Overview of Adaptive Machine Learning Methods: Towards Virtual 6D Phase Space Diagnostics

Science and Applications of Plasma-Based Accelerators

Wednesday, May 18

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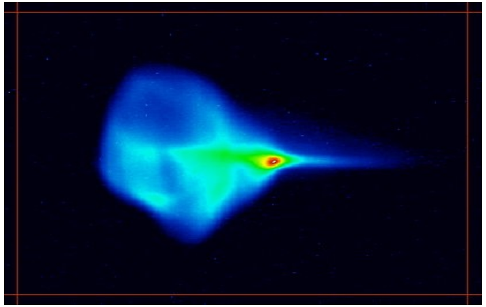
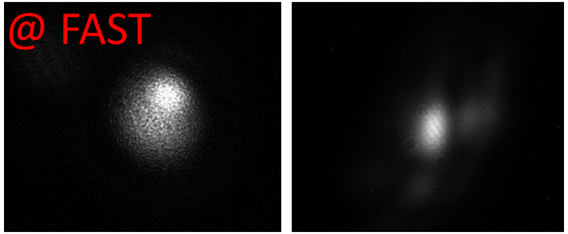
Initial Beam Distributions are Time-Varying and Beam Dynamics are Governed by Complex Collective Effects

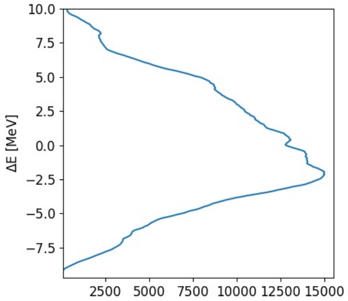
- Wakefields, Space charge, Coherent synchrotron radiation



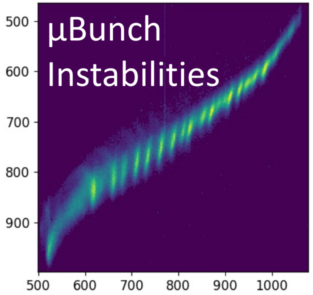
Typical 2D (x,y) beam profile, not a simple Gaussian.

