Applications of Machine Learning to Analysis and Computation for Particle Accelerators

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Outline

- Overview of accelerators, their applications, and why we're interested in ML
- Current efforts to apply ML to accelerators
  - *Anomaly detection and data cleaning*
  - *Virtual diagnostics and on-line modeling*
  - *Surrogate modeling and optimization*
- Summary

Particle accelerators and their applications

Electron Accelerators

E-Beam sources
(Electron sources for a range of applications)

- Cancer treatment
- Polymer linking
- Wastewater treatment

Free electron lasers
(Highly tunable coherent photon sources ranging from IR to Hard X-Ray)

- Basic research
- Directed energy
- Industrial research

Synchrotron light sources
(Tunable photon sources usually in the x-ray)

- Basic research (NSLS-II, APS)
- Materials science, biology, etc.

Hadron accelerators

Proton accelerators

- High flux neutron sources (SNS)
- Accelerator driven subcritical reactors
- Basic research (fixed target and colliders)
- Cancer treatment

Ion accelerators

- Basic research (nuclear physics)
- Cancer treatment
- Isotope production

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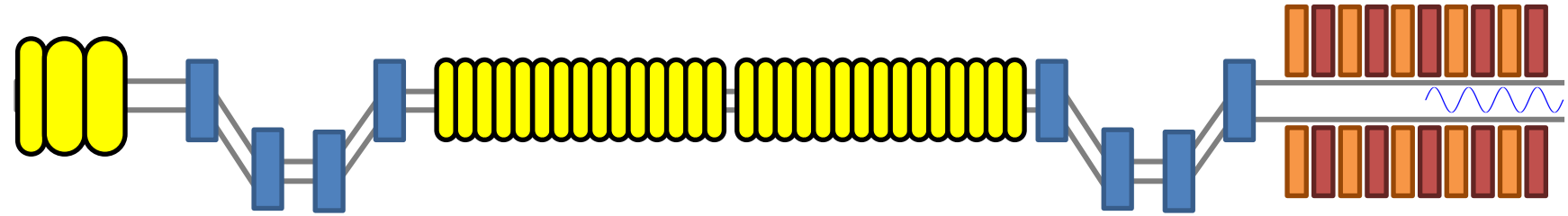
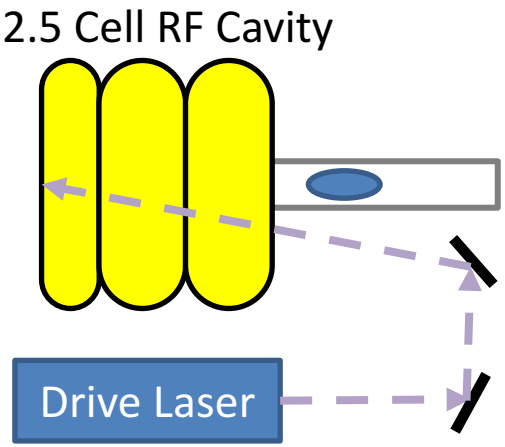
See DOE Report "Accelerators for America's Future"
(https://science.energy.gov/~/media/hep/pdf/accelerator-rd-stewardship/Report.pdf)

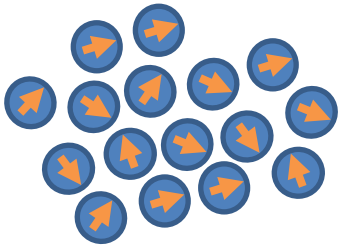
Electron sources for context



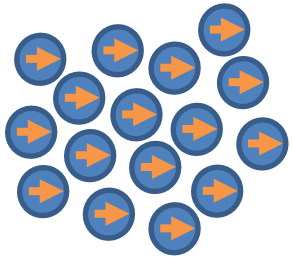


Emittance: a measure of beam quality

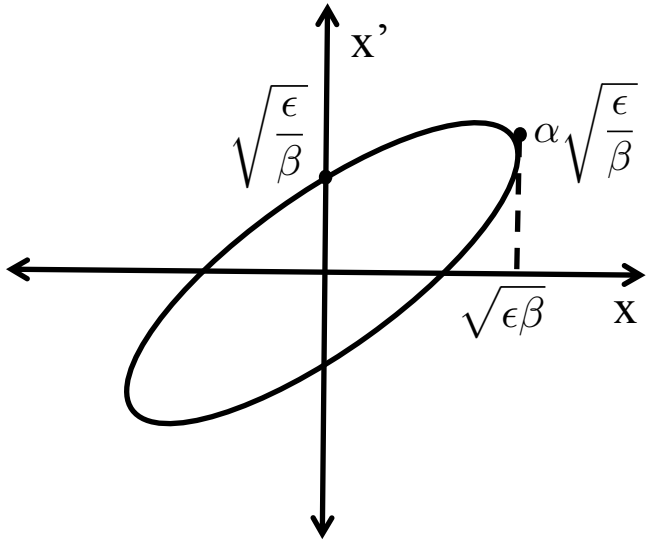
High degree of disorder – high emittance



Low degree of disorder – low emittance



- Beam ellipse in x-x' phase space with important parameters noted:
- Beta – beam envelope function
- Alpha – change in the beam envelope function
- Epsilon – beam emittance



Why are we interested in machine learning?

- Accelerator facilities rely heavily on human operators for tuning/control

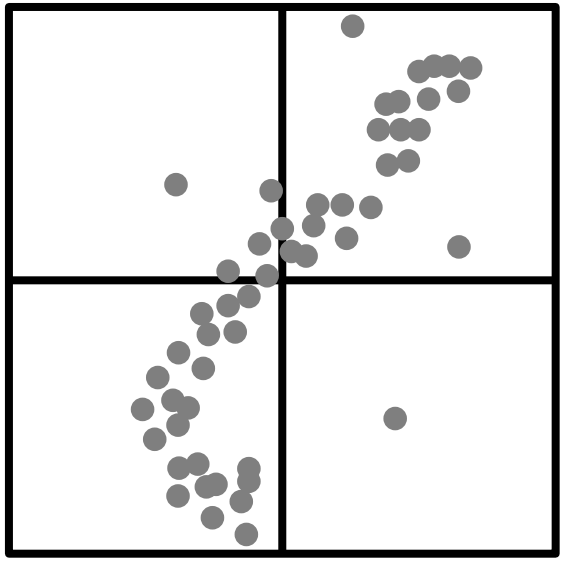
- Modeling and control of these machines is challenging
  - *Nonlinear systems with large parameter spaces*
  - *Variety of diagnostics (e.g. beam images), but these are limited and number, and some are not continuously available for use*
  - *Time-varying/ non-stationary behavior*

- Strong incentives for improving control (and understanding system)
  - *High user demand → want to switch between custom user requests quickly*
  - *High cost for unintended down-time → personnel time, user time, scientific output*
  - *Achieve challenging beam setups for new science goals*

Fast, accurate accelerator models → aid operation, model-based control, prototyping and experiment planning, design of new setups

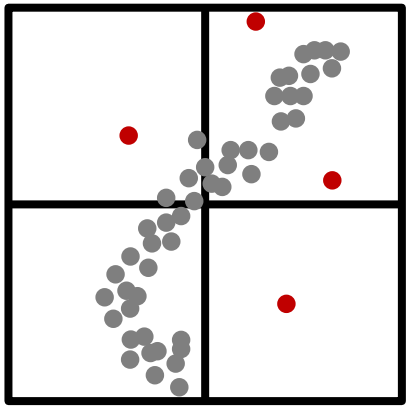
Application: Data Cleaning

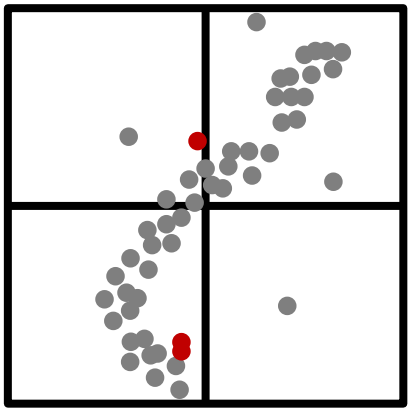
What do we mean by data cleaning?



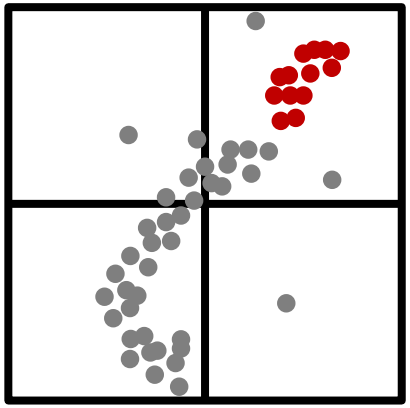
Raw data
(measurement or
simulation)

Obvious Outliers
(bad data or simulation run)





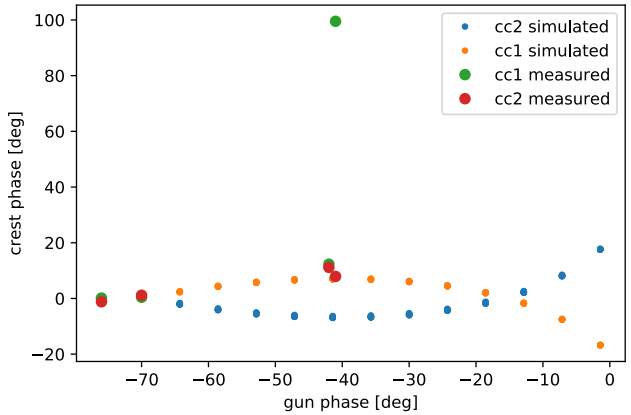
Subtle Outliers
(possible anomalies)

