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

Ji Qiang

Nuclear Physics Accelerator R&D, PI Exchange Meeting
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Project members:

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

Outline:

1) Introduction

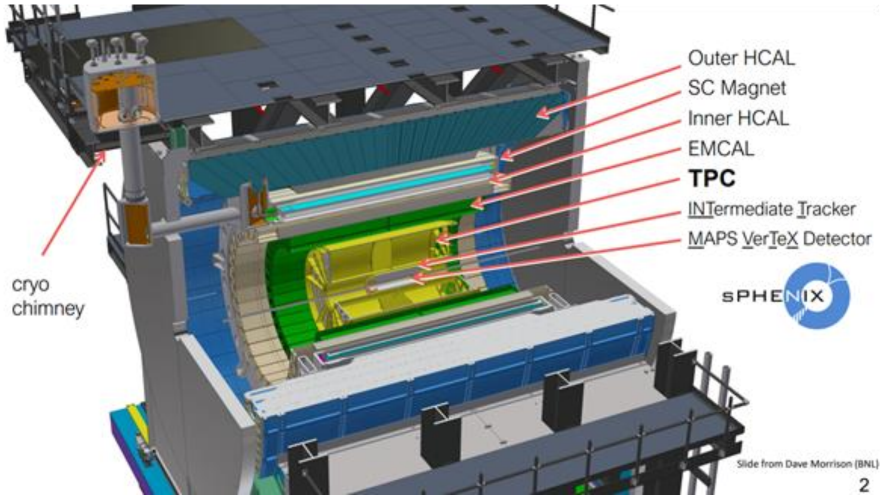
2) Current project status

3) Future work

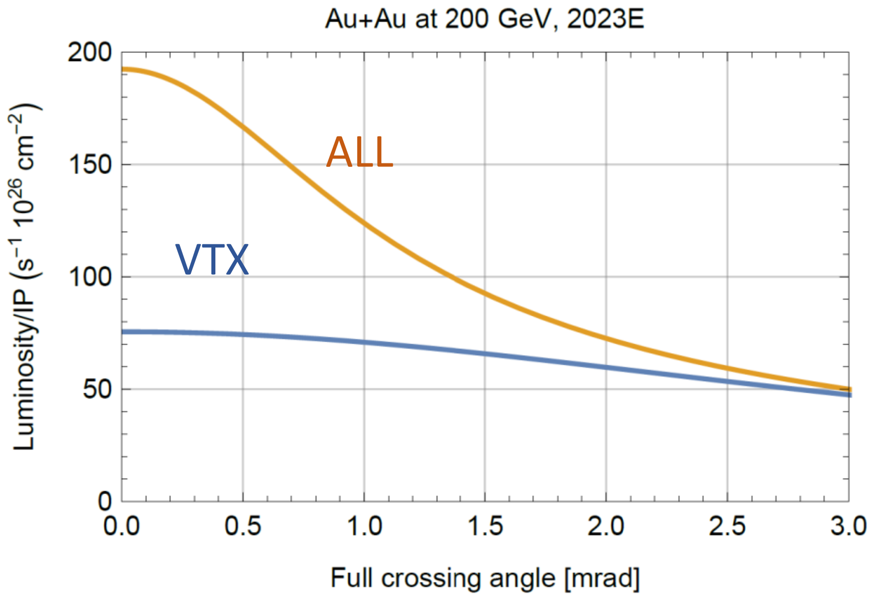
4) Summary of expenditures

Luminosity Optimization Needed at the New RHIC Jet Detector

- New jet detector sPHENIX is being commissioned in 2023.
- 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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Year 2:
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.

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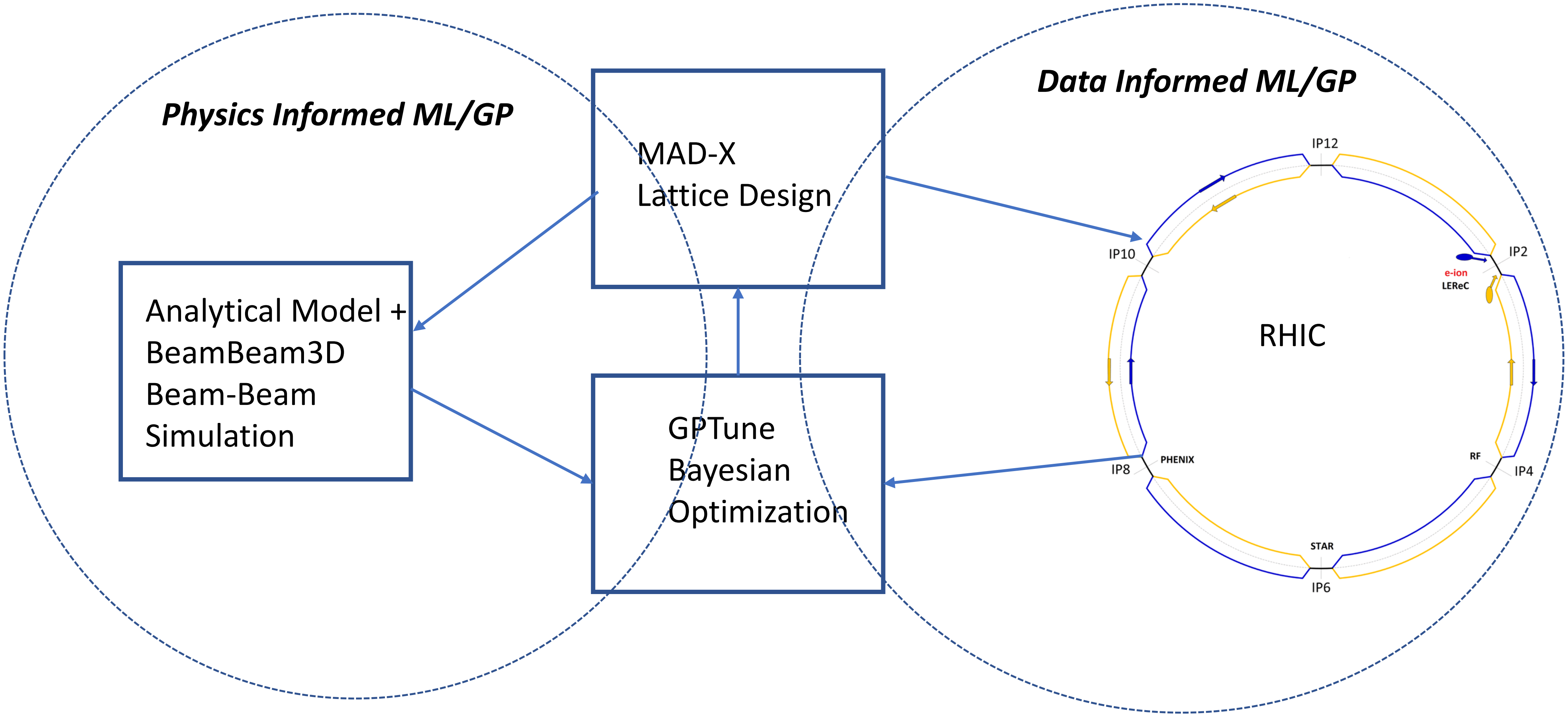
Q3: Update the optics tuning model with the experimental data, improve the tuning strategy; Apply to RHIC measurement data to test the model using RHIC's accelerator physics experiment (APEX) time.

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.

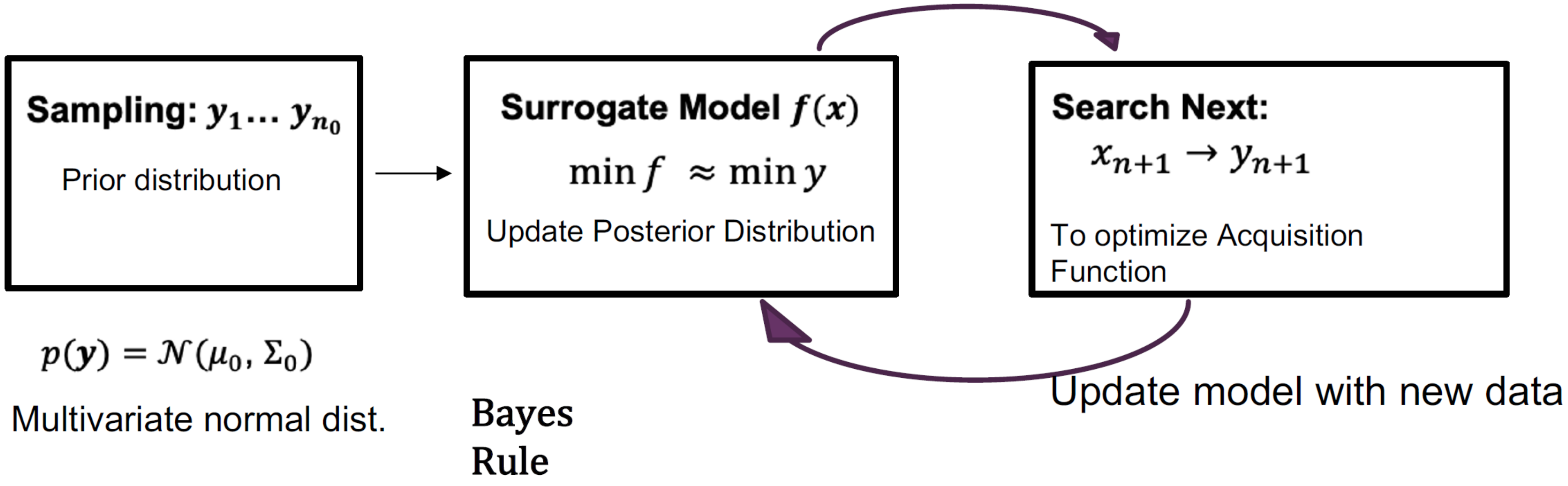
Advanced Modeling Framework for RHIC Lum. Optimization



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

Bayesian Optimization

- 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



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

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

Gaussian Process:

- 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: $K_{\mathrm{Matern}}(x, x') = \frac{2^{1-\nu}}{\Gamma(\nu)}\left(\frac{\sqrt{2\nu}|d|}{\ell}\right)^{\nu} K_\nu\left(\frac{\sqrt{2\nu}|d|}{\ell}\right)$

Search Phase

- Where to place the new point(s)?
- Given a new sample point, need quickly update the model

Search for a point to maximize Acquisition Function

(… another optimization problem, but easier)

- Balance between exploitation and exploration
  - **Exploitation**: local search within promising regions
  - **Exploration**: global search of new regions with more uncertainty
- **Expected Improvement (EI)** – most commonly used AF.

