





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

Ji Qiang

Nuclear Physics Accelerator R&D, PI Exchange Meeting Dec.7, 2023

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





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

Courtesy of W. Fischer

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).
- \succ 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.

Major Deliverables and Schedule

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.

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.

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



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)

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

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

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

covariance is large if two points are close

(Can use other kernels ...) Matérn:
$$K_{ ext{Matern}}(x, x') = rac{2^{1-
u}}{\Gamma(
u)} \left(rac{\sqrt{2
u}|d|}{\ell}
ight)^{
u} K_{
u} \left(rac{\sqrt{2
u}|d|}{\ell}
ight)$$

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

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

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

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

(Jones et al. 1998)

1D Example:



- 5 initial samples4 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_m eeting_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

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



Test of the GPTune Optimization Software with the Analytical Model

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



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

objective function $oldsymbol{f}:\mathbb{R}^n$ $\min_{oldsymbol{x}\in X}oldsymbol{f}(oldsymbol{x})$ $X \subseteq \mathbb{R}^n$ feasible set



17

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:

- change the target s^{*}, beta^{*} within 'deltas.dat' file;
- 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:

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

GPTune is ready for testing with scripts:

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

APEX Test of s* Online Control Script at IR12



- 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 \boldsymbol{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

Duration	1000	2000	2000	100		100	500	65000	400	1000	1000
RampTime	15000	52000	400	2500	320	10	4000	15000	2000	3000	10000
Start of Duration	15000	68000	70400	74900		78200	82300	97800	164800	168200	179200
Start of Ramp	0	16000	70000	72400	750	00	78300	82800	162800	165200	169200
	57										
-											
Anode	-200	-200	-200	9600		13800	16098	20400	18100	-200	-200
LowerAnode1oF2	-200	-200	-200	4800		6900	8049	10200	9050	-200	-200
UpperAnode2oF2	0	0	0	4800		6900	8049	10200	9050	0	(
CathodeBias	-100	-14000	-14000	-14000	- 1	14000	-16400	-18300	-18300	-17100	-10
	5										
ad		E20	E20	620	E20	62	50 E2	A E2A	E20	-	
172		500	500	500	500	53	0 150	0 1500	1500	0	
312	0	5200	5200	5200	5200	520	× 100	0 5200	5100	0	
014	0	6300	6300	6300	6300	636	0 660	0 6600	6500	0	
TE	0	7700	7200	7700	7700	776	270	0 7700	7700	0	
TE	0	6700	6700	6700	6700	670	700	0 7000	6800	0	
017	0	6500	6500	6500	6500	660	700	0 7800	6800	0	
Ev. DT7	0	0	0	0	0	005	0 100	0 0	0000	0	
178	0	8900	8900	8900	8900	890	890	0 8900	8900	0	
Fy DT8		0	0	0	0	0.05	0	0 0	0000	0	
119	0	8400	8400	8400	8400	870	890	0 8900	8900	0	
Ex.DT9	0	0	0	0	0		0	0 0	0	0	
0110	0	8900	8900	8900	8900	890	890	0 8900	8900	0	
					_						
	[s]										
0112	7000	12200	12200	12200 1	2200	1180	0 1120	0 11200	11200	7000	
Ex.DT12	12300	12300	12300	12300 1	2300	1230	0 1230	0 12300	12300	12300	
0113-17	2000	9900	9900	9900	9900	820	780	0 7800	7200	2000	
Ex,DT13-17	9800	13300	13300	13300 1	3300	1330	00 1330	0 13300	13300	9800	
DT18	4000	6700	6700	6700	6700	1010	0 1100	0 11000	8900	4000	
Ex.DT18	1900	4000	4000	4000	4000	400	800	0 8000	1900	1900	
0119	4000	7100	7100	7100	7100	710	0 710	0 7100	6000	4000	
0120	2800	3000	3000	3000	3000	300	300	0 3000	3000	2700	
0121	1150	2000	2000	2000	2020	202	202	0 2020	2020	1150	
	<u>م</u>										
IonExtractor	-5000	-9300	-9300	-9300 -	9300	-934	10 -934	0 -9340	-9340	-5000	
ReflectorRepeller	0	Ó	0	Ő	Ó		0	0 0	0	0	
IonLens0-20kV	-3400	-34500 -	34500 -	34500 -3	4500	-3450	-3450	0 -34500	-34500	-34000	
IonLens20-40kV	310	3120	3120	3120	3120	-1020	-1320	0 -13200	-9200	3100	
Def1P1atBias	-96	-720	-720	-720	-720	-287	79 -287	9 -2879	-2879	-960	
6PoleX	-	-47	-47	-47	-47	34	17 34	7 347	347	-47	
16PoleY	-16	-104	-164	-104	164		7 7	3 73	73	-164	

