Toward Automated Multi-Fidelity Model Calibration

For Accelerator Physics Simulations

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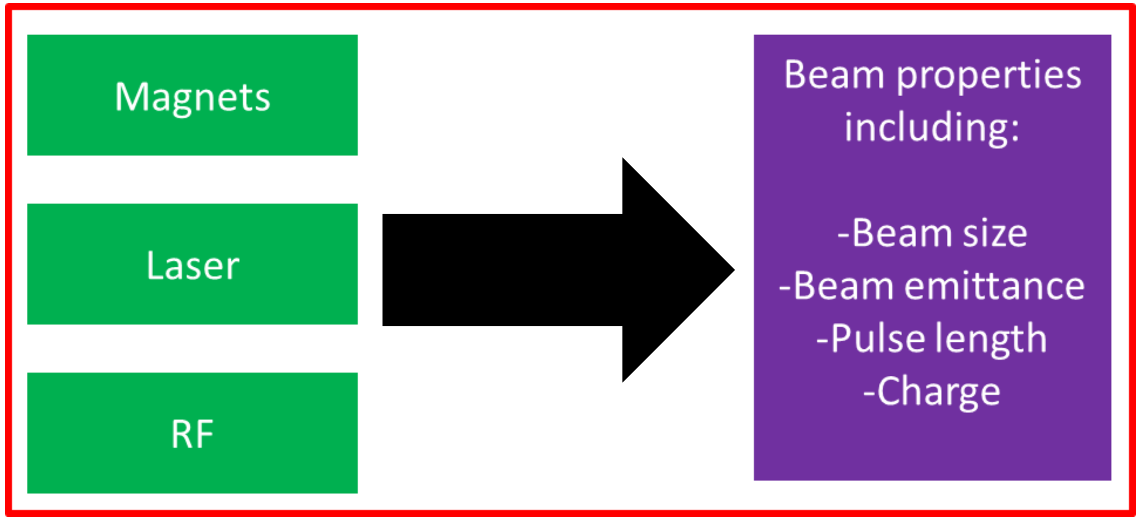
SLAC NATIONAL ACCELERATOR LABORATORY

Stanford University | U.S. DEPARTMENT OF ENERGY

Goals & Definitions



Model: predicts beam behavior given accelerator settings.

Key concept: **simulation-based surrogate model**:

- Data-driven model, but predicts simulation results
- Fast & incorporates nuances of simulation
- Differentiable!
- Downside: only valid within span of training data
- Downside: more sources of error

Model typology:

- Physics-based simulations
  - Slow (seconds to hours on desktop CPU or cluster) but accurate
- Transfer matrices or mathematical model
  - Fast but simple
- Data-driven model
  - Can be fast (ms on desktop CPU/GPU), but incorporates nuances of data
  - Differentiable!

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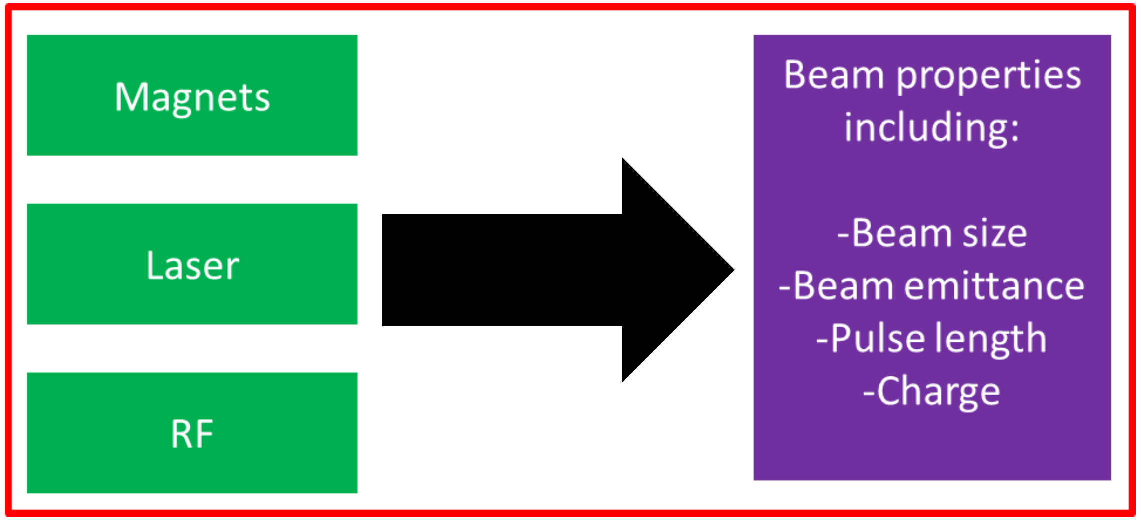

Model: predicts beam behavior given accelerator settings.

Need accurate models for high precision accelerator control!

Physics-Based Simulations

Analytic Model

Data-Driven Model

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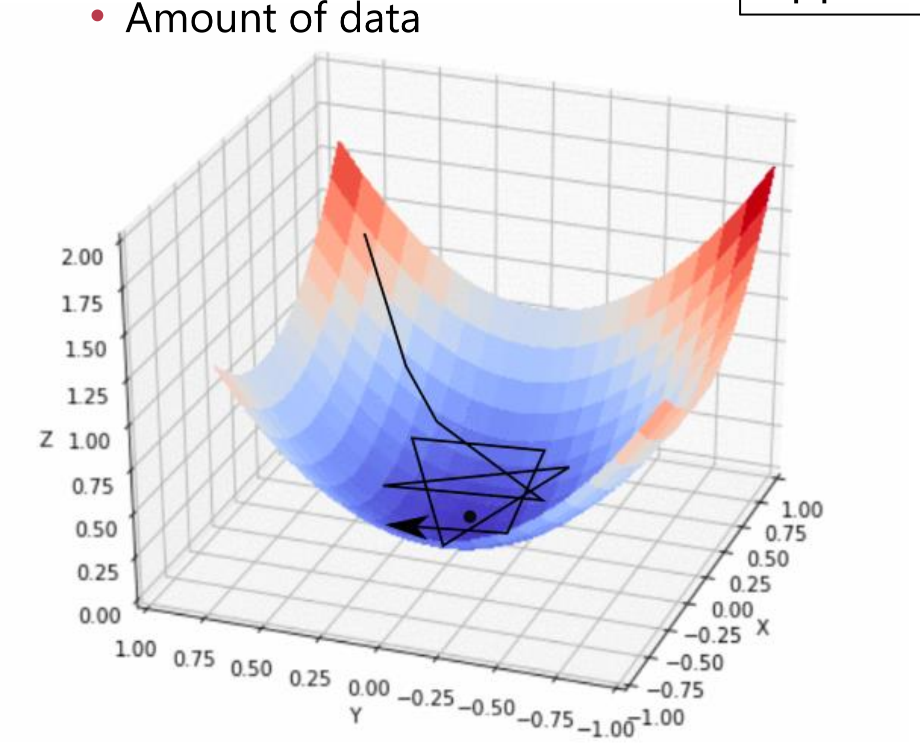
Accurate Model Predictions Required!

