ML-Based Model Calibration Methods

For Accelerator Physics Simulations

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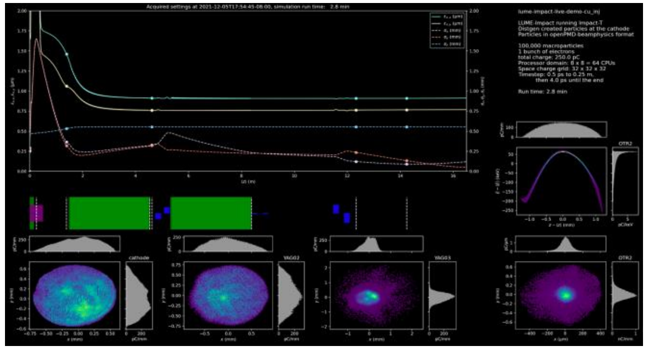
On behalf of the SLAC ML team

2024-03-08

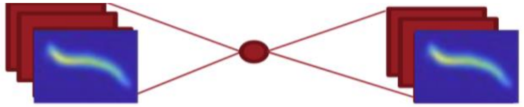
High Performance Accelerator Models Are Central to AI/ML Efforts

Online prediction with physics sims and **fast/accurate ML models**

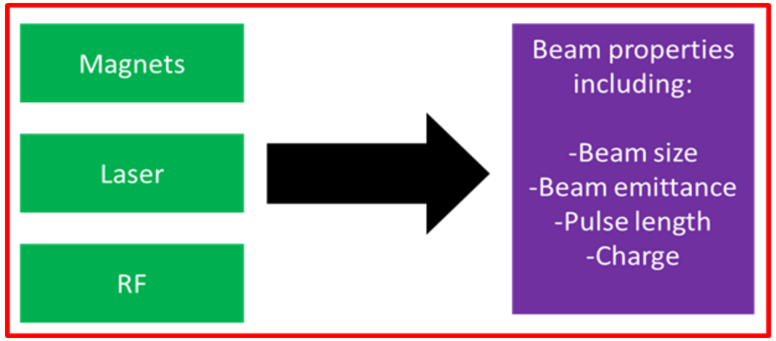


Representation learning

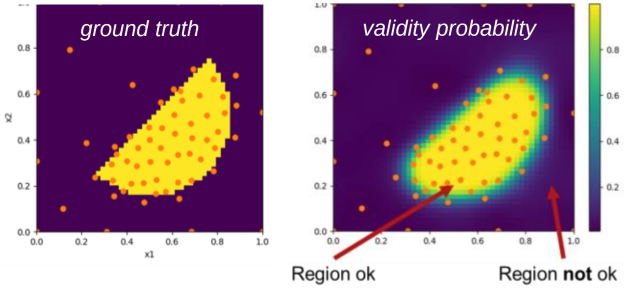
(e.g. better ways of modeling beams)



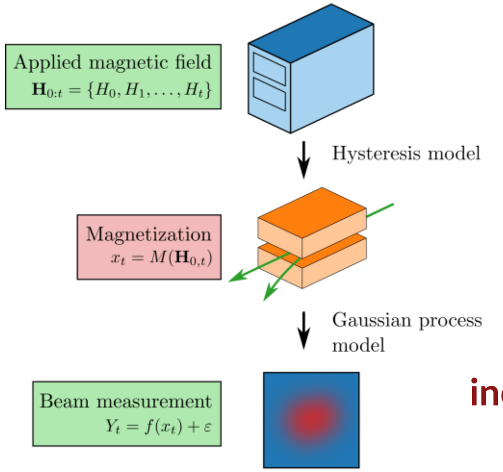
Accelerator Models



Roussel et. al. *Nat. Comm.* **2021**



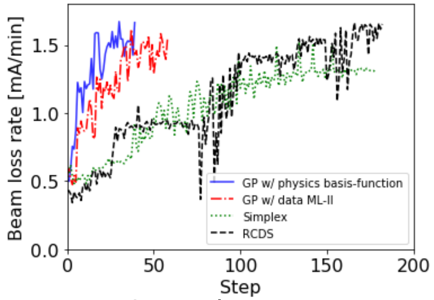
Output constraints learned on-the-fly



Roussel et. al. *PRL*. **2022**

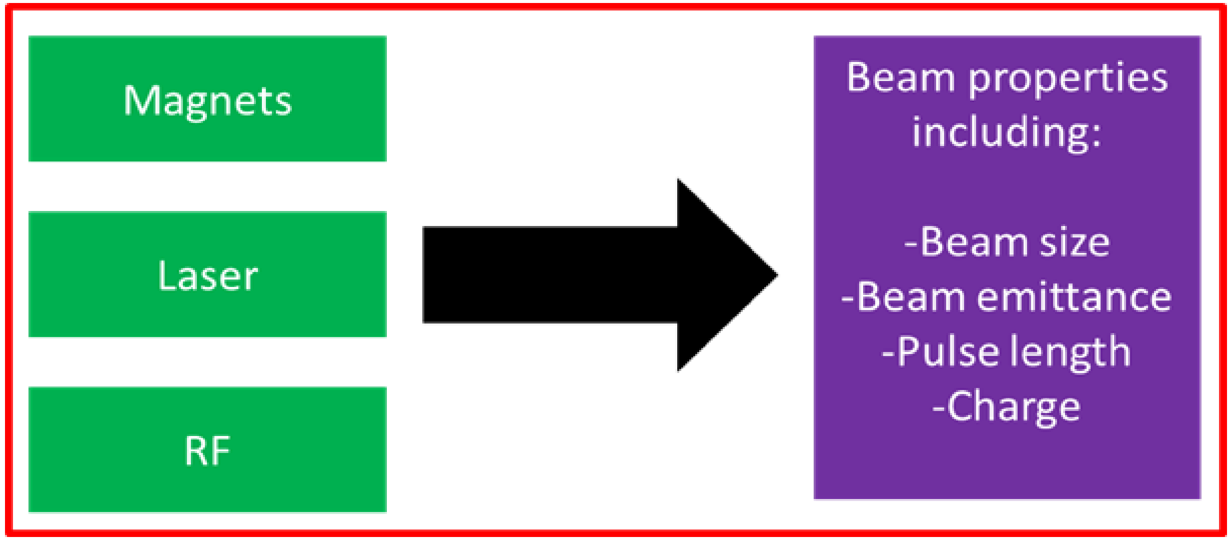
Combining physics and ML, including differentiable simulators

Efficient optimization and characterization

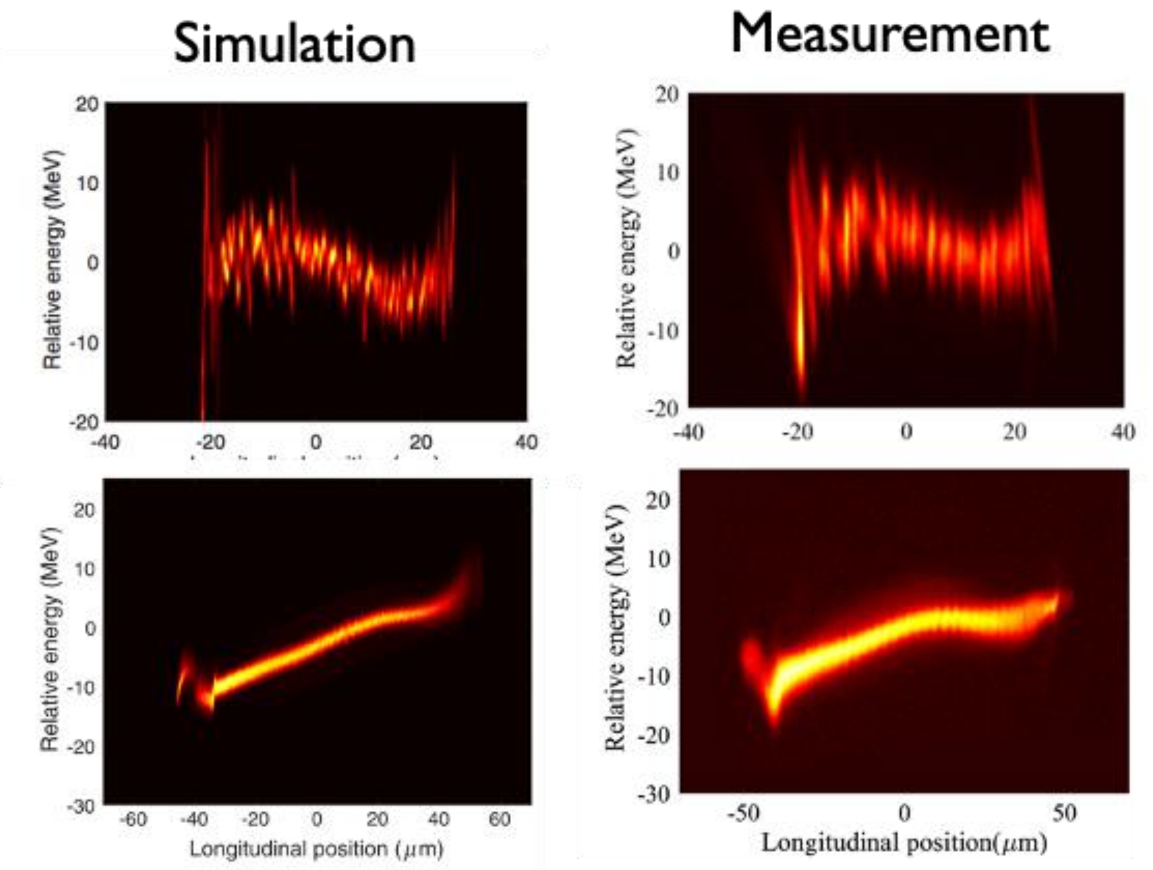


Hanuka et. al. PRAB , **2021**

Fast-Executing, Accurate System Models



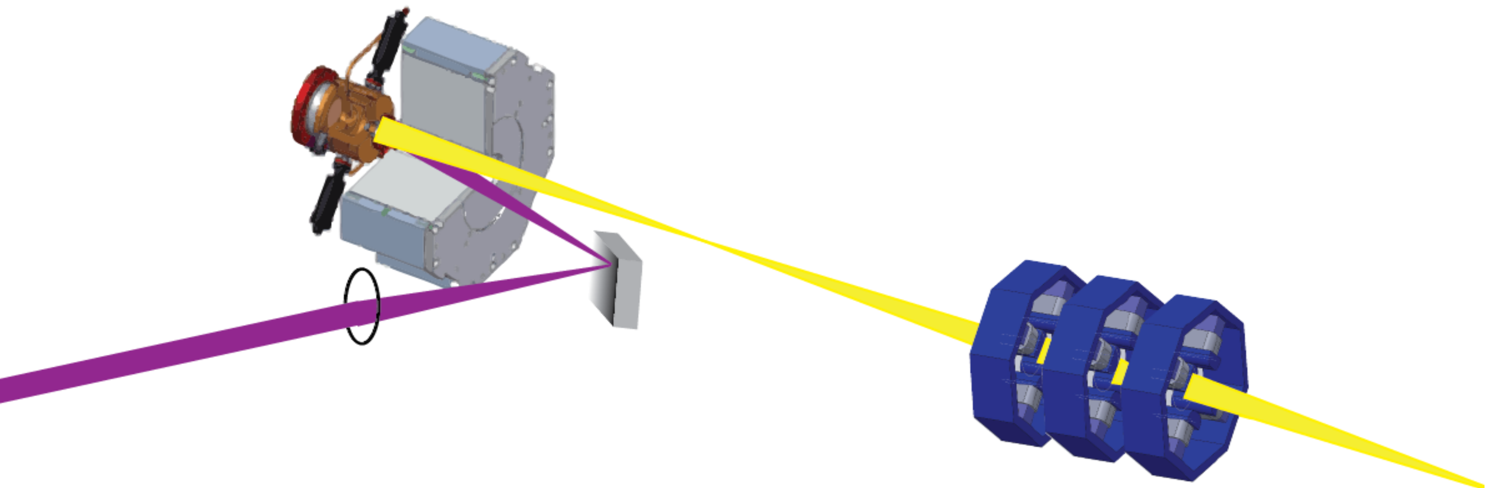
Accelerator simulations that include nonlinear and collective effects are powerful tools, but they can be computationally expensive

