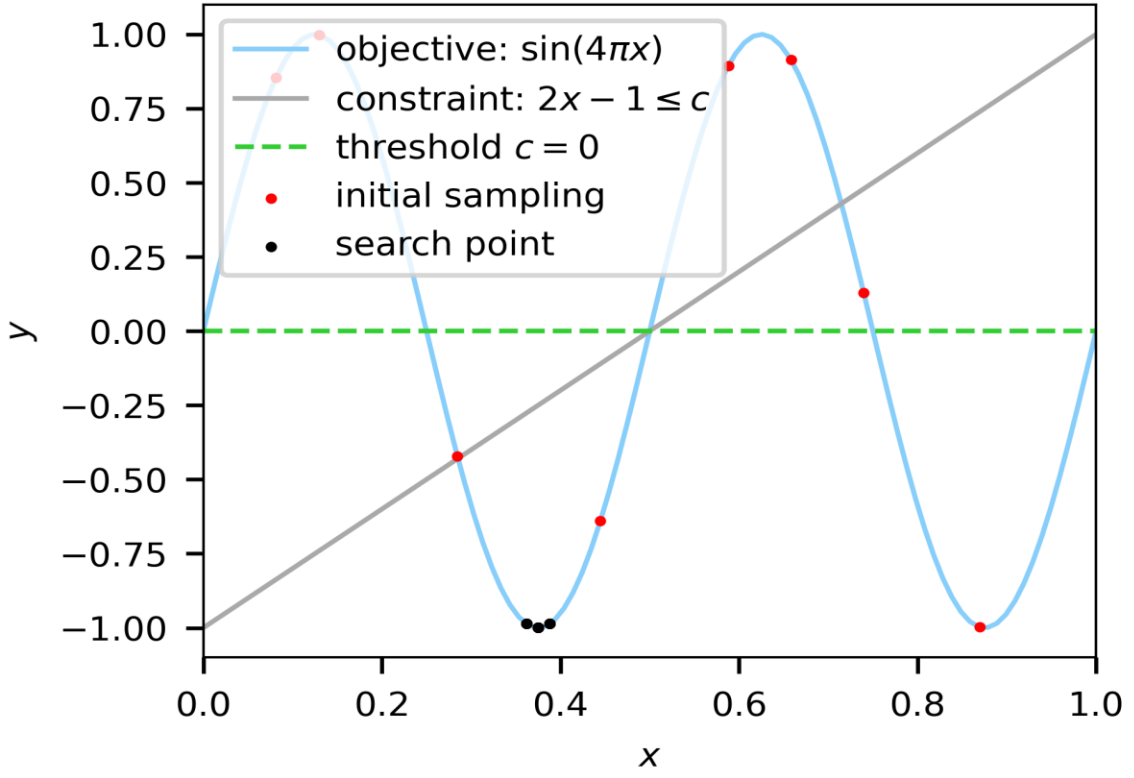
Verification of Bayesian Optimization with Black Box Constraints

f = sin(4π x)
g = 2x-2



- feasible domain for x is between 0 and 1.

f = sin(4π x)
g = 2x-1



- feasible domain for x is between 0 and 0.5.

Application of Bayesian Optimization with Black Box Constraints to a RHIC Example

Minimize: $$f(\mathbf{x}^n) = -\gamma_x(\mathbf{x}^n, s_{ip}) \cdot \gamma_y(\mathbf{x}^n, s_{ip})$$

X: the quadrupole strength of two lattice elements *bo7_qd3* and *bo7_qf4*

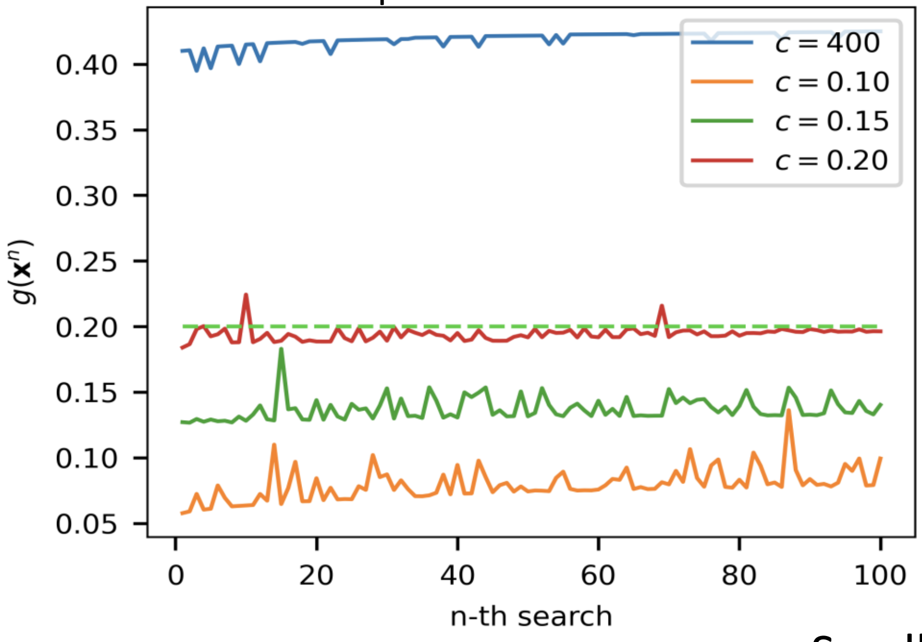
where $\gamma_x(\cdot,\cdot)$ and $\gamma_y(\cdot,\cdot)$ are horizontal and vertical Twiss functions

$$g(\mathbf{x}^n) = \max_{i \in I_c}\left(\max \Delta\beta_x(\mathbf{x}^n, s_i), \Delta\beta_y(\mathbf{x}^n, s_i)\right) \leq c$$