$$\arg\min \|d_{obs} - f(x_1, x_2, \ldots, x_n)\|_1$$

- Considerations: choosing an approach
  - Model execution time/cost
  - Model types
  - Desired information
  - Amount of data

Consider Goals & Applications!



https://blog.paperspace.com/intro-to-optimization-in-deep-learning-gradient-descent/

Goal: Calibrate Models

Goal: Automated Approach

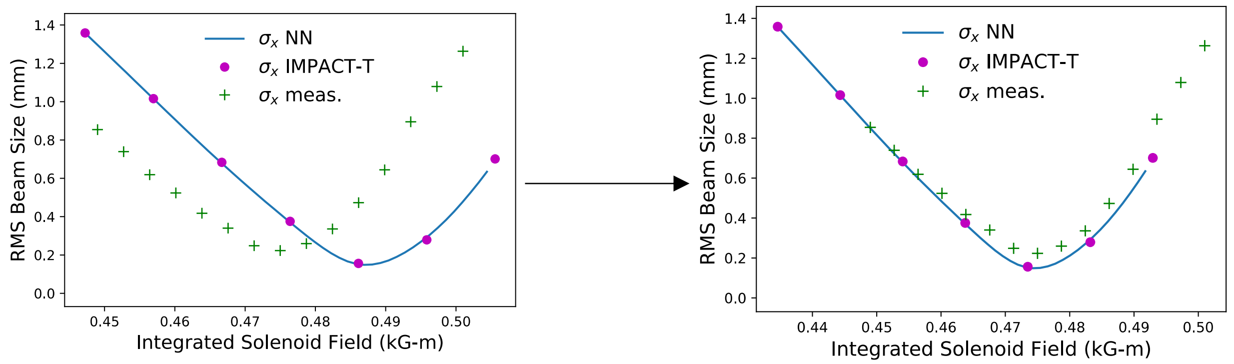
Challenge: Collective Effects

Challenge: Slow Simulation Execution

Challenge: Uncertainty Quantification

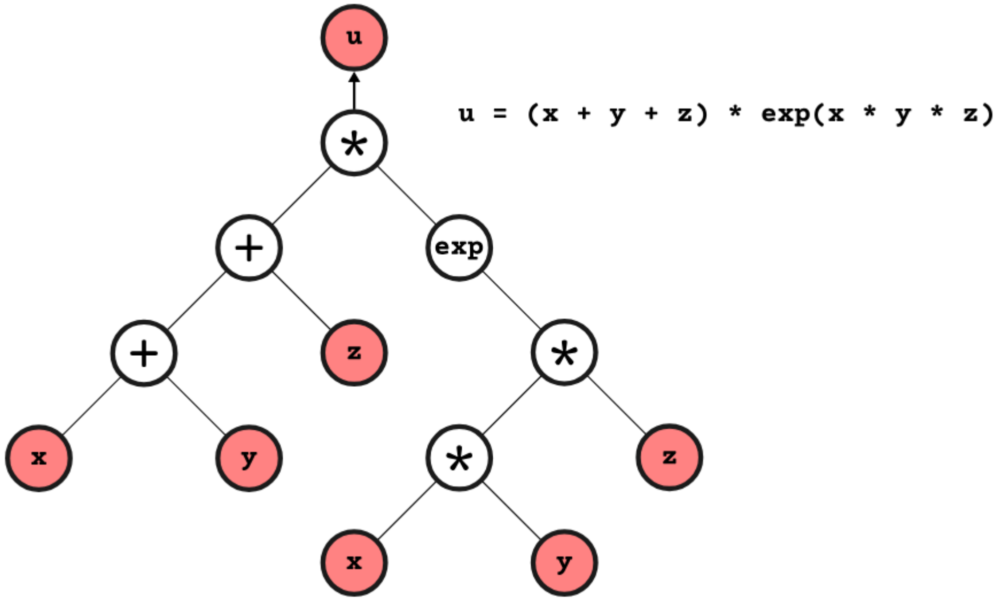
Challenge: Lots of Information in Tails of Beam

Challenge: Simulation Differentiability



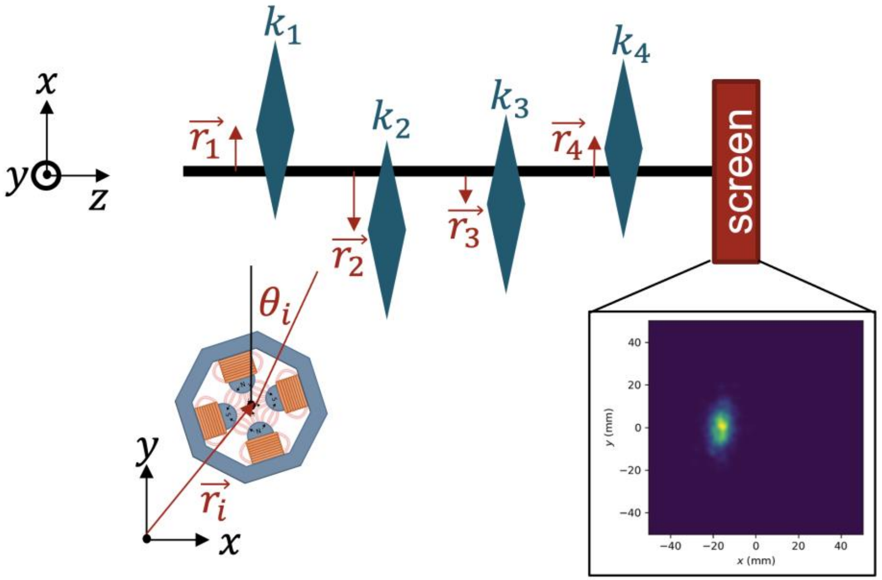
Differentiable Programming & Simulation

- Keeping track of derivatives
- Critical concept in ML
- For model calibration, allows for quick optimization using autodiff



https://autodiff.github.io/

- Using differentiable simulator to track derivatives
- Ongoing work using Bmad-X and Cheetah
- Basic example/proof of concept here:
  - https://github.com/bmad-sim/Bmad-X/blob/main/docs/examples/optimization/model-calibration-and-differentiable-histograms.ipynb



J. Gonzalez-Aguilera et al. Proc. of IPAC 2023 [10.18429/JACoW-IPAC2023-WEPA065](https://doi.org/10.18429/JACoW-IPAC2023-WEPA065)