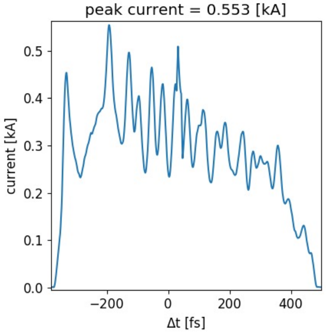


Time-Varying Input Beam

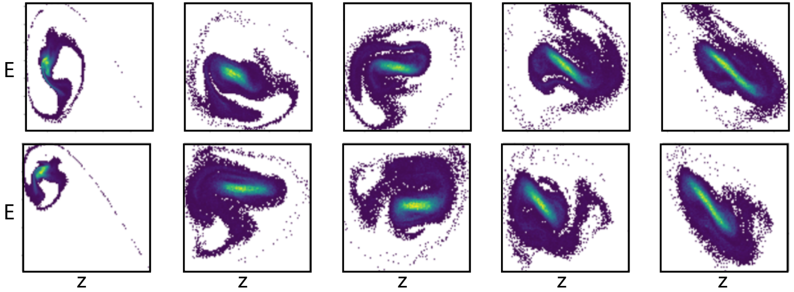


EuXFEL

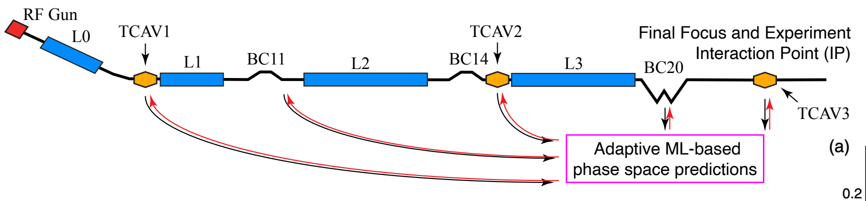


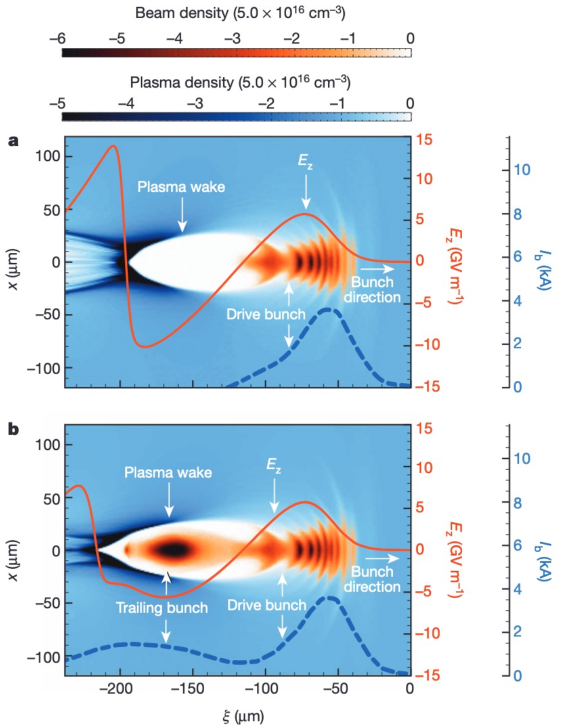


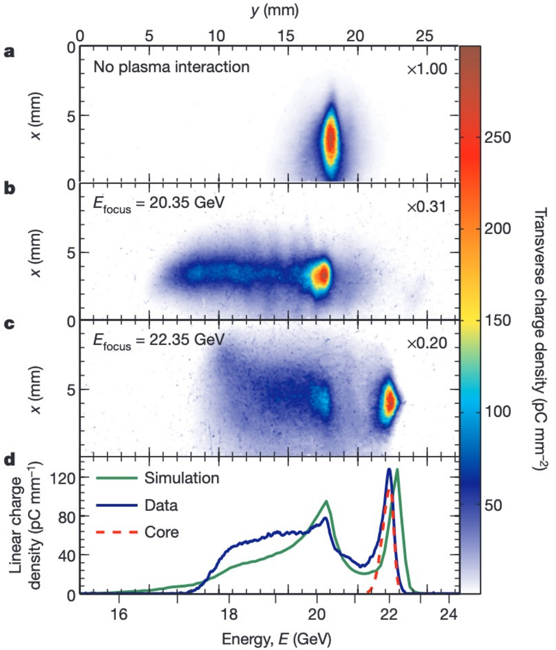
LANSCE: Space Charge



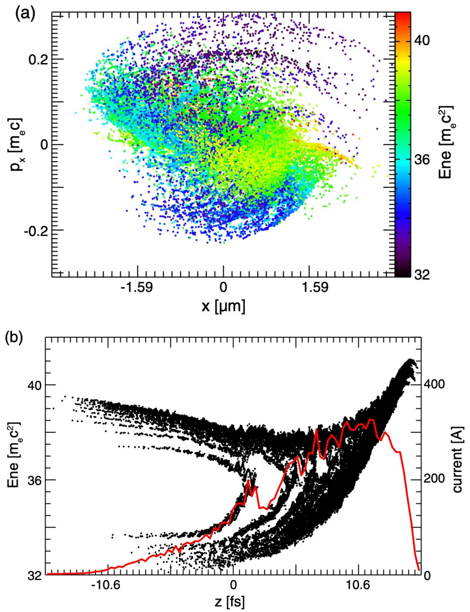
Goal: Develop Adaptive ML-based Virtual Diagnostics to Observe the Complex Phase Space Dynamics of Beam-driven Plasma Wakefield Acceleration





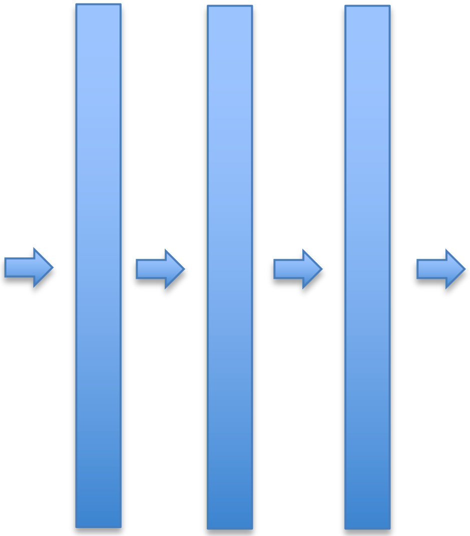


Litos, M., et al. "High-efficiency acceleration of an electron beam in a plasma wakefield accelerator." *Nature* 515.7525 (2014): 92-95.

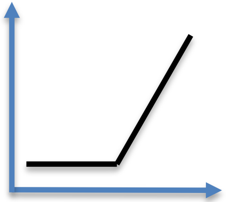


Xu, X. L., et al. "Low emittance electron beam generation from a laser wakefield accelerator using two laser pulses with different wavelengths." *Physical Review Special Topics-Accelerators and Beams* 17.6 (2014): 061301.

Quick Intro to Neural Networks



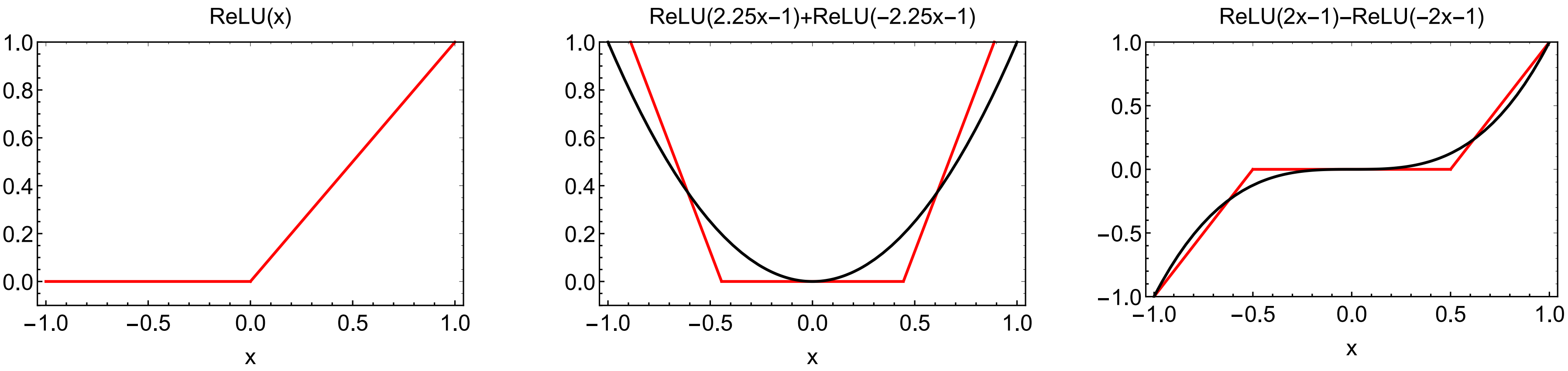
$$\begin{bmatrix} x_1^i \\ x_2^i \end{bmatrix} \begin{bmatrix} w_{11}^1 & w_{12}^1 \end{bmatrix} + b_1^1 = x_1^i w_{11}^1 + x_2^i w_{12}^1 + b_1^1$$