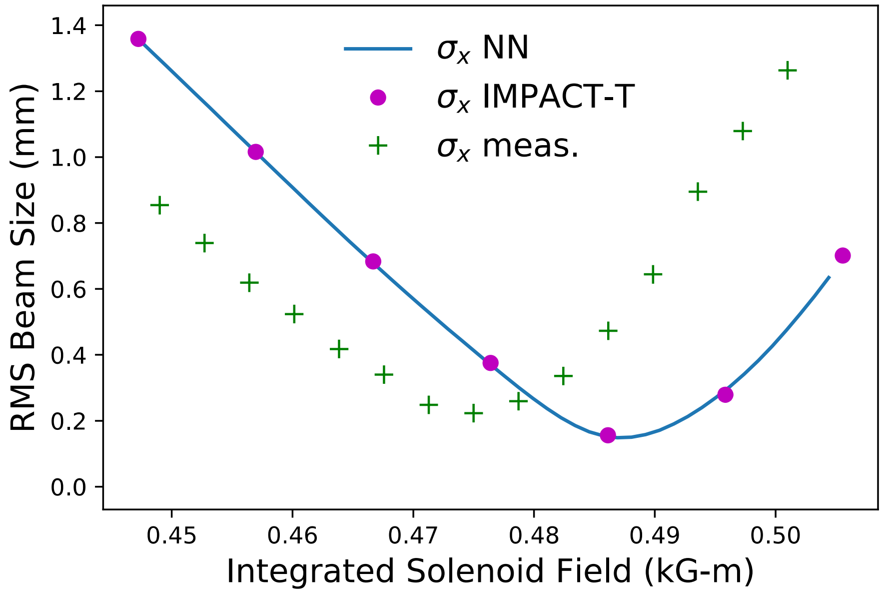


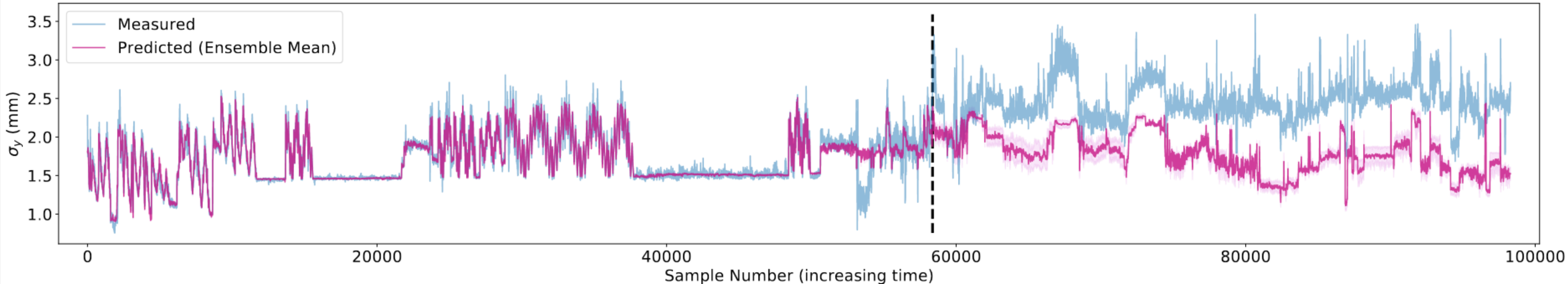
10 hours on thousands of cores at NERSC!