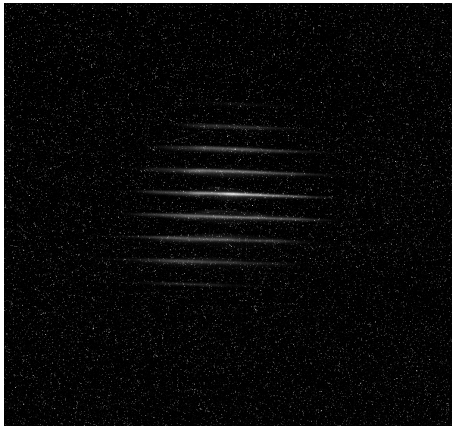


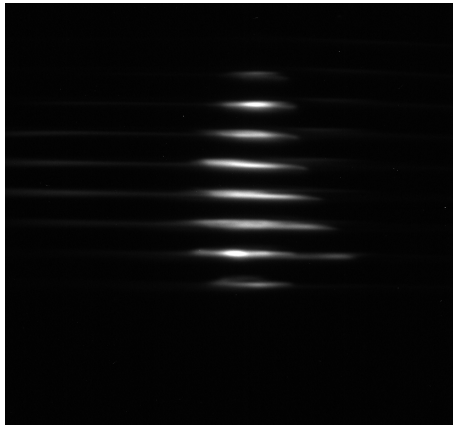
Discontinuities
(change in calibration or
machine state)

Case study: Simulations of the FAST Accelerator

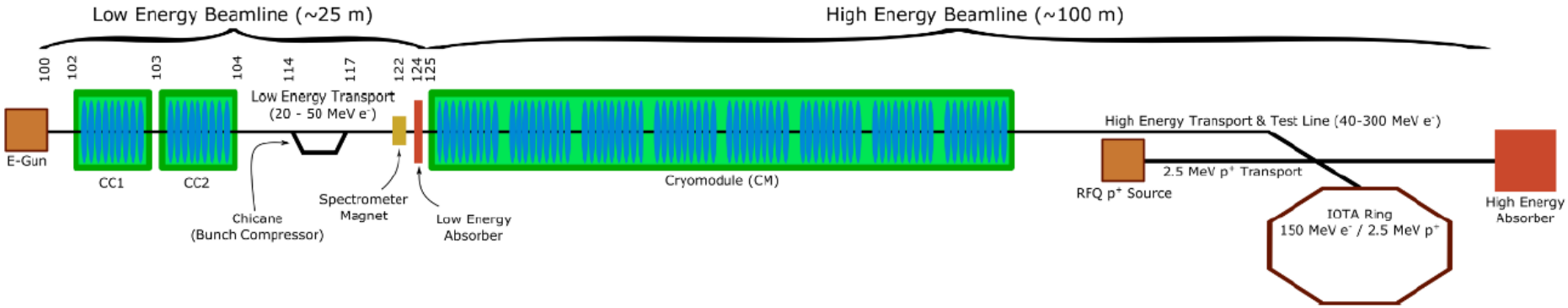
- Explore the use of unsupervised learning for automatic data cleaning using case studies:
  - *Start simple*
    - Batch simulation scans
  - *Increase complexity:*
    - Classification of machine drift
    - Multi-slit emittance measurements (images)

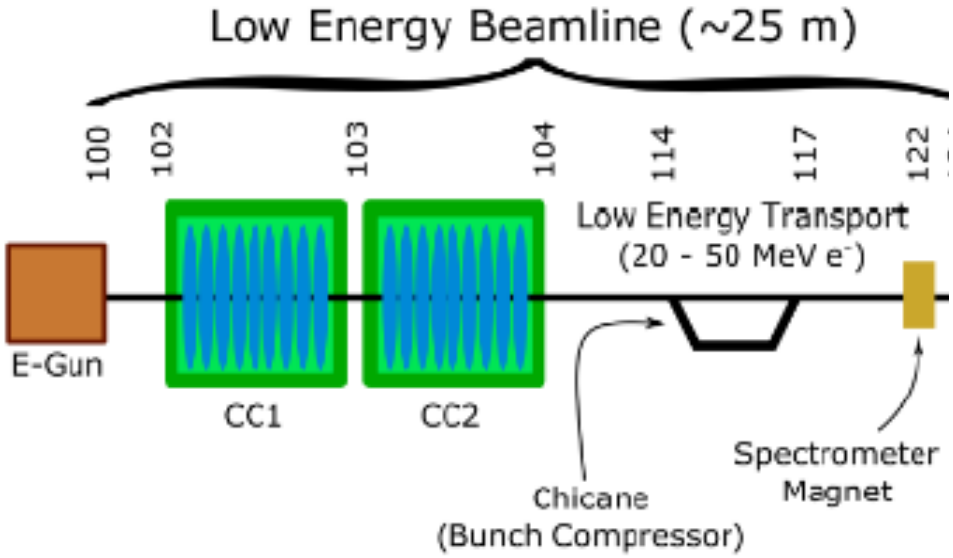






The Fermilab Science and Technology Facility

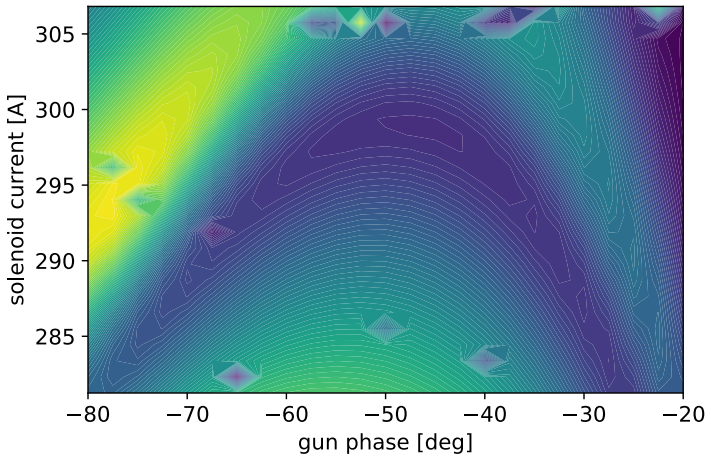


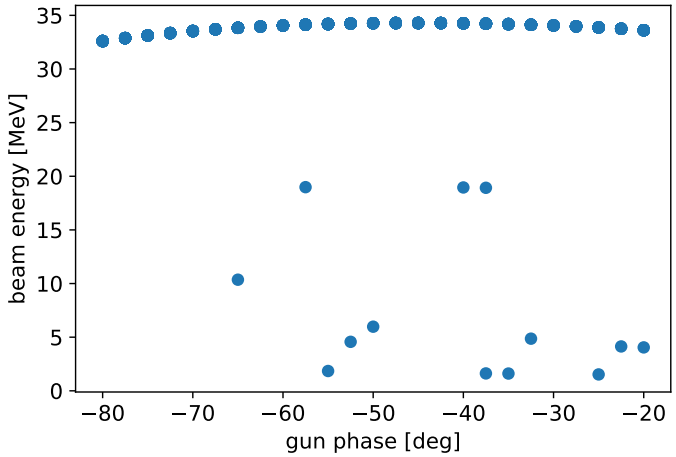


- Simulations start at the cathode and run up to x117
- Photo-cathode RF Electron Gun accelerates the beam to 4.5 MeV
- Superconducting RF cavities accelerate the beam to ~40 MeV