  For a proposed point x_i^*, expected difference from current best is

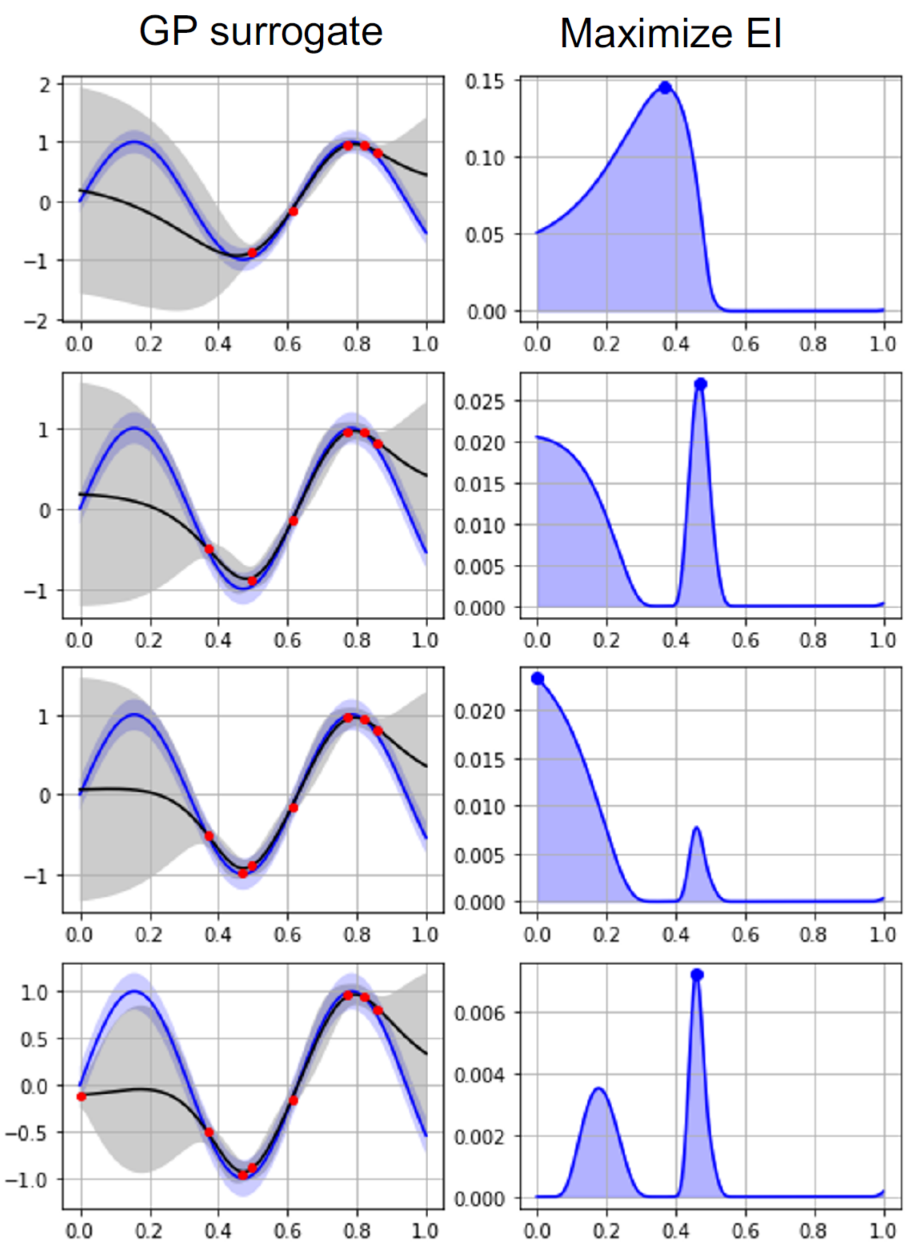
$$\Delta(x_i^*) = \mu_i^* - y_i^{min}$$

$$EI(x_i^*) = \mathbb{E}\left[\left[y_i^* - y_i^{min} \right]^+ \right] = \sigma_i^* \varphi\left(\frac{\Delta(x_i^*)}{\sigma_i^*}\right) + |\Delta(x_i^*)| \Phi\left(\frac{\Delta(x_i^*)}{\sigma_i^*}\right)$$

  - $\varphi(.)$: probability density function
  - $\Phi(.)$: cumulative distribution function

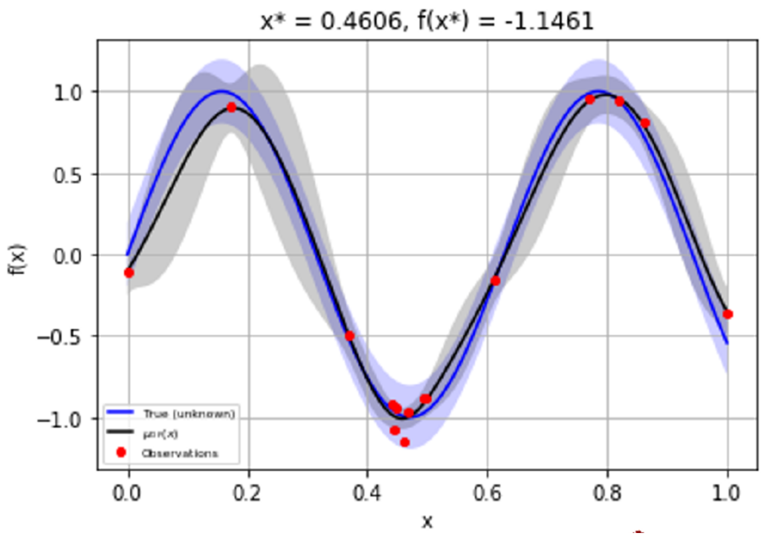
(Jones et al. 1998)

1D Example:



5 initial samples
4 additional steps

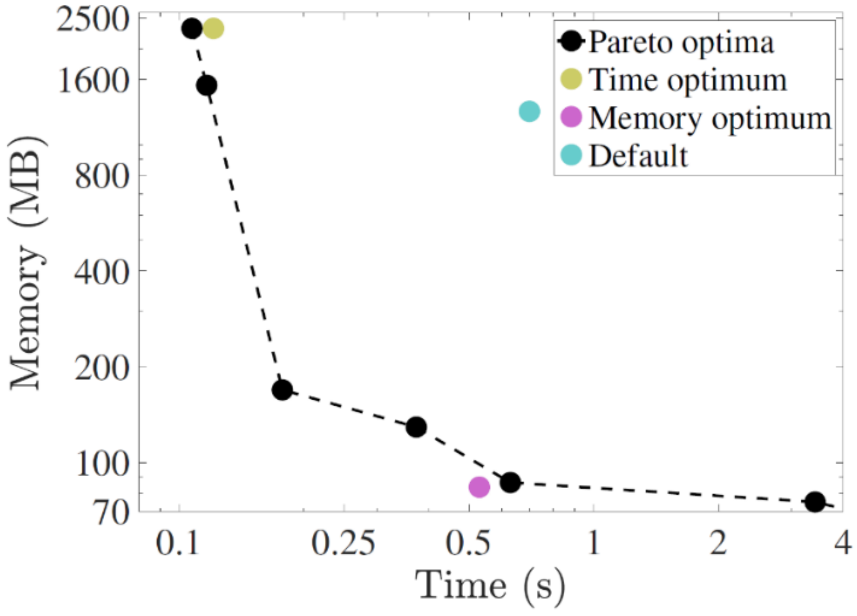
- Blue line: true function
- Red dots: function evaluations
- Black line: mean function of the fitted surrogate model
- Grey shaded area is 95% confidence interval



Bayesian Optimization Software Package: GPTune

Some features of GPTune include:

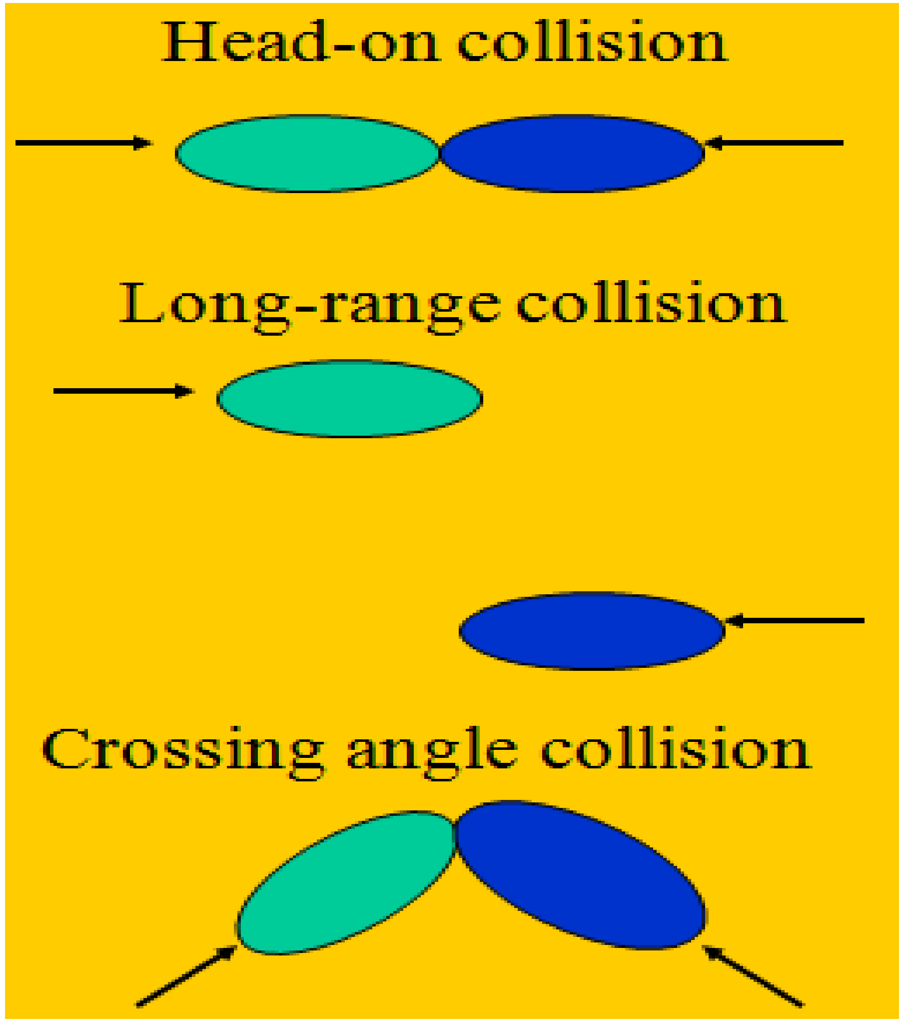
(1) relies on dynamic process management for running applications with varying core counts and GPUs
(2) can incorporate coarse performance models to improve the surrogate model
(3) allows multi-objective tuning such as tuning a hybrid of computation, memory and communication
(4) allows multi-fidelity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



Application:
Conduct parameter optimization for several HPC codes. The most notable result is for the multiscale production-level full-blown simulation codes, M3D-C1 and NIMROD that are used in the fusion Tokamak design.

https://github.com/mkturkcan/GPTune
https://nimrodteam.org/meetings/team_mtg_5_21/nimrod_meeting_YangLiu.pdf

BeamBeam3D: A Parallel Colliding Beam Simulation Code



Some key features of the BeamBeam3D

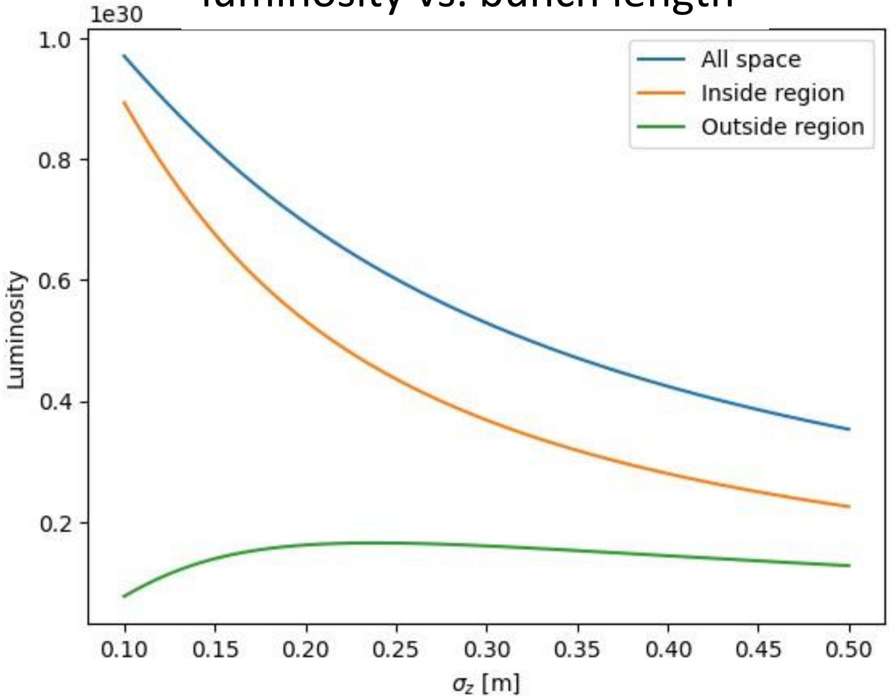
- Multiple-slice model for finite bunch length
- New algorithm -- shifted Green function -- efficiently models long-range collisions
- Parallel particle-field based decomposition to achieve perfect load balance
- Lorentz boost to handle crossing angle
- Arbitrary closed-orbit separation
- Multiple bunches,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

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

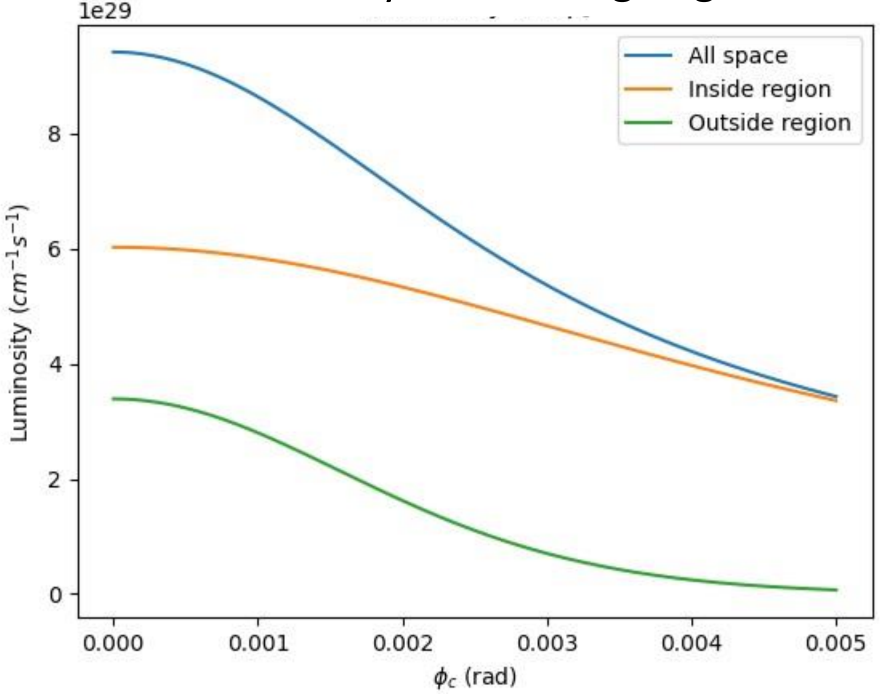
Analytical Model of Luminosity with Crossing Angle Collision

$$L = \cos^2(\frac{\phi}{2}) f N_1 N_2 \int_{-D}^{D} \frac{ds}{4\pi^{3/2}\sigma_x^2\sigma_y\sigma_z\sqrt{\frac{\cos^2(\frac{\phi}{2})}{\sigma_x^2} + \frac{\sin^2(\frac{\phi}{2})}{\sigma_z^2}}} \exp(-s^2(\frac{\sin^2(\frac{\phi}{2})}{\sigma_x^2} + \frac{\cos^2(\frac{\phi}{2})}{\sigma_z^2}))$$