J. Qiang, et al., PRSTAB30, 054402, 2017

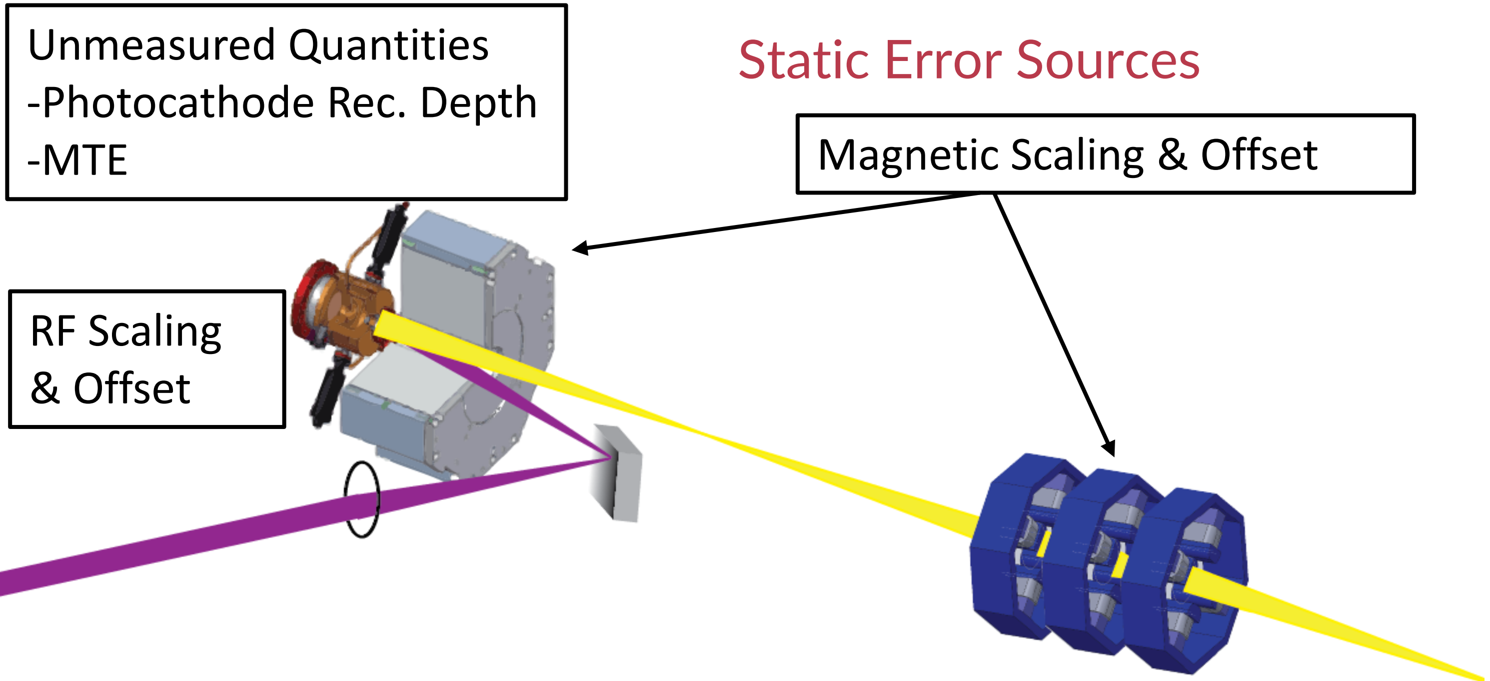
Model Calibration

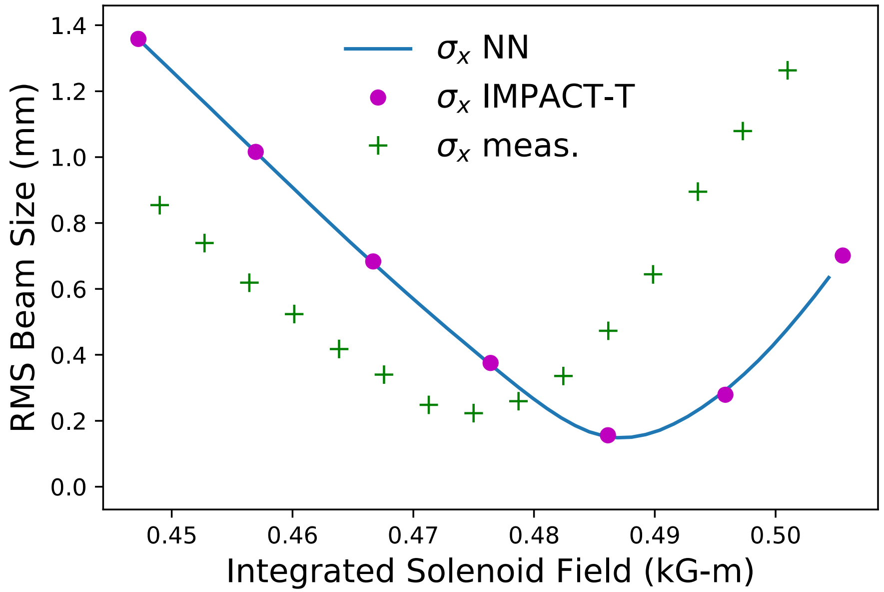


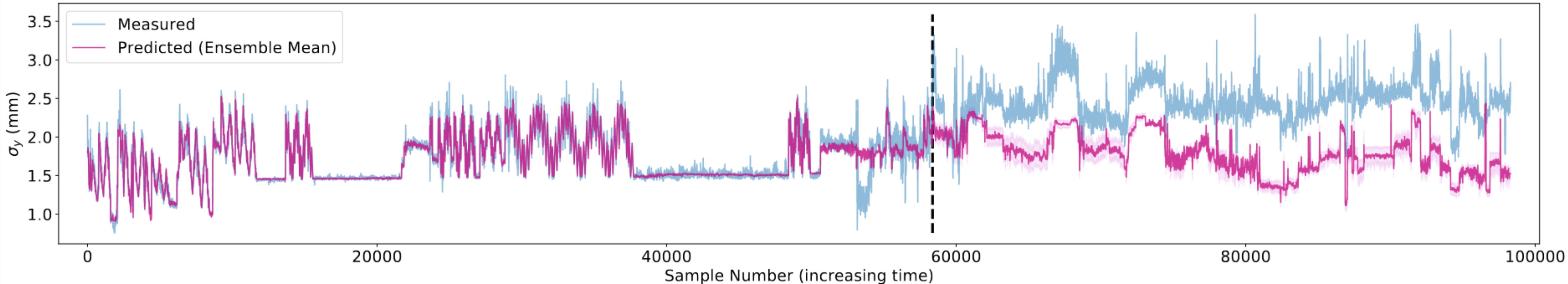




Model Calibration





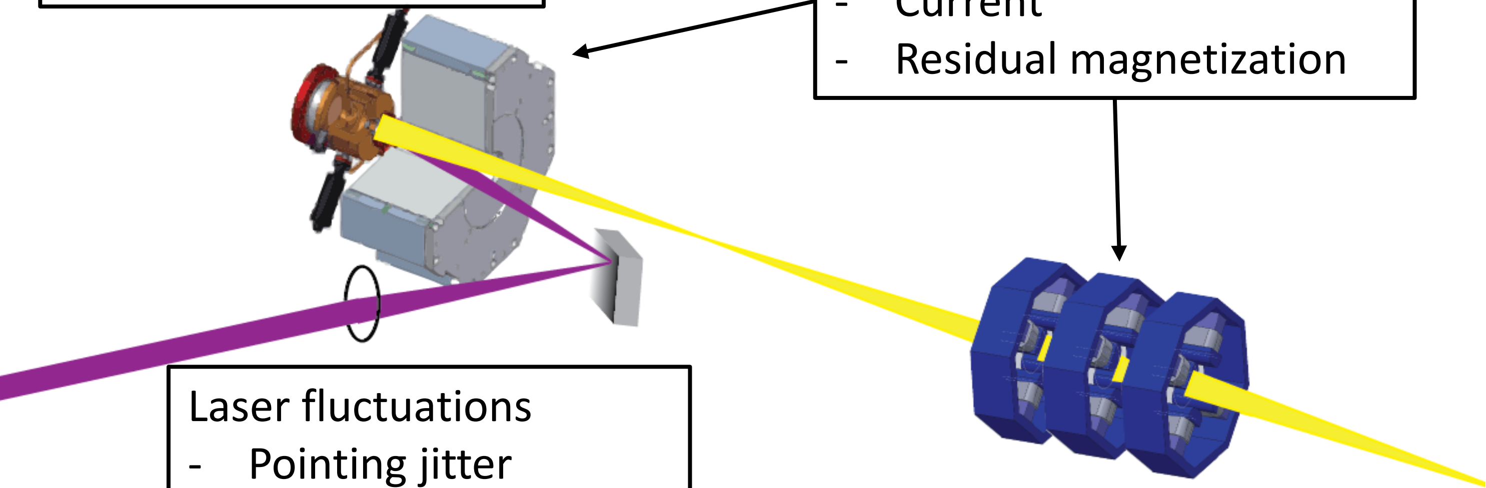


Model Calibration

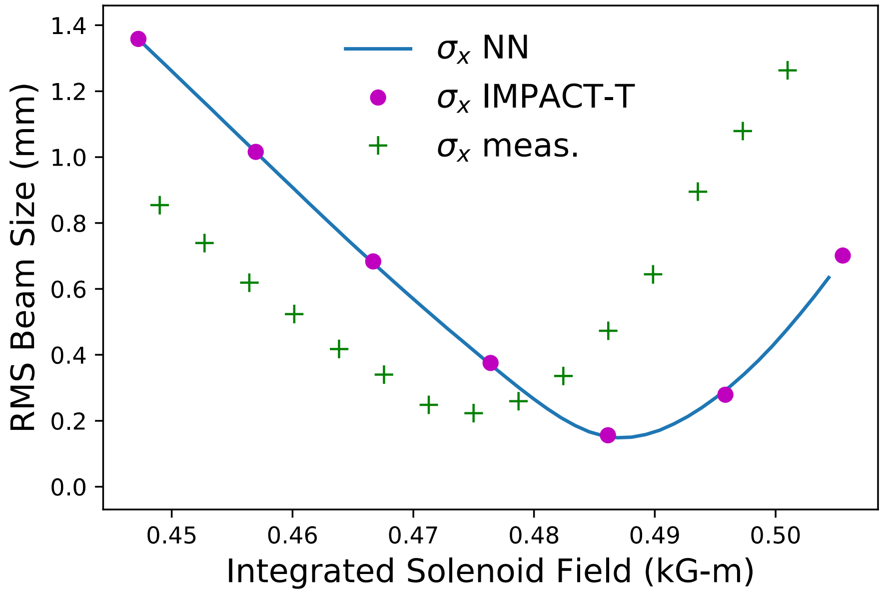
RF fluctuations
- Phase & Amplitude
- Amplifier drift

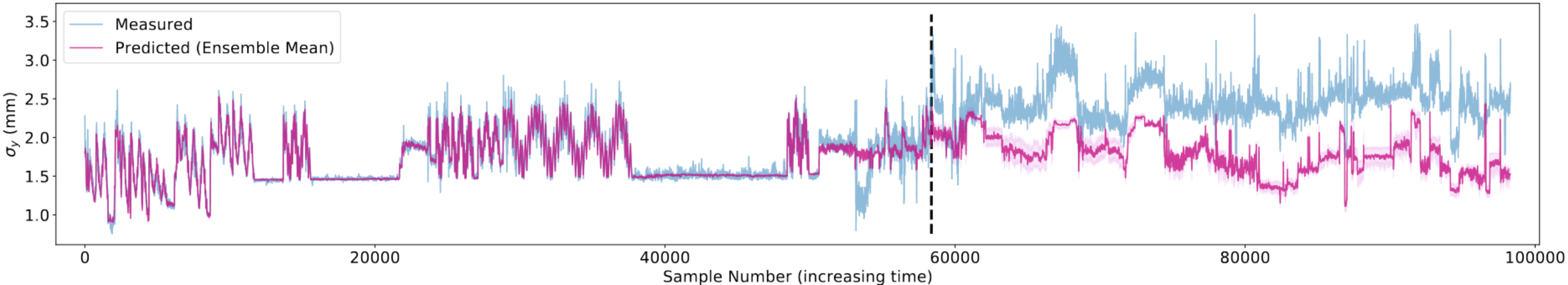
Time-Varying Error Sources

Magnet fluctuations
- Current
- Residual magnetization



Laser fluctuations
- Pointing jitter
- Intensity fluctuations

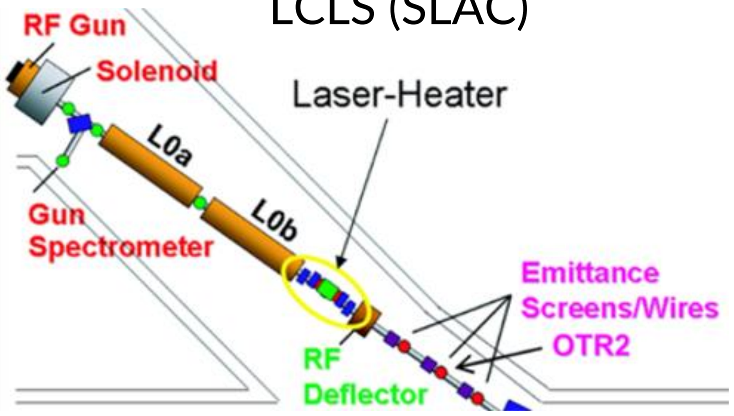


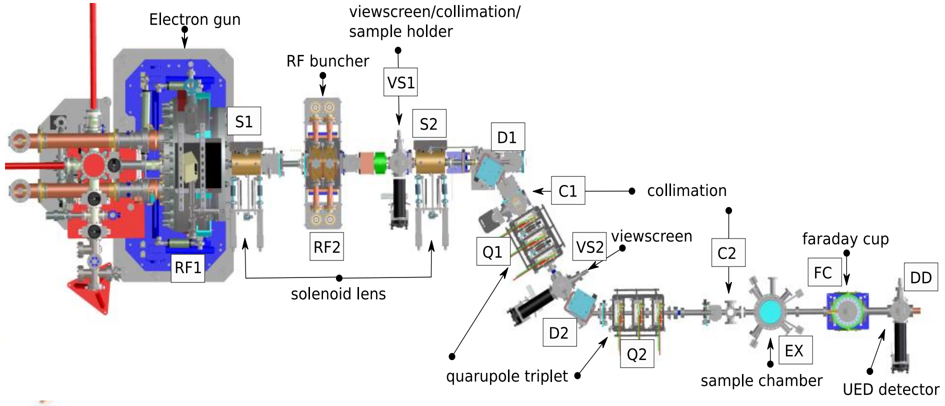


Outline

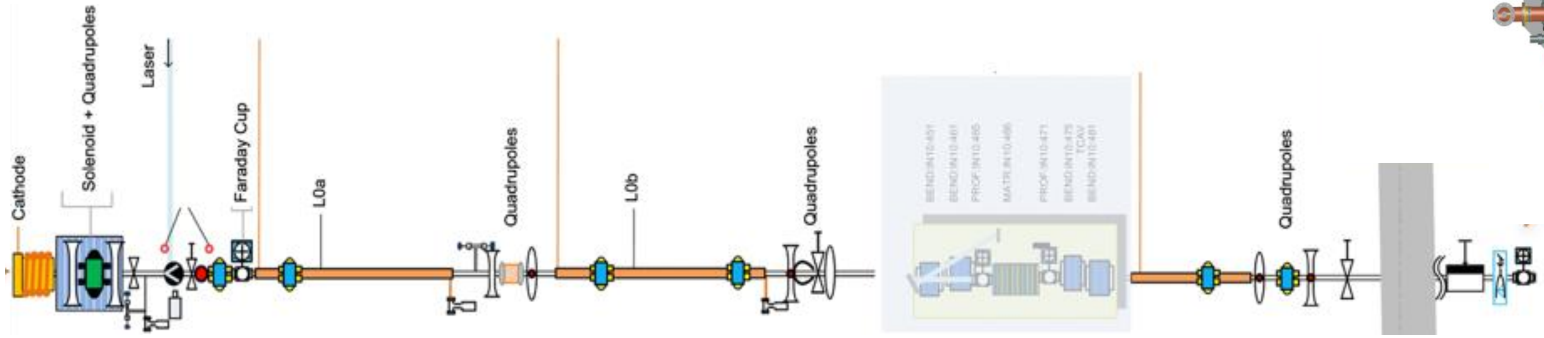
- Framing the problem
- Three examples:
  - MCMC at HiRES (LBNL)
  - Learning scaling factors & offsets at LCLS (SLAC)
  - Ongoing FACET-II (SLAC) model calibration
- Outlook

LCLS (SLAC)





HiRES (LBNL)