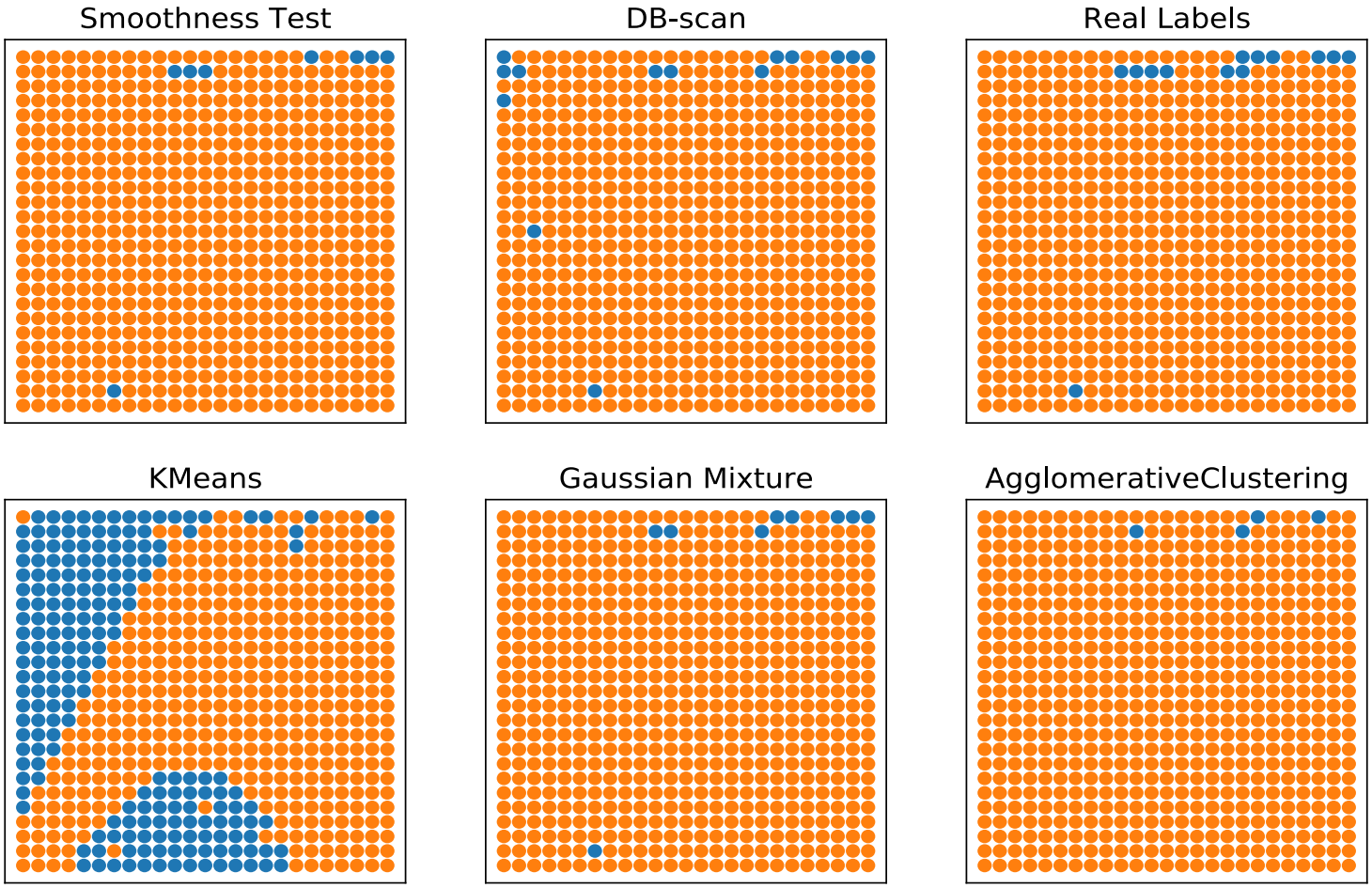
2-D Simulation scan data

- 2-D scan of gun-phase and solenoid strength
  - *Run on high performance computing, (Linux cluster with 100 cores)*
  - *Some simulations terminated unexpectedly*
  - *Remove unwanted data from dataset*
- Energy is the cleanest indicator of good vs. bad
  - *Use this to label dataset but exclude from clustering analysis*





Identification of bad simulation runs



Orange: Identified good run
Blue: Identified bad run

Identification of bad simulation runs

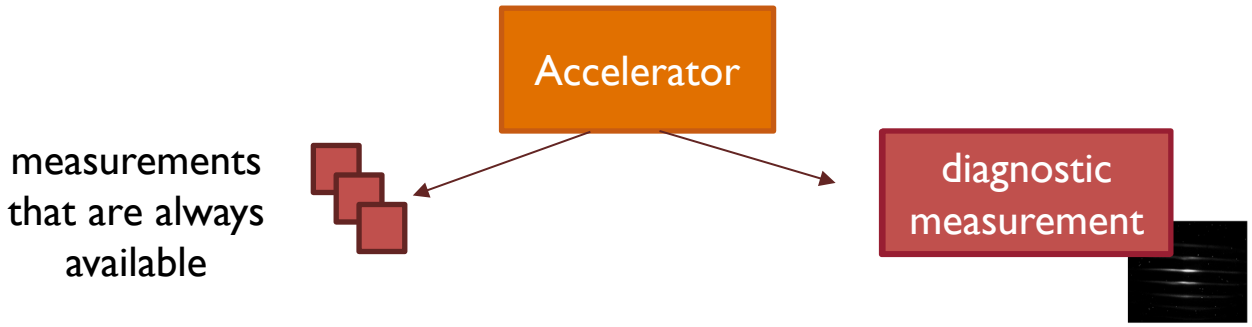
	K-means	DB-Scan	Gaussian Mix	Agglo	Smoothness
Percentage Correct	67.2%	98.6%	99.4%	98.6%	99.2%
Correctly Identified Bad Runs	3/13	9/13	9/13	4/13	8/13
False Positive	10/13	4/13	4/13	9/13	5/13
False Negative	195/612	5/612	0/612	0/612	0/612

False Positive: Predicted to be good but are actually bad. False Negative: Predicted to be bad but are actually good

- DB-Scan/Gaussian Mixture/Smoothness have similar performance
- K-means and Agglomerative are both poor performers
- Gaussian mixture is a very good option for this dataset as specification of hyper-parameters is easiest and zero false positives

Application:
Virtual Diagnostics and On-line Modeling

What is a virtual diagnostic?



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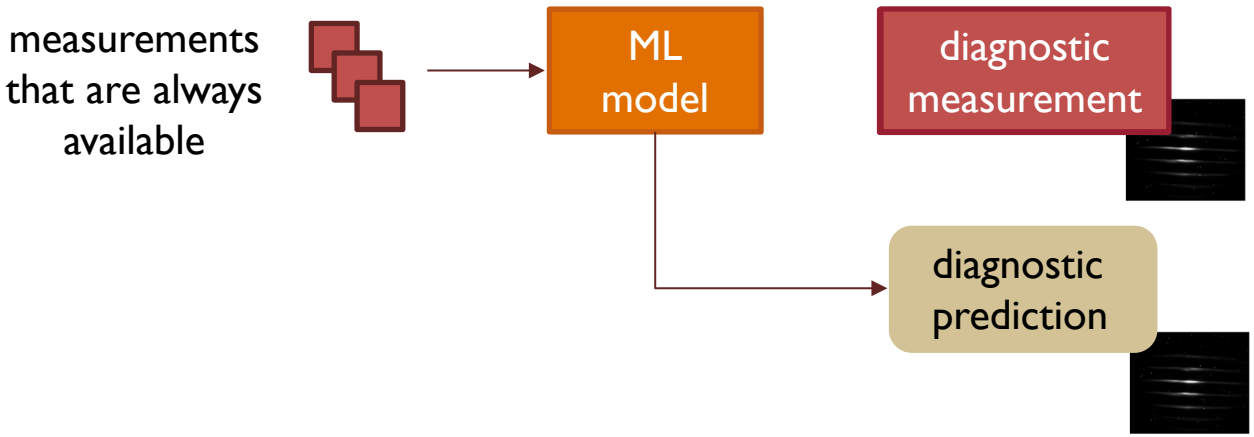

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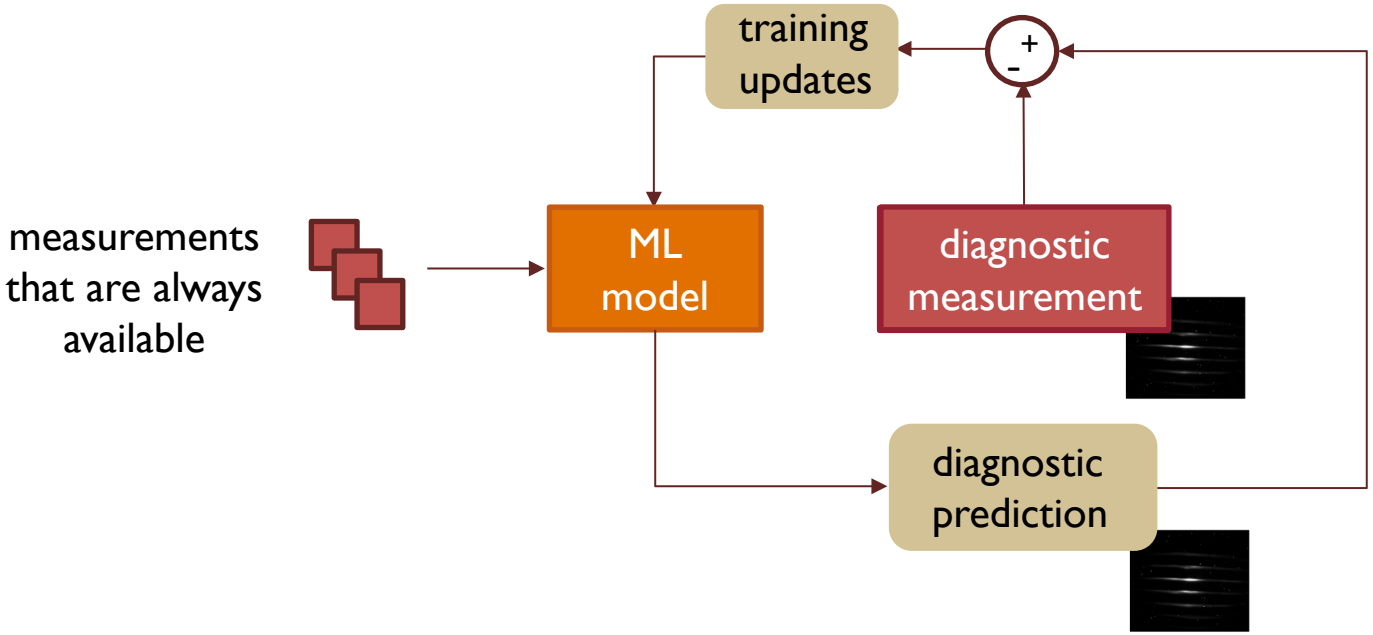
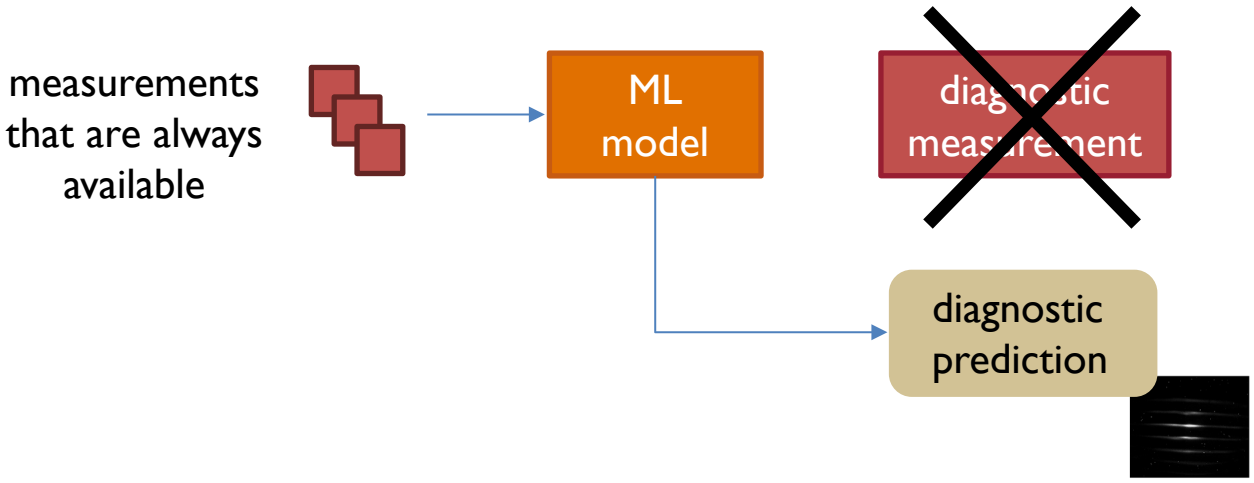


What is a virtual diagnostic?