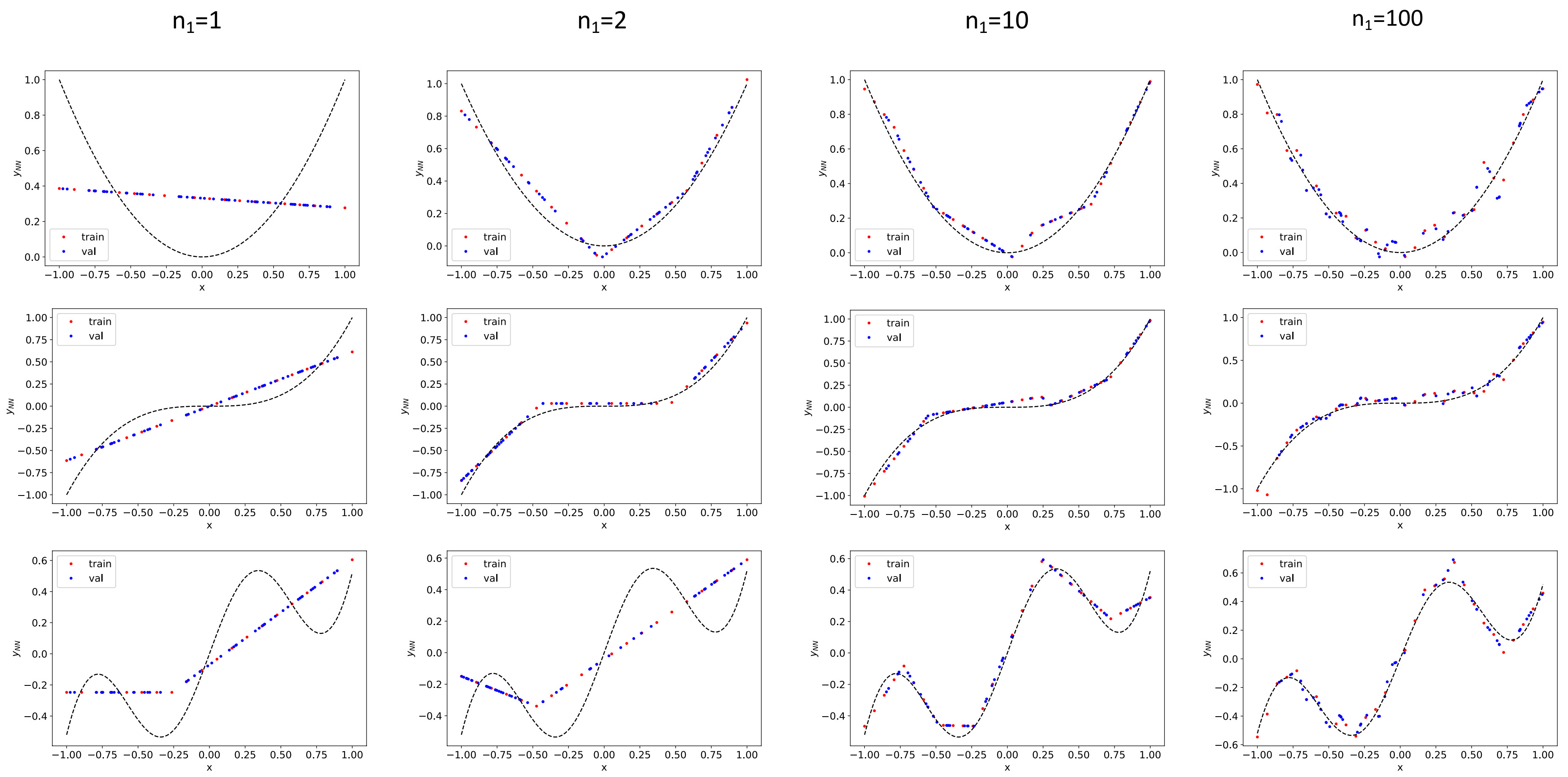


ReLU

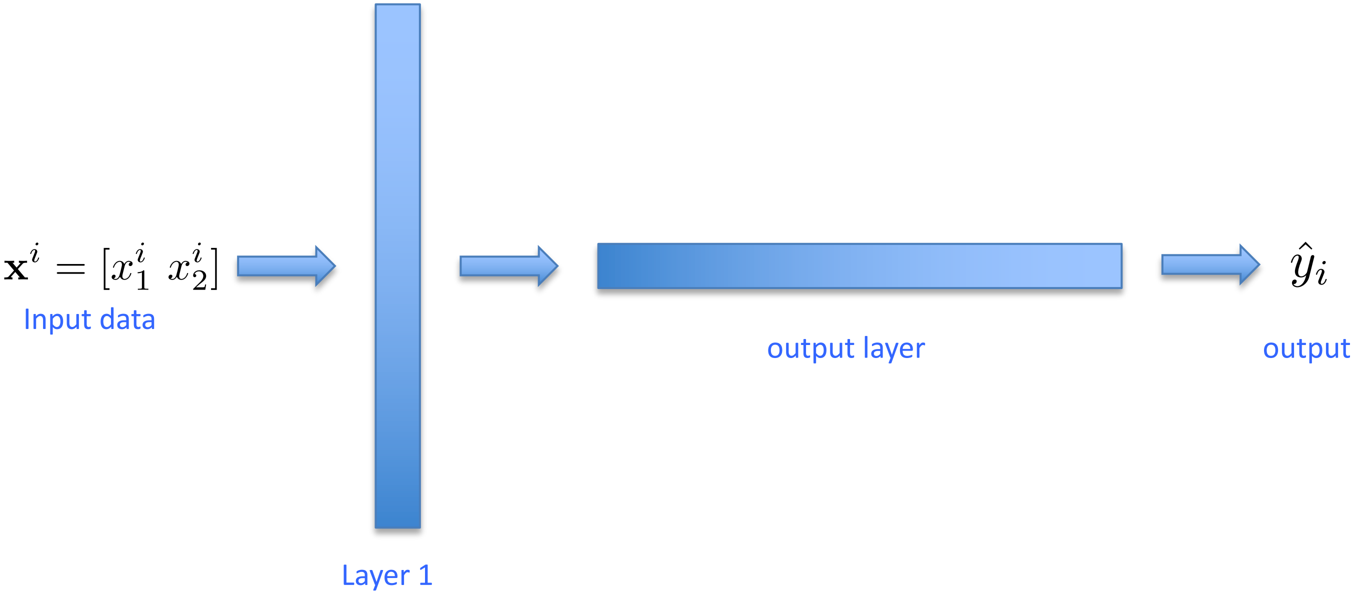
$$\text{ReLU}(x) = \max\{0, x\}$$

$$\text{ReLU}\left(x_1^i w_{11}^1 + x_2^i w_{12}^1 + b_1^1\right)$$


ReLU(x)
ReLU(2.25x−1)+ReLU(−2.25x−1)
ReLU(2x−1)−ReLU(−2x−1)
1.0
0.8
0.6
0.4
0.2
0.0
0.5
−0.5
−1.0
x