luminosity vs. bunch length

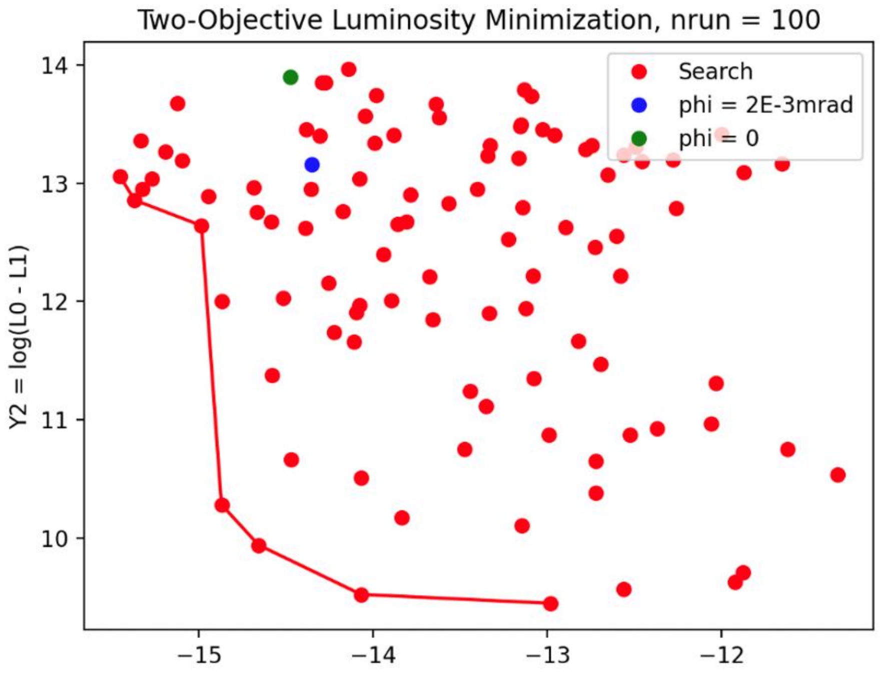


luminosity vs. crossing angle



Test of the GPTune Optimization Software with the Analytical Model

$\beta_{x,y}$ and σ_z	$[0.1, 1]$m
ϕ	[0,5] mrad



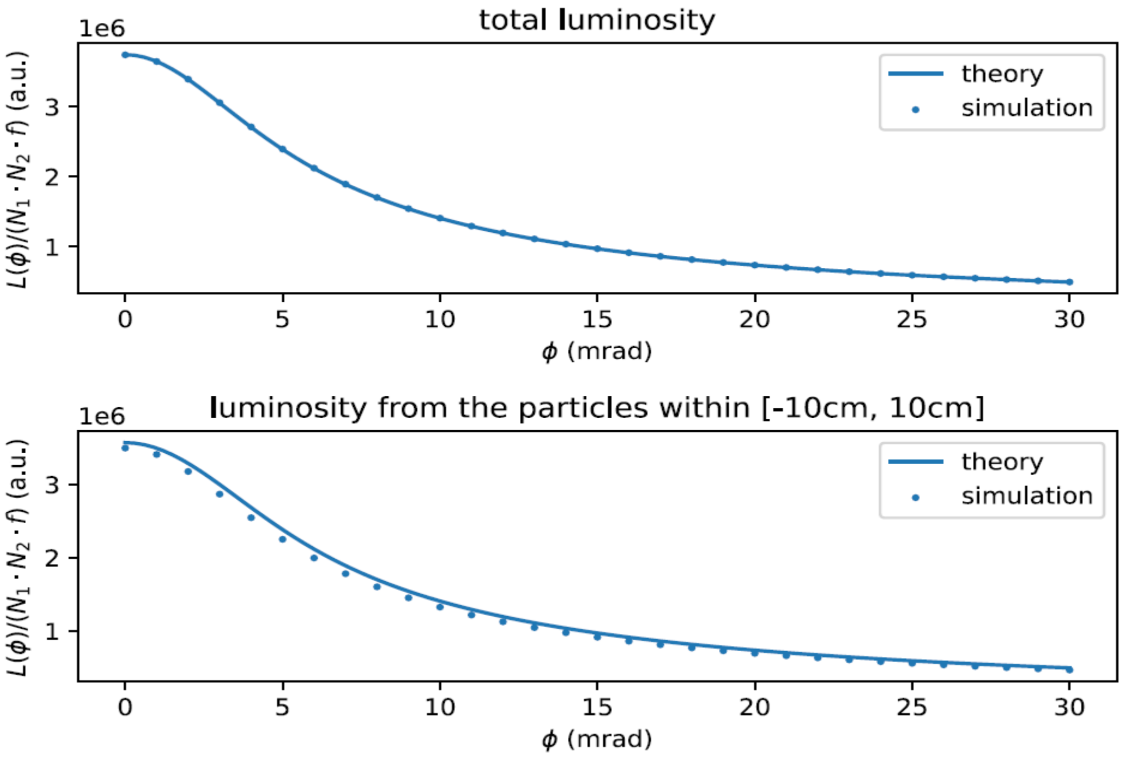
background

$Y_1 = -log(L_1)$

Vertex signal

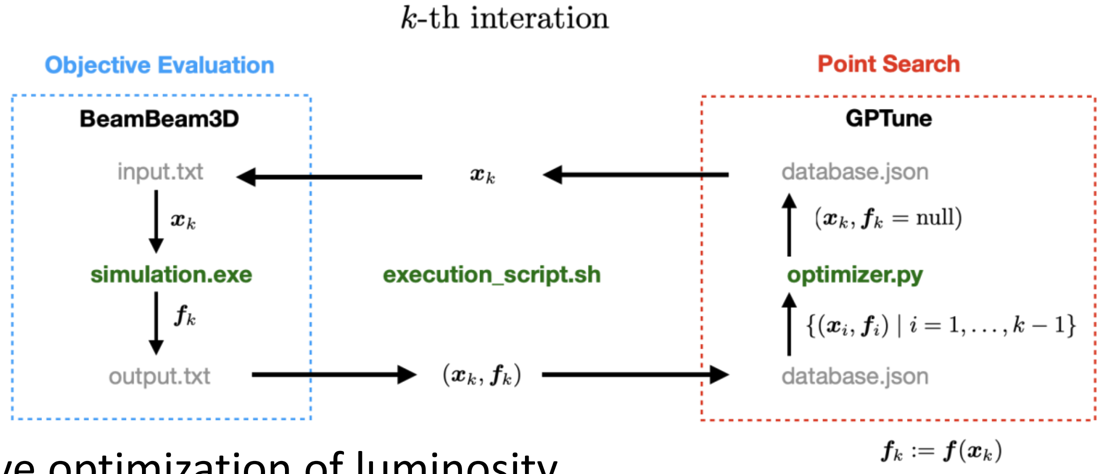
First Principle Numerical Model Is Needed to Include Nonlinear Effects

- Analytical model doesn't include nonlinear effects such as amplitude dependent tune modulation.
- In this project, we have modified the BeamBeam3D to include those nonlinear effects.
- Excellent agreement between the numerical simulation and the analytical model is attained for a simple example.

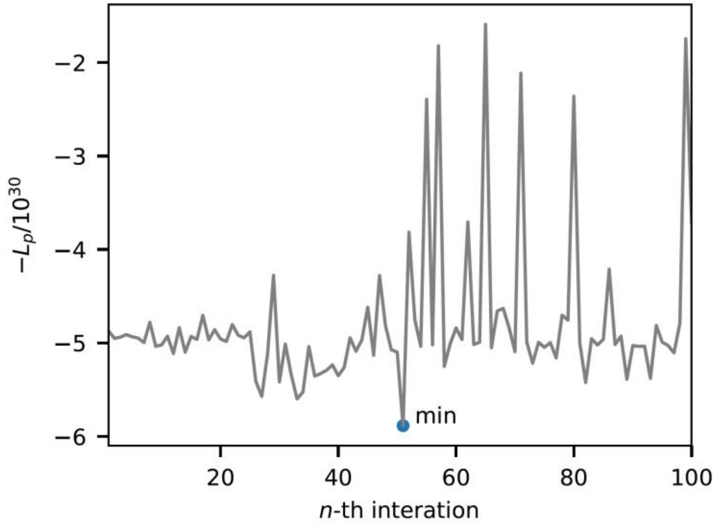


Test of GPTune Optimization Software with Numerical Simulation

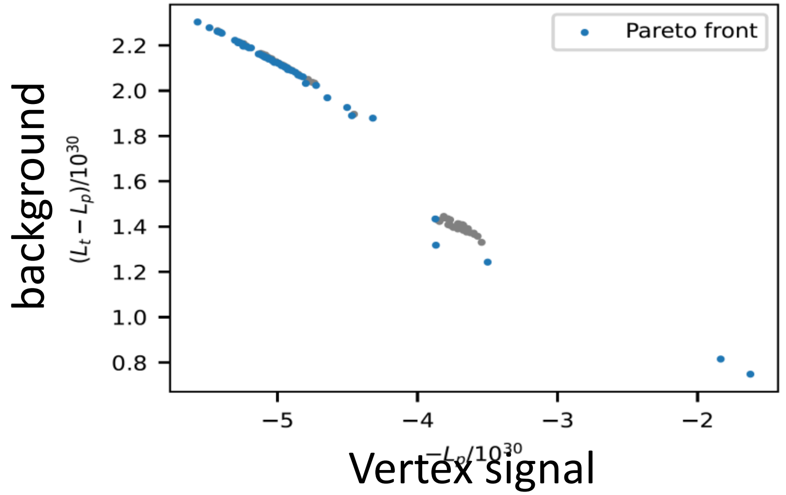
$$\min_{\boldsymbol{x} \in X} \boldsymbol{f}(\boldsymbol{x}) \qquad \boldsymbol{f} : \mathbb{R}^n \to \mathbb{R}^m \ \text{objective function} \qquad X \subseteq \mathbb{R}^n \ \text{feasible set}$$