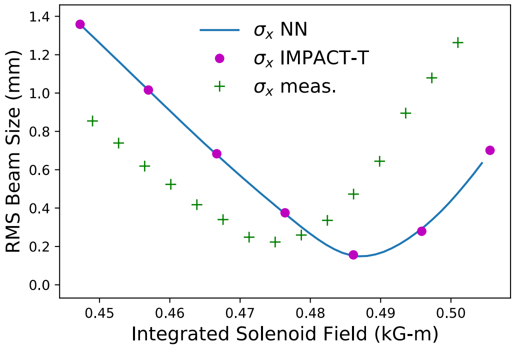
FACET-II (SLAC)

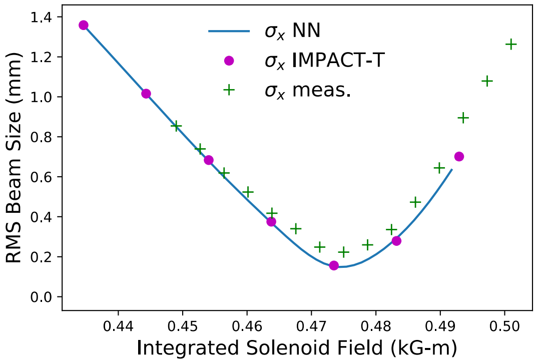
The Inverse Problem for Model Calibration

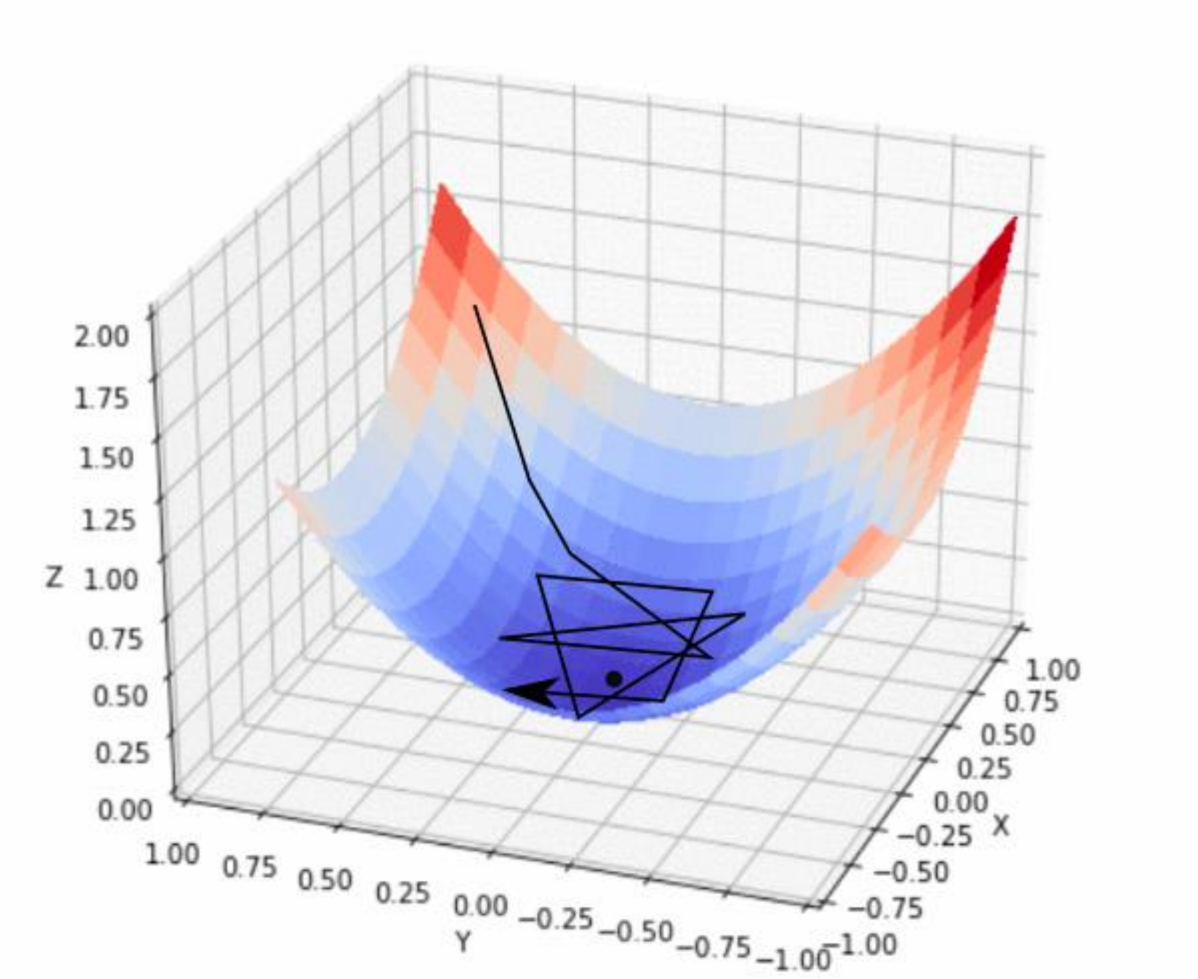
$$\arg\min \|d_{obs} - f(x_1, x_2, \ldots, x_n)\|_1$$

- Zeroth order solution: parameter scan
  - But with multiple dimensions, becomes untenable
- Considerations: choosing an approach
  - Model execution time/cost
  - Model types
  - Desired information
  - Amount of data

Consider Applications!



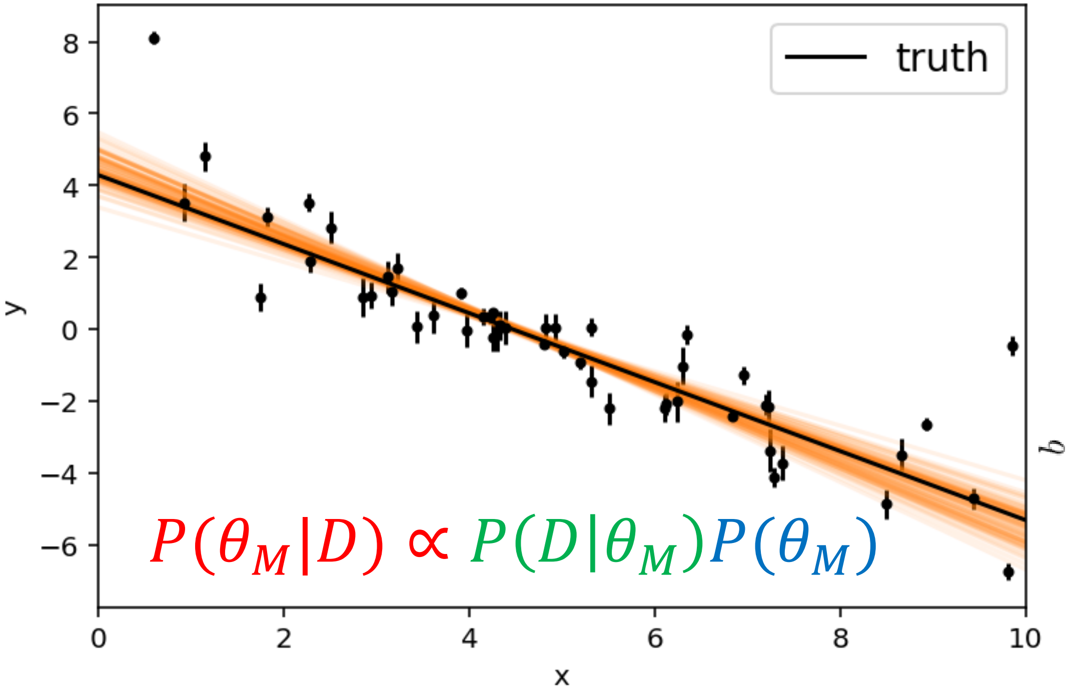


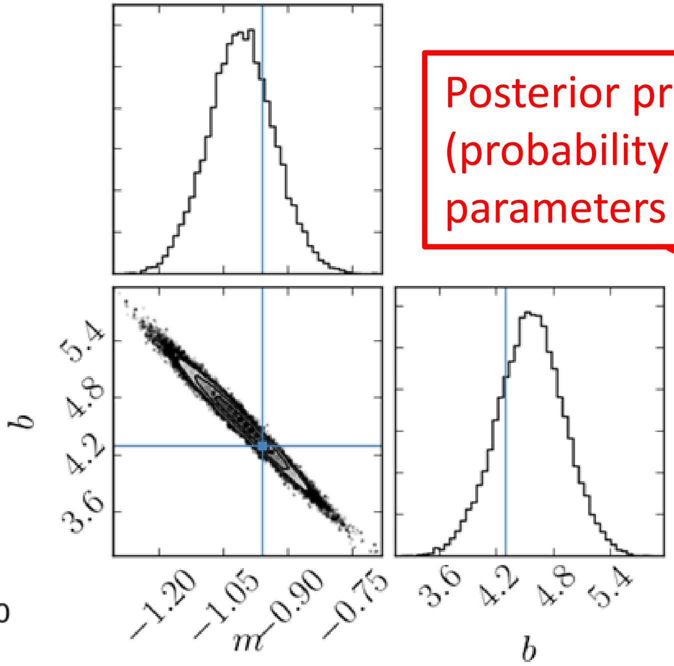


https://blog.paperspace.com/intro-to-optimization-in-deep-learning-gradient-descent/

Full Prob. Distributions: Markov Chain Monte Carlo (MCMC)

Figures adapted from https://emcee.readthedocs.io/





Likelihood function

Posterior probability (probability of model parameters given data)

Prior probability

$$P(\theta_M|D) = \frac{P(D|\theta_M)P(\theta_M)}{P(D)}$$

Probability of evidence (data): impractical to estimate

- Initialize walkers and have them update based on probability of proposed move
- Goodman and Weare "stretch move" proposal [1] (with Metropolis-Hastings [2] acceptance rule)
- Markov chain: future step depends only on current step

Advantages & Disadvantages

- **Full posterior probability distribution for optimization variables**
- Generally slower than optimization
  - **Requires fast-executing model**

[2] W. Hastings, Biometrika, 57: 97–109 (1970)
[1] J. Goodman and J. Weare, Communications in applied mathematics and computational science 5, 65 (2010)