Real diagnostic no longer available:

- *destructive, cannot use during normal operations*
- *slower update rate than desired*
- *moved to another location (e.g. cost constraints)*



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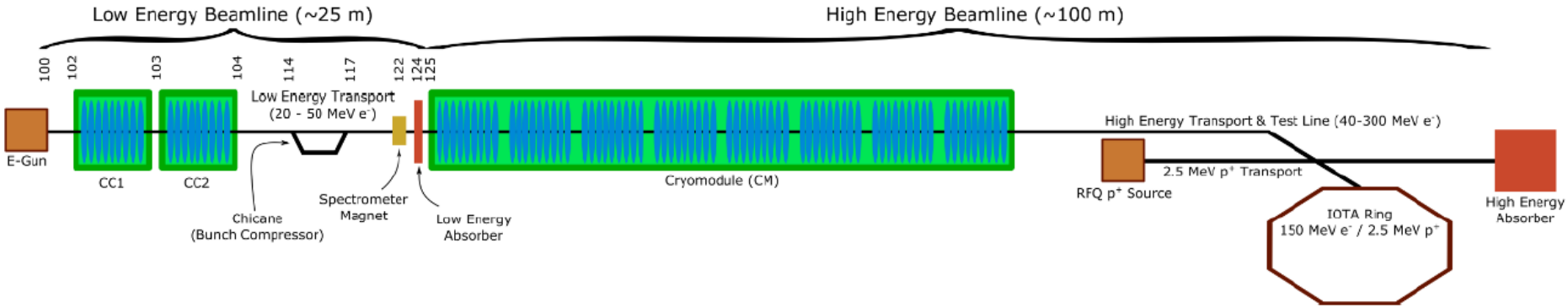
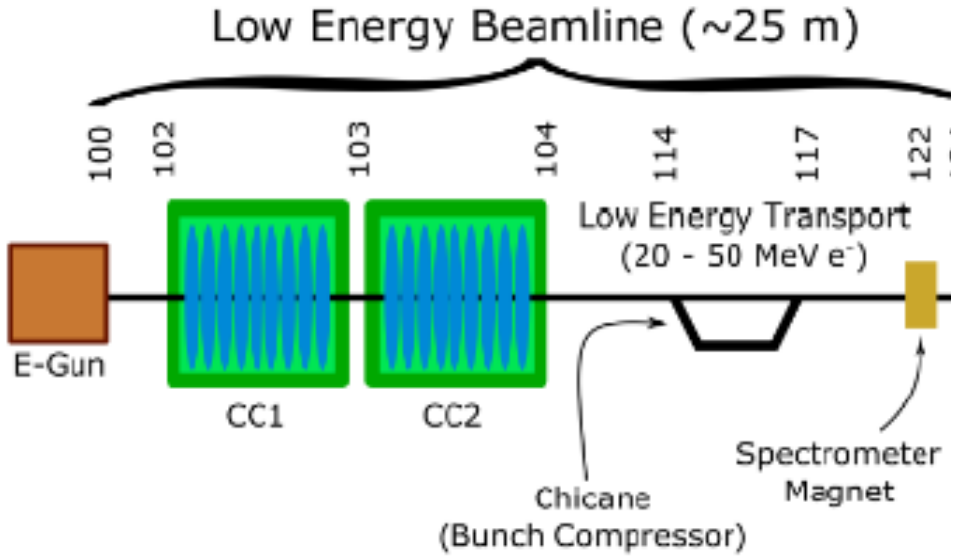
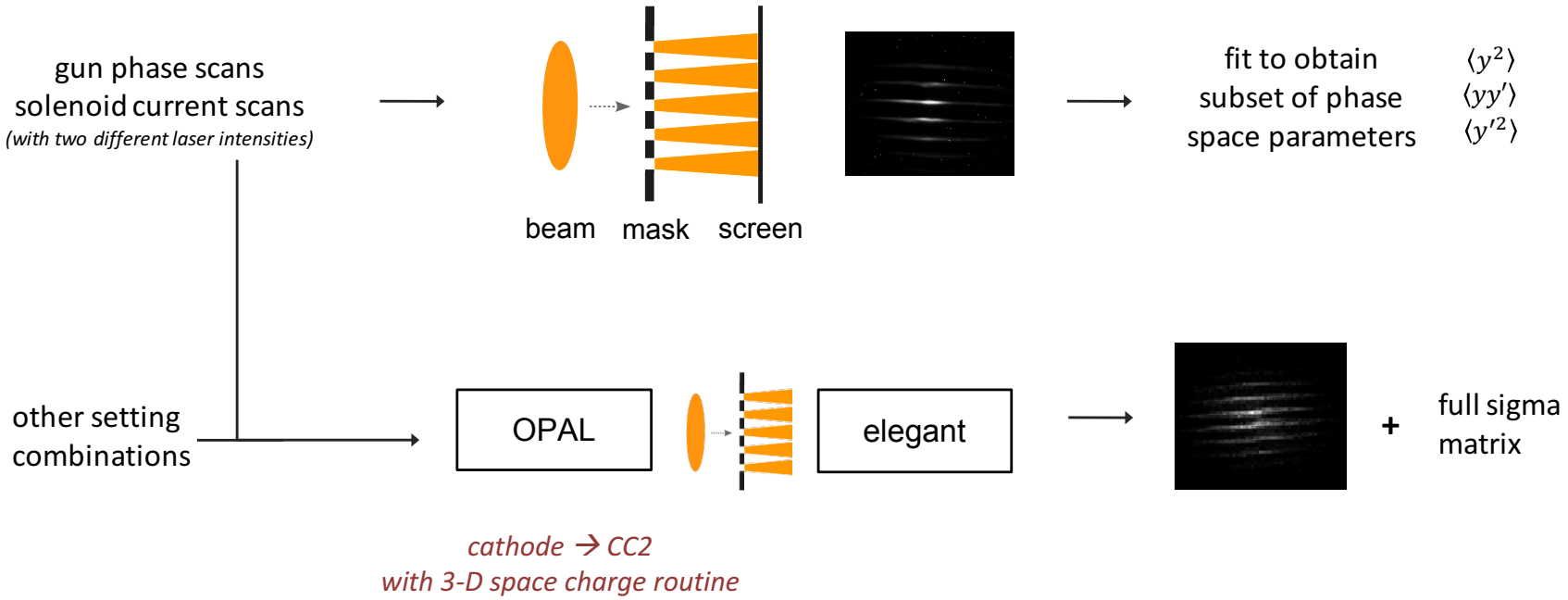




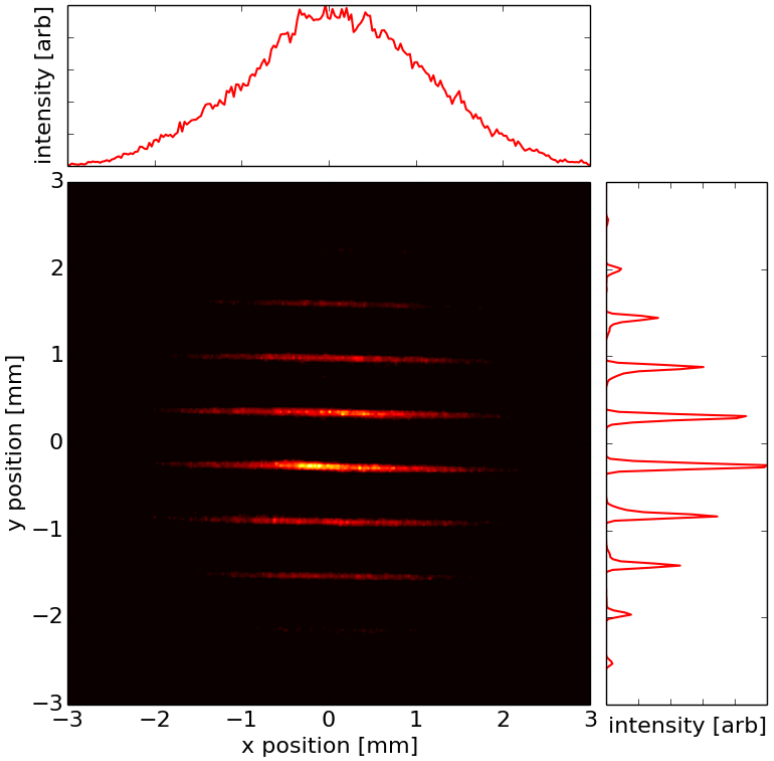
- 1.3 GHz photocathode RF gun
  - *PITZ style gun with solenoid and bucking coil*
  - *Beam accelerated to ~4 MeV*
- 1.3 GHz 9-cell Tesla type cavities
  - *Beam accelerated to ~35 MeV*