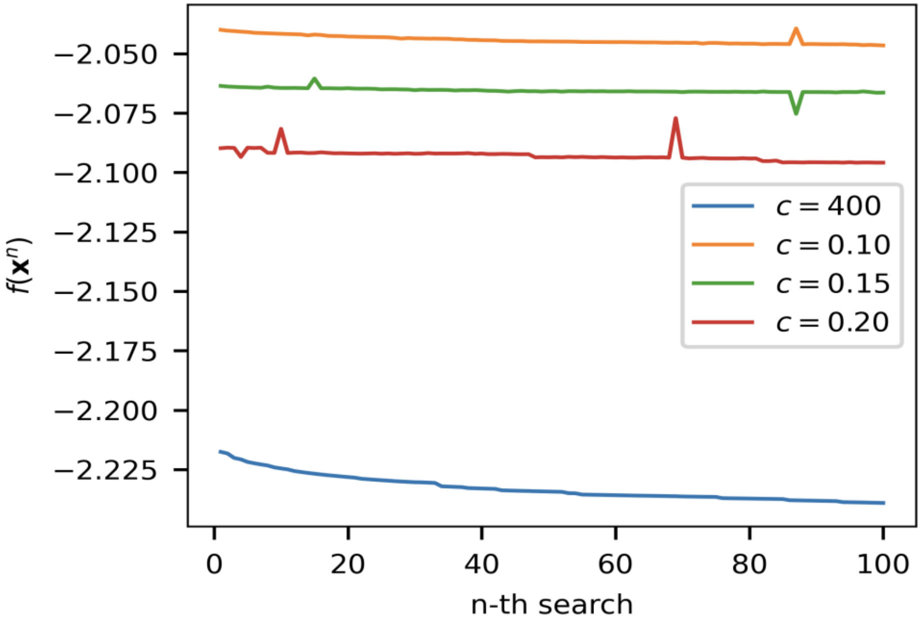
$$\Delta\beta_k(\mathbf{x}^n, s) := \left|\frac{\beta_k(\mathbf{x}^n, s) - \beta_k(\mathbf{x}^0, s)}{\beta_k(\mathbf{x}^0, s)}\right| \quad k \in \{x, y\}.$$

Here, the set I_c denotes the index set for the lattice elements *bo6_qd1*, *bo7_qd1*, *bo10_qd1*, *bo11_qd1*, and *bo2_qd1*.

Value of the constraint equation at each optimization step for the problem with different *c*



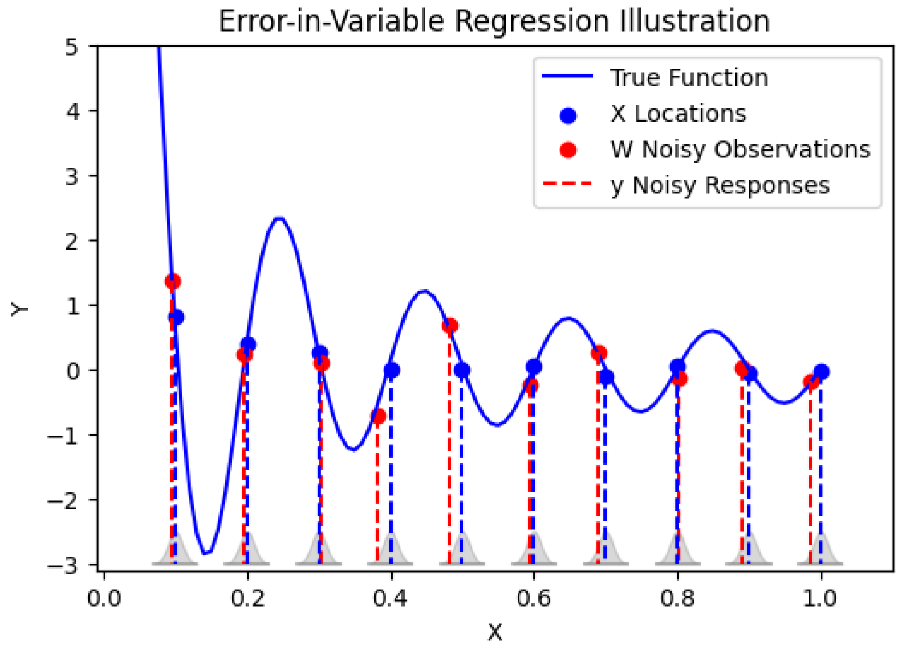
Value of the objective function at each optimization step for the problem with different *c*



- Smaller objective function is achieved with weaker constraints.

New Feature in GPTune: Wasserstein-Based Kernels for Inputs with Uncertainties

- Functions with input uncertainty
  - Assume a collection of function samples $(x_i, y_i), i \leq n$ with observation errors $\epsilon_i \sim N(0, u_i^2)$ and input errors $\delta_i \sim N(0, \sigma_i^2)$
  $$y_i = f(x_i + \delta_i) + \epsilon_i$$
  - For d-dimensional problems:
  $$y_i = f\left(x_{i,1} + \delta_{i,1}, \dots, x_{i,d} + \delta_{i,d}\right) + \epsilon_i$$
  - δ_i^d represents known or unknown uncertainty, in e.g., control knobs of accelerators



Wasserstein-Based Gaussian Process (WGP)