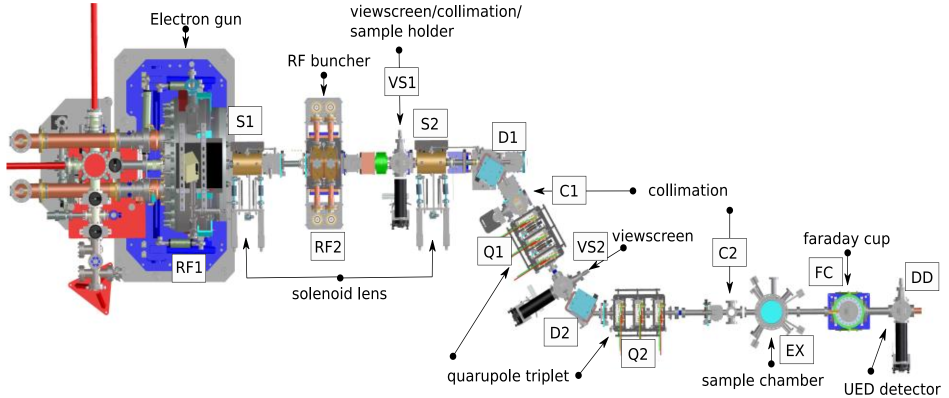
Example Problem and the Prescription

Example Problem

HiRES (LBNL) gun: matching beam dynamics (GPT) simulation to real data (using NN surrogate model)

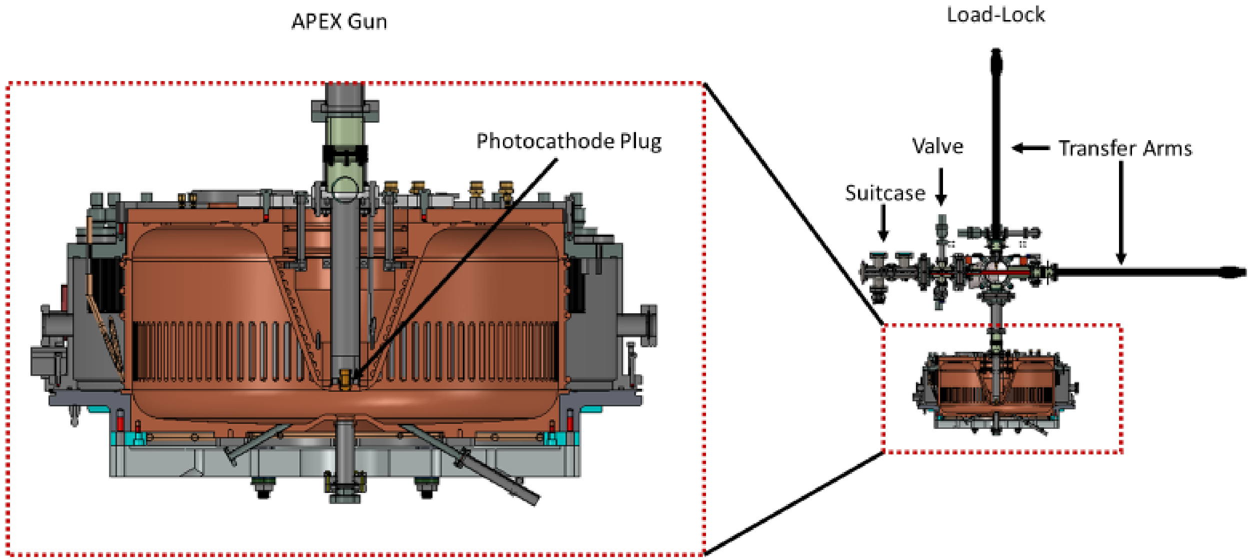
Find the following parameters based on beam second order moments in solenoid scan:

- Cathode MTE
- Beam energy
- Solenoid quadrupole moment
- Solenoid skew quadrupole moment
- Cathode recession depth



The Prescription

- Run GPT in parallel for rough parameter scan
- Train NN surrogate model
- MCMC sampling of surrogate model to match model to data



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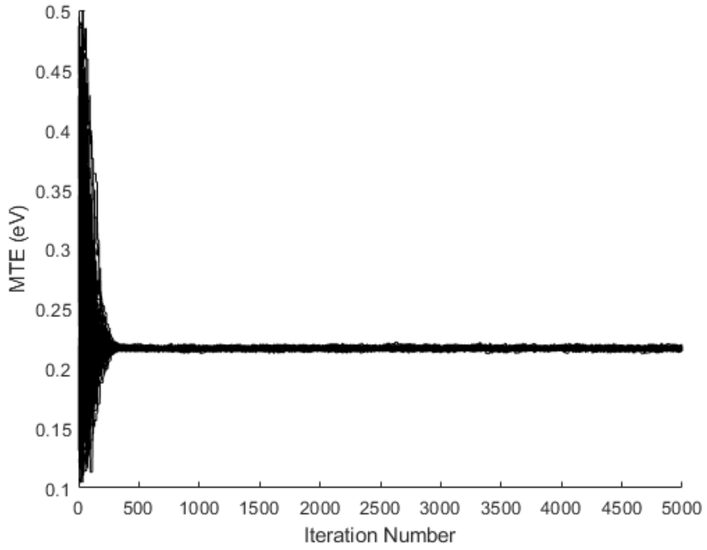
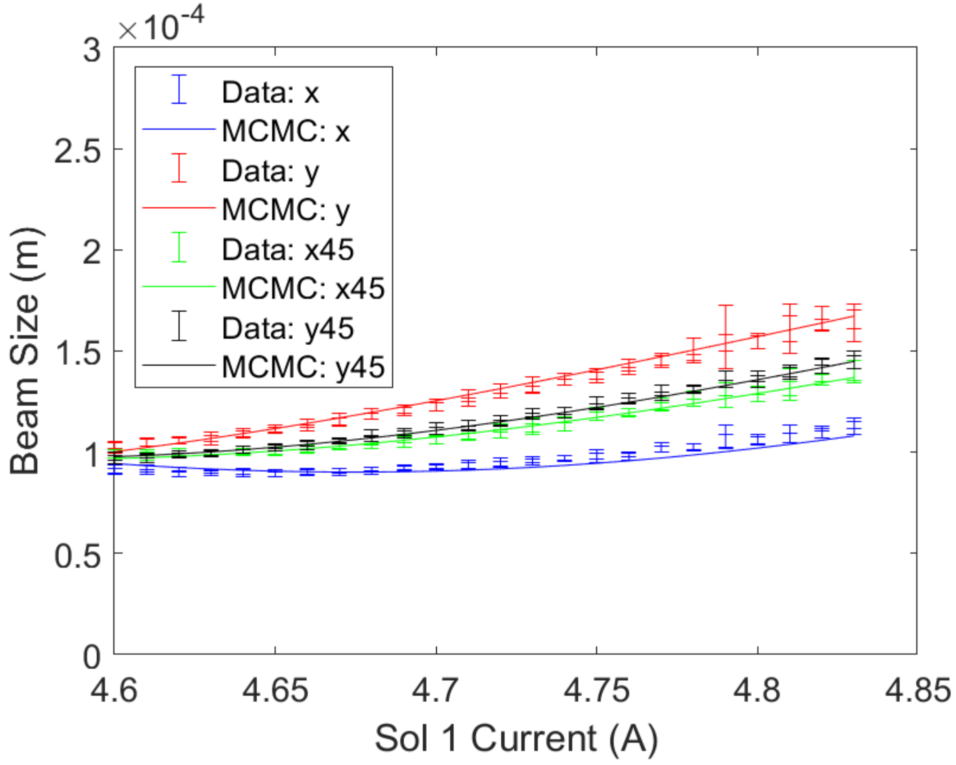
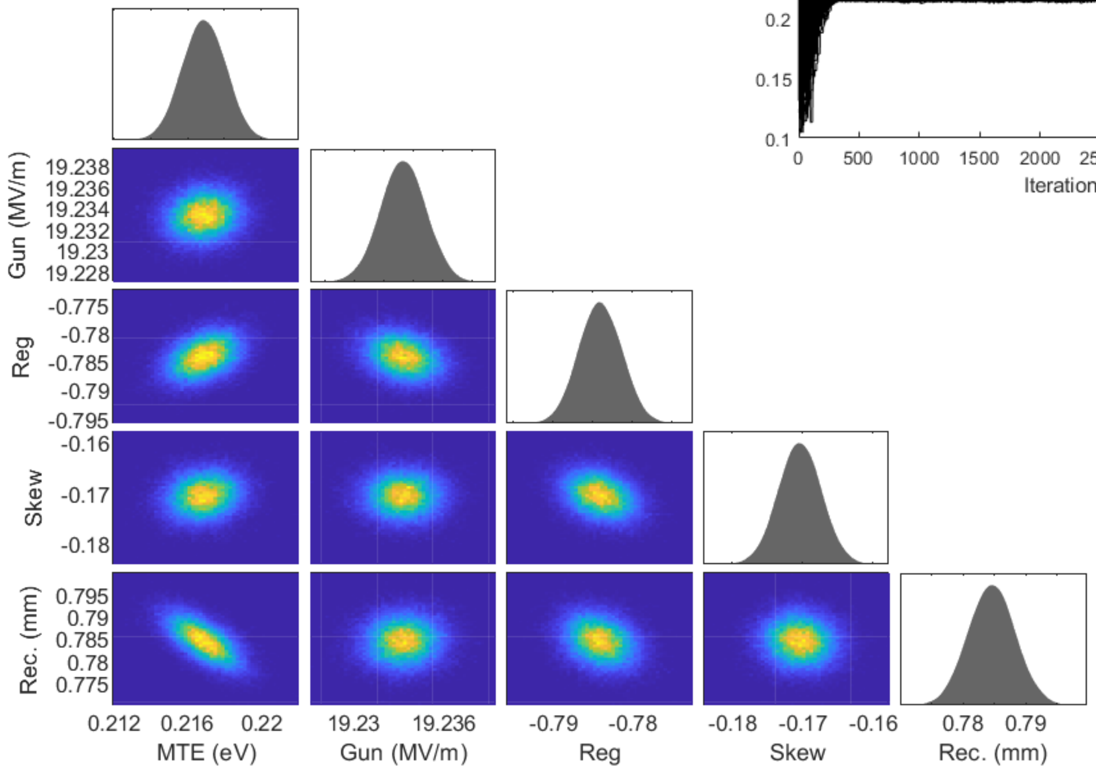
Comparison with local optimization

Below: Plot of posterior distributions
Middle: Walker positions throughout scan
Right: Plot of simulated solenoid scan (with data for comparison)