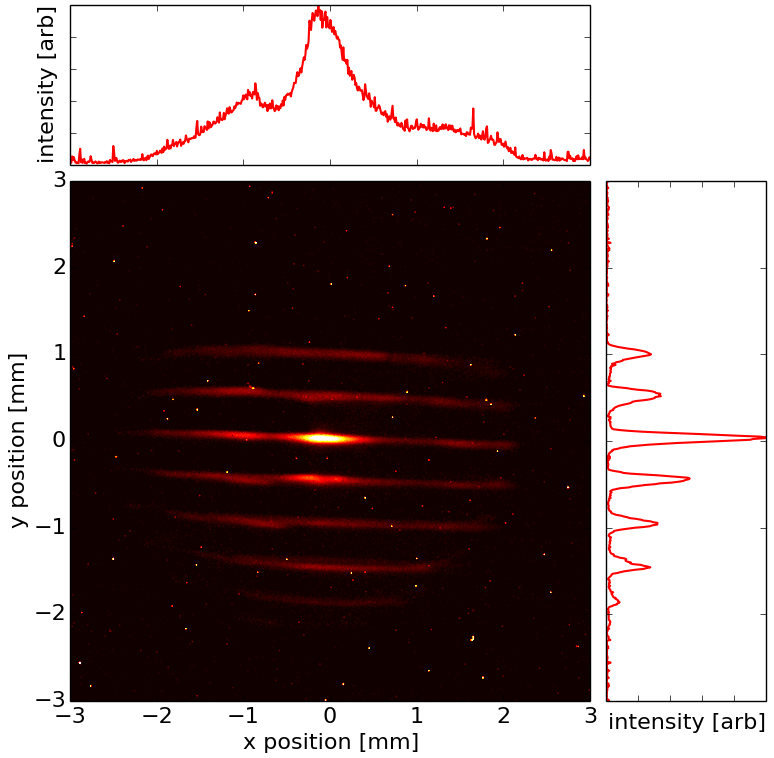
Developing our simulation model



Comparison of simulations and measurements

- Simulating the multi-slit diagnostic
  - *Export beam distribution at X107, apply mask, propagate to X111*
  - *Generate simulated images from 2-d histograms*
  - *Process images in the same manor as is done on the machine*
  - *Compare simulated images with measured images and compare processed results*





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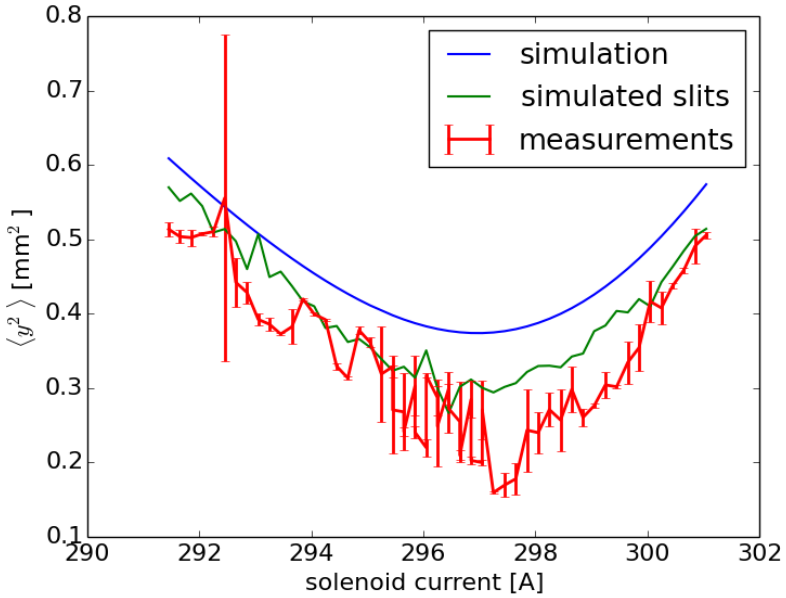
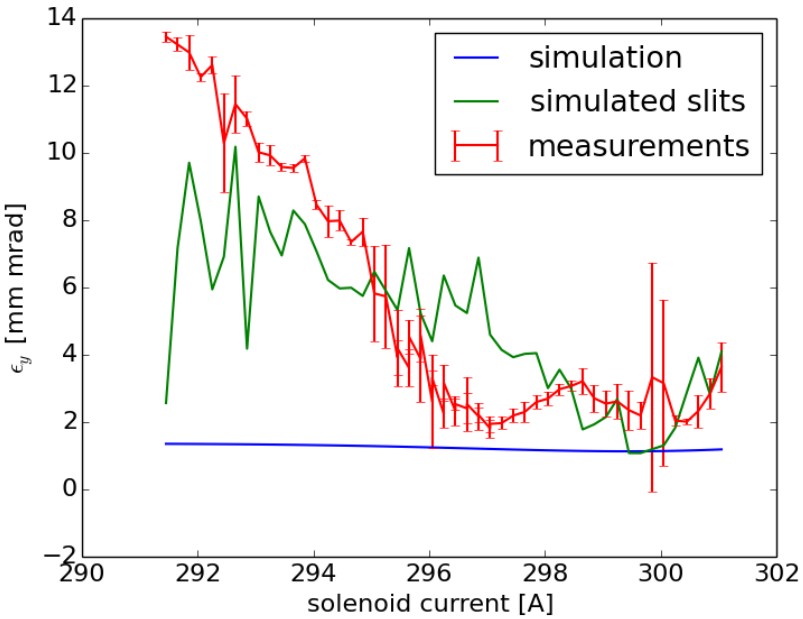
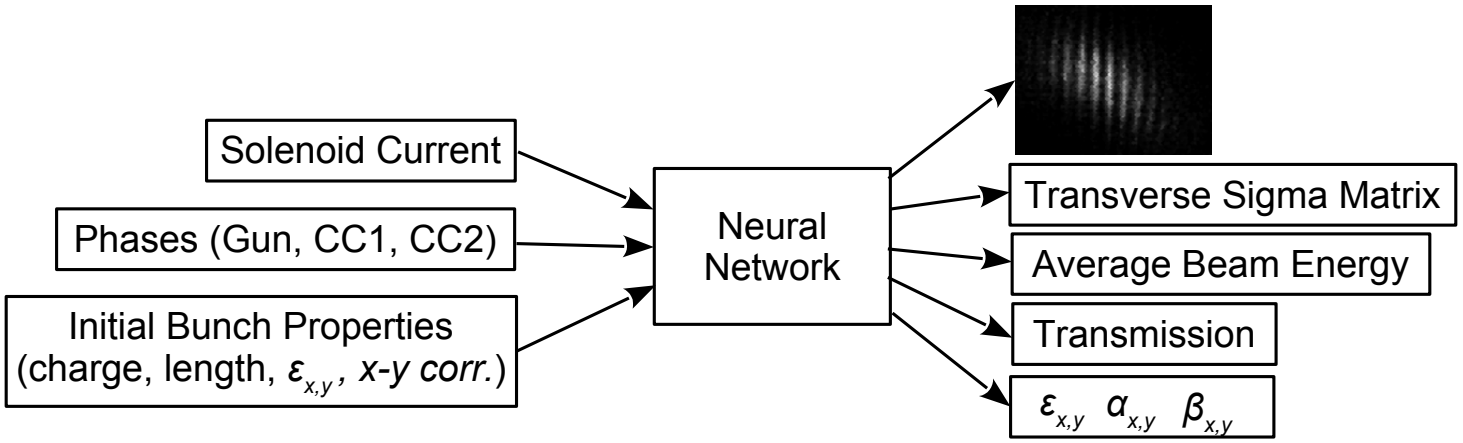


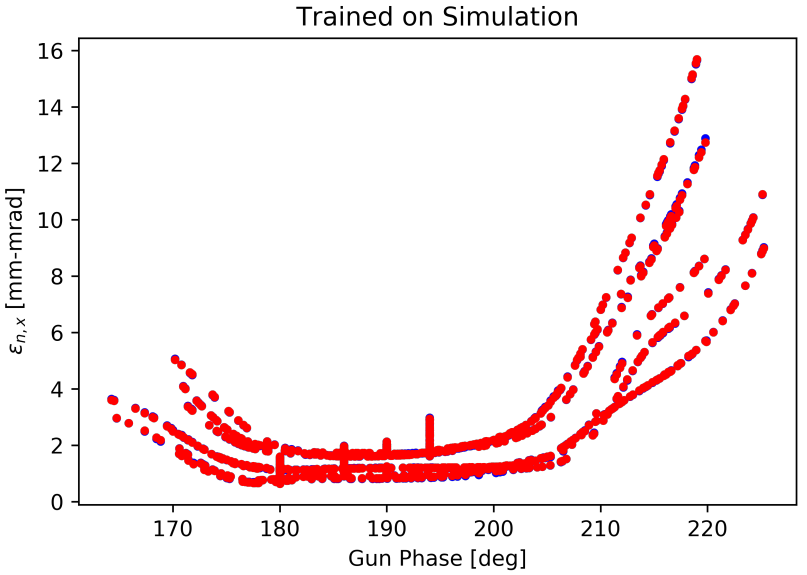


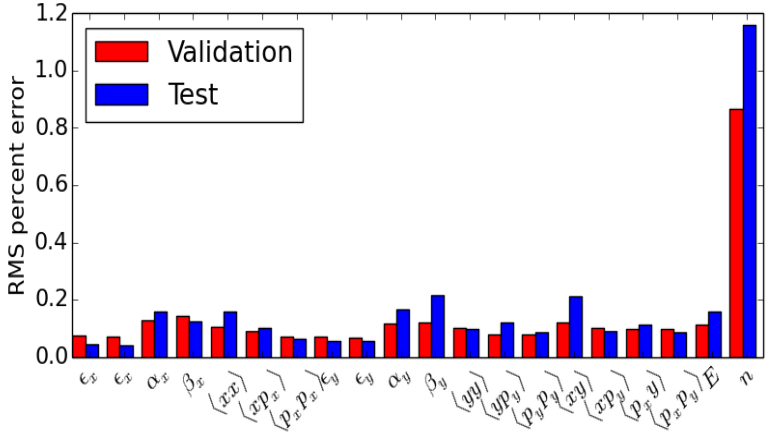
Neural Network Modeling



NN Architecture and performance

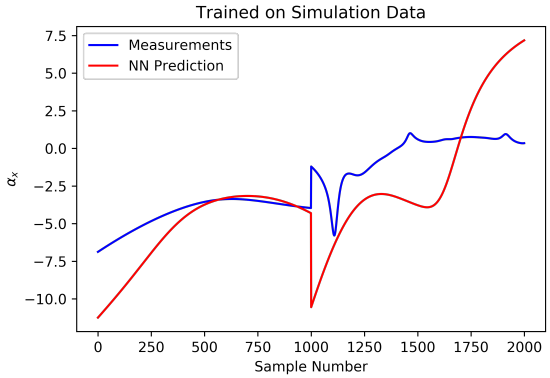
- Data separated into Training, Validation, and Test sets
  - *Training set: used directly in training*
  - *Validation set: not used in weight updates, but used during training to assess model fit (e.g. avoid overfitting)*
  - *Test set: data not used at all during training, sometimes outside range of training data*
- Noise added to the data before training
- Performance across validation and test set
  - *Top: prediction and simulation as a function of gun phase*
  - *Bottom: rms percent error between neural network and simulations*
- All output parameters perform well except transmission
  - *All transmission is 100% in our range of simulations so this is dominated by noise added during training*