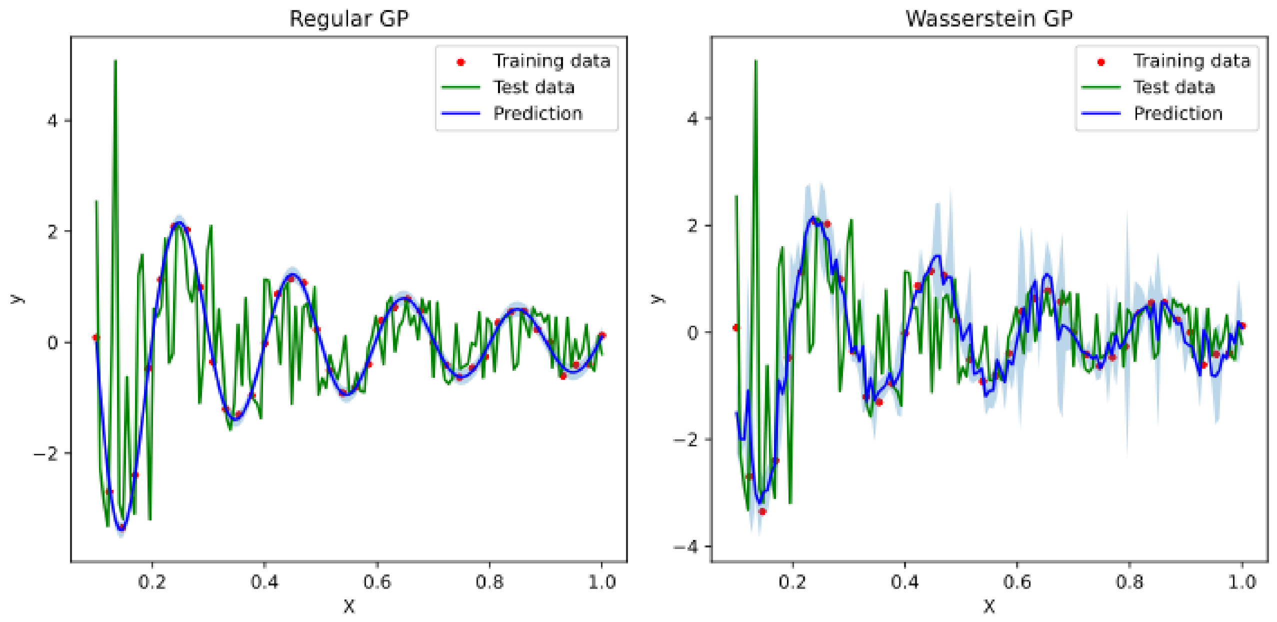
- Wasserstein distance between two normal distributions $x_1 \sim N(\mu_1, \sigma_1^2)$, $x_2 \sim N(\mu_2, \sigma_2^2)$

$$r_W(x_1, x_2) = \sqrt{(u_1 - u_2)^2 + (\sigma_1 - \sigma_2)^2}$$

- Assume f follows a GP: $f(x) \sim GP(0, K(x, x'))$, with Wasserstein-distance-based kernels:

$$K(x, x') = \gamma^2 \prod_{k=1}^{d} \exp\left(-\frac{r_W(x_k, x'_k)^2}{2l_k^2}\right)$$

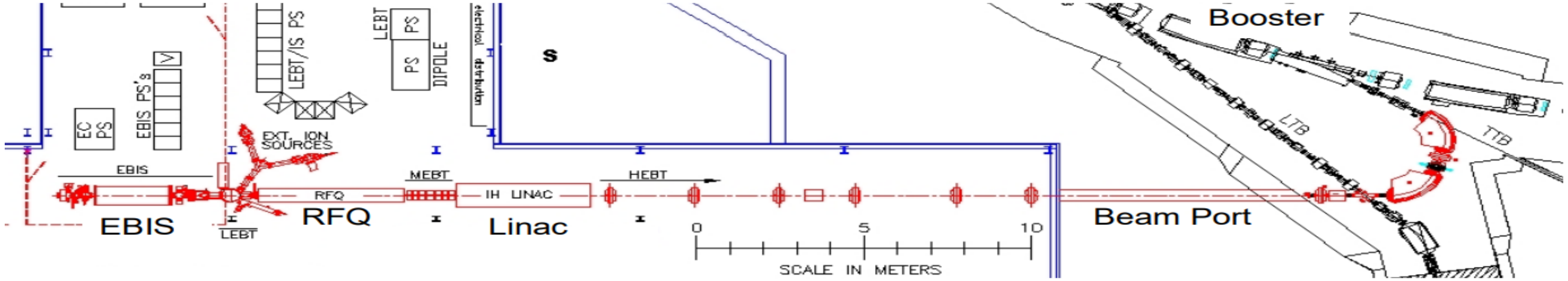
- The log-likelihood function can be optimized w.r.t. l_k and γ^2 via e.g., MCMC

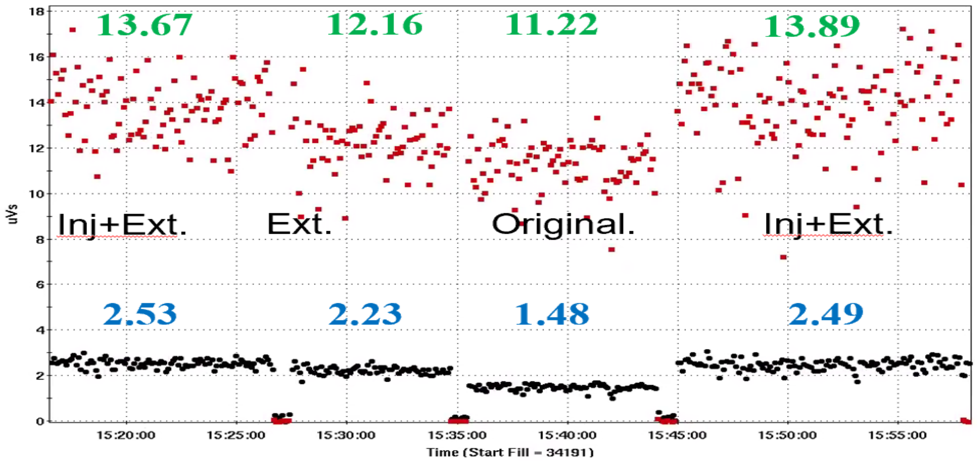


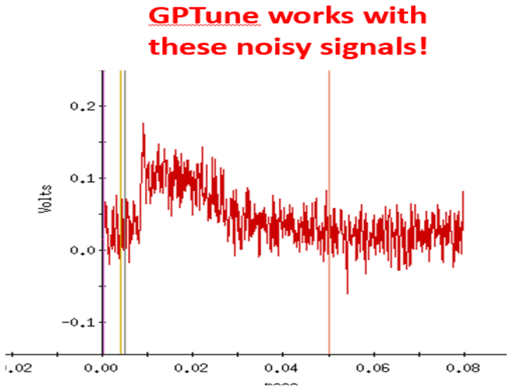
WGP provides more accurate confidence intervals

- WGP is available in GPTune, supporting multi-task and multi-objective optimizations

Online Bayesian Optimization Improves EBIS Performance







Intensity detector	Original	Ext. optimized with xf14	Gain	+ Inj. Optimized with FC96	Total Gain
xf14 (uVs)	1.48	2.23	42~50%	2.53/2.49	68~71%
fc96 (uVs)	11.22	12.61	8.4%	13.67/13.89	22-24%