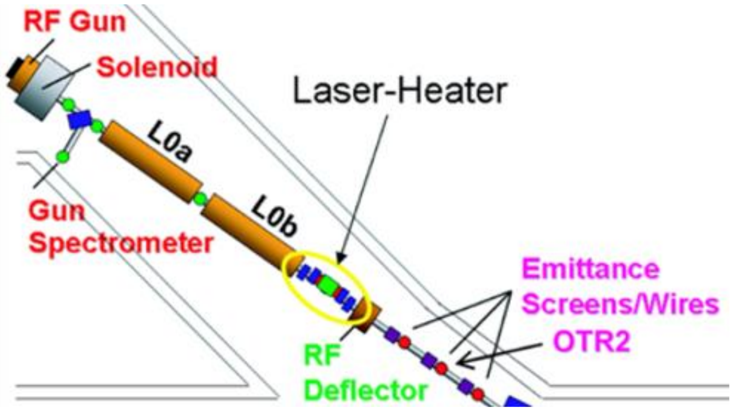


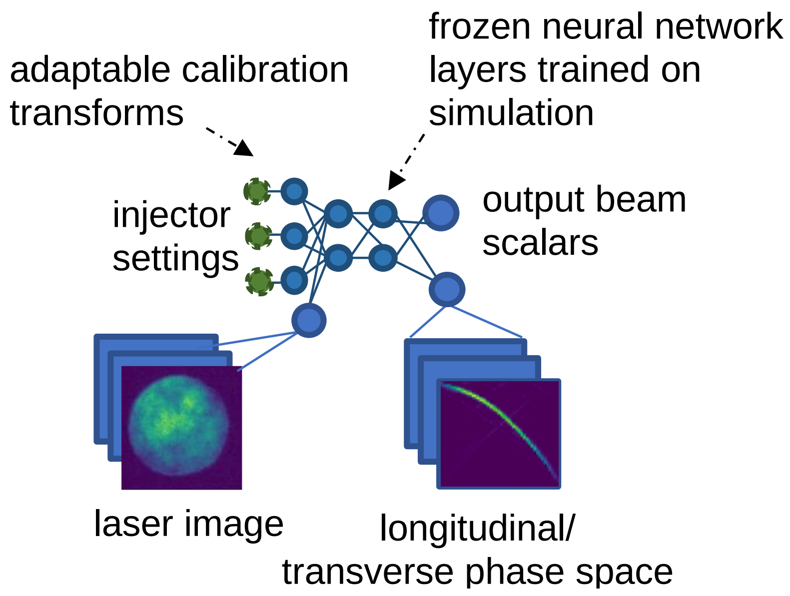


Parameter	Fmincon Value	MCMC Mean	MCMC Error
MTE (eV)	0.217	0.217	0.001
Field (MV/m)	19.233	19.233	0.002
Rec Depth (mm)	0.785	0.784	0.004
QCurr	-0.784	-0.784	0.003
SQCurr	-0.170	-0.171	0.003

LCLS Injector Calibration with a NN

- Trained neural network model on IMPACT-T
  - MOGA on the emittance and random sampling
- Freeze main representation, learn **scaling and offset** via **back-propagation**
- Linear approach: interpretability
  - Fast way of identifying possible error sources simultaneously
  - Similar to transfer learning, but interpretable





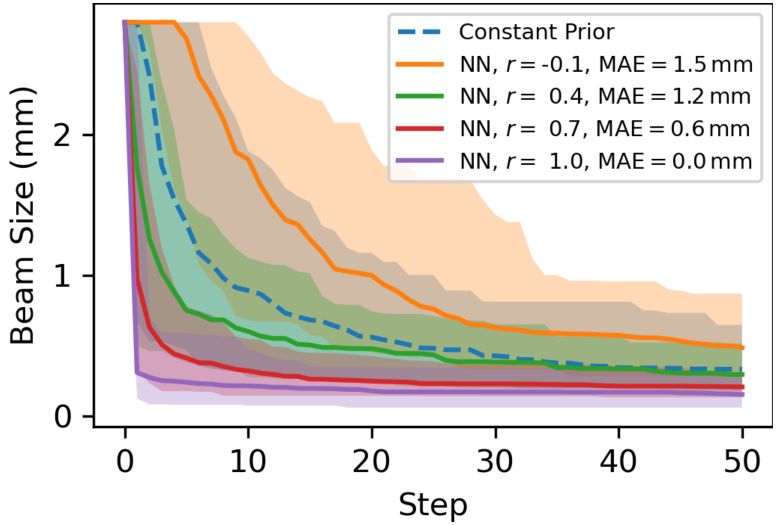
Inputs
Laser radius
Laser spot sizes
Pulse length
Charge
Solenoid
L0A phase
L0B phase
SQ quad
CQ quad
6 matching quads

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

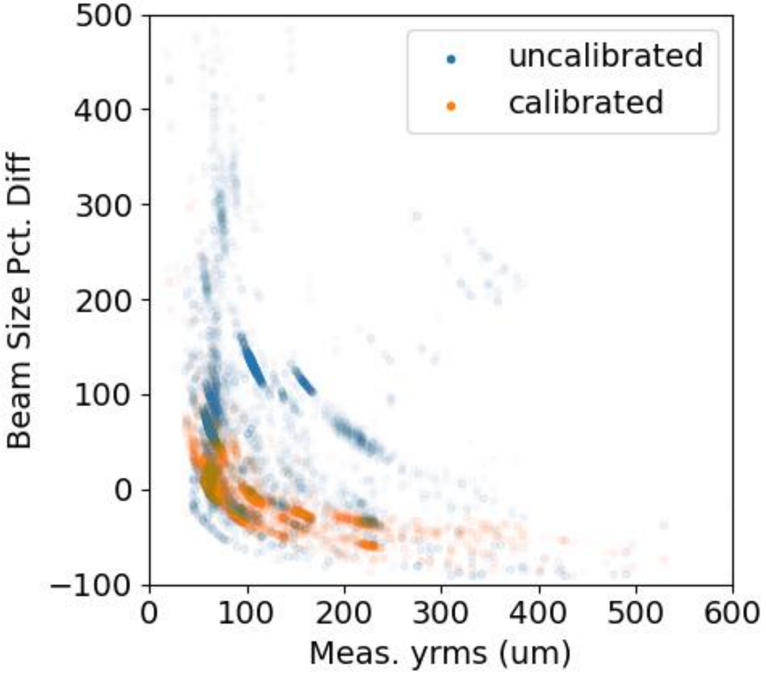
Recall Wednesday's talk from T. Boltz

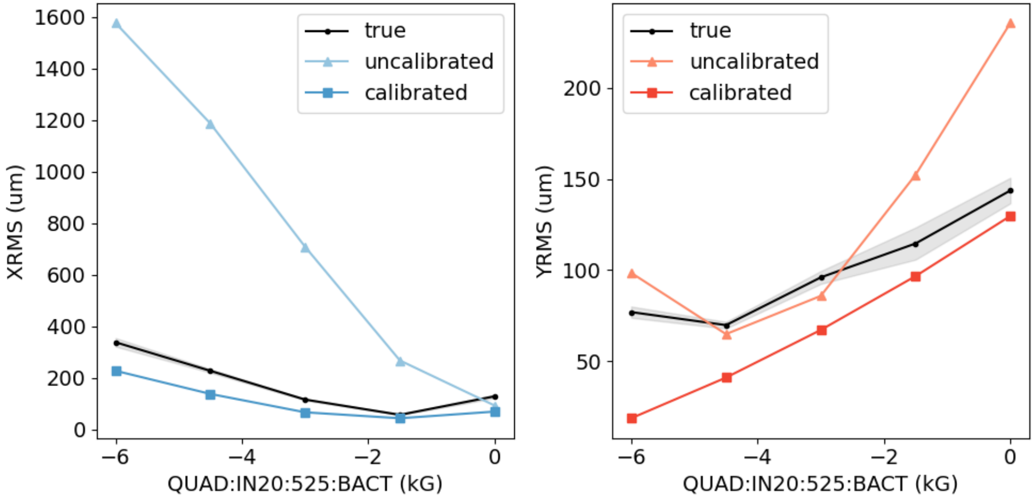
LCLS Example: Model Calibration for BO with NN Priors

- **Quality of the prior mean model is important to BO performance**
- Need to account for all changes in parameters/inputs over time
- Number of required samples depends heavily on the data distribution