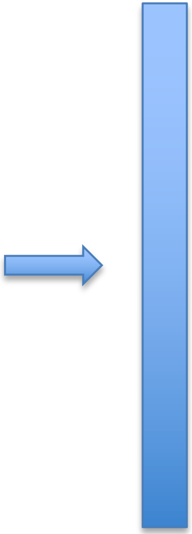

n1=1
n1=2
n1=10
n1=100
train
val
x
yNN

$$\mathbf{x}^i = [x_1^i \ x_2^i], \quad \mathbf{X} = \begin{bmatrix} \mathbf{x}^1 \\ \mathbf{x}^2 \\ \vdots \\ \mathbf{x}^N \end{bmatrix} = \begin{bmatrix} x_1^1 & x_2^1 \\ x_1^2 & x_2^2 \\ & \vdots & \\ x_1^N & x_2^N \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}$$



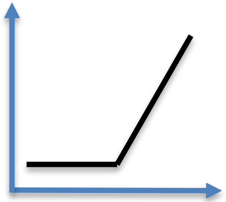
$$\mathbf{x}^i = [x_1^i \;\; x_2^i]$$

Input data



Layer 1

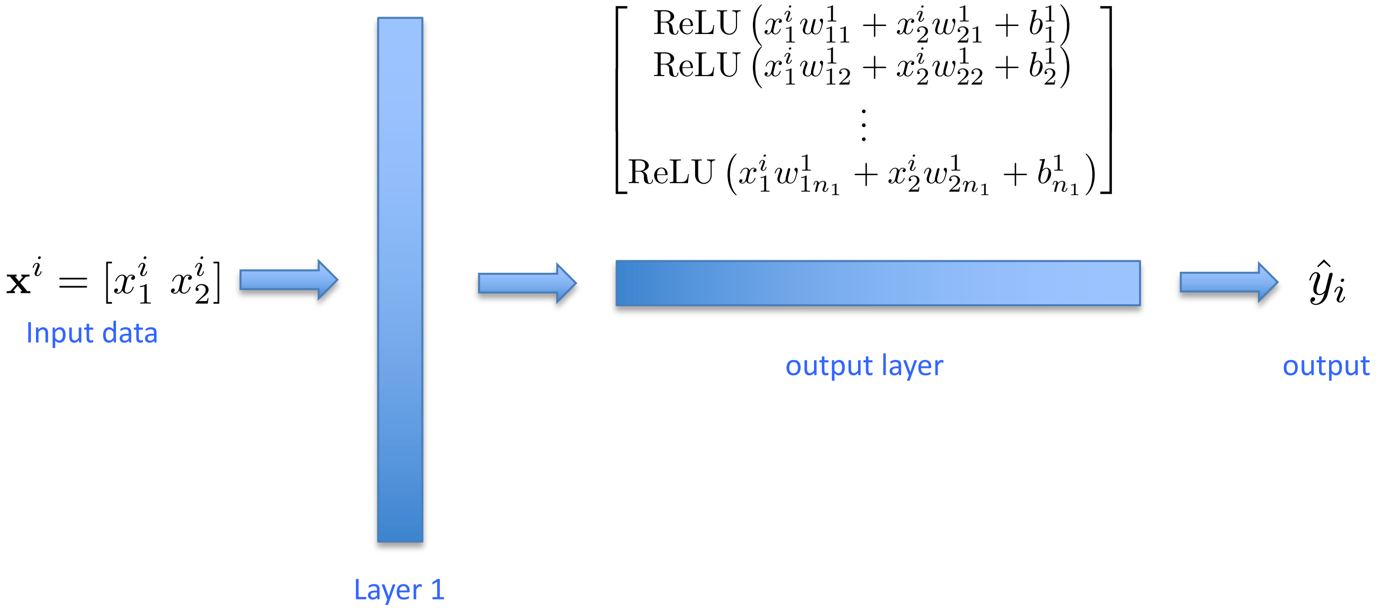
$$\begin{bmatrix} x_1^i \\ x_2^i \end{bmatrix} [w_{11}^1 \;\; w_{12}^1] + b_1^1 = x_1^i w_{11}^1 + x_2^i w_{12}^1 + b_1^1$$