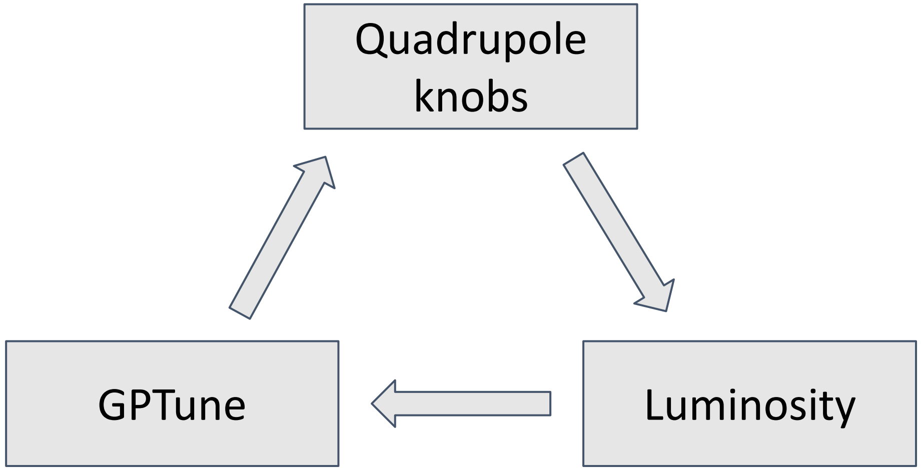
Online Optimization of Luminosity in RHIC

- Optimize the luminosity by correcting its loss of geometric overlap due to beam optics mismatch.
- There are 17 tuning quadrupoles at interaction region, most of them are independent and with tight tuning range.
- There are 4 targeting objectives. In order not to disturb the optics function outside the interaction region and IBS rate in the entire ring, additional 9 constraints have to be satisfied.
- **It is inefficient to use optimizer (GPTune) directly on all 17 quadrupole knobs, instead, GPTune controls the change of s* and use model to calculate correct quadrupole settings. (Dimension Reduction)**

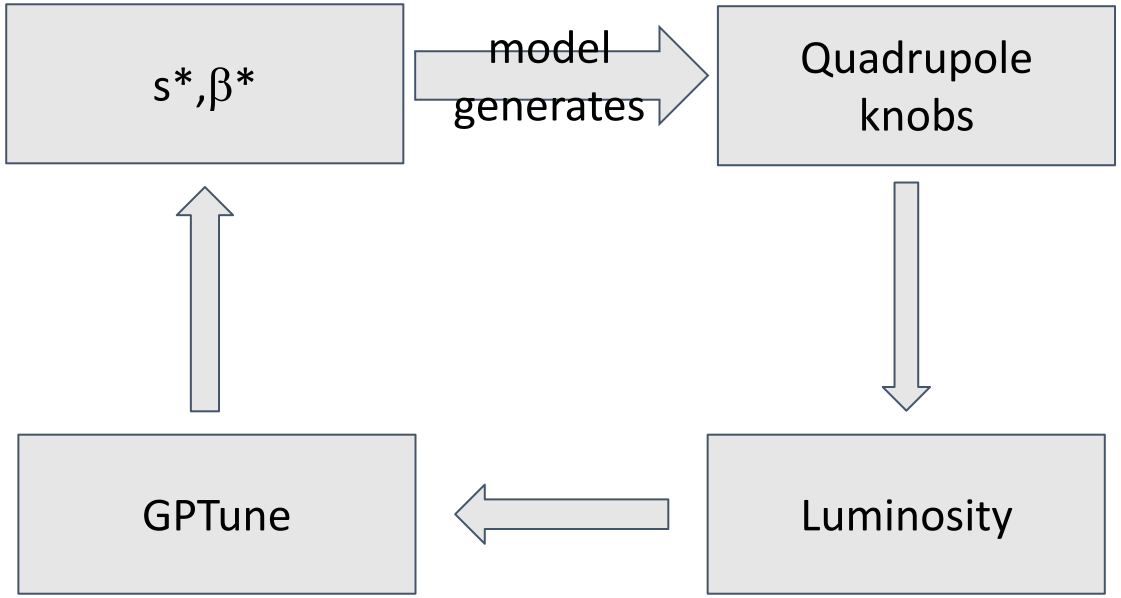
	@ IR boundary (6+0)			@IP (1+4)			Global (2+0)
Constraints	$\beta_{x/y}$	$\alpha_{x/y}$	η, η'			η	$\nu_{x/y}$
targets				$\beta^*_{x/y}$	$s^*_{x/y}$		