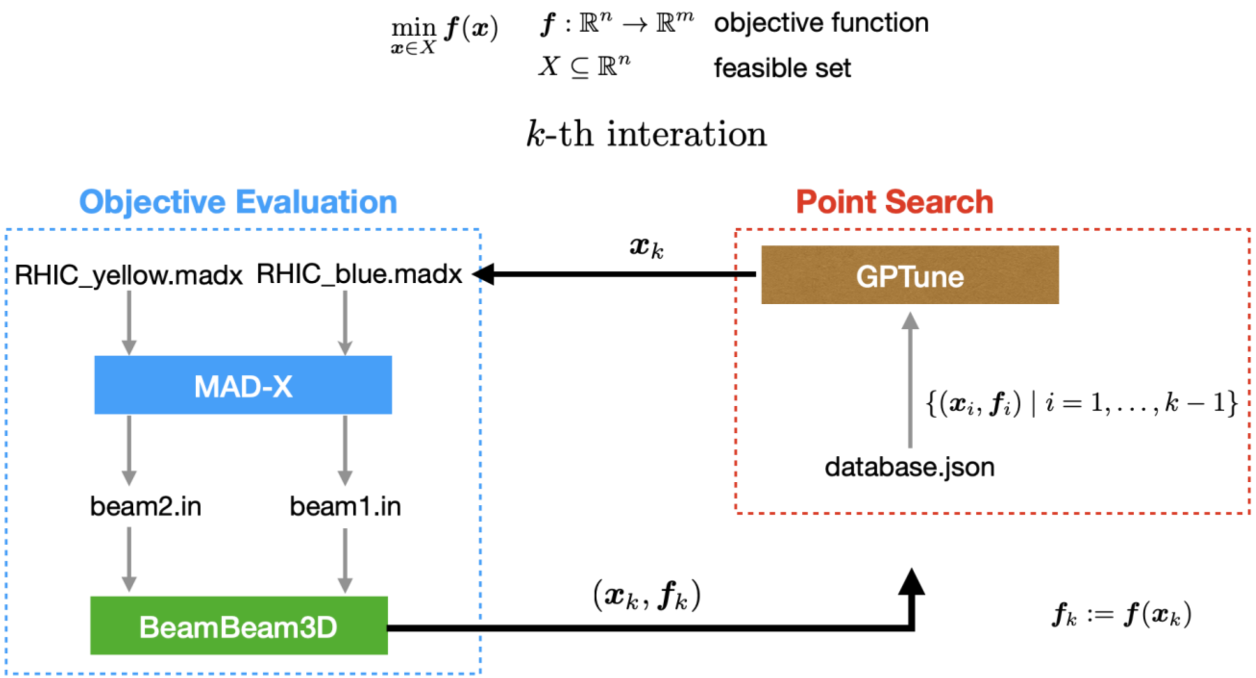
single objective optimization of luminosity

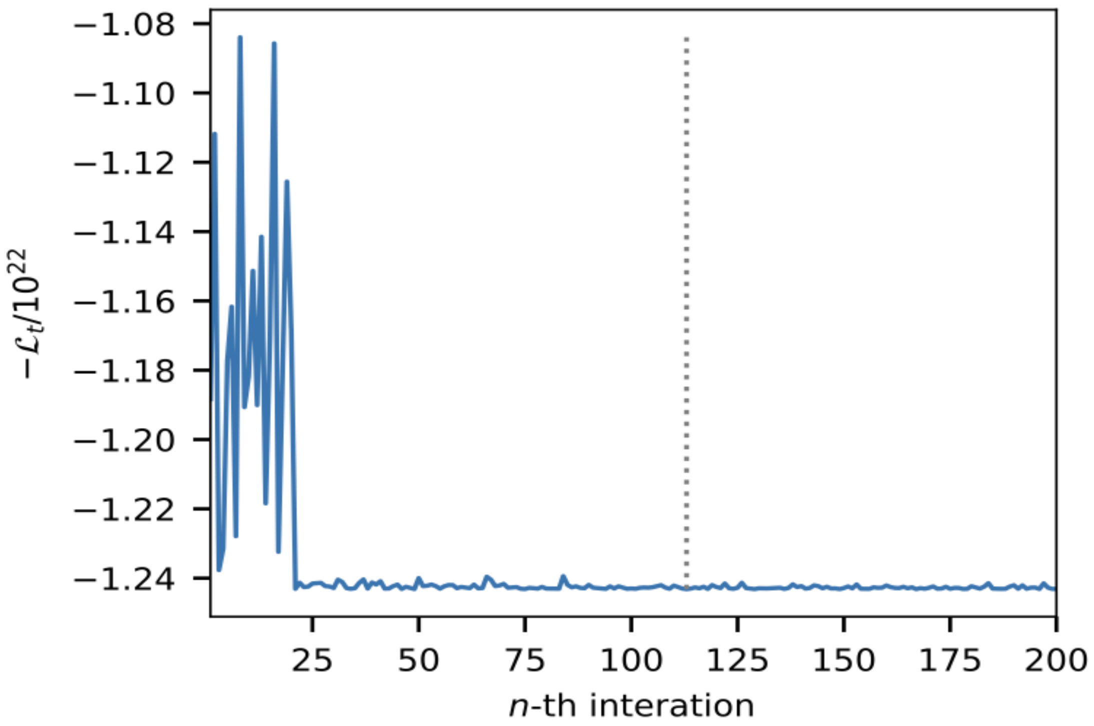


multiple objective optimization of signal and background



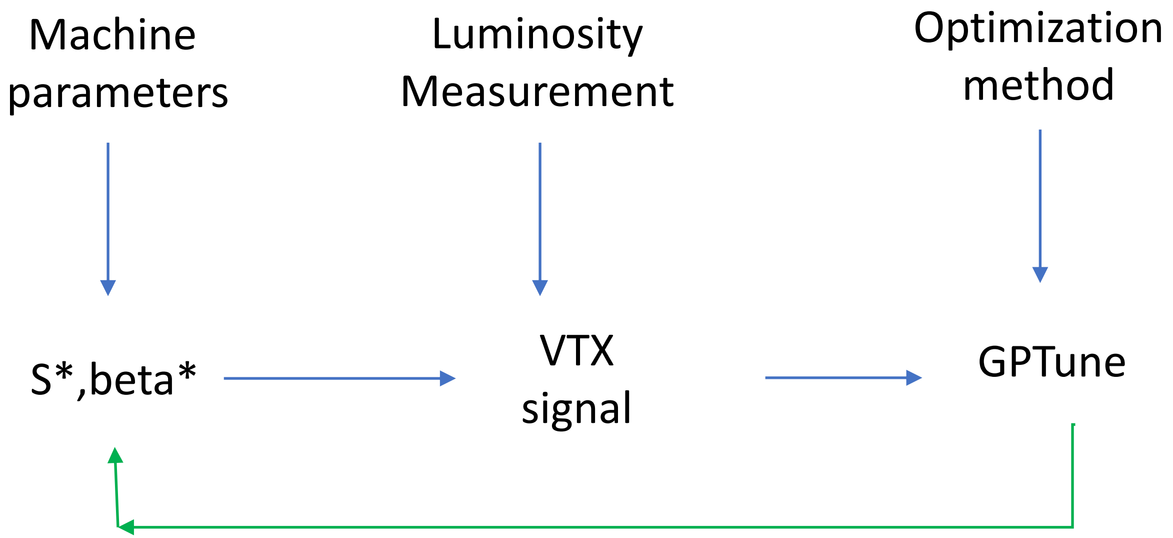
Bayesian Optimization of RHIC Luminosity with Numerical Simulation





- The optimization of the lattice setting with respect to the luminosity is performed for the head-on collision of two Au-Au beams in the Relativistic Heavy Ion Collider (RHIC). The parameters of the lattice setting with only two variables ΔS_x and ΔS_y.
- The value of the objective function converges when more optimization steps are executed. This implies the value of the objective function is minimized and hence the total luminosity L_t is maximized.

Integration of GPTune with Control Scripts for Online Luminosity Optimization



S* and beta* changing scripts: ready for testing:

1. change the target s*, beta* within 'deltas.dat' file;
2. run 'madx job.madx_Au16-e0::store' command, will get 'IP8knob.dat' file;
3. run 'CreateSend.IP8' command, will get 'SendTrim.IP8' file;
4. run 'SendTrim.IP8' command.

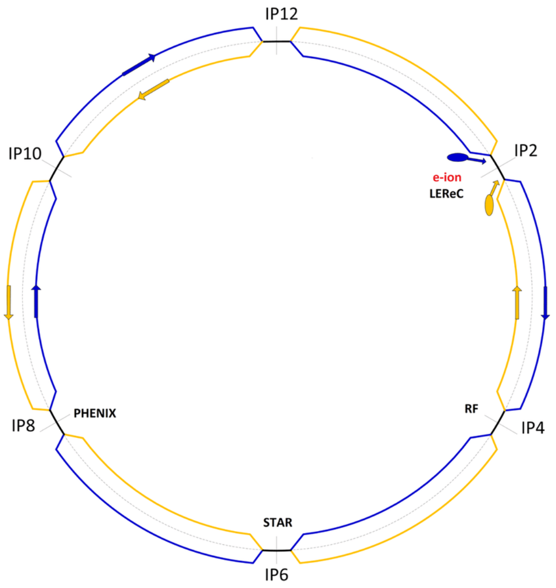
Vertex (VTX): contacted with sPHINEX colleagues:

1. Did it with PHENIX before
2. Send the vertex data in several ways.

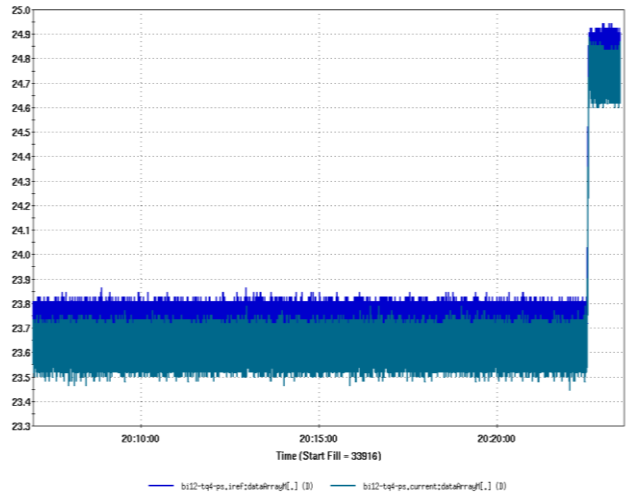
GPTune is ready for testing with scripts:

1. Installed and tested
2. Did optimization with EBIS beam line and attained some good results

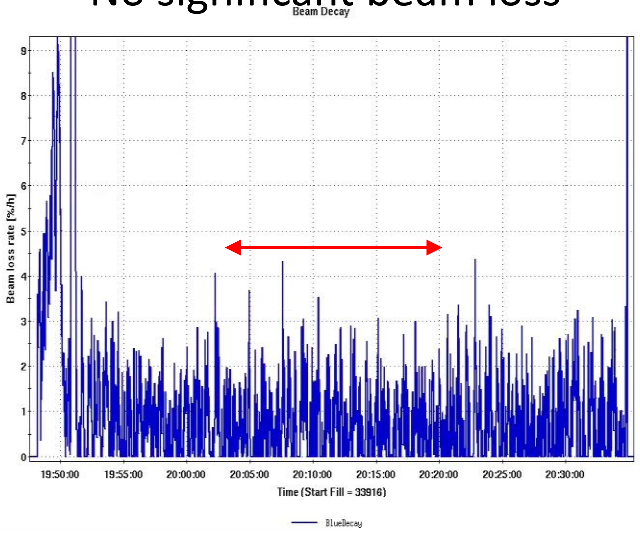
APEX Test of s* Online Control Script at IR12



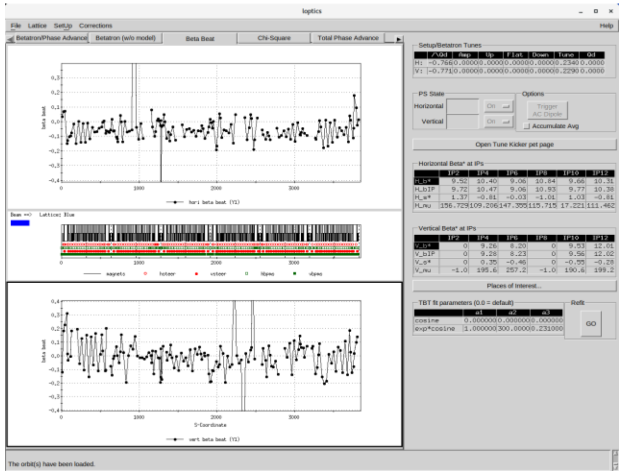
electric current for s* control



No significant beam loss



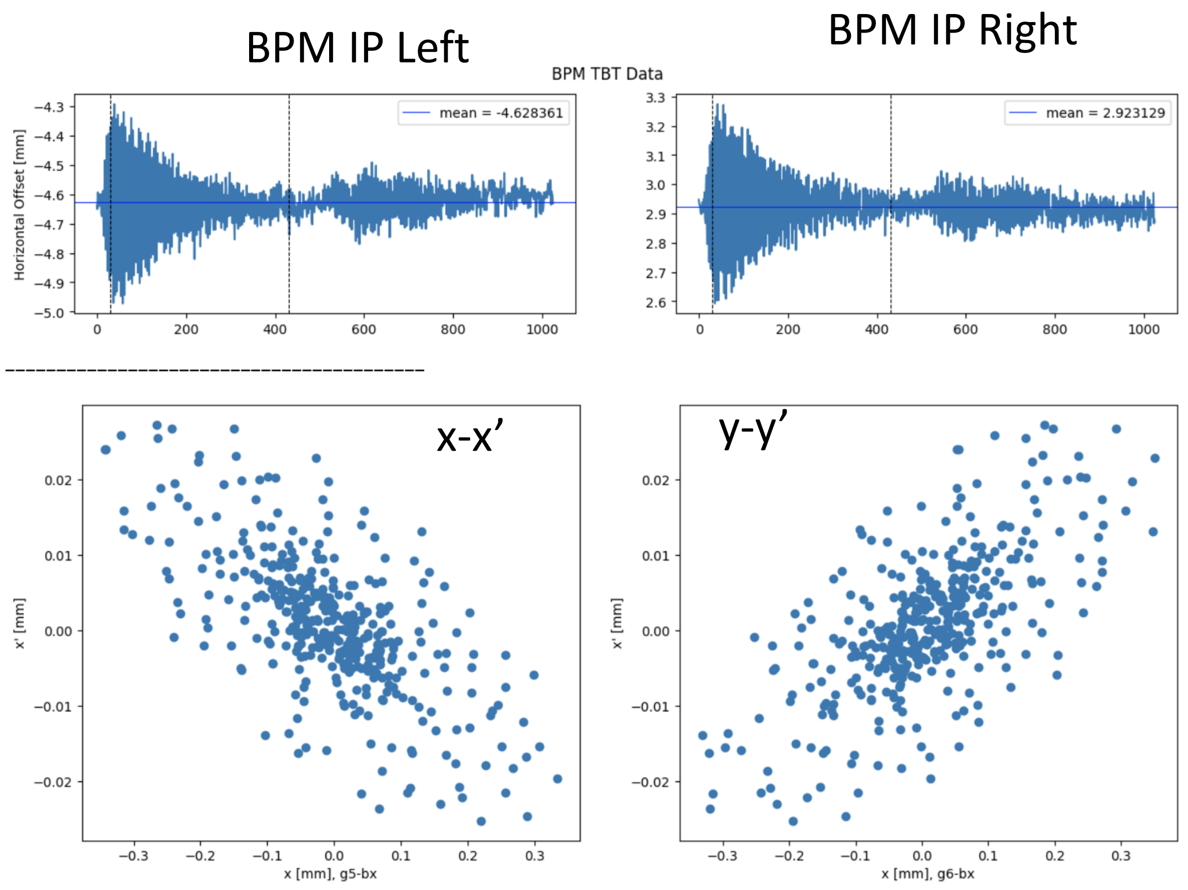
S* measurement



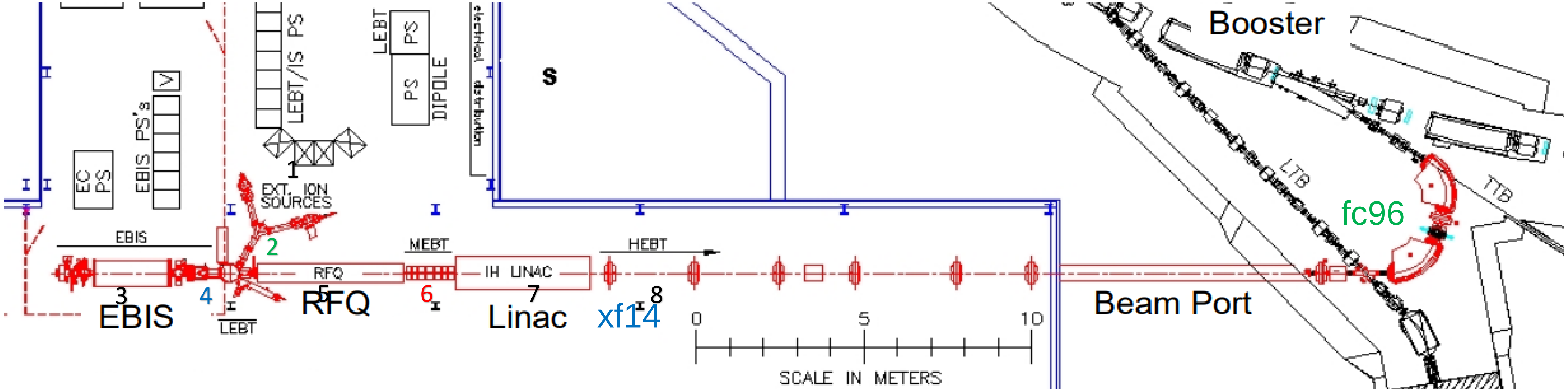
- Successfully test the s* script at store (IR12).
- No additional significant beam loss during +/- 0.5 m s* change.
- Will explore a large safety range next time at IR12 without separation bump.
- Offline data analysis: MADX (online) model vs. machine measurements.