Prescription for Non-Differentiable Models

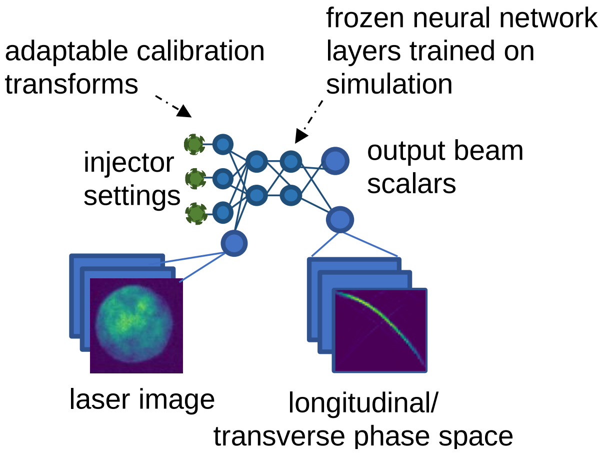
T. Boltz et al. arXiv:2403.03225v4

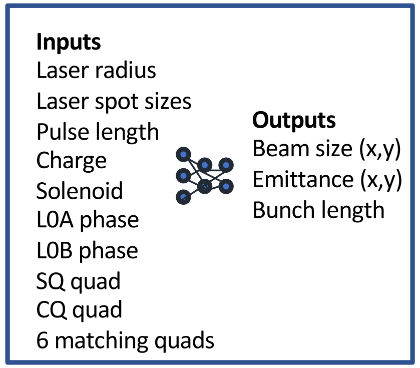
But what do we do if simulations are not differentiable? (General case…)

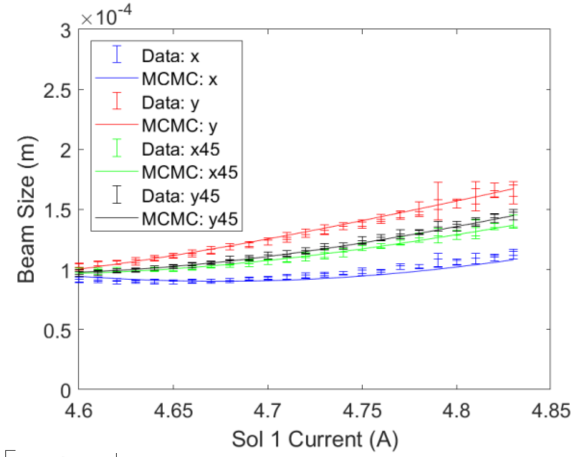
1) Make differentiable surrogate models → quick optimization, slow to train
2) Direct optimization on non-differentiable model

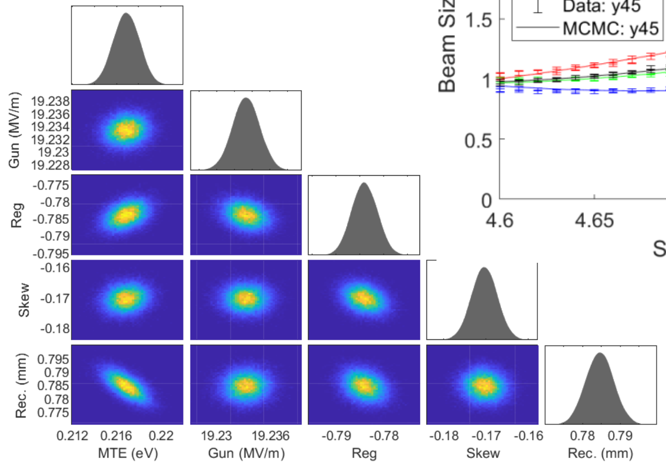
Accelerator Inputs (Sample "entire" space) → Simulation Model (Non-Differentiable) → Beam Properties

Surrogate Model (Differentiable)









F. Cropp Ph.D. Thesis

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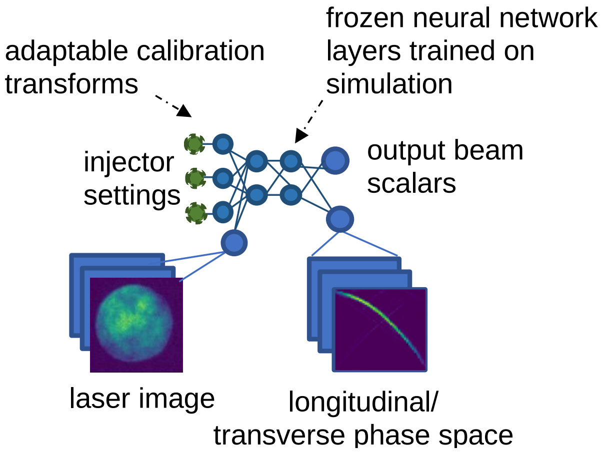


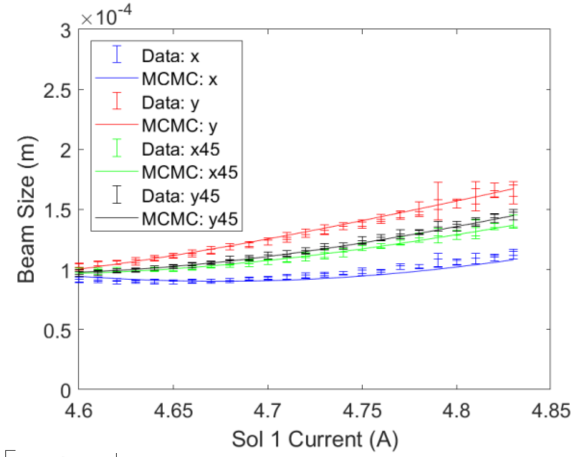
Inputs
Laser radius
Laser spot sizes
Pulse length
Charge
Solenoid
L0A phase
L0B phase
SQ quad
CQ quad
6 matching quads

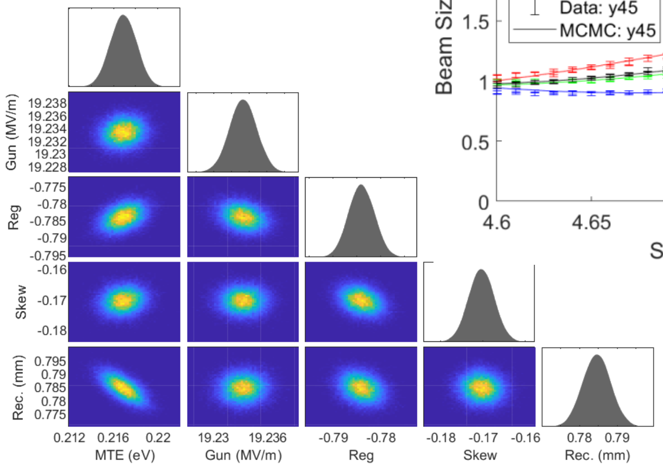
Outputs
Beam size (x,y)
Emittance (x,y)
Bunch length

Accelerator Inputs (Sample "entire" space) → Simulation Model (Non-Differentiable) → Beam Properties

Modified Inputs (from exp. Settings) → Surrogate Model (Differentiable) → Beam Properties Compared with Real Data

Or regular training with backpropagation





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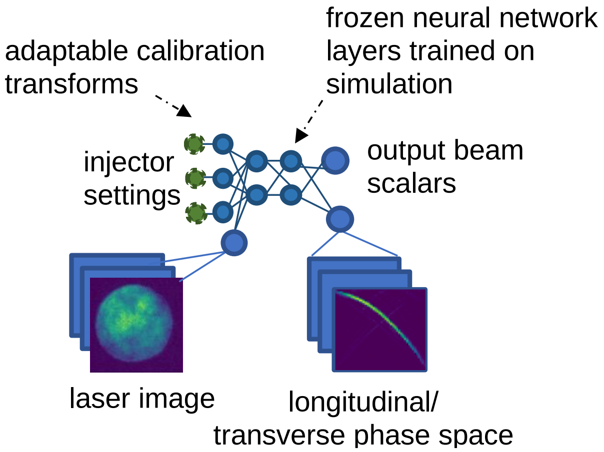