Online RHIC Optimization Diagram

Brute Force Method



Model Based Method in this Project

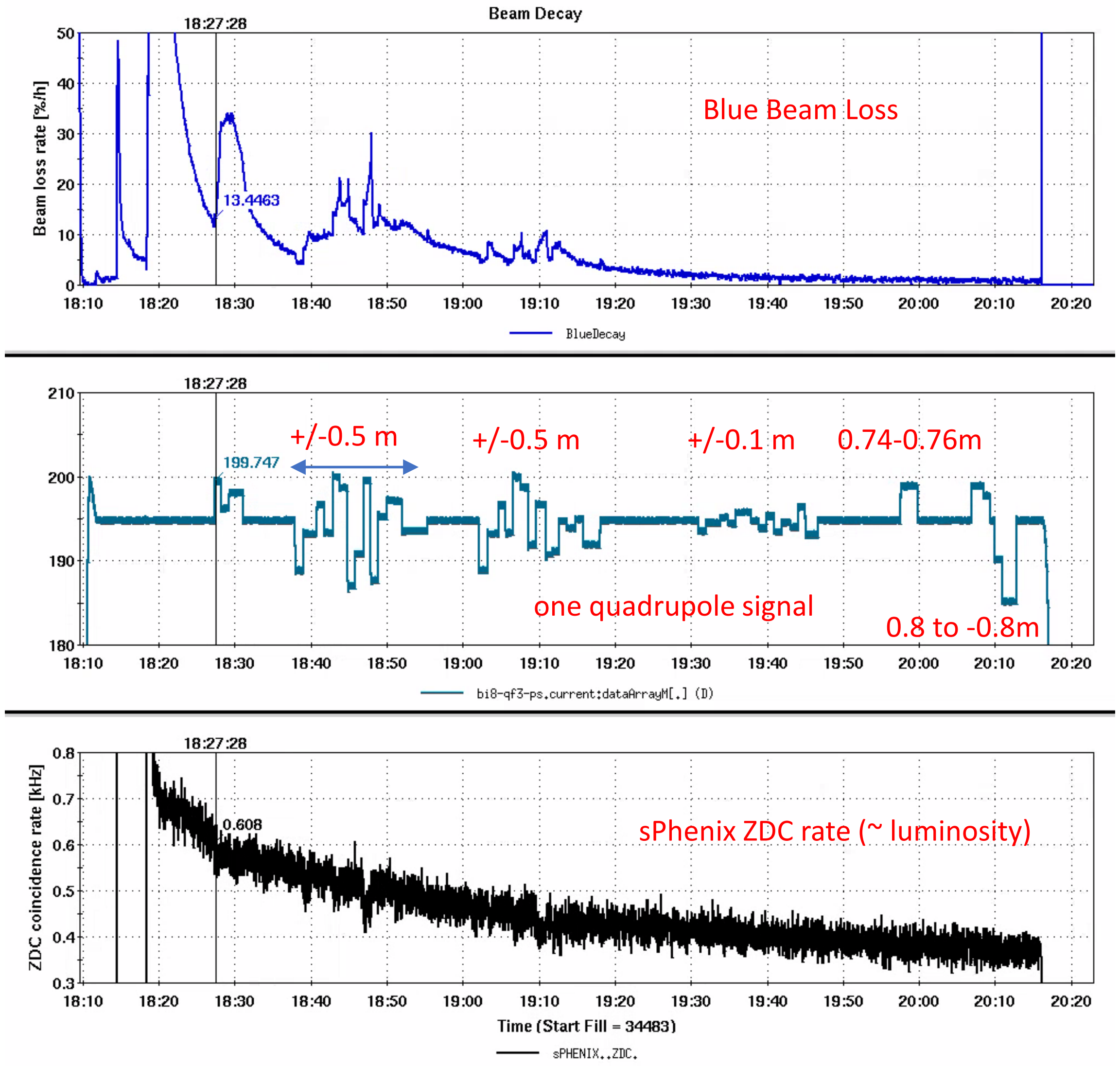


Brute Force Method
Pros:
-- direct acting on the targeting objective
Cons:
-- higher dimension
-- change global RHIC accelerator parameters

Model Based Method
Pros:
-- lower dimension
-- maintain global RHIC accelerator parameters
Cons:
-- potential mismatch between model prediction and real settings

First sPhenix ZDC Online Optimization Experiment

GPTune Used Signal

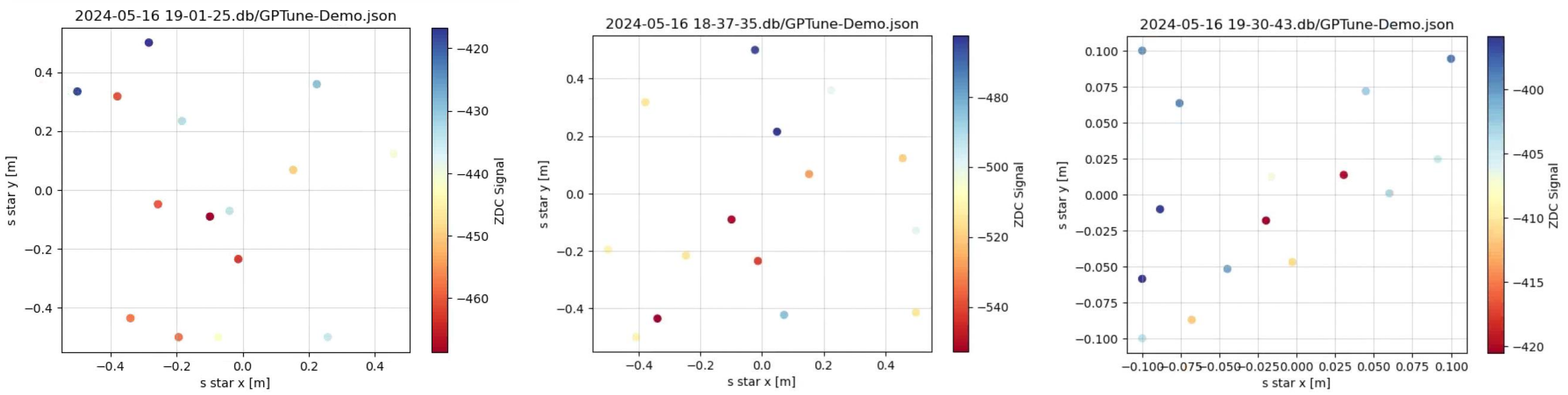


- S*: +/-0.5 m without decay compensation
- S*: +/-0.5 m; +/-0.1 m.
- S*(x plane): 0.74-0.76m; 0.8m->0.4m->0m->-0.4m->-0.8m.
- S* > 0.8 m, MADX didn't find solutions.

  - Beam loss is acceptable.
  - ZDC rate was changed. Didn't see any visible improvement with ± 10% pp noise.
  - With +/- 0.8m, it is expected 17% change for ZDC rate.
  - GPTune works with std ±10% (pp) noisy signals ±15%!