Offline Data Analysis:

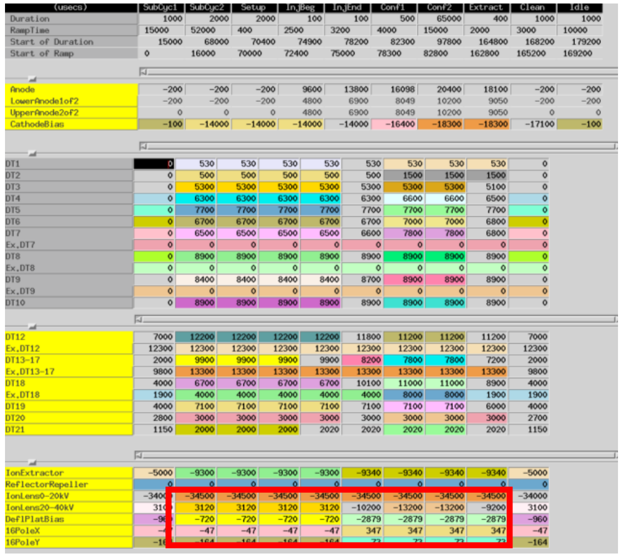
- Model dependent method (used in RHIC measurement):
  - BPM amplitudes are fit to the RHIC lattice model, ~ 15% beta beat.
  - Get IP lattice and convert to β^* and s^*.
- Model independent approach (excluding effects outside IR):
  - Every IP have BPM on each side, i.e. drift space between them.
  - Phase space can be retrieved directly
  - β^* and s^* calculated similarly
  - Accuracy limited by BPM noise and machine decoherence.
- Developing pseudo-knob for changing s^* for next experiment

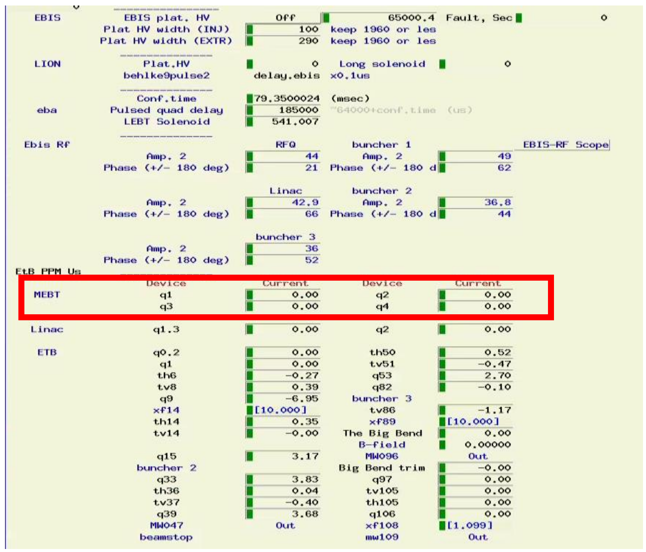


Test of GPTune for EBIS Intensity Optimization



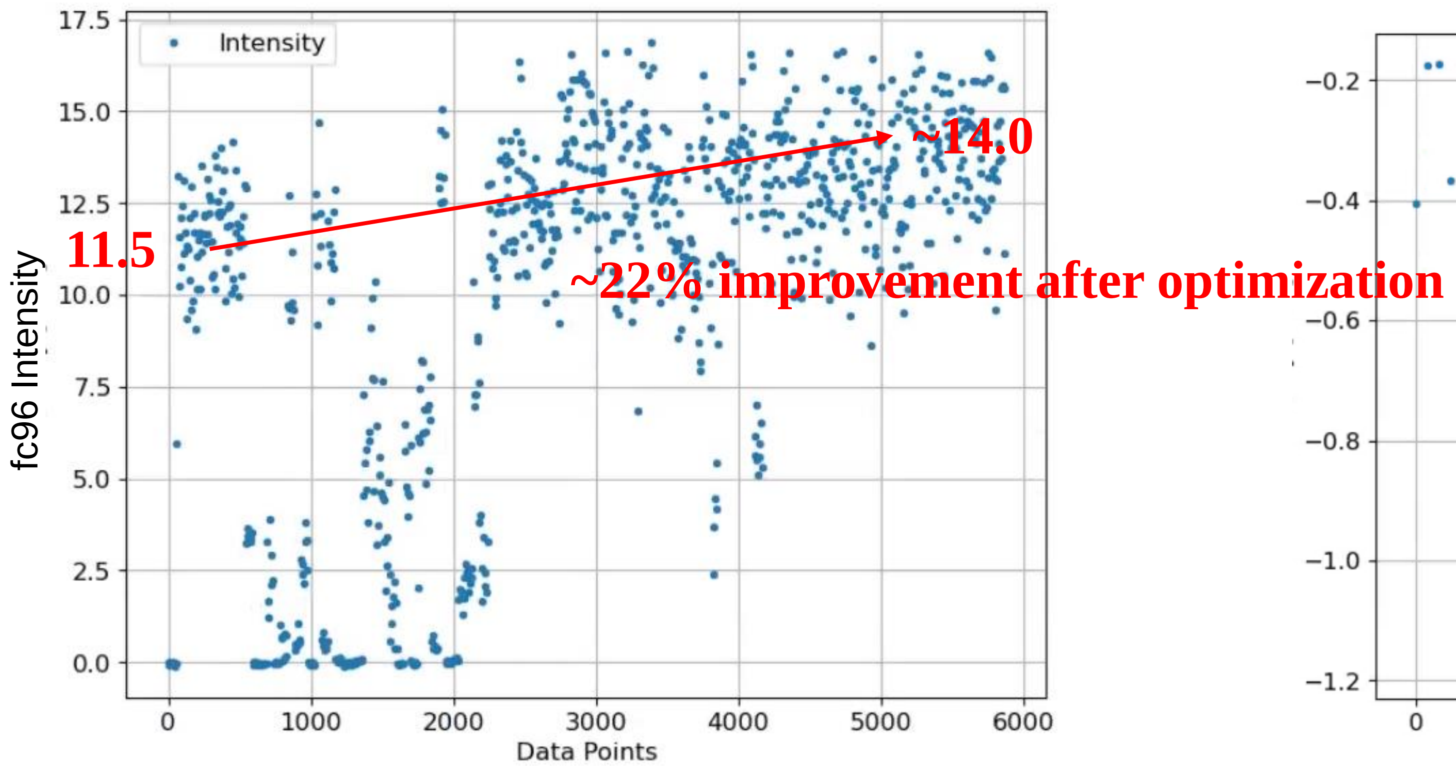
1. LION
2. EBIS Injection Line (fc96)
3. EBIS
4. EBIS Extraction line (xf14)
5. RFQ
6. MEBT
7. Linac
8. HEBT

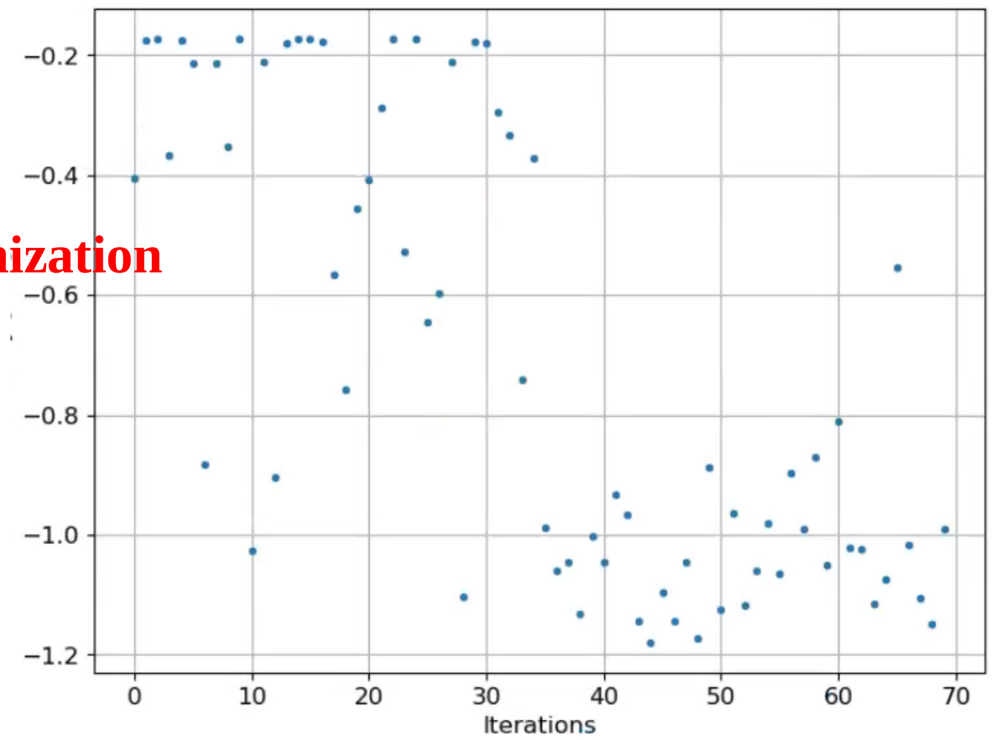




Acknowledge Robert-Demolaize, Takeshi Kanesue, Masahiro Okamura, John Morris's help in the RHIC experiments.

