ISBN: 978-3-95450-247-9 ISSN: 2673-5490 doi: 10.18429/JACoW-IPAC2024-THPC72

ADVANCED MODELING AND OPTIMIZATION OF NUCLEAR PHYSICS COLLIDERS*

Y.-K. Kan, X. Li, Y. Liu, J. Qiang†, Lawrence Berkeley National Laboratory, Berkeley, CA, USA
X. Gu, Brookhaven National Laboratory, Upton, NY, USA
W. Fung, Y. Hao, Michigan State University, East Lansing, MI, USA

Abstract

High energy colliders provide a critical tool in nuclear physics study by probing the fundamental structure and dynamics of matter. Optimizing the collider's machine parameters is both computationally and experimentally expensive. A fast and robust optimization framework that includes both beam-beam and the detailed machine lattice will be crucial to attaining the best performance of the collider. In this paper, we report on the development of an integrated framework that includes an advanced Bayesian optimization software GPTune, a self-consistent beam-beam simulation code BeamBeam3D, and the detailed lattice model from MAD-X. Application results to the RHIC facility optimization are also presented.

INTRODUCTION

The high energy collider, Relativistic Heavy Ion Collider (RHIC) is a critical device in the study of quak-gluon plasma in nuclear physics. To maximize the potential of scientific discovery, it is important to optimize the parameters of the collider to attain higher luminosity. Increasing luminosity has many limiting factors from the beam dynamics point of view. Among them, the beam-beam effect, the electromagnetic interactions from the opposing beams, has been a strong limitation for most colliders, due to its nonlinear nature. Depending on the distinctive feature of the detector, the total luminosity may not be the only parameter indicating the performance of the collider. As prioritized in the 2015 NSAC Long Range Plan (LRP) [1], a state-of-art jet detector, named 'sPHENIX' [2], was commissioned at IR8 of RHIC, and started taking physics data in 2023. The acceptance of sPHENIX demands the collision point located at a longitudinal window $|s| < 0.1$m from the interaction point (IP), which imposes additional challenges in tuning and optimizing the performance of RHIC. In this paper, we report on progress of developing an integrated computational framework and application of this framework to RHIC optimization. A schematic plot of this framework is shown in Fig. 1. It consists of two optimization workflow circles: the left circle includes the Bayesian optimization software GPTune [3], the accelerator lattice optics program, MAD-X [4], and the analytical and beam-beam simulation tools. The right circle contains the RHIC collider, and the optimization software and the lattice program. The left circle optimizes the RHIC luminosity based on simulations. The right circle optimizes

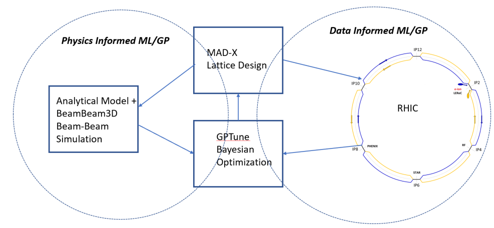

Figure 1: Schematic plot of the computational framework for a nuclear physics collider (RHIC) luminosity optimization.

the RHIC luminosity based on experimental measurements. The left circle can generate sufficient amount of data to train parameters inside the optimizer. The trained optimizer will then be used for the right circle direct RHIC luminosity. The left circle provides a transfer learning for the right circle and will improve the optimization convergence speed.

BEAM-BEAM SIMULATION TOOL

Besides the analytical model, we also used a self-consistent simulation code, BeamBeam3D [5, 6], based on the particle-in-cell method, that was developed in our previous studies to simulate the beam-beam effect. This code includes a self-consistent calculation of the electromagnetic forces (beam-beam forces) from two colliding beams (i.e. strong-strong modeling), linear and nonlinear transfer maps for beam transport between collision points, a stochastic map to treat radiation damping, quantum excitation, an arbitrary orbit separation model, and a single map to account for chromaticity effects. Here, the beam-beam forces are calculated by solving the Poisson equation using an FFT-based algorithm. The parallel implementation is done using a particle-field decomposition method to achieve a good load balance. It has been applied to studies of the beam-beam effect at several colliders [7–9].