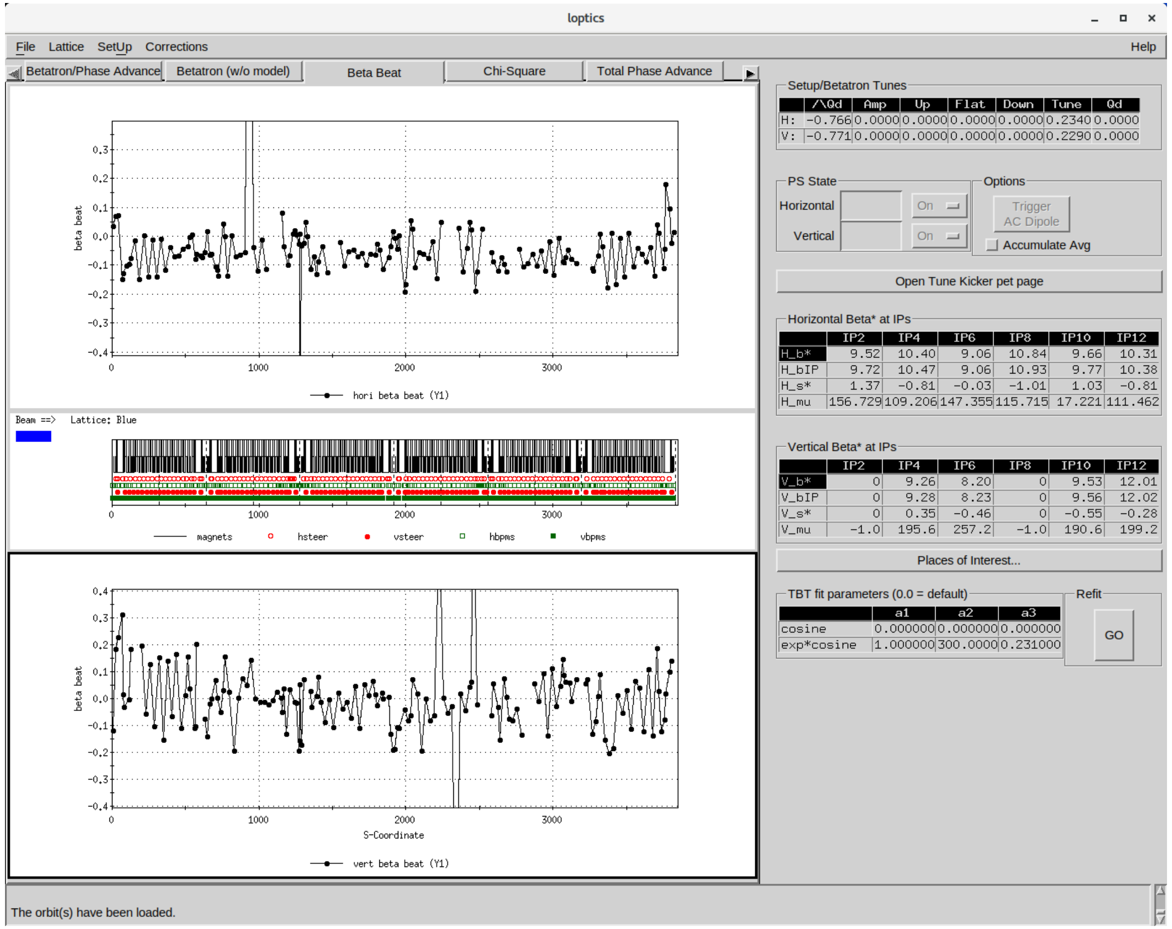
- Integrated GPTune optimization framework, control software and experimental measurement loop worked.
- Didn't observe significant luminosity signal (ZDC rate) improvement during optimization.

Analyzing First Online Optimization Experiment Shows Imperfection in S* setting



- Three sets of experiment show some correlation between zero s* values and higher (red) zdc rate (proportional to luminosity), but with significant spreads.
- **Imperfection in setting s* is too large to optimize luminosity in 10% level.**
- Need to improve the control of s* for the next luminosity optimization experiment.

Experimental Measurements Show Measured S* Different from Intended S*



Base line measurement: s*x = -0.81m, s*y = 0.28m

Intend to move s*x -> 0.5 m: s*x = -1.30m, s*y = -0.48

Intend to move s*x -> -0.5m: s*x = -1.09m, s*y = -0.40

Intend back to base line1: s*x = -1.62m, s*y = -0.28m

Intend back to base line2: s*x = -0.89m, s*y = -0.20m

- Significant differences observed between the expected settings and the real measured settings.

Improvement in Optics Control @ IP

We have to improve the optics control to make optics measurement and tuning reproducible.

Tuning:

- Use traditional model match show large discrepancy.
- We developed tuning strategy using optics response matrix (from model)

Optics $\Delta O = B\Delta I$ Current

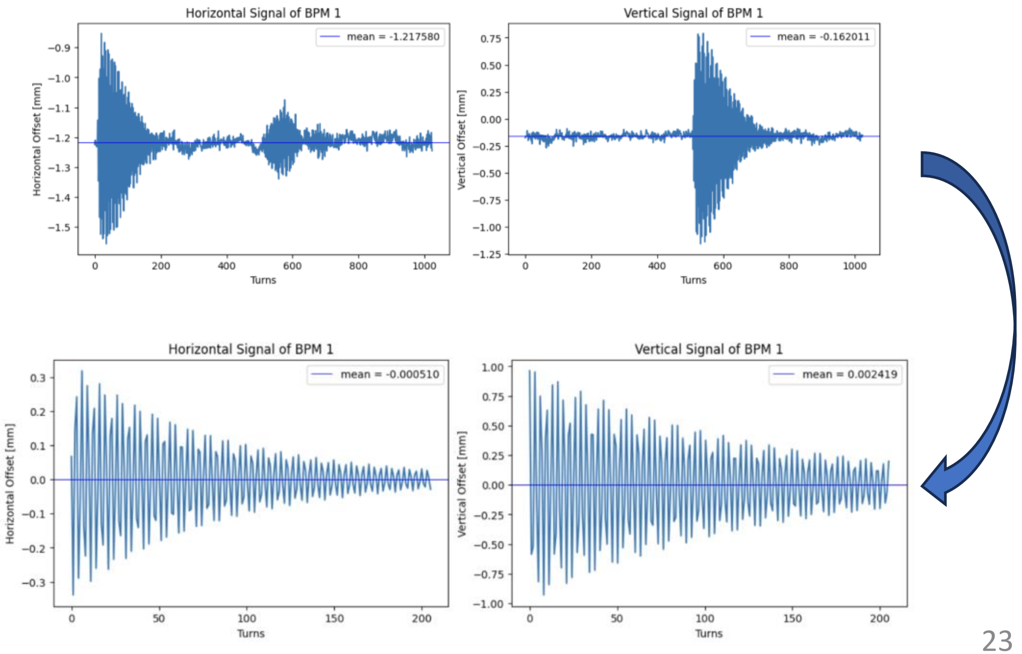
Response

$$\Delta I = B^{-1}\Delta O - \mathrm{null}(B)C$$

- Adjust C to satisfy current limits.