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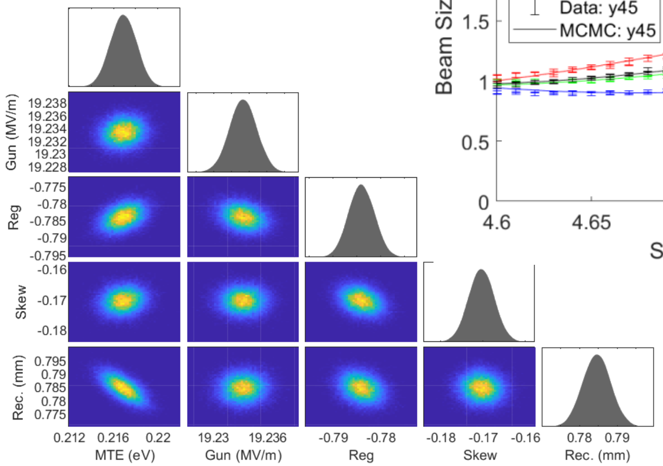

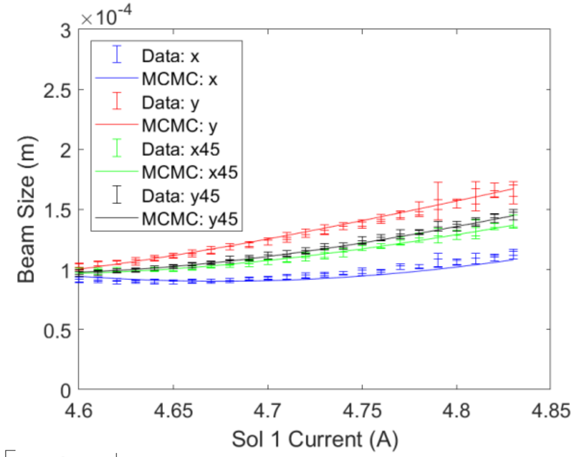

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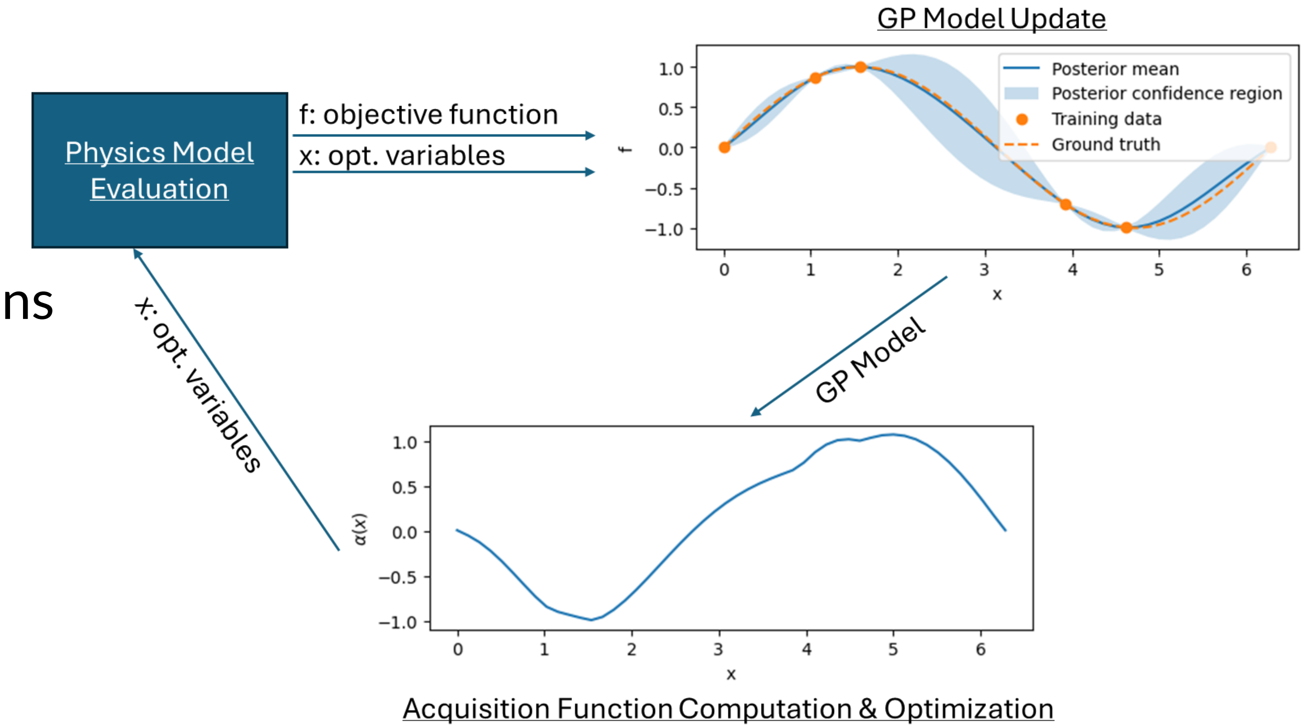
Multi-Fidelity Optimization

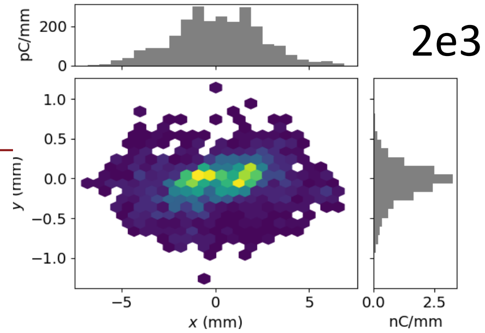
- Information theoretic approach to simulations
- Learn correlations between different model fidelities
- Use multi-fidelity Bayesian optimization to select model fidelity and next optimization variables



Number of Particles (N)	2e3	2e4	2e5
Num. Space Charge Grids	8	16	32
Execution time	19 sec	3 min	28 min
σ_x (um)	2316	2463	2575
σ_y (um)	263	345	386
Norm x/y emit (um)	14.4/8.9	15.8/10.6	16.7/11.4

Example of multifidelity from design optimization:
A. Ferran Pousa et al. PRAB, 2023

N= 2e3



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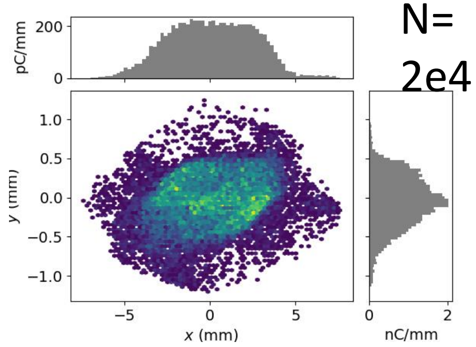