ReLU

$$\text{ReLU}\left(x_1^i w_{11}^1 + x_2^i w_{12}^1 + b_1^1\right)$$

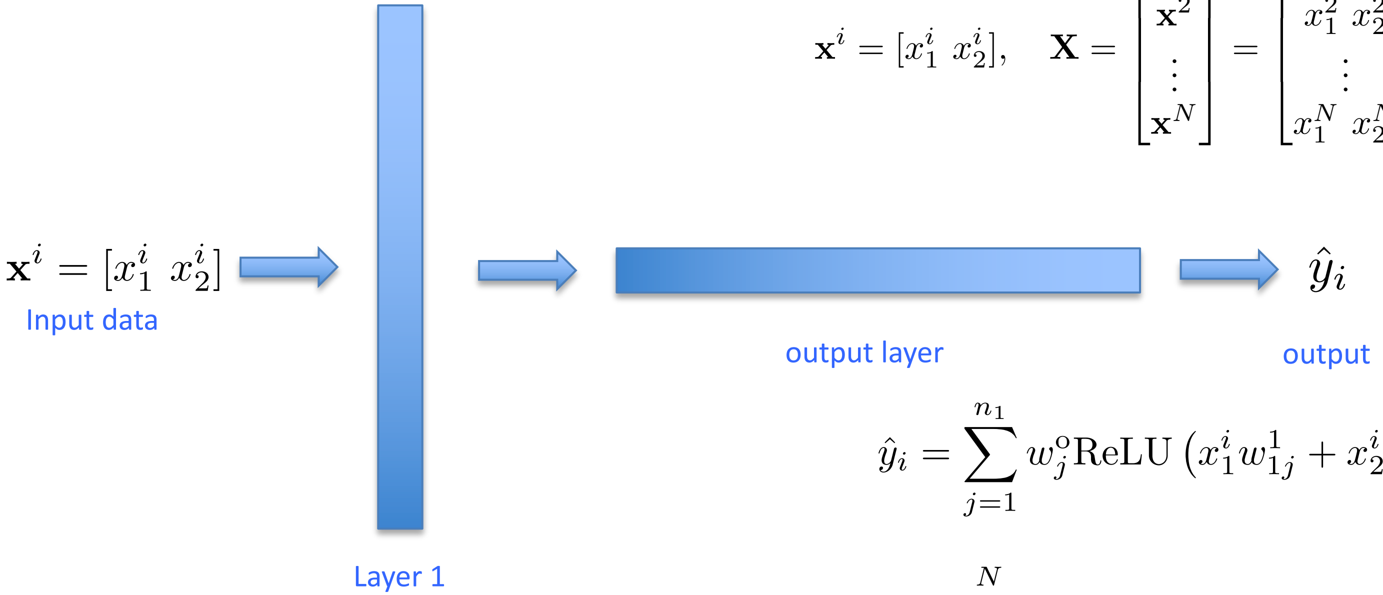
$$\begin{bmatrix} w_{11}^1 & w_{12}^1 \\ w_{21}^1 & w_{22}^1 \\ \vdots & \\ w_{1n_1}^1 & w_{2n_1}^1 \end{bmatrix} \begin{bmatrix} x_1^i \\ x_2^i \end{bmatrix} + \begin{bmatrix} b_1^1 \\ b_2^1 \\ \vdots \\ b_{n_1}^1 \end{bmatrix} = \begin{bmatrix} x_1^i w_{11}^1 + x_2^i w_{21}^1 + b_1^1 \\ x_1^i w_{12}^1 + x_2^i w_{22}^1 + b_2^1 \\ \vdots \\ x_1^i w_{1n_1}^1 + x_2^i w_{2n_1}^1 + b_{n_1}^1 \end{bmatrix} \Longrightarrow \begin{bmatrix} \text{ReLU}\left(x_1^i w_{11}^1 + x_2^i w_{21}^1 + b_1^1\right) \\ \text{ReLU}\left(x_1^i w_{12}^1 + x_2^i w_{22}^1 + b_2^1\right) \\ \vdots \\ \text{ReLU}\left(x_1^i w_{1n_1}^1 + x_2^i w_{2n_1}^1 + b_{n_1}^1\right) \end{bmatrix}$$



$$[w_1^{\text{o}} \; w_2^{\text{o}} \; \dots \; w_{n_1}^{\text{o}}] \begin{bmatrix} \text{ReLU}\left(x_1^i w_{11}^1 + x_2^i w_{21}^1 + b_1^1\right) \\ \text{ReLU}\left(x_1^i w_{12}^1 + x_2^i w_{22}^1 + b_2^1\right) \\ \vdots \\ \text{ReLU}\left(x_1^i w_{1n_1}^1 + x_2^i w_{2n_1}^1 + b_{n_1}^1\right) \end{bmatrix} + b^{\text{o}}$$

$$\hat{y}_i = \sum_{j=1}^{n_1} w_j^{\text{o}} \text{ReLU}\left(x_1^i w_{1j}^1 + x_2^i w_{2j}^1 + b_j^1\right) + b^{\text{o}}$$

$$\mathbf{x}^i = [x_1^i \ x_2^i], \quad \mathbf{X} = \begin{bmatrix} \mathbf{x}^1 \\ \mathbf{x}^2 \\ \vdots \\ \mathbf{x}^N \end{bmatrix} = \begin{bmatrix} x_1^1 & x_2^1 \\ x_1^2 & x_2^2 \\ & \vdots \\ x_1^N & x_2^N \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}$$