Dataset	N. Data Points
train	36020
val	17671
test	10011





Science and Technology Facilities Council
ISIS Neutron and Muon Source

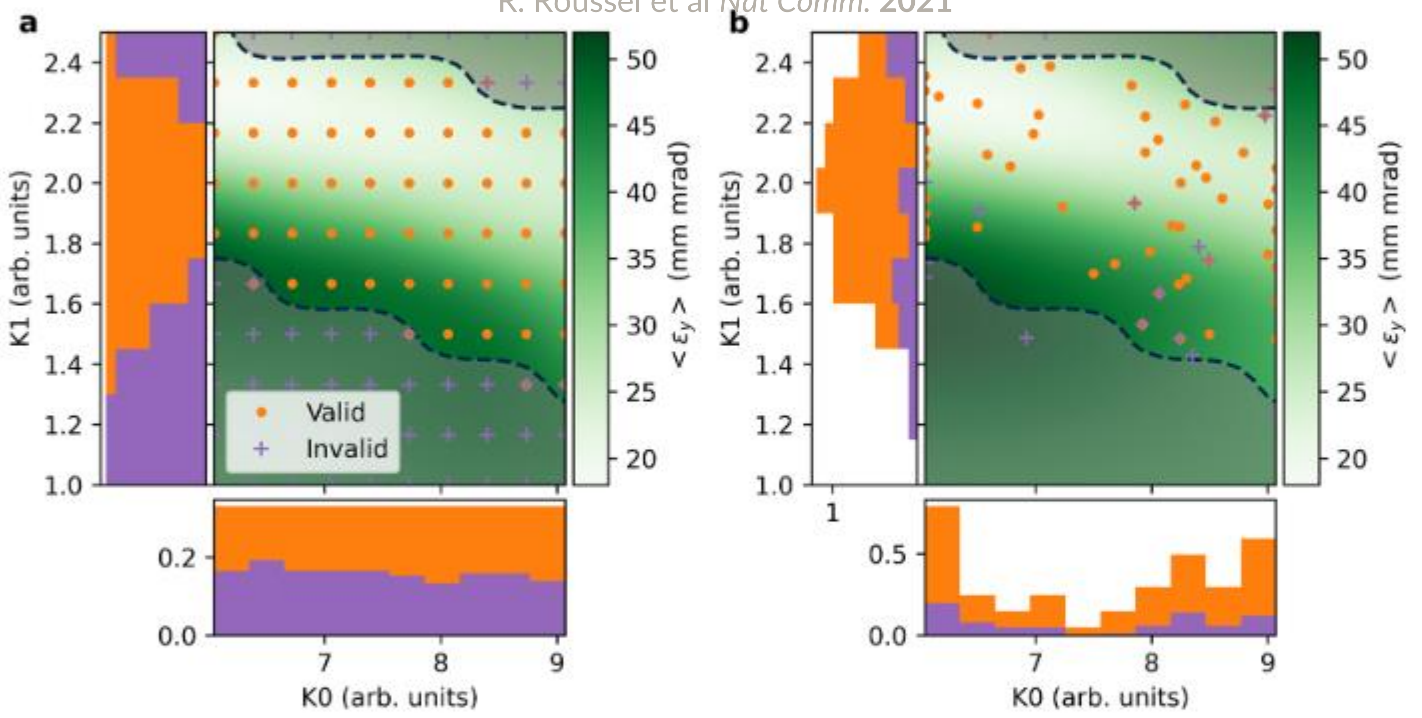
SLAC

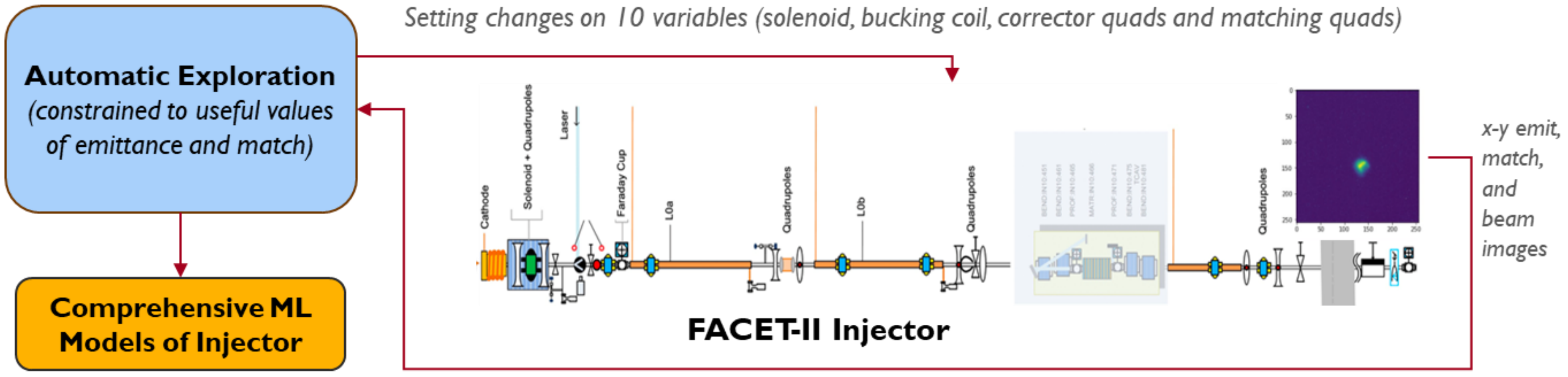
T. Boltz et al. arXiv:2403.03225

Well-distributed data

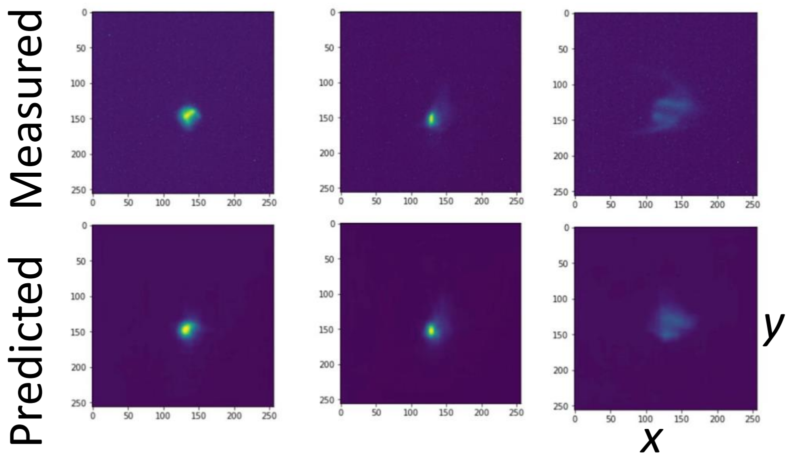
R. Roussel et al *Nat Comm.* 2021

- Bayesian Exploration for **efficient exploration**:
  - Time efficient
  - Well-distributed data
- FACET-II: **2 hrs for 10 variables compared to 5 hrs for 4 variables with N-D parameter scan**
- Data was used to train neural network model of injector response predicting x-y beam images.
- GP ML model from exploration predicts emittance and match.



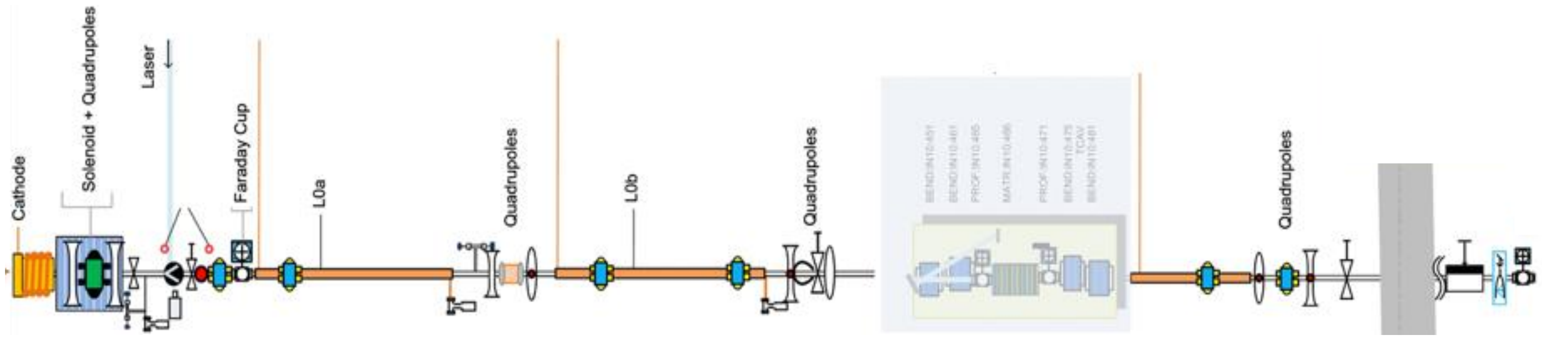


transverse beam profile



SLAC

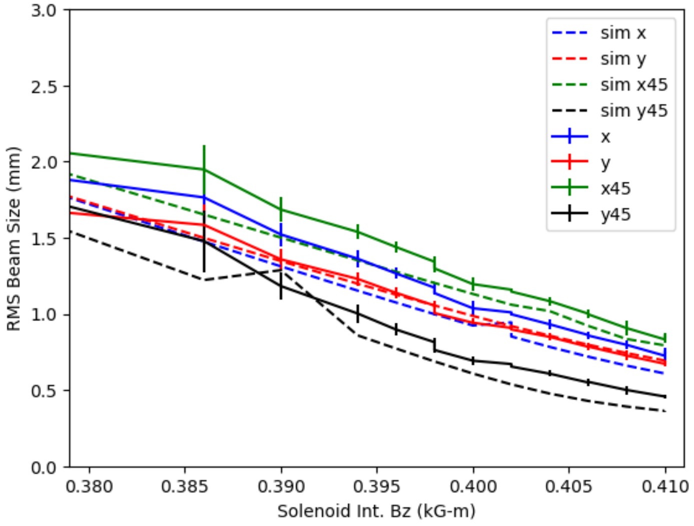
In Progress: FACET-II Model Calibration

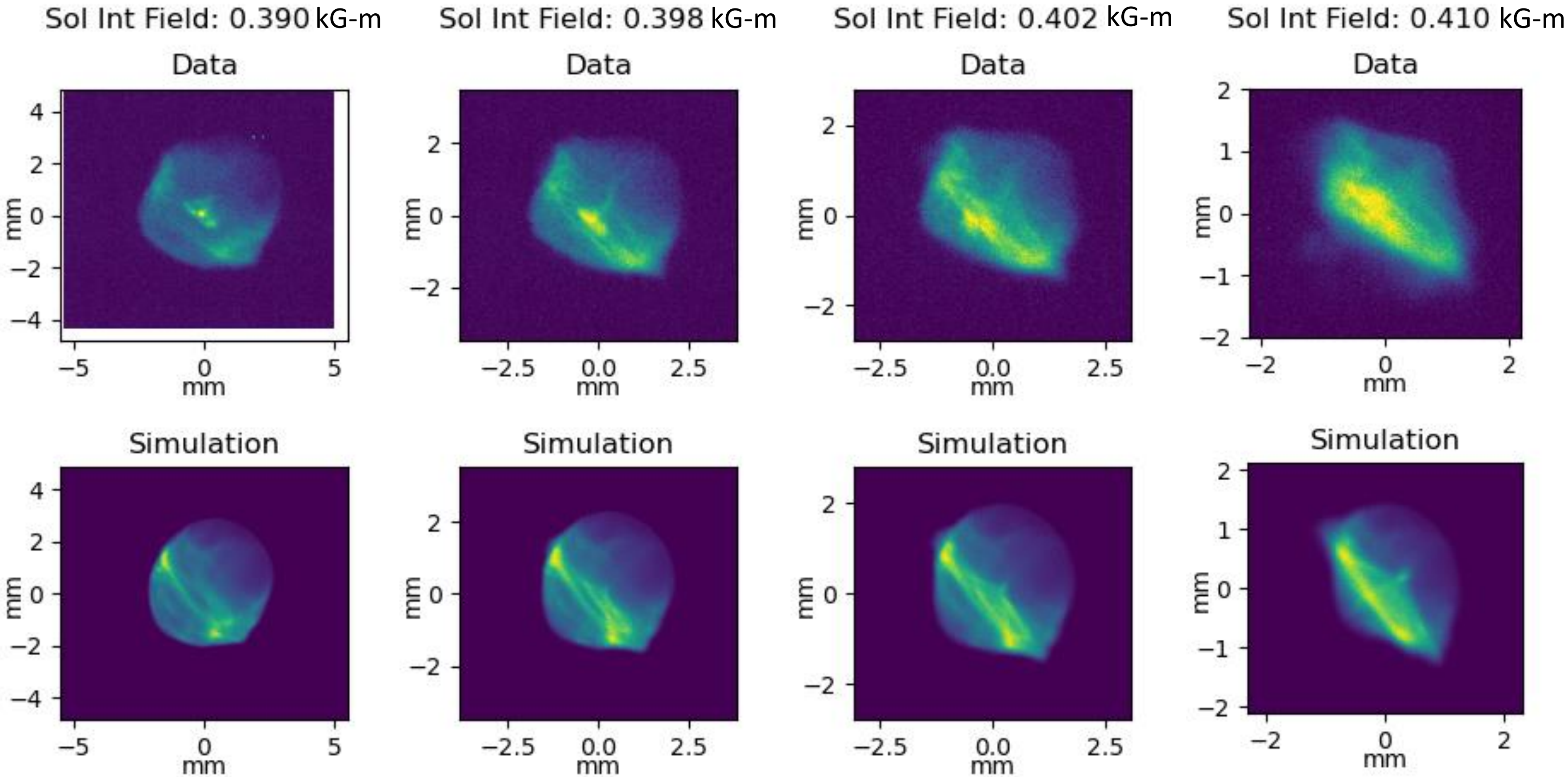


- High charge beams --> plasma experiments
- Want start-to-end simulations so users can optimize their experiments

Second-Order Moments from Solenoid Scan (Below)

Selected Images from Solenoid Scan (Right)