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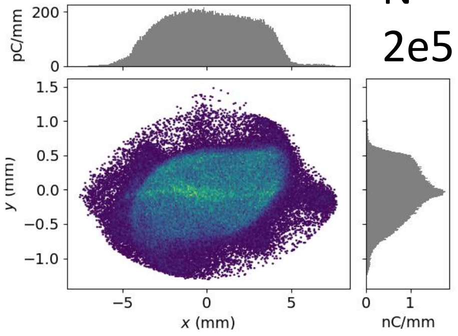

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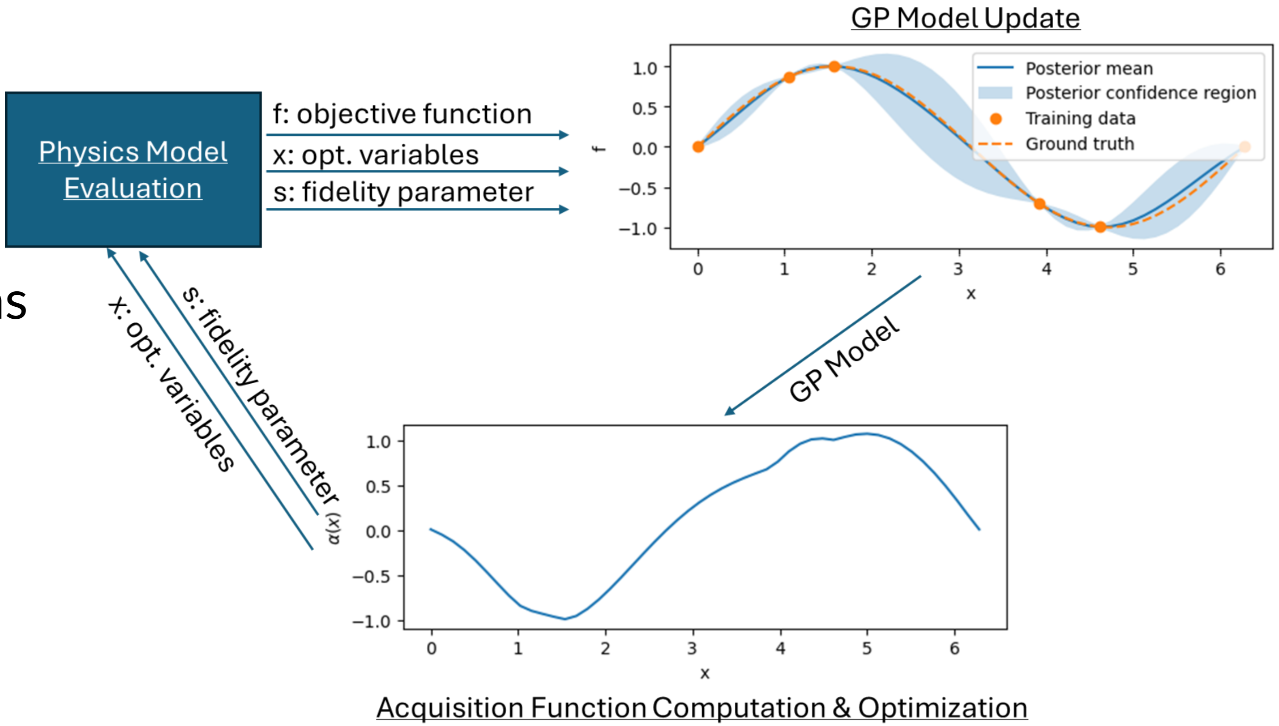

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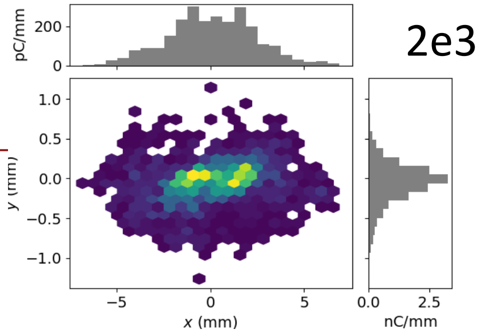

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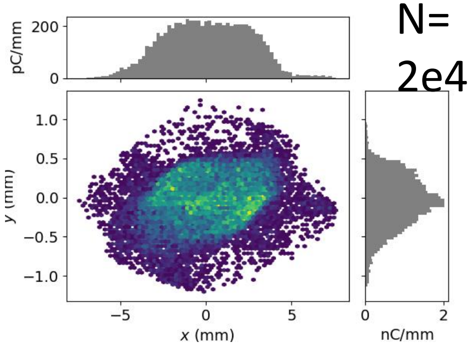

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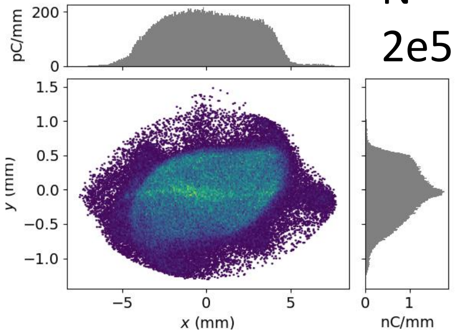
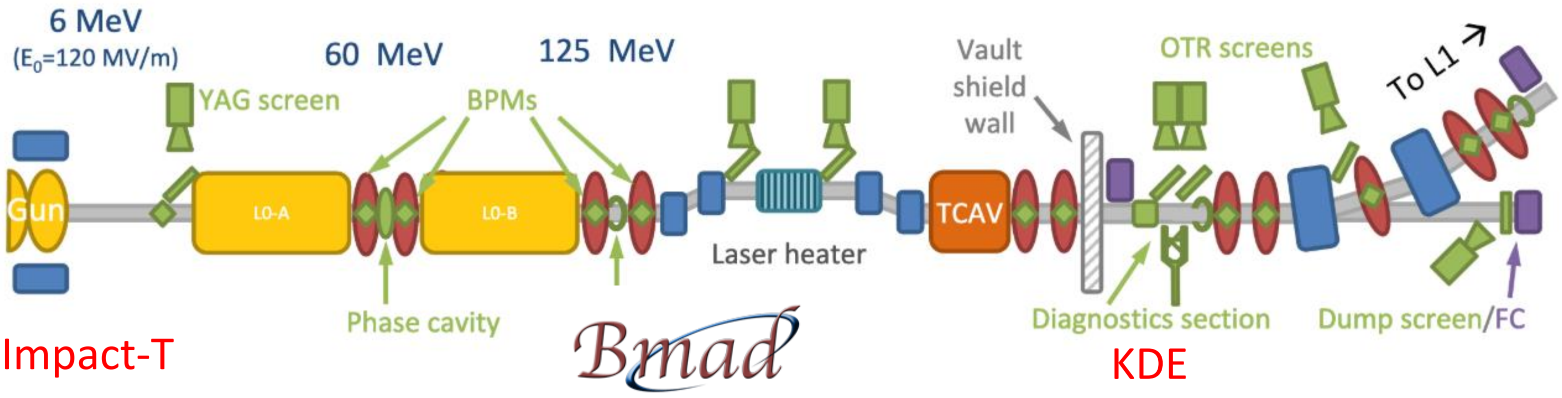