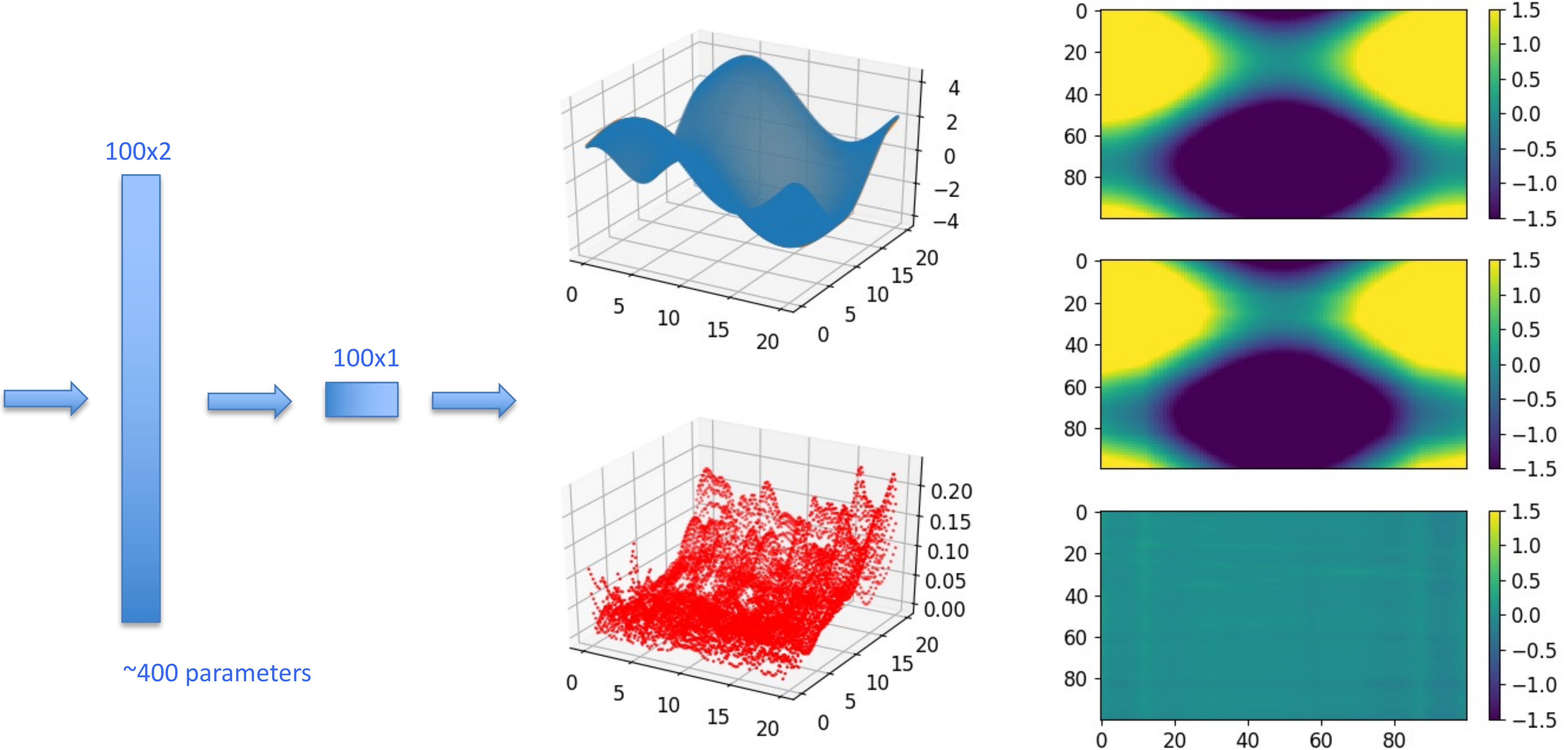


$$\hat{y}_i = \sum_{j=1}^{n_1} w_j^{\text{o}} \text{ReLU}\left(x_1^i w_{1j}^1 + x_2^i w_{2j}^1 + b_j^1\right) + b^{\text{o}}$$

$$C = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2, \quad p \Longrightarrow p - \delta \nabla_p C$$

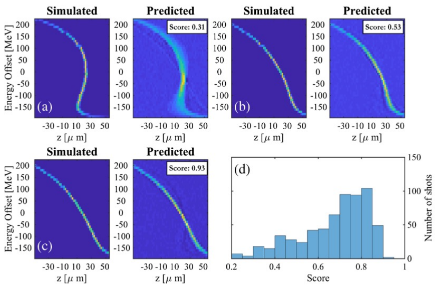
$$\nabla_{w_{kj}^1} C = 2 \sum_{i=1}^{N} (y_i - \hat{y}_i) \frac{\partial \hat{y}_i}{\partial w_{kj}^1} = 2 w_j^{\text{o}} \sum_{i=1}^{N} (y_i - \hat{y}_i) \begin{cases} x_k^i, \text{ if } & \text{ReLU}\left(\sum_{k=1}^2 x_k^i w_{kj}^1 + b_j^1\right) > 0 \\ 0, \text{ if } & \text{ReLU}\left(\sum_{k=1}^2 x_k^i w_{kj}^1 + b_j^1\right) < 0 \end{cases}$$

$$f(x,y) = 2\left[\sin(0.6x) + \cos(0.6y)\right]$$

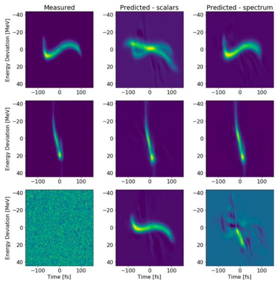


ML for Accelerators is a Growing Field
Many Applications as Virtual Diagnostics

LCLS, LCLS-II, FACET-II

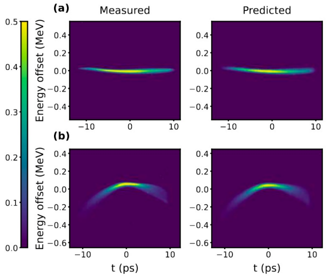


Emma, C., et al. "Machine learning-based longitudinal phase space prediction of particle accelerators." *Physical Review Accelerators and Beams* 21.11 (2018): 112802.



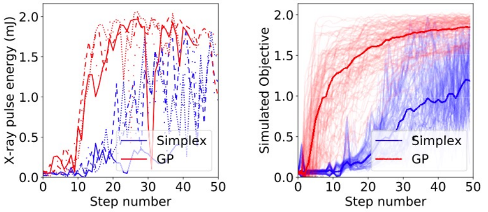
Hanuka, Adi, et al. "Accurate and confident prediction of electron beam longitudinal properties using spectral virtual diagnostics." *Scientific Reports* 11.1 (2021): 1-10.

EuXFEL



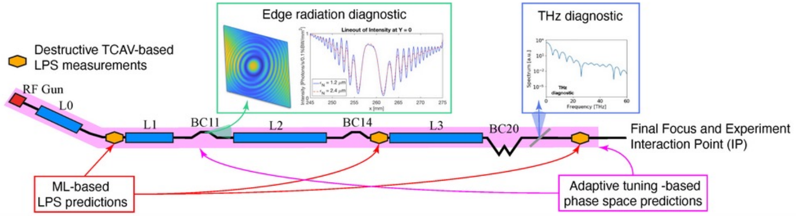
Zhu, Jun, et al. "Deep Learning-Based Autoencoder for Data-Driven Modeling of an RF Photoinjector." *arXiv preprint arXiv:2101.10437* (2021).

Duris, Joseph, et al. "Bayesian optimization of a free-electron laser." *Physical review letters* 124.12 (2020): 124801.