EBIS	EBIS plat, HV	OFF	65000.4	Fault, Sec	0
	Plat HV width (INJ)	100	keep 1960 or let	3	
	Plat HV width (EXTR)	290	keep 1960 or le		
LION	Plat,HV	•	Long solenoid	•	
	beh1ke9pu1se2	delay.ebis	x0.1us		
	Conf.time	79,3500024	(msec)		
eba	Pulsed quad delay	185000	"64000+conf.time	a (us)	
	LEBT Solenoid	541,007			
Ebis Rf		RFQ	buncher 1	-	EBIS-RF Scope
	Amp, 2	44	Amp. 2	49	
	Phase (+/- 180 deg)	21	Phase (+/- 180 4	62	
		1.1000	humahan 0		
	0	LINAC	Duncher 2	20.0	
	Phone (1/- 180 dec)	42.0	Phane (+/- 190	4 44	
	Thanke (47 - 100 deg)		11111111 (177- 100 1		
		buncher 3			
	Amp. 2	36			
	Phase (+/- 180 deg)	52			
tB PPM Us	time to be ag				
	Device	Current	Device	Current	
MEBT	q1	0.00	q2	0.00	
and the second sec	q3	0.00	q4	0.00	
Linac	q1.3	0.00	q2	0.00	
ETR	a0 2	. 0.00	+650	0.52	
LID	40.2		CITOO	0.02	
		0.00	1 1 1 1 1	-0.47	
	tb6	0.00	tv51	-0.47	
	th6 tv8	0.00	453 482	-0.47	
	44 th6 tv8 a9	0.00 -0.27 0.39 -6.95	tv51 q53 q82 buncher 3	-0.47 2.70 -0.10	
	th6 tv8 q9 ×f14	0.00 -0.27 0.39 -6.95	tv51 q53 q82 buncher 3 tv86	-0.47 2.70 -0.10	
	44 th6 tv8 q9 ×f14 th14	0.00 -0.27 0.39 -6.95 [10.000] 0.35	tv51 q53 q82 buncher 3 tv86 ×f89	-0.47 2.70 -0.10 -1.17 [10,000]	
	44 th6 tv8 q9 ×f14 th14 tv14	0.00 -0.27 0.39 -6.95 [10.000] 0.35 -0.00	tv51 q53 q82 buncher 3 tv86 xf89 The Big Bend	-0,47 2.70 -0,10 -1,17 [10,000] 0,00	
	44 th6 ty8 q9 xf14 th14 tv14	0,00 -0,27 0,39 -6,95 [10,000] 0,35 -0,00	tv51 q53 q82 buncher 3 tv86 xf89 The Big Bend B-field	-0,47 2.70 -0,10 -1,17 [10,000] 0,00 0,00000	
	44 th6 tv8 q9 ×f14 th14 tv14 q15	0.00 -0.27 0.39 -6.95 [10.000] 0.35 -0.00 3.17	tv51 q53 q82 buncher 3 tv86 xf89 The Big Bend B-field MM096	-0,47 2,70 -0,10 -1,17 [10,000] 0,00 0,00000 Out	
	44 46 49 xf14 414 414 415 buncher 2	0.00 -0.27 0.39 -6.95 [10.000] 0.35 -0.00 3.17	tv51 q53 q82 buncher 3 tv86 ×f89 The Big Bend B-field MM096 Big Bend trim	-0,47 2,70 -0,10 -1,17 [10,000] 0,000 0,00000 0ut -0,00	
	416 406 49 xf14 4114 414 415 buncher 2 433	0.00 -0.27 0.39 -6.95 [10.000] 0.35 -0.00 3.17 3.83	tv51 q53 q82 buncher 3 tv86 ×f89 The Big Bend B-field MM096 Big Bend trim q97	-0.47 2.70 -0.10 [10.000] 0.000 0.00000 Out -0.00 0.000	
	416 416 49 4114 4114 4114 4114 4115 50000000000000	0.00 -0.27 0.39 -6.95 [10.000] 0.35 -0.00 3.17 3.83 0.04	tv51 q53 q82 buncher 3 tv86 ×f89 The Big Bend B-field MM096 Big Bend trim q97 tv105	-0.47 2.70 -0.10 (10.000) 0.000 0.0000 0ut -0.00 0.000 0.000	
	th6 tv8 q9 xF14 th14 tv14 q15 buncher 2 q33 th36 tv37	0,00 -0.27 0.39 -6.95 [10,000] 0.35 -0.00 3.17 3.83 0.04 -0.40	tv51 q53 q82 buncher 3 tv86 ×R89 The Big Bend B-field MM096 Big Bend trim q97 tv105 th105	-0.47 2.70 -0.10 -1.17 [10.000] 0.000 0.0000 0.000 0.000 0.000 0.000	
	44 tv6 q0 xF14 tv14 tv14 q15 buncher 2 q33 tv37 q39	0,00 -0.27 0,39 -6.95 [10,000] 0.35 -0.00 3.17 3.83 0.04 -0.40 3.68	tv51 q53 q82 buncher 3 tv86 xf89 The Big Bend B-field MM006 Big Bend trim q7 tv105 th105 q106	-0.47 2.70 -0.10 -1.17 [10.000] 0.000 0.000 0.000 0.000 0.000 0.000 0.000	
	th6 tv8 q9 xF14 tv14 q15 buncher 2 q33 th36 tv37 q39 PM047	0,00 -0.27 0.39 -6.95 -0.00 3.17 3.83 0.04 -0.40 3.68 0.04	tv51 q53 q82 buncher 3 tv86 ×F89 The Big Bend B-field HM096 Big Bend trim q97 tv105 tv105 q106 ×f108	-0.47 2.70 -0.10 -1.17 [10.000] 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000	

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



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

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.

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.

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!