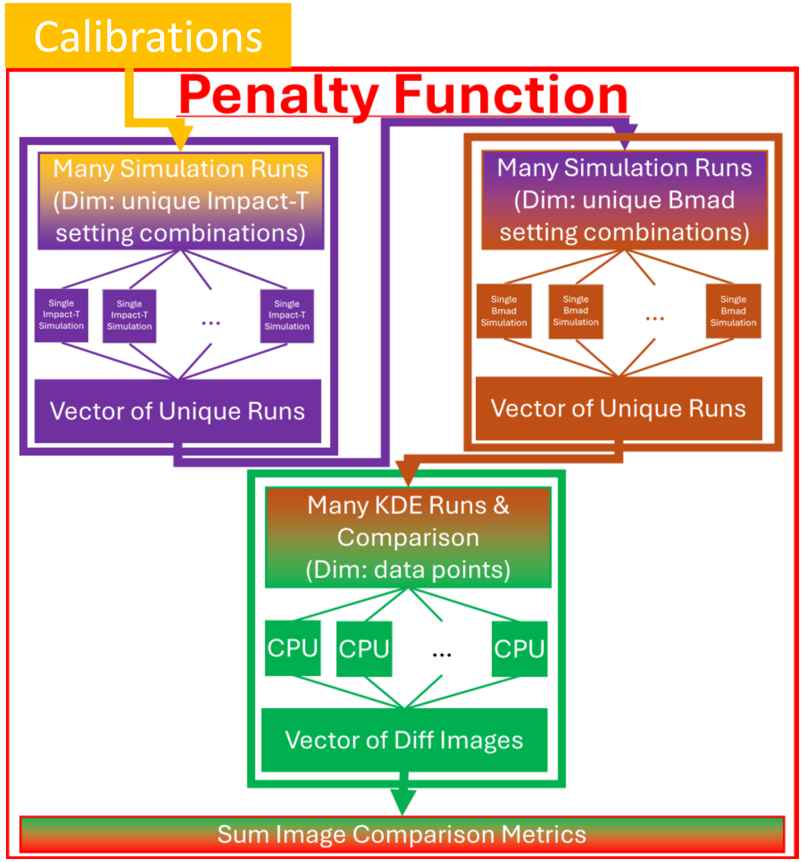
Approach

Containerized Impact-T to Bmad Pipeline Available at SLAC

Xopt

FACET-II injector (SLAC)

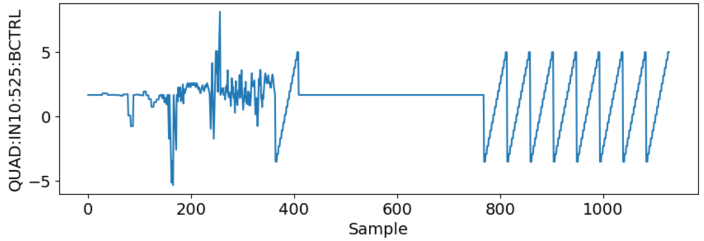


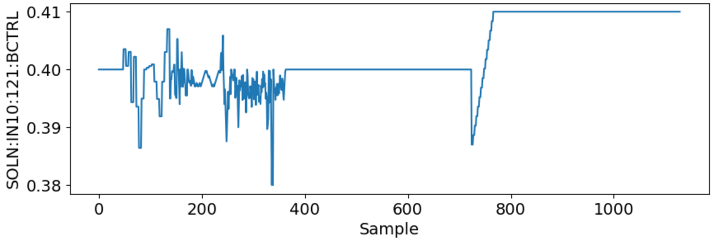


Wrapped in Xopt

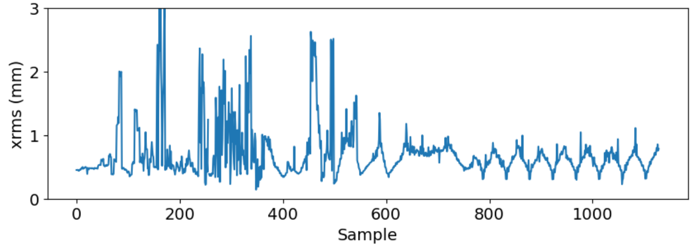
- Many optimizers available, including Bayesian Optimization (BO), MOGA
- Can compare to data at multiple screens
- Using all open-source tools: Lume-Impact, Bmad/Pytao, FastKDE, Xopt
- Balancing multiple fidelities (images vs. beam sizes)
  - Focused initially on high-fidelity and low-fidelity case