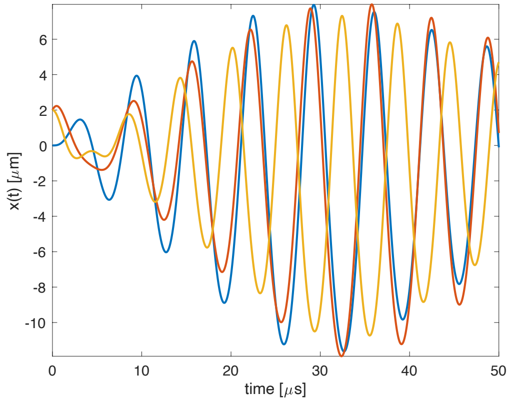
(a) Live 12 quadrupole optimization

(b) Simulated 12 quadrupole optimization



Emma, Claudio, et al. "Virtual diagnostic suite for electron beam prediction and control at FACET-II." *Information* 12.2 (2021): 61.

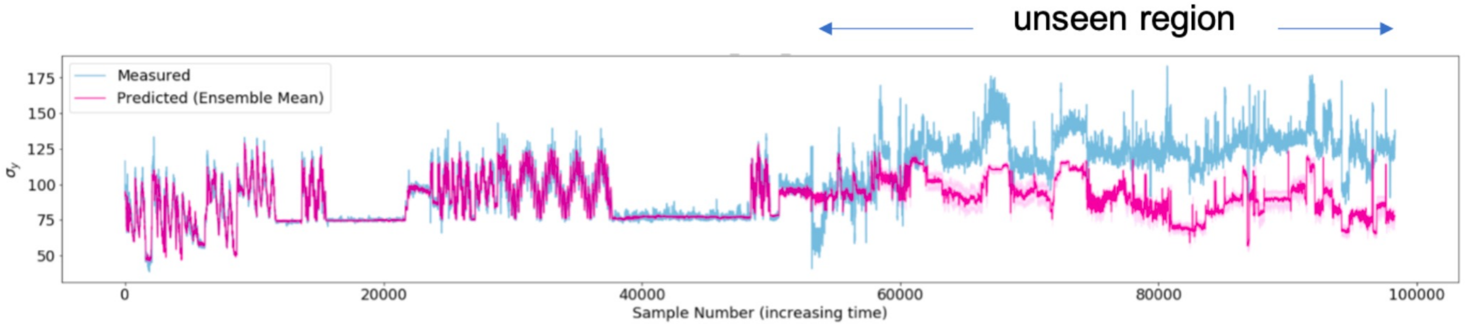
Need for robust machine learning techniques for time-varying systems (systems with distribution drift)



Simple numerical example: nonlinear simple harmonic oscillator with time-varying inputs and parameters.

$$\ddot{x}(t) = -w^2\left[x(t) + \epsilon x^2(t)\right] - b\dot{x}(t) + f(t)$$

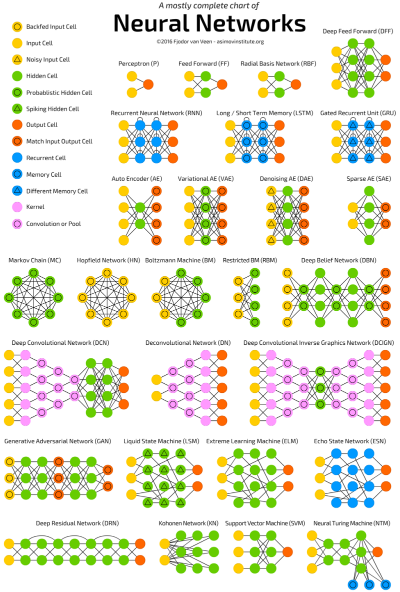
- This is a 1D analytically known system, but as soon as there are even small changes to the initial position, velocity, or non-linear coefficient ε, the trajectories change wildly. Clearly trying to memorize a model of an accelerator with thousands of nonlinear components ("Digital Twins") should be done very carefully and with a lot of skepticism since learning a single 1D system is impossible if it changes with time.



Example shared by researchers from SLAC: time-varying system shows limitations of traditional ML approaches. - Neural network predicting σ_y beam size at some test stand.

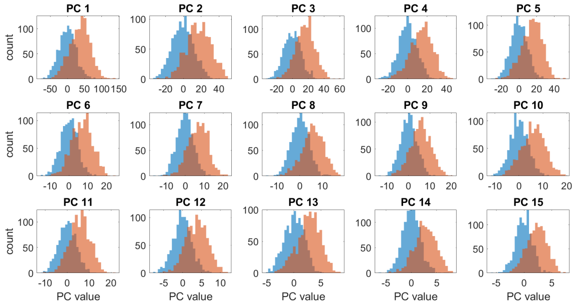
Adaptively machine learning is being developed to provide real-time diagnostics for time-varying systems

Machine Learning

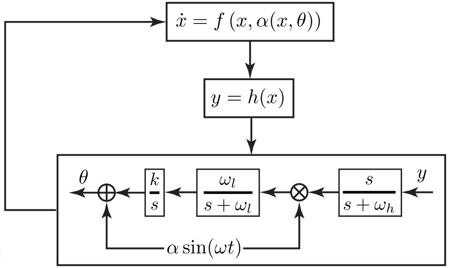


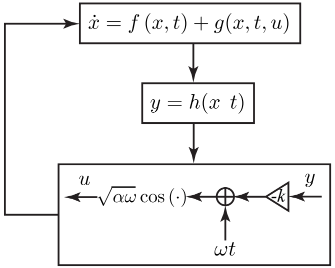
- Neural Networks
- Deep RL

Adaptive Machine Learning for Time-Varying systems with distribution shift



Model—Independent Feedback



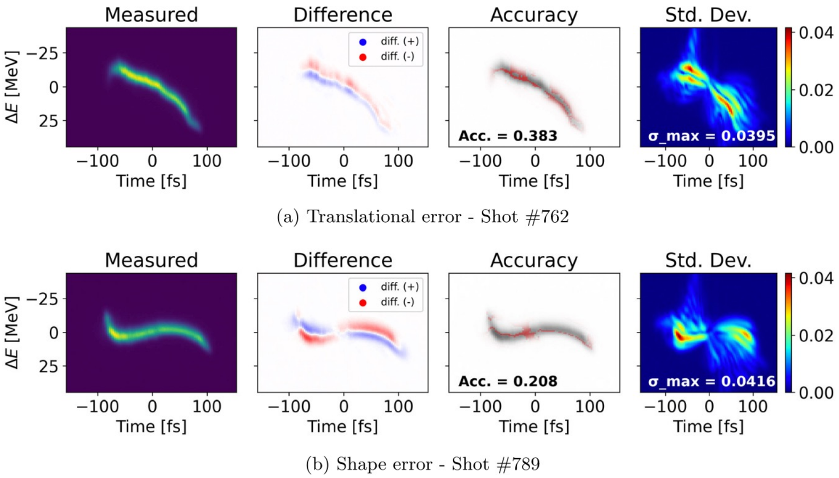


- Adaptive Control
- Extremum Seeking

Uncertainty quantification is important to try to understand how much a model can be trusted if things change