BAYESIAN OPTIMIZATION

Bayesian optimization (BO) is an attractive machine learning technique particularly well-suited for optimization for an expensive "black-box" function with limited function evaluation points. In the context of this study, the black-box function can be either a simulation code or an experiment from an accelerator operation. Through the Bayesian approach, we can obtain a fast machine learning surrogate model, as well as the uncertainty of the model's prediction. Bayesian optimization employs the Bayes Theorem of setting a prior over the objective function and combining it with evidence to get a posterior function [10]. A popular surrogate model

* Work supported by the U.S. DOE under Contract No. DE-AC02-05CH11231.
† jqiang@lbl.gov

ISBN: 978-3-95450-247-9 ISSN: 2673-5490 doi: 10.18429/JACoW-IPAC2024-THPC72

for Bayesian optimization is Gaussian Processes (GP), a non-parametric stochastic model of distribution over functions. GP takes the set of input values t, and their function values $F(t)$ (from analytical model, simulation, or measurement) and assumes they are sampled from a Gaussian distribution with

$$F(t) \sim GP(\mu(t), \Sigma(t, t')) \tag{1}$$

in Eq. (1), where μ is the mean function and Σ is the kernel function, also known as covariance function, that characterizes the correlation as a function of the "similarity" between two samples. Then GP is used in the acquisition function to propose a new sampling point that is likely to yield improvement. The prediction from the acquisition function represents an automatic trade-off between exploration and exploitation. Popular acquisition functions include expected improvement (EI), maximum probability of improvement (MPI), and upper confidence bound (UCB) [11]. This optimization technique performs well with limited number of objective function evaluations. Moreover, it is likely to do well even in settings where the objective function has multiple local maxima and noise.

In this study, we employed a Bayesian optimization software called GPTune [3]. Several useful 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 optimization, (4) allows multi-fidelity tuning to better utilize the limited resource budget, and (5) supports checkpoints and reuse of historical performance database.

BAYESIAN OPTIMIZATION OF THE RHIC LUMINOSITY

In this study, we first developed a fast analytical model to calculate luminosity for optimization. Given the colliding bunch parameters, the luminosity L of two colliding bunches within a longitudinal window position [-D,D] can be written as:

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

in Eq. (2), where σ is the colliding beam RMS size in each direction, ϕ is half crossing angle of collision, N_1 and N_2 are bunch intensities of each colliding bunch, and f is the revolution frequency. Figure 2 shows the peak luminosity, the luminosity inside the window, and the luminosity outside the window as a function of bunch length and a function of crossing angle. It is seen that shorter bunch length leads to larger luminosity inside the window and smaller luminosity outside the window. A larger luminosity inside the window and a smaller luminosity outside the window help maximize signal to noise ratio in the application. From Fig. 2(bottom) it is seen that larger crossing angle results in larger ratio

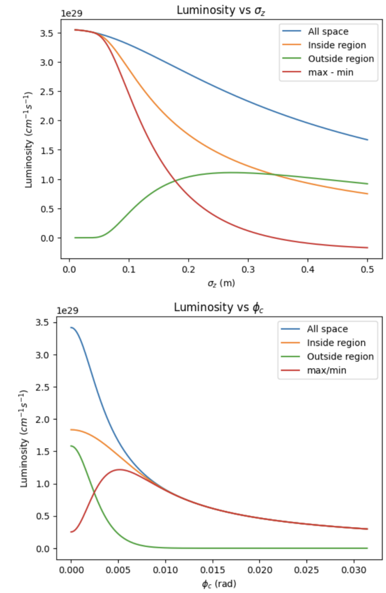

Figure 2: Peak luminosity as a function of bunch length (top) and of crossing angle (bottom) from the analytical model.

of luminosity inside the window to luminosity outside the window. However, this also results in smaller total peak luminosity. In the machine operation, it is desirable to maximize the luminosity inside the window and minimize the luminosity outside the window.

Figure 3 shows two-objective optimization of the luminosity inside the window (-log(L_1)) and the luminosity outside the window (log($L_0 - L_1$)) with respect to Twiss parameters β_x, β_y, bunch length σ_z, and the crossing angle. The non-dominated solutions are connected with a solid line. There exists a minimum (-log(L_1)) around -30, beyond which the outside window luminosity will increase rapidly.