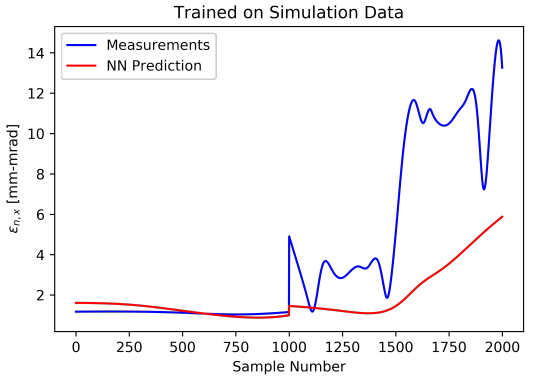


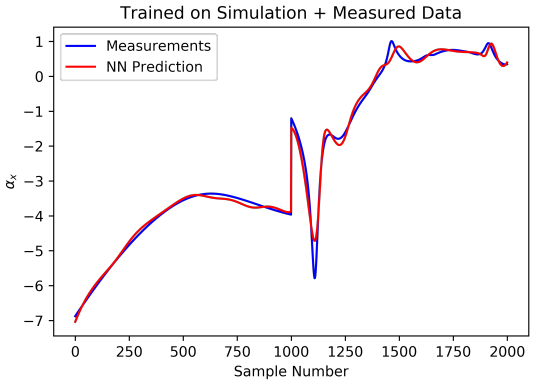


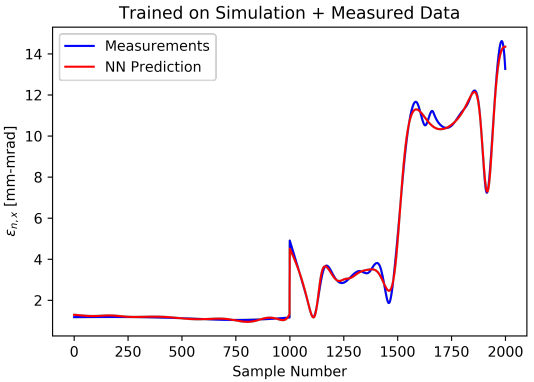
Updating the network with measurements

- Compare network trained on simulations to measurements: top
  - *Note this model was trained on rms parameters from simulations, not the simulated multi-slit measurement*
- Updating with measurements: bottom
  - *Bottom Left: Alpha as a function of sample number for updated dataset*
  - *Bottom Right: Normalized emittance as a function of sample number for updated dataset*









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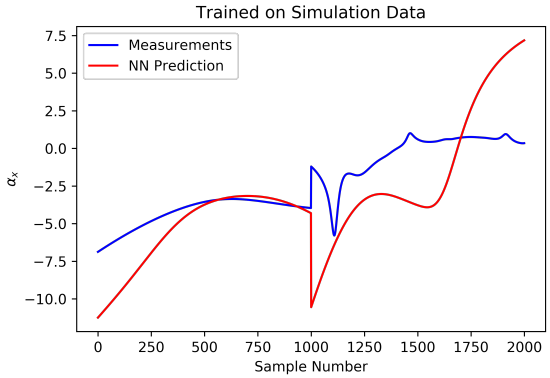
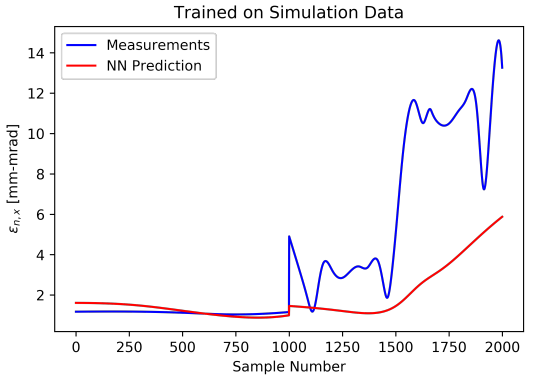
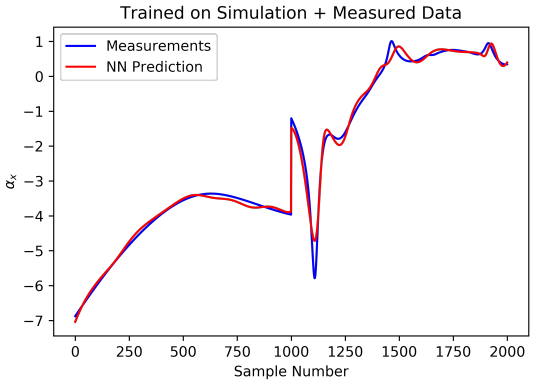
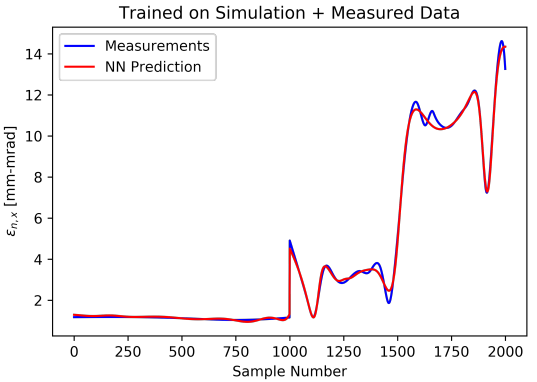
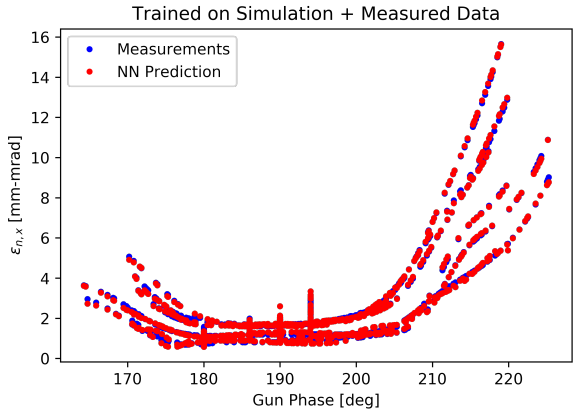