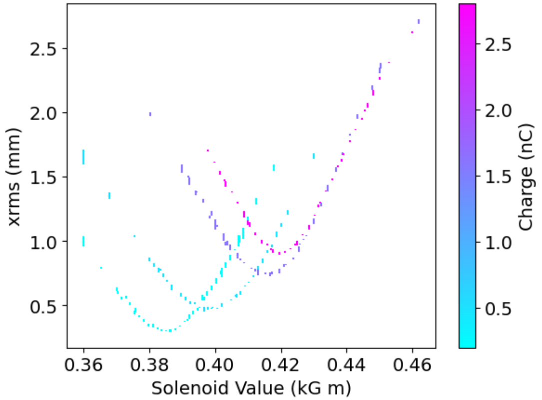
Test Problem



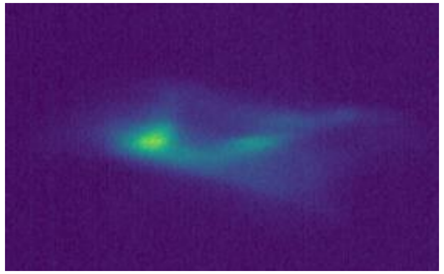


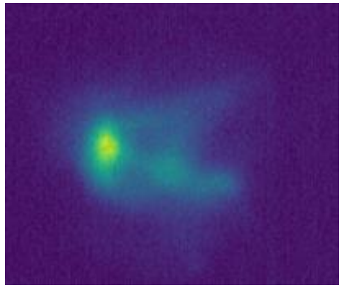
Bayesian Exploration

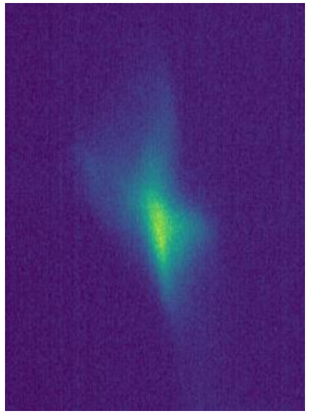


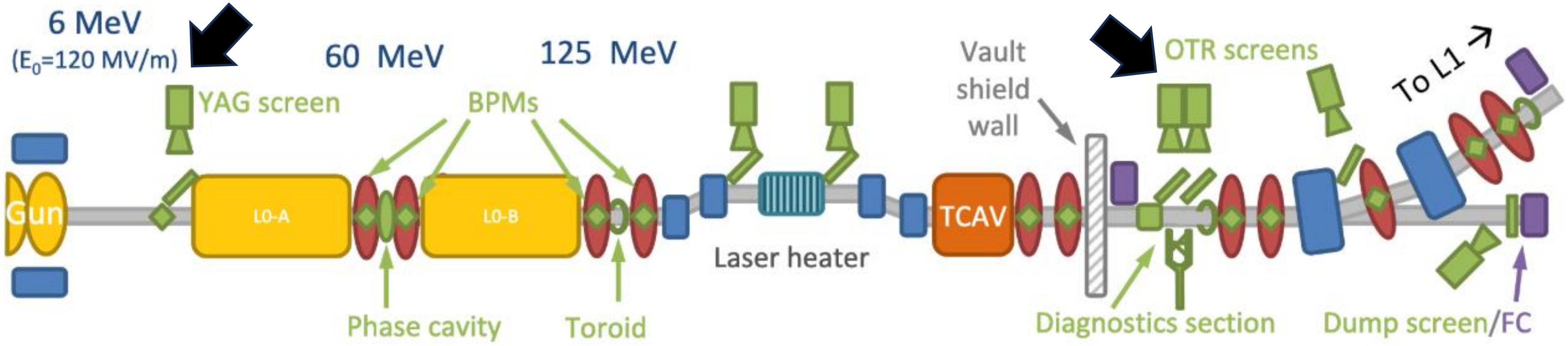


- FACET-II injector (SLAC)
- Parameters varied using multiple techniques:
  - Bayesian Exploration — Roussel et. al. *Nat. Comm.* **2021**
  - Parameter scans
- Images saved on two screens
- 6 datasets taken months apart over past 1+ year

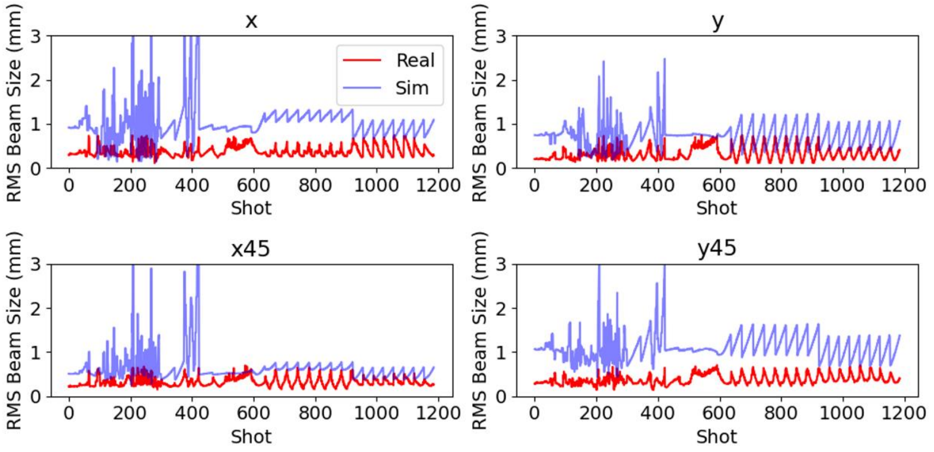




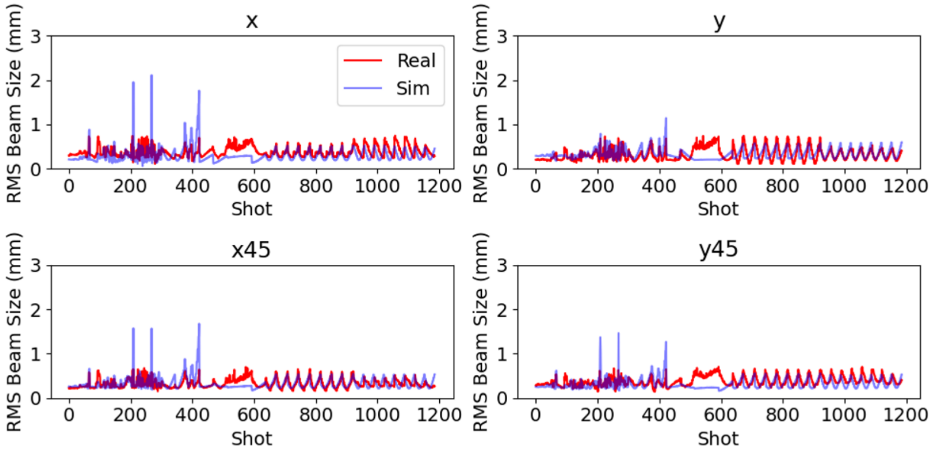




Preliminary Results



Nominal calibration



Improved calibration

BO Optimization on the following parameters (scaling & offset):

- Quad calibration x6
- Solenoid calibration
- Gun, linacs (x2) amplitudes & phases
- Initial pulse length

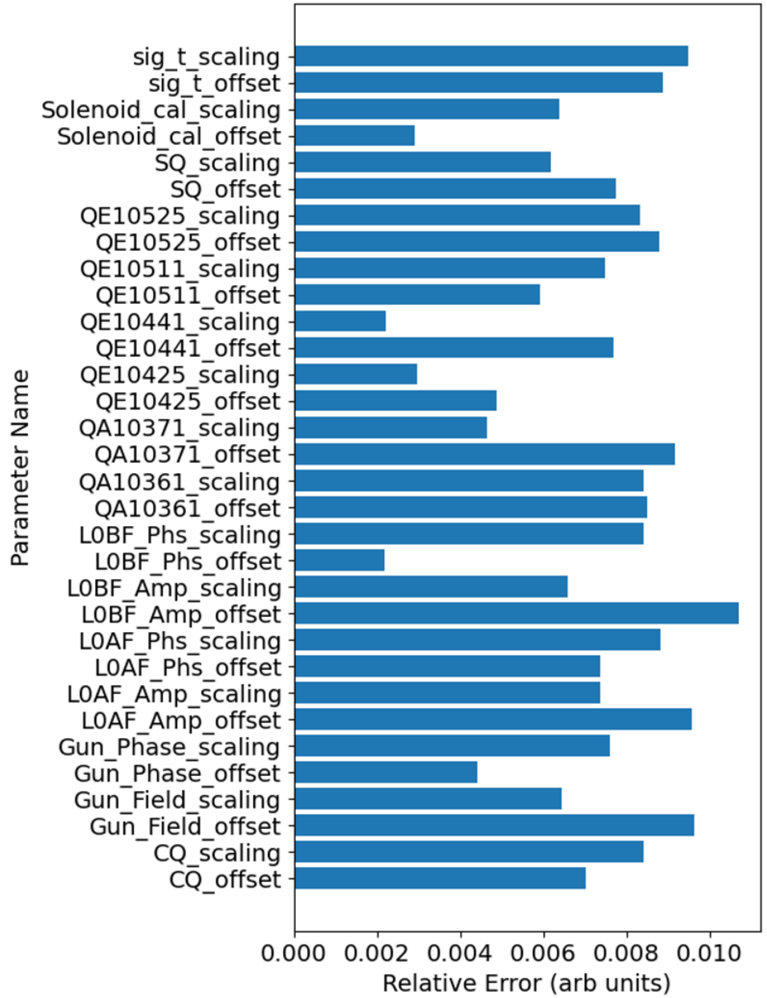
BE data, 400 points for optimization, evaluated on all points taken that day, including some parameter scans