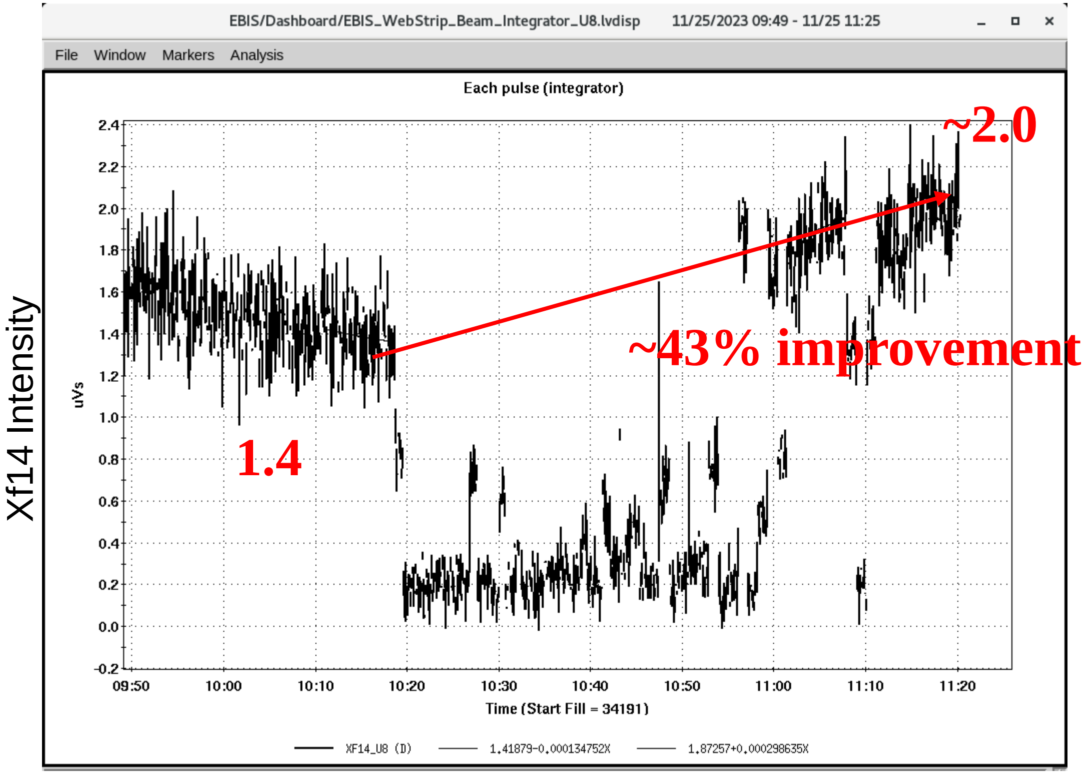
EBIS Injection Online Optimization with 9 Control Knobs

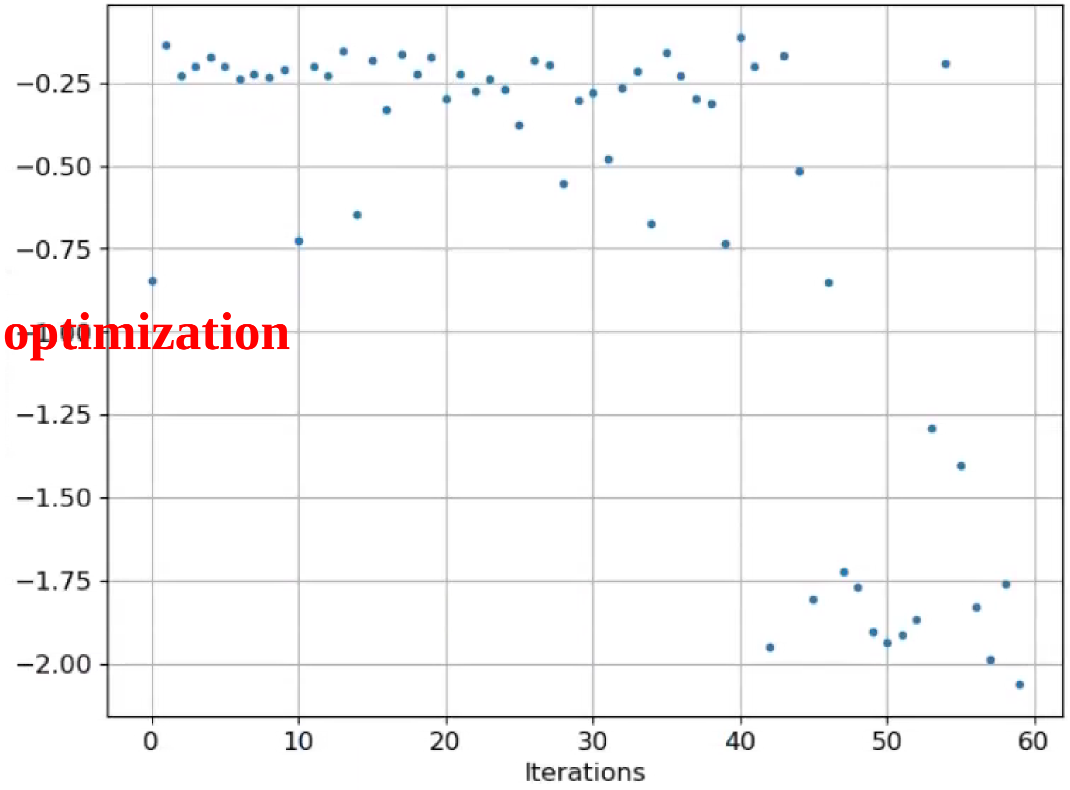




- script ran from 12:33 to 13:36 (~63 min)
- 1 beam / supercycle [6.6 s]; it takes 2 supercycles for the powers settle down;4 supercycles for measurement.
- fc96 measurement was used for injection optimization
- 9 control parameters after 70 iterations

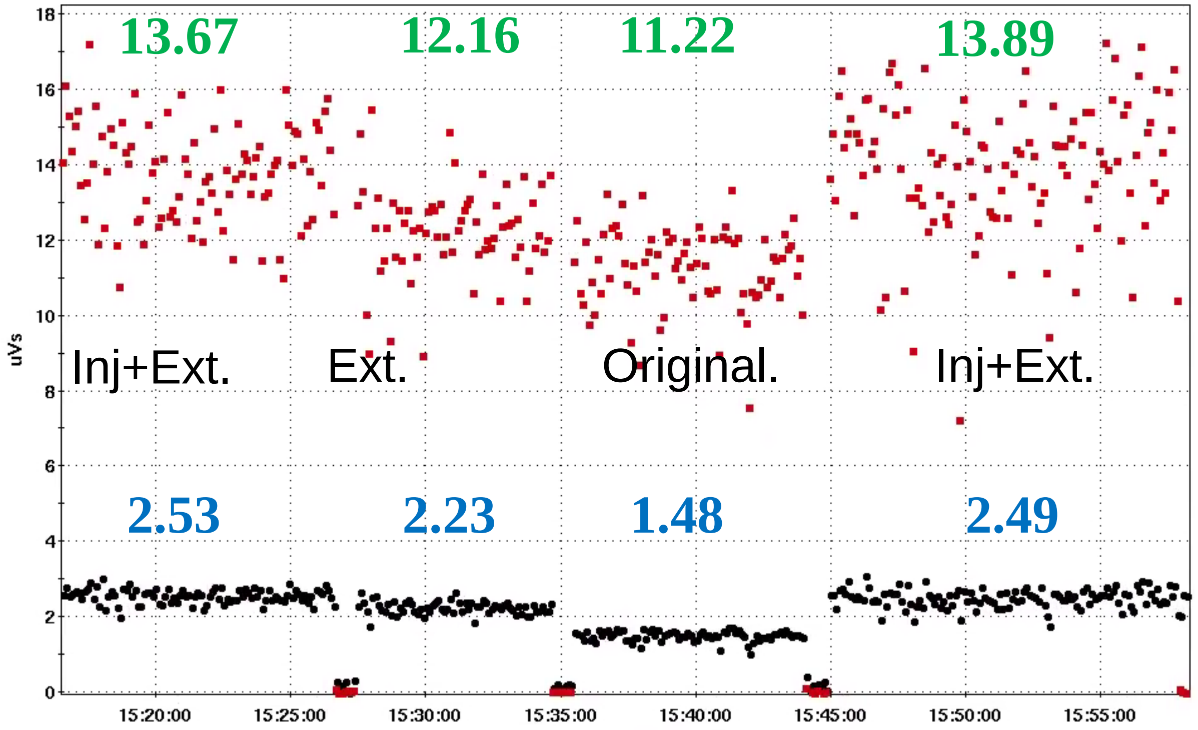
EBIS Extraction Online Optimization with 10 Knobs



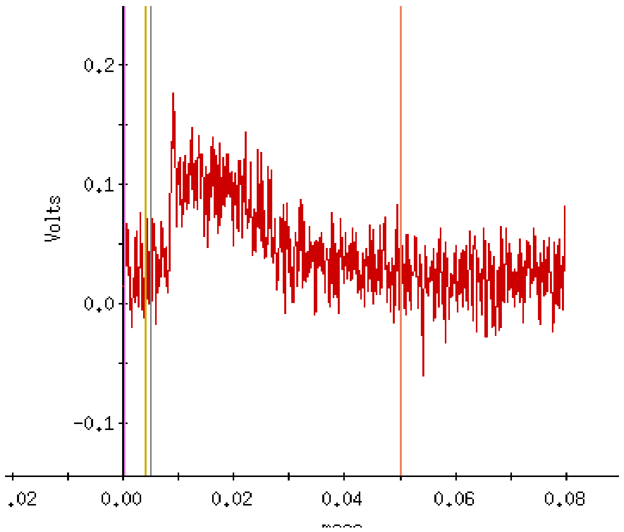


- script ran from 10:18 to 11:15 (~57 min)
- 2 beam / supercycle [6.6 s].
- xf14 measurement was used for extraction optimization.
- 10 control parameters after 60 iterations

Online Optimization Improves EBIS Performance



GPTune works with these noisy signals!



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%

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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			349

Thank You!