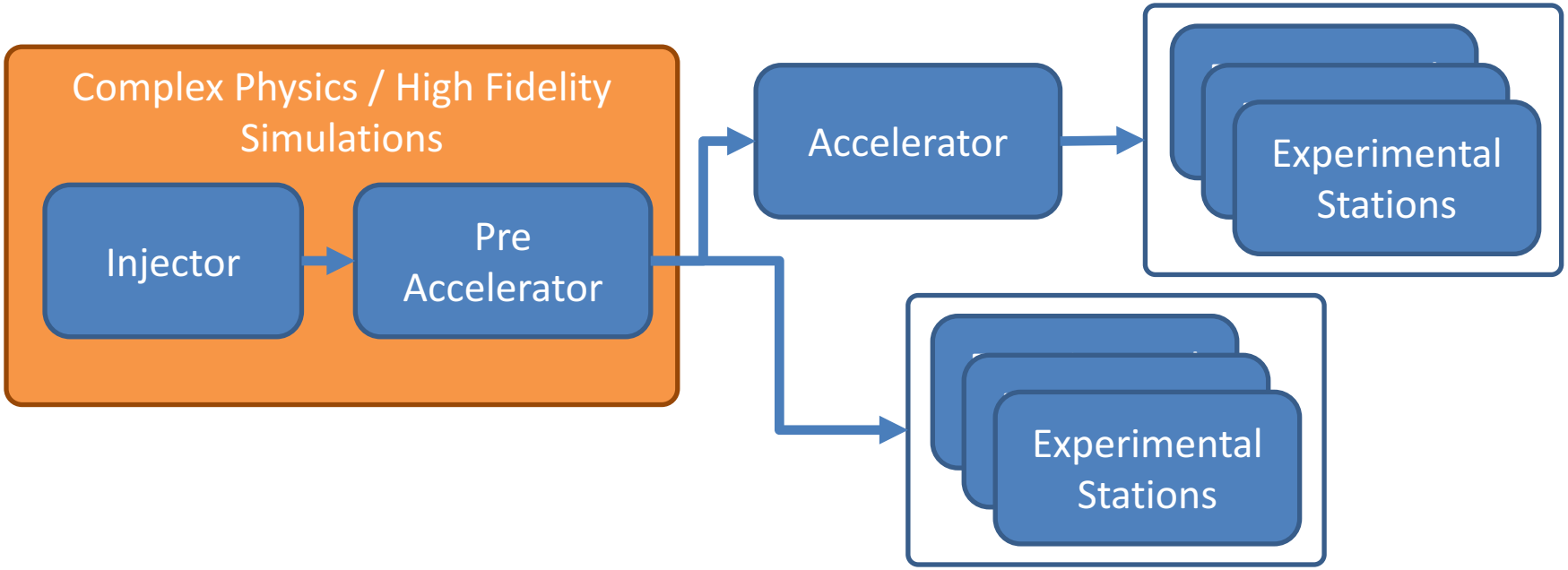




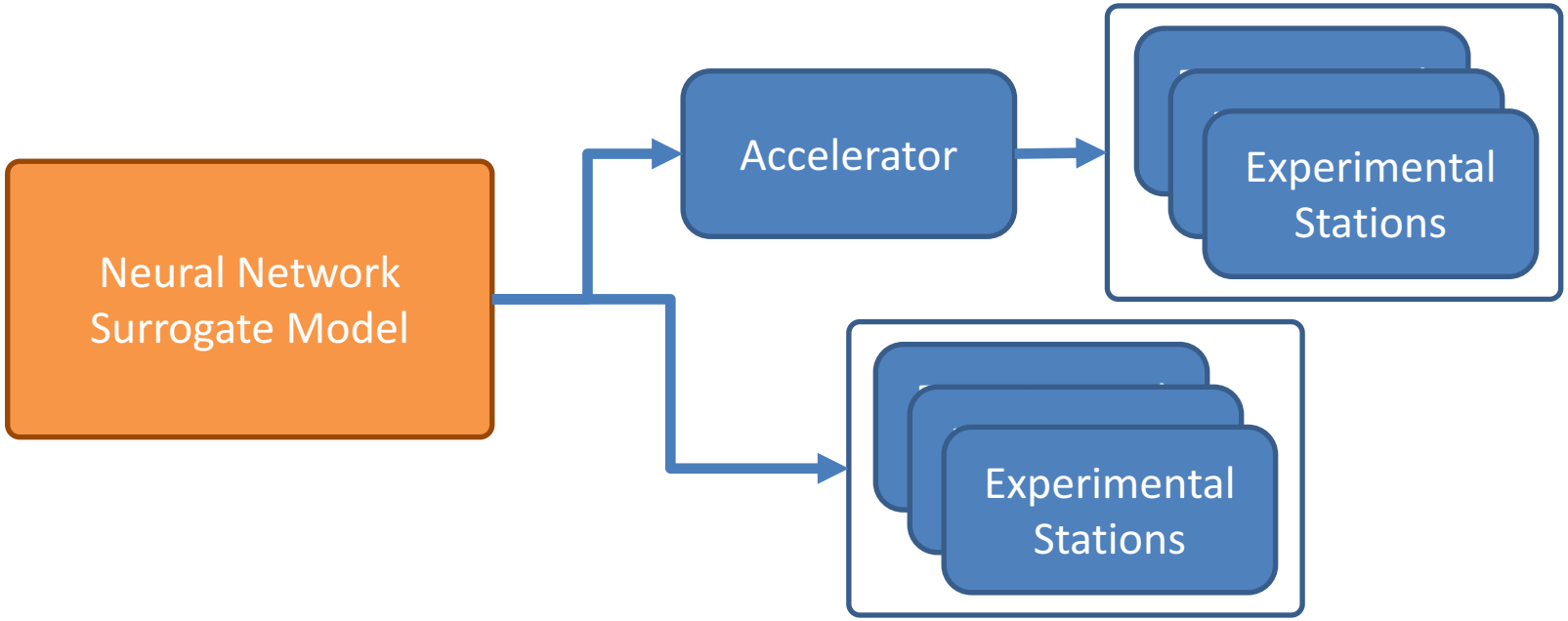
- Network retains the information from the simulations
  - *Left: comparison of network prediction for phase scan data from before and after updating with measurements*

Application:
Surrogate Modeling and Optimization

Surrogate Modeling



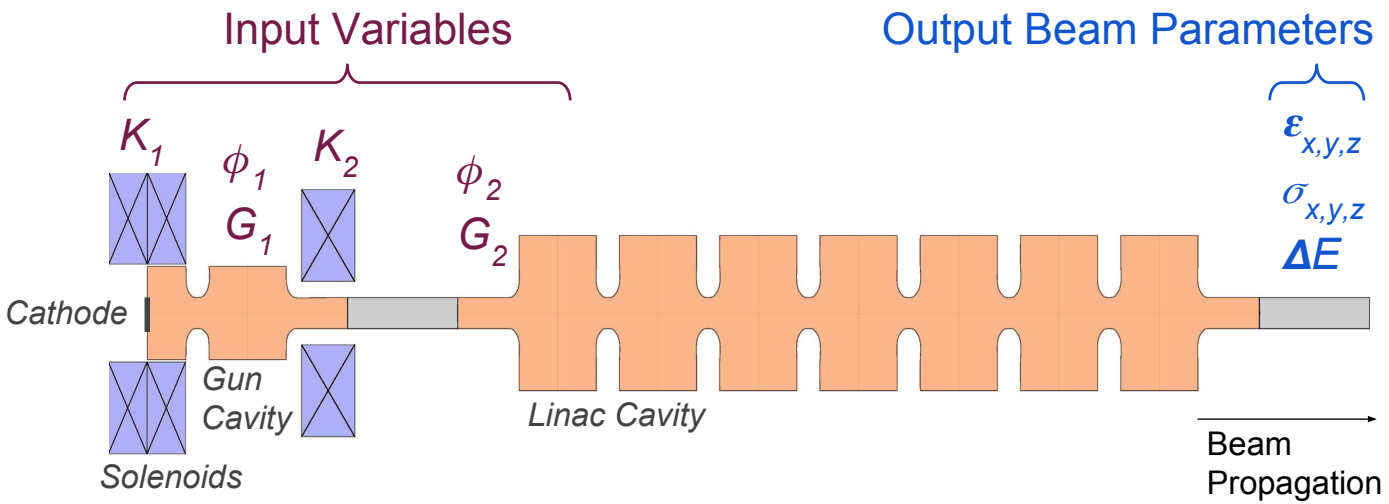
Surrogate Modeling



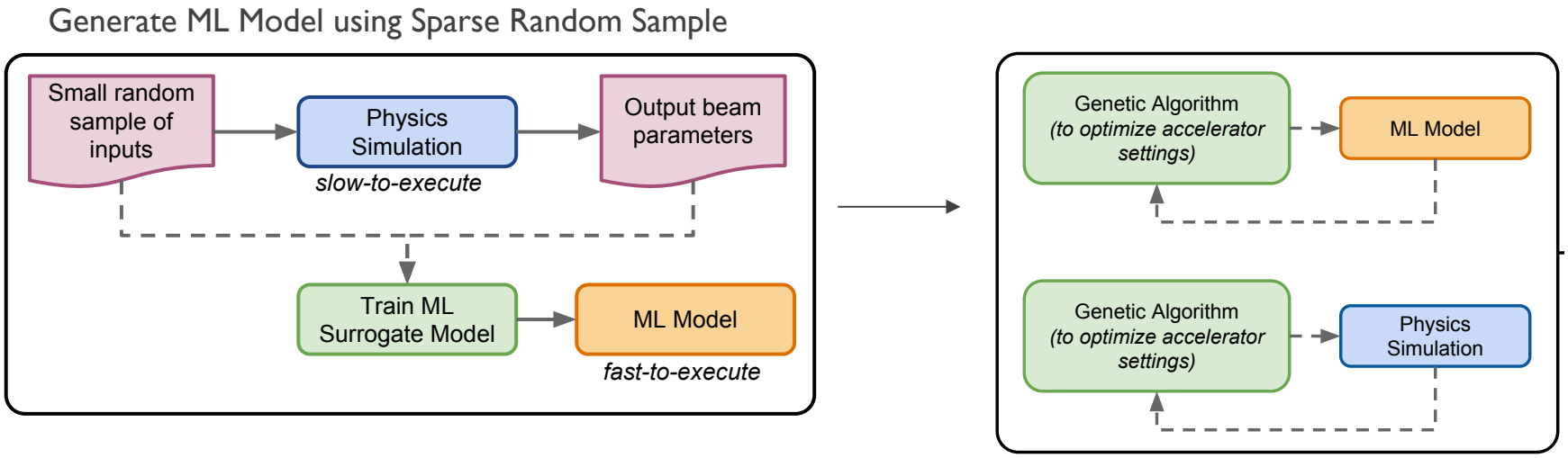
Injector Surrogate Modeling and Optimization

Test Case: Argonne Wakefield Accelerator Injector

OPAL simulation (PIC) : 3D space charge 3D field maps	NSGA-II for optimization: 200 generations ~350 individuals	100 - 5K random points for training