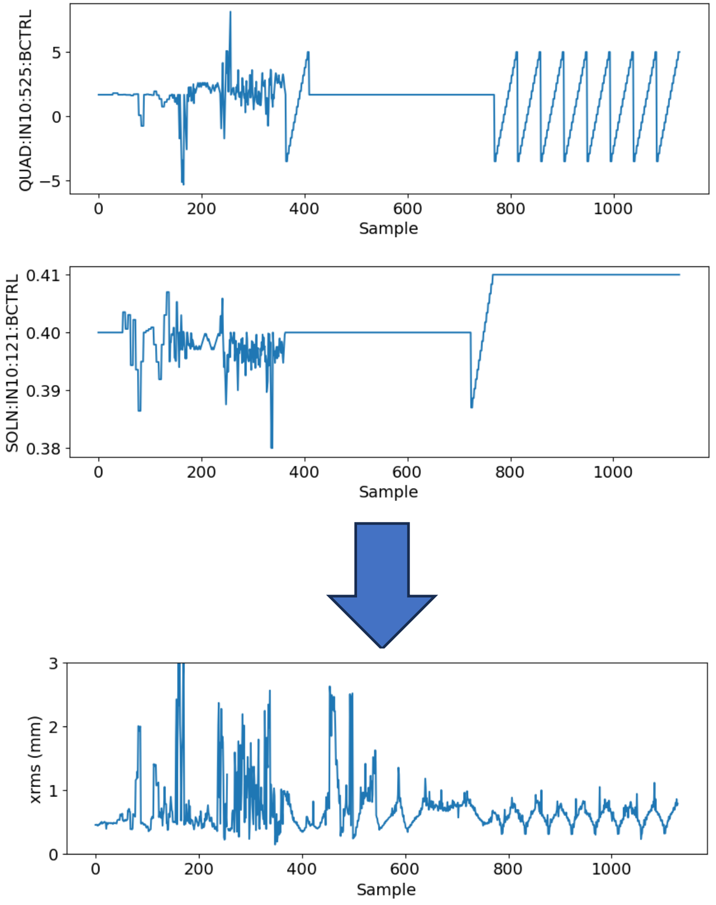




Recall Wednesday’s talk from R. Lehe

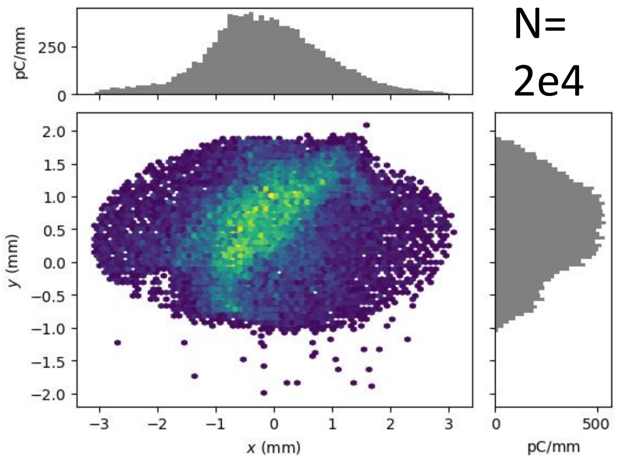
FACET-II & Multifidelity Optimization

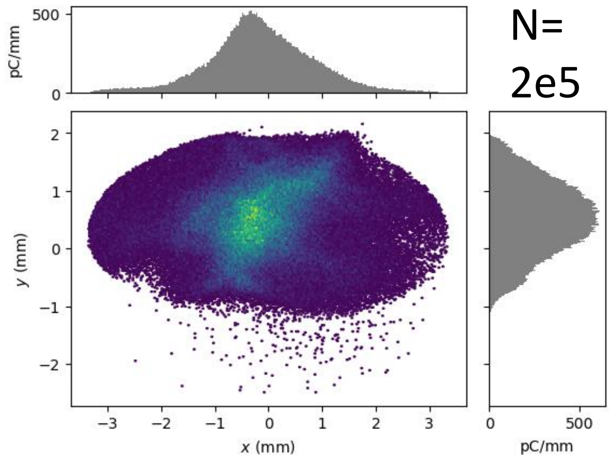
Bayesian Exploration

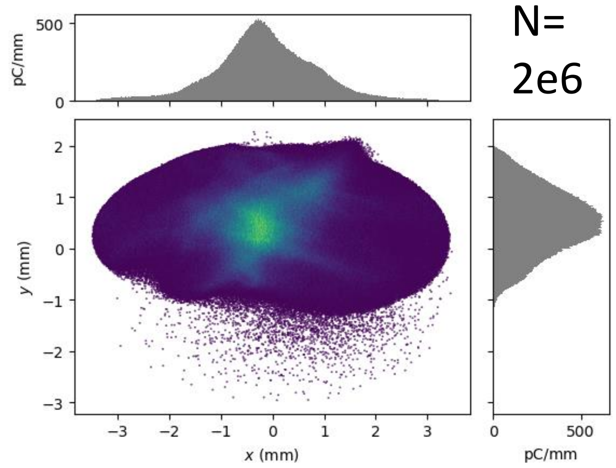


- Information theoretic approach to simulations
- Learn correlations between different model fidelities
- Use multi-fidelity Bayesian optimization to select model fidelity

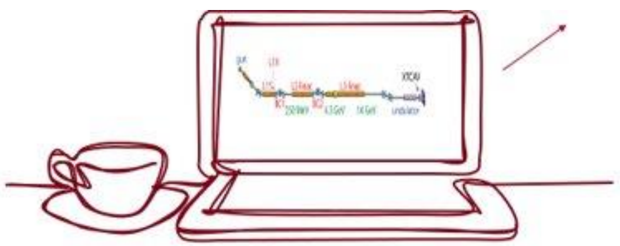
Number of Particles (N)	2e4	2e5	2e6
Space Charge Grid Size	16	32	64
Execution time	~1 min	~2.5 min	~25 min
σ_x (um)	1026	1018	1017
σ_y (um)	654	623	614
Norm x emit (um)	9.26	8.87	8.77





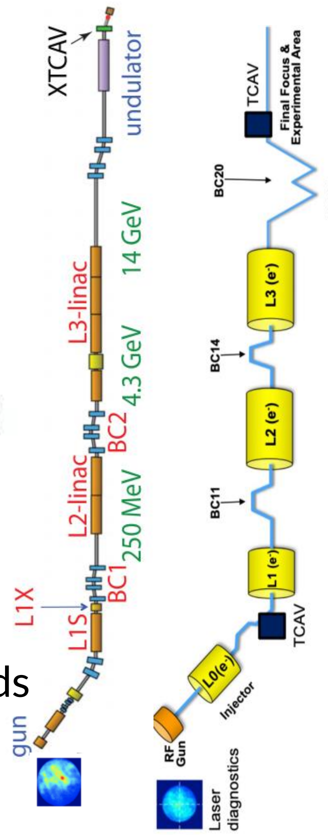


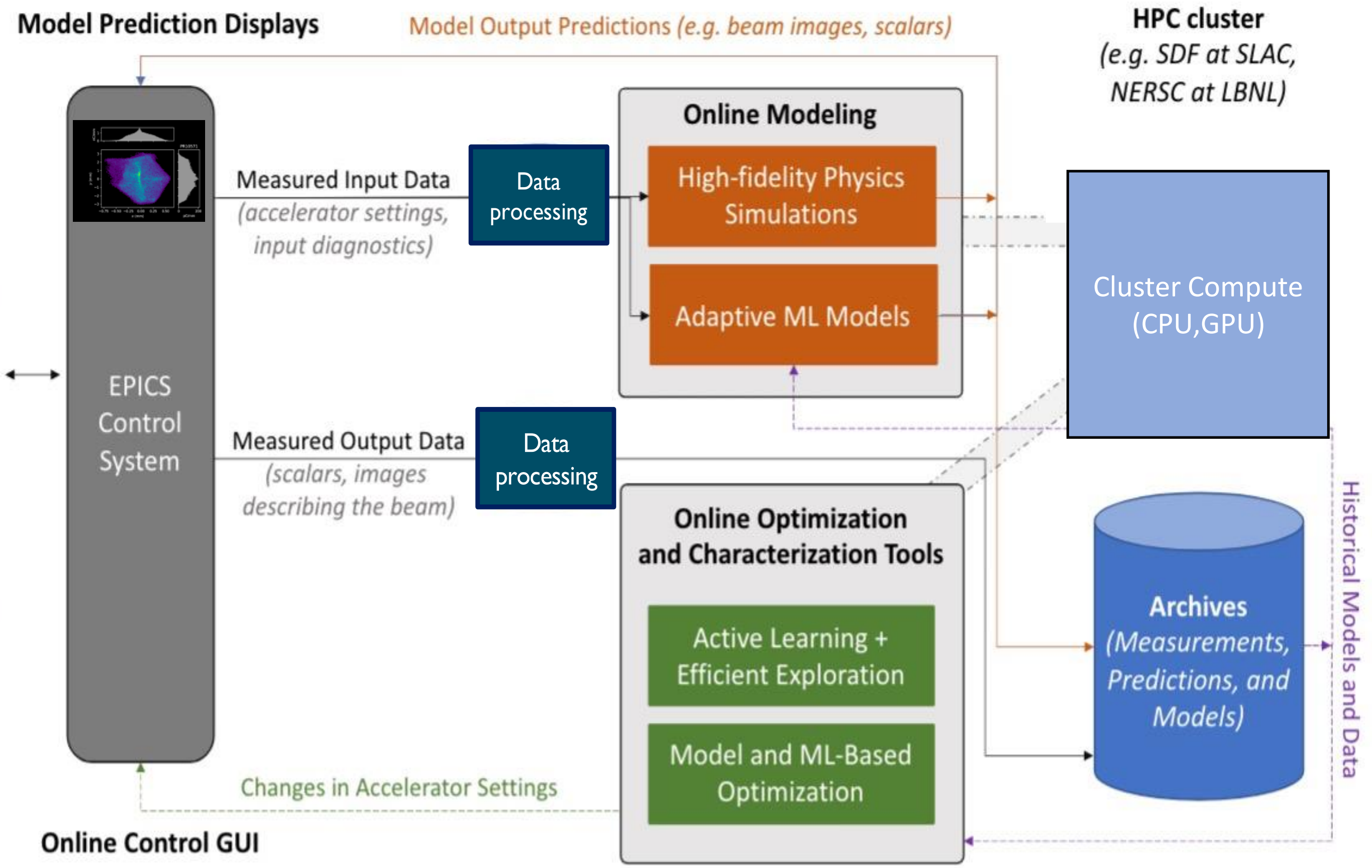
Future: Full Integration of AI/ML Optimization, Modeling, and Physics Simulations



digital twins + online modeling
(fast sims, differentiable sims, model calibration)

- Ultimately, model calibration → full digital twin
- Infrastructure being built to these ends





Part of a larger effort

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

Differentiable simulations, including Bmad

Model calibration for RHIC

Acknowledgements

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Questions?