Measurement:

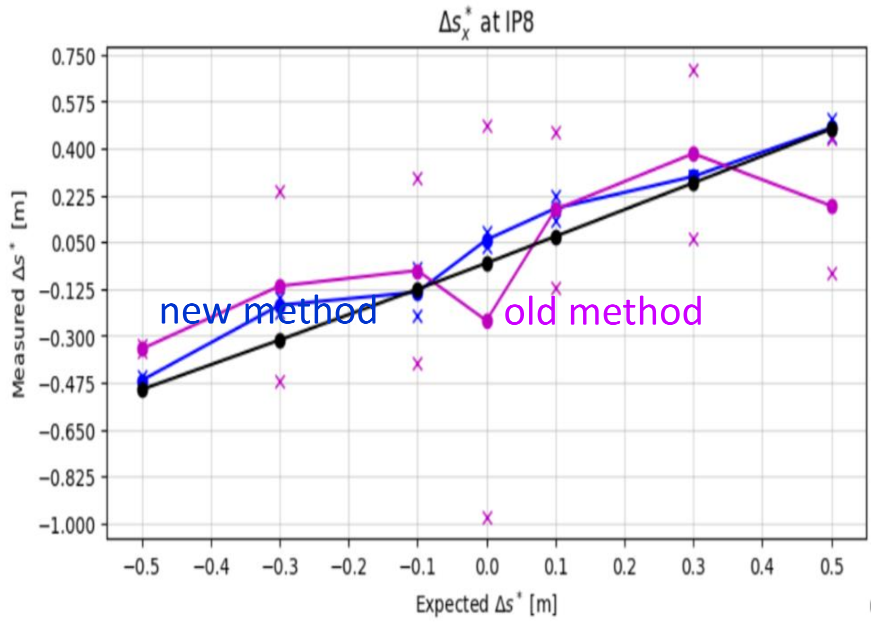
- We took advantage of the correlations of BPMs to reduce the noise in data using Dynamic Mode Decomposition.

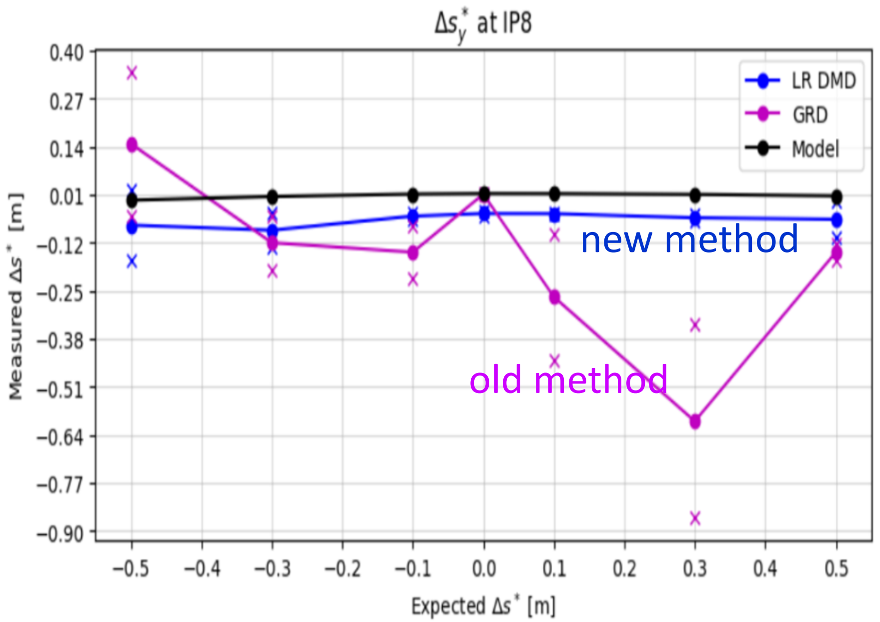


Experimental Test the Improved Optics Control

Resulting change in s^*_x

- 12 Datasets: Δs^*_x = [-.5, -.3, -.1, 0, .1, .3, .5]m
- Want relative data to follow trend: only IP8 horizontal should change
- WF_New and GRD_Old method able to keep trend on average everywhere
- Able to show on **average that Δs^*_x increases while Δs^*_y** is fairly constant (**blue vs black**)
- WF_New method **has less spread**:
  - Preprocessing
  - Linear optimization method may seem sufficient for [-.5, .5]m





- New method shows good tracking with model prediction

Global Accelerator Parameters Stay Reasonable during the Experimental Test

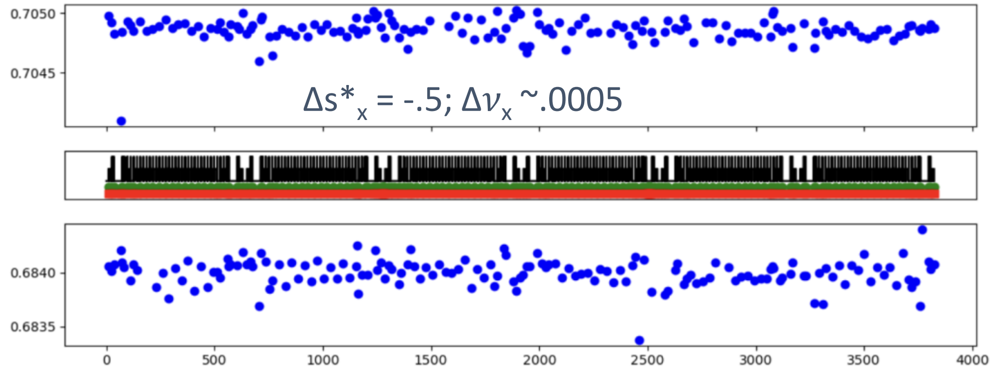
Tune Variation (one constraint)

- Larger tune spread is seen as Δs^*_x increases.
- This tune variation is reasonable even with significant s* variation.
- This small tune variation can be compensated with feedback control.