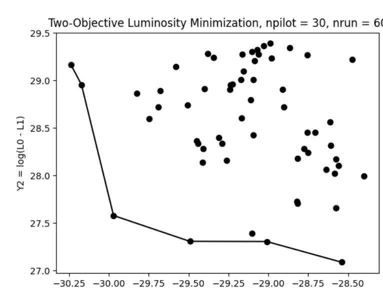

Figure 3: Two-objective luminosity optimization using the analytical model and the GPT tune optimizer.

Besides the analytical model, we also developed a numerical model based on BeamBeam3D to calculate the luminosity. The numerical model can include linear chromaticity and amplitude dependent tune modulation in the simulation. It accounts for the dynamic beta effect during the collision. Figure 4 shows the luminosity as a function of crossing angle from the above analytical model and from the BeamBeam3D

ISBN: 978-3-95450-247-9 ISSN: 2673-5490 doi: 10.18429/JACoW-IPAC2024-THPC72

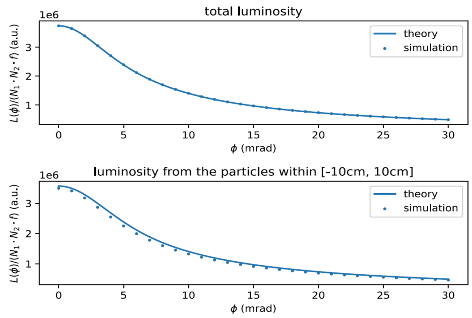

Figure 4: Total luminosity as function of crossing angle from the analytical model and from the simulation (top) and the window luminosity from the analytical model and from the simulation (bottom).

numerical simulation. Both models agree with each other very well in these cases.

Figure 5 shows a flow diagram of the integration of the lattice optics program MAD-X, the beam-beam simulation code BeamBeam3D, and the Bayesian optimization software GPTune. Here, the predicted control parameters from the

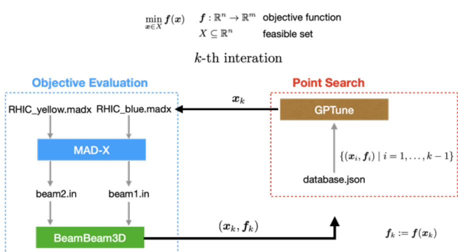

Figure 5: Flow diagram of the integration of the optics calculation, luminosity simulation, and the Bayesian optimization framework (GPTune).

GPTune Bayesian optimization are passed to the MAD-X optics program to calculate corresponding parameters used in the BeamBeam3D code. The BeamBeam3D then calculates luminosity and passes it to the GPTune for further luminosity optimization. Figure 6 shows that the negative

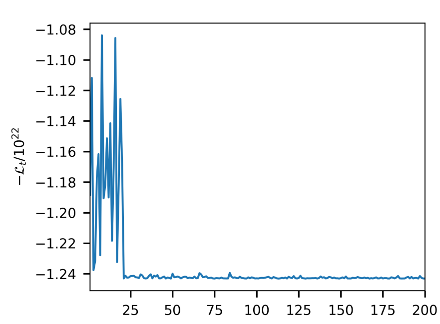

Figure 6: A test of the luminosity optimization using the above workflow.

luminosity evolution during the Bayesian optimization process (with respect to colliding location s_x^* and s_y^*) using the above optimization flow. A minimum value is attained after 25 iterations.

TEST OF BAYESIAN OPTIMIZATION ON RHIC INJECTOR

In the paper, we didn't get a chance to apply the GPTune to RHIC luminosity optimization. As a test of real accelerator optimization, we integrated the GPTune optimizer with the RHIC injector control system, and optimized the beam intensity from the injector [12]. Figure 7 shows a schematic plot of the RHIC linac injector. There are 9 control parameters in the EBIS injection line and 10 control parameters in the EBIS extraction line. These parameters are used in the GPTune optimizer to maximize the beam intensity signal at two location measurements, fc96 and xf14. Here, we

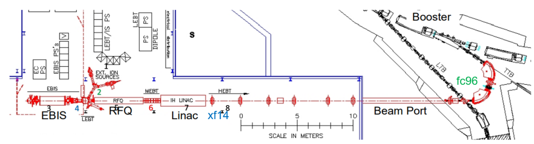

Figure 7: A schematic plot of the RHIC injection linac.