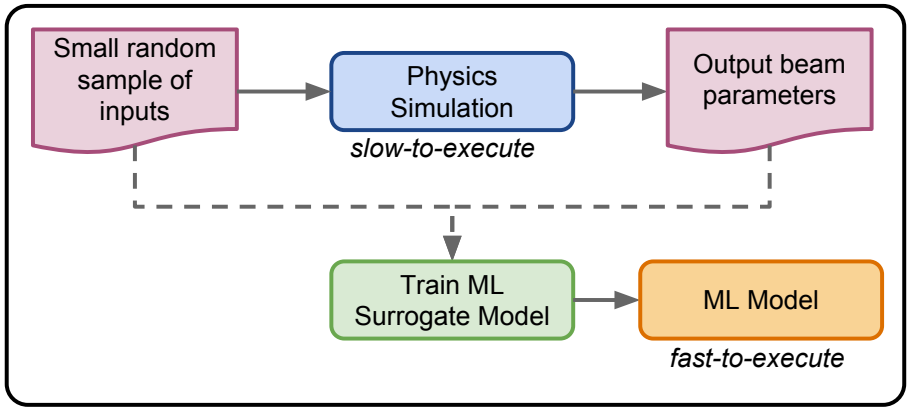


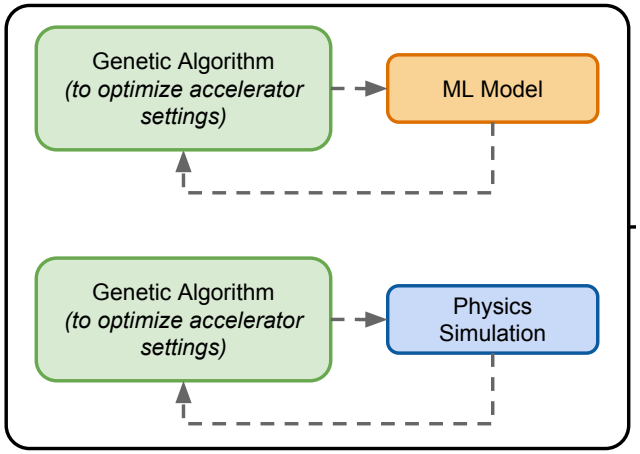
Injector Surrogate Modeling and Optimization



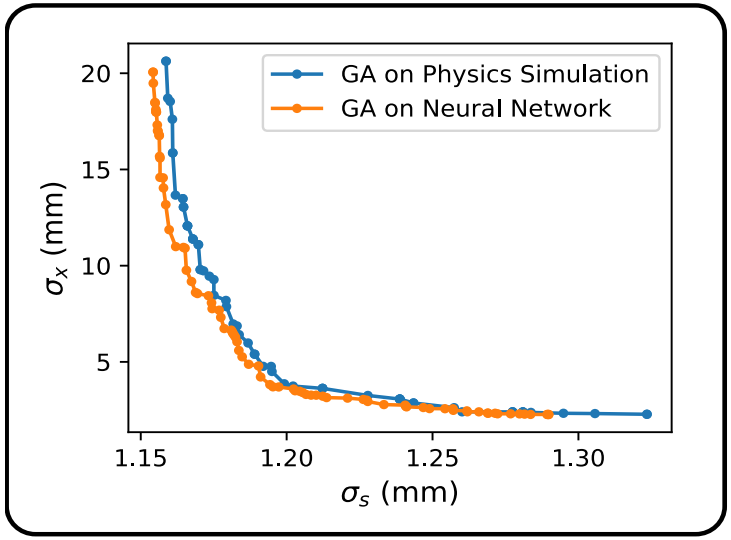
Injector Surrogate Modeling and Optimization

Generate ML Model using Sparse Random Sample





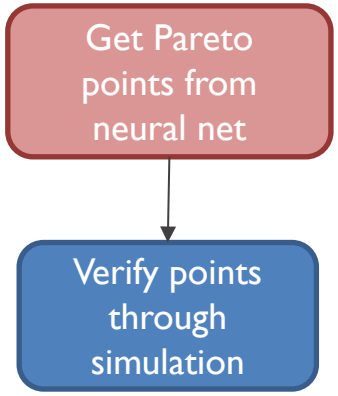
Compare Resulting Pareto Fronts

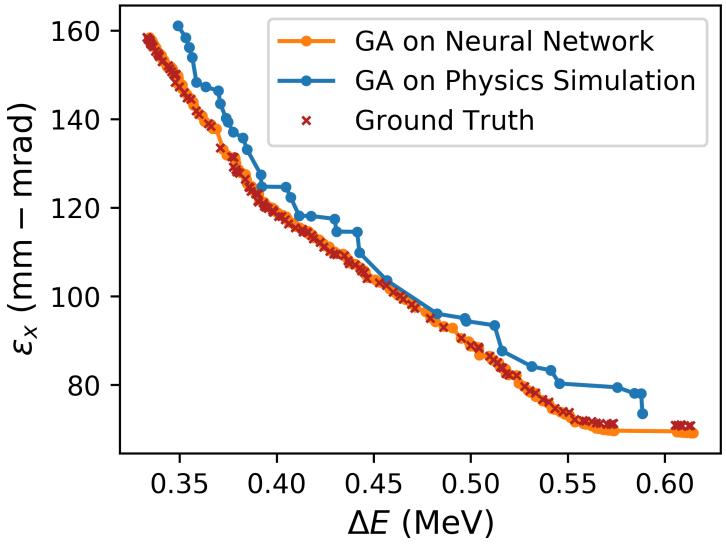


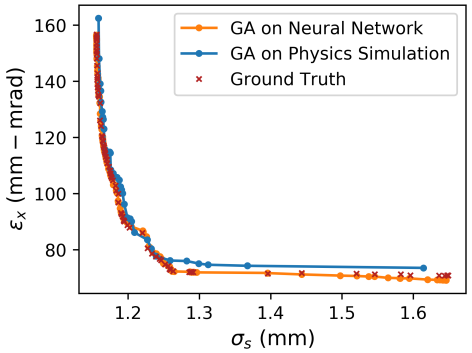
Verifying pareto front from the neural network

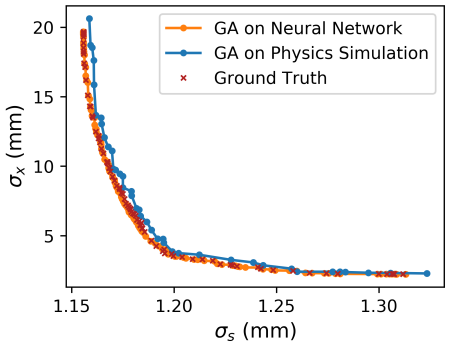
In some cases, optimization over simulation takes too long to converge

→ *validate Pareto front from neural network more directly*









Neural network gave a ***better*** **approximation of the Pareto front** than the naïve GA on the simulation

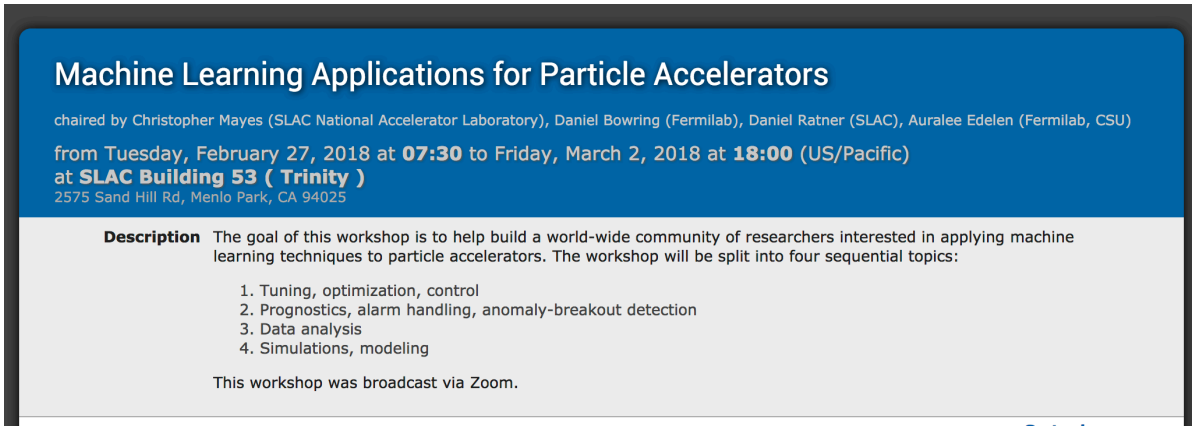
Required **13x fewer simulations** and had **10^6 times faster execution** in the optimization

→ ***In addition to creating a surrogate model, this is a way to speed up optimization for new designs***

Accelerator workshops on ML

https://indico.psi.ch/event/6698/

https://www.cockcroft.ac.uk/events/ICPA/



https://indico.fnal.gov/event/16327/other-view?view=standard

Publications

J. P. Edelen A. L. Edelen, and D. Edstrom "Methods for Data Cleaning" 2nd ICFA Mini Workshhop on Machine Learning for Particle Accelerators (Feb 2019)

J. P. Edelen, A. L. Edelen, and D. Edstrom "Neural Network Based Virtual Diagnostics at FAST" Contributed Oral at the Fermilab Workshop on Megawatt Rings (May 2018)

A.L. Edelen et al. "Results and Discussion of Recent Applications of Neural Network-Based Approaches to the Modeling and Control of Particle Accelerators" Proc. IPAC 2018 (THYGBE2)

A.L. Edelen et al " Neural Network Virtual Diagnostic and Tuning for the FAST Low Energy Beamline" IPAC 2018 (SUSPL054)

J.P. Edelen, A.L. Edelen & D. Edstrom, "Neural network modeling and virtual diagnostics at FAST," presented at ICFA Beam Dynamics Mini-Workshop: Machine Learning Applications for Particle Accelerators (SLAC, 2018).

A. Edelen et al. "Opportunities in Machine Learning for Particle Accelerators". In: (2018) arXiv: 1811.03172 [physics.acc-ph].

A. L. Edelen et al. "Using Neural Network Control Policies For Rapid Switching Between Beam Parameters in a Free Electron Laser". In: Proceedings of the 2017 Deep Learning for Physical Sciences workshop at the Neural Information Processing Systems Conference. 2017.

A. L. Edelen et al. "Neural Networks for Modeling and Control of Particle Accelerators" In: IEEE Transactions on Nuclear Science 63.2 (Apr. 2016), pp. 878–897. issn: 0018-9499.

A.L. Edelen, S.G. Biedron, S.V. Milton & J.P. Edelen, , "First steps towards incorporating image based diagnostics into particle accelerator control systems using convolutional neural networks," Proc. North American Part. Accel. Conf., TUPOA51 (2016)