Model:

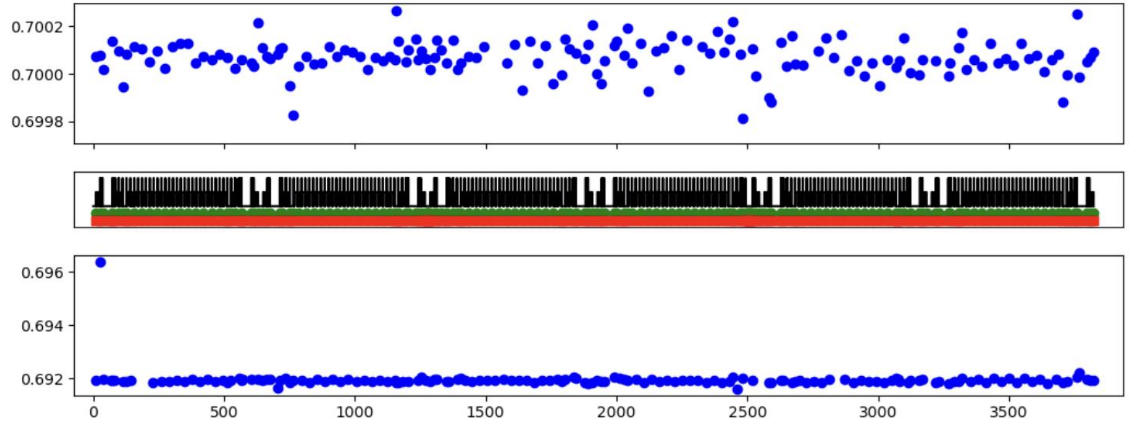
```
ssx = -0.5
horizontal tune before: 0.6934846999999991
horizontal tune after: 0.6985311500000009
Difference: 0.005046450000001812

Vertical tune before: 0.6904881299999985
Vertical tune after: 0.6852685899999997
Difference: -0.005219539999998801
```

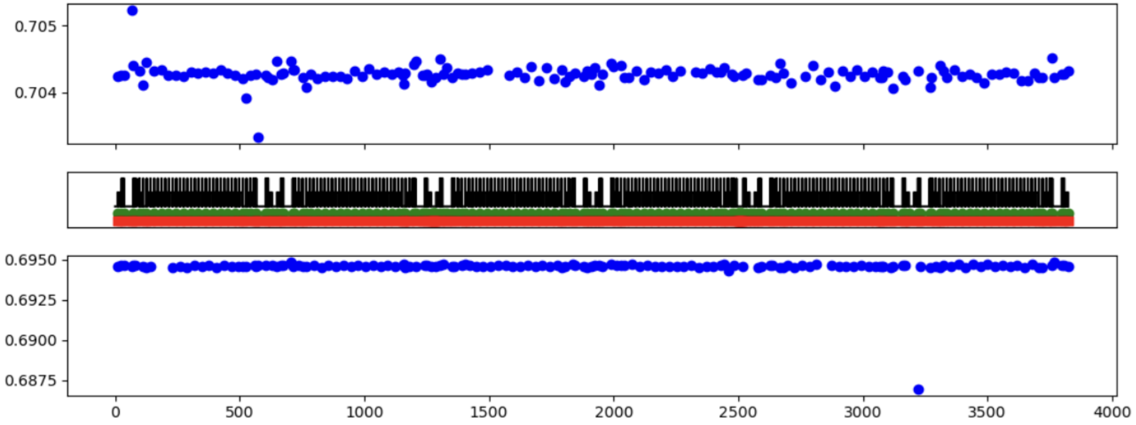


$\Delta s^*_x = -.5$; $\Delta \nu_x$ ~.0005

$\Delta s^*_x = 0$; $\Delta \nu_x$ ~.0002



$\Delta s^*_x = .5$; $\Delta \nu_x$ ~.005



Summary

- **Demonstrated consistent control in changing Δs^*_x between [-.5, .5]m with minimum variation in Δs^*_y**
  - While minimizing beta beat and variation in beta around the ring

- The maximum variation in the tune was still large (~0.01), when changing Δs^*_x =.5m
  - Although this is not a big issue without collision, we need to turn on tune feedback in later experiments

- Able to fit and retrieve s* and beta* with reasonable uncertainty

- Future Experiments:
  - Change Δs^* in both directions
  - On-line Bayesian optimization to maximize luminosity using s* as knobs

The new optics tuning method has important applications in the EIC operation due to x10 reduction of vertical beta function at IP!

Major Deliverables and Schedule

Year 1:

- ✓ Q1: Develop data manipulation package that can be used to extract and label data from RHIC measurements, and to interface with the simulation packages; Build an analytical luminosity model from integration, including the hourglass effect, crossing angle and IP optics.

- ✓ Q2: Modify the existing beam-beam simulation code to include the requirements of sPHENIX; Interlink the analytical model with RHIC optics model and the GPTune framework.

- ✓ Q3: Connect the GPTune to the simulation tools; Test the beam in RHIC for luminosity optimization using GPTune (without sPHINEX detector knobs).

- ✓ Q4: Analyze the initial experimental data and benchmark the analytical model; Build models and control knobs to maximize the performance of RHIC, especially the sPHENIX experiment**;** Explore new prior functions and kernel functions in the GPTune based on the physics knowledge.

Major Future Deliverables and Schedule

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- ✓ Q3: Update the optics tuning model with the experimental data, improve the tuning strategy; Apply to RHIC measurement data to test the model using RHIC's accelerator physics experiment (APEX) time.

Q4: Continue to apply optimization to the RHIC measurement control knobs using RHIC 's accelerator physics experiment (APEX) time; Test beam with updated optimization strategy and further improve sPHINEX performance.

Summary of expenditures by fiscal year (FY):

	FY22 ($k)	FY23 ($k)	Totals ($k)
a) Funds allocated	490	490	980
b) Actual costs to date	490	305	795

Thank You!