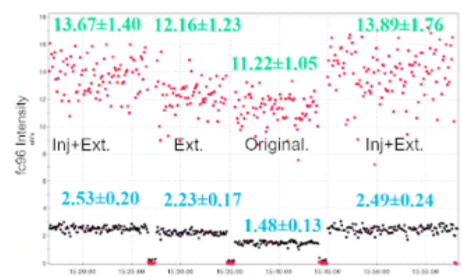

Figure 8: Optimization results with different settings: Inj + Ext, Ext only, and Original.

compared the intensity under three settings: 1) Inj + Ext: Power supplies optimized for both injection and extraction lines; 2) Ext: Power supplies optimized only for extraction with original injection setting; 3) Original: Original settings without any optimization. The optimization results for these three different settings are shown in Fig. 8. In Fig. 8, the red and black dots represent the measurements at fc96 and xf14, respectively. The green and cyan numbers represent the average beam intensities with their deviations for the fc96 and xf14 measurements. We observed significant intensity gain after optimization: 1) xf14 measurement: 42% for extraction-only optimization and 68 – 71% for combined optimization; 2) fc96 measurement: 8.4% for extraction-only optimization and 22 – 24% for combined optimization. Figure 8 also reveals substantial noise of the beam intensity signal. The standard deviation is 10%, and the peak-to-peak deviation is 15%. This optimization demonstrated GPTune's outstanding capability to handle noisy signals, an important feature for many experimental settings.

ISBN: 978-3-95450-247-9 ISSN: 2673-5490 doi: 10.18429/JACoW-IPAC2024-THPC72

REFERENCES

[1] A. Aprahamian, A. Robert, H. Caines, G. Cates, J. A. Cizewski, V. Cirigliano, D. J. Dean, A. Deshpande, R. Ent and F. Fahey, *et al.* "Reaching for the horizon: The 2015 long range plan for nuclear science", 2015. https://www.osti.gov/biblio/1296778

[2] Y. Kim, "The Detector Development and Physics Program in sPHENIX Experiment at RHIC", *Nucl. Phys. A*, vol. 982, pp. 955–958, Feb. 2019. doi:10.1016/j.nuclphysa.2018.10.075

[3] GPTune, https://gptune.lbl.gov/.

[4] MAD-X, https://mad.web.cern.ch/mad/.

[5] J. Qiang, M. A. Furman, and R. D. Ryne, "Strong-strong beam-beam simulation using a Green function approach", *Phys. Rev. Spec. Top. Accel Beams*, vol. 5, no. 10, p. 104402, Oct. 2002. doi:10.1103/physrevstab.5.104402

[6] J. Qiang, M. A. Furman, and R. D. Ryne, "A parallel particle-in-cell model for beam–beam interaction in high energy ring colliders", *J. Comput. Phys.*, vol. 198, no. 1, pp. 278–294, Jul. 2004. doi:10.1016/j.jcp.2004.01.008

[7] J. Qiang, "Terascale Beam-Beam Simulations for Tevatron, RHIC and LHC", in *Proc. PAC'05*, Knoxville, TN, USA, May 2005, paper ROPA006, pp. 535–539.

[8] J. Qiang, M. A. Furman, R. D. Ryne, W. Fischer, and K. Ohmi, "Recent advances of strong–strong beam–beam simulation", *Nucl. Instrum. Methods Phys. Res., Sect. A*, vol. 558, no. 1, pp. 351–355, Mar. 2006. doi:10.1016/j.nima.2005.11.045

[9] J. Qiang *et al.*, "Simulation of beam–beam interaction with crab cavities for LHC upgrade", *Nucl. Instrum. Methods Phys. Res., Sect. A*, vol. 900, pp. 53–59, Aug. 2018. doi:10.1016/j.nima.2018.05.055

[10] B. Shahriari, K. Swersky, Z. Wang, R. P. Adams, and N. de Freitas, "Taking the Human Out of the Loop: A Review of Bayesian Optimization", *Proc. IEEE*, vol. 104, no. 1, pp. 148–175, Jan. 2016. doi:10.1109/jproc.2015.2494218

[11] J. Snoek, H. Larochelle, R. P. Adams, *arXiv*. doi:10.48550/arXiv.1206.2944

[12] X. Gu *et al.*, "Enhancing beam intensity in RHIC EBIS beam line via GPTune machine learning-driven optimization", presented at the IPAC'24, Nashville, TN, USA, May 2024, paper MOPC25, this conference.