Low fidelity, moment-based calibration

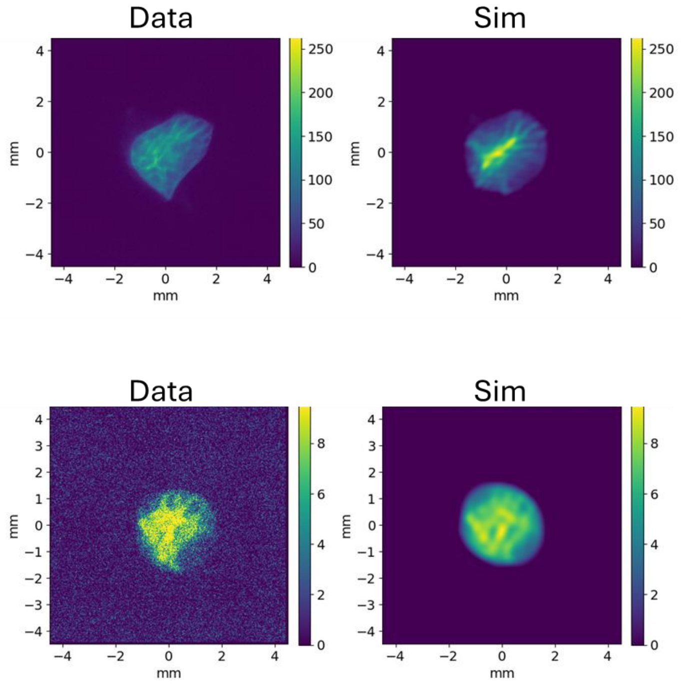
Right: Uncertainty quantification from GP model

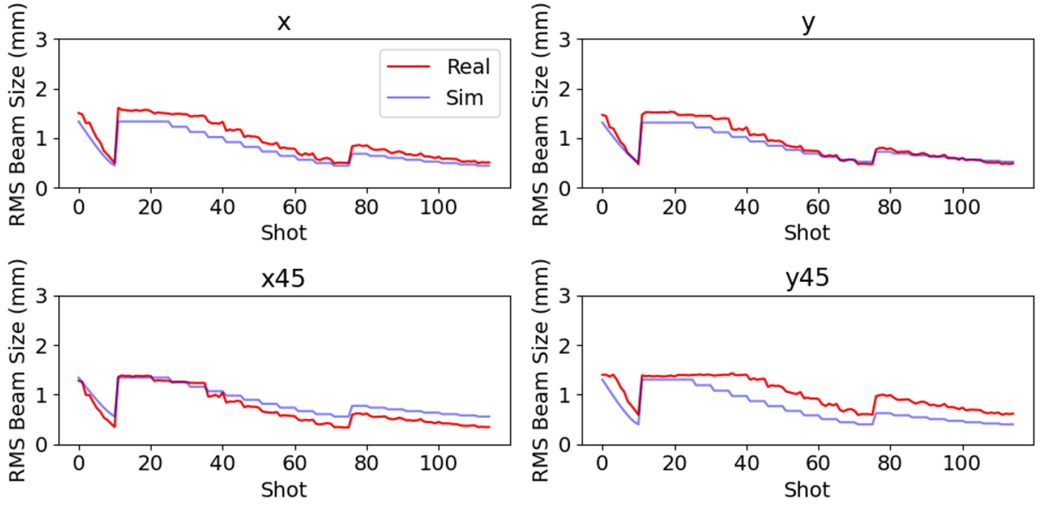
Sources of error include:

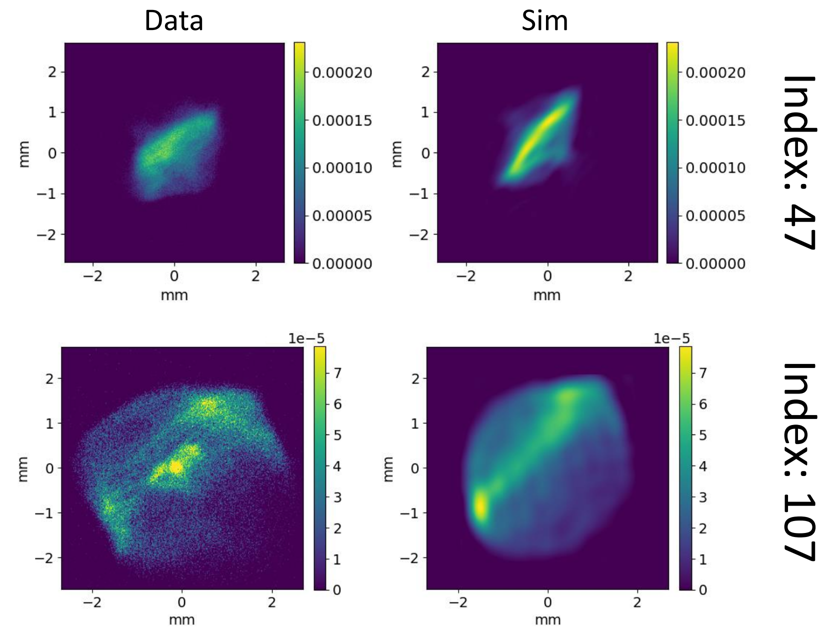
- Unmeasured parameter fluctuations (time varying)
- Image fitting & moment calculations



Preliminary Results (Upstream Screen)







Below: Example images from first screen. Predictions about pixel calibration confirmed by measurement. (Later data-set)

Note different simulation fidelities!

Above and right: Optimized calibrations from previous slide (downstream screen) checked on upstream screen

Conclusion

- Evaluating the efficacy of direct model calibration using efficient ML-based techniques:
  - BE
  - BO
- Infrastructure for optimization built and operational
- Preliminary optimization → working, but is it more efficient than training a surrogate model?
- Initial studies with two-tier multi fidelity approach are underway → many technical aspects to resolve
- Future: more efficient treatment of simulation fidelities
- Once relevant nonlinear collective effects are implemented in differentiable sims (Cheetah), faster gradient-based methods could be used
- Part of a larger effort: see right

Interoperable standards and tools for end-to-end accelerator simulations

Differentiable simulations, including Bmad

Model calibration for RHIC

Acknowledgements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(SLAC)


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(SLAC)

Claudio Emma
(SLAC)


Zihan Zhu
(SLAC)

Dylan Kennedy
(SLAC)


Nathan Majernik
(SLAC)


Sanjeev Chauhan
(Duke U.)


Chris Mayes
(xLight, Inc./SLAC)


Juan Pablo Gonzalez-Aguilera
(U. Chicago)


Brendan O'Shea
(SLAC)

SLAC