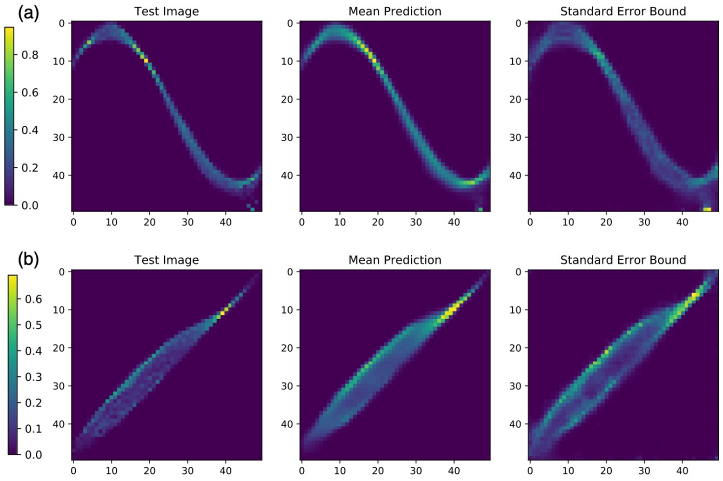
(Research led by Adi Hanuka)

Ensembles of Deep Neural Networks



LCLS-II measured longitudinal phase space predictions.

Bayesian Neural Networks

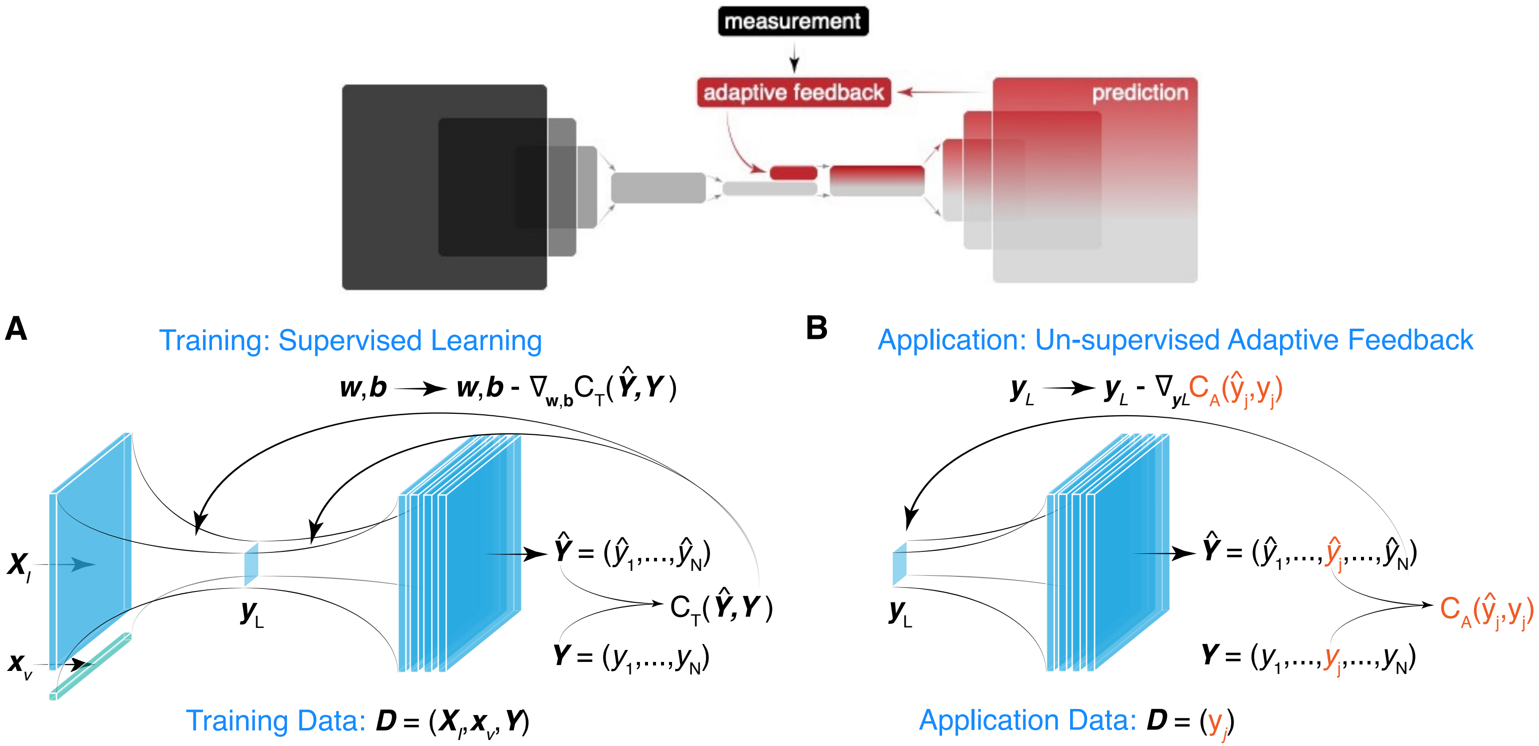


LCLS-II longitudinal phase space simulations predictions.

Convery, O., Smith, L., Gal, Y., & Hanuka, A. (2021). Uncertainty quantification for virtual diagnostic of particle accelerators. *Physical Review Accelerators and Beams*, *24*(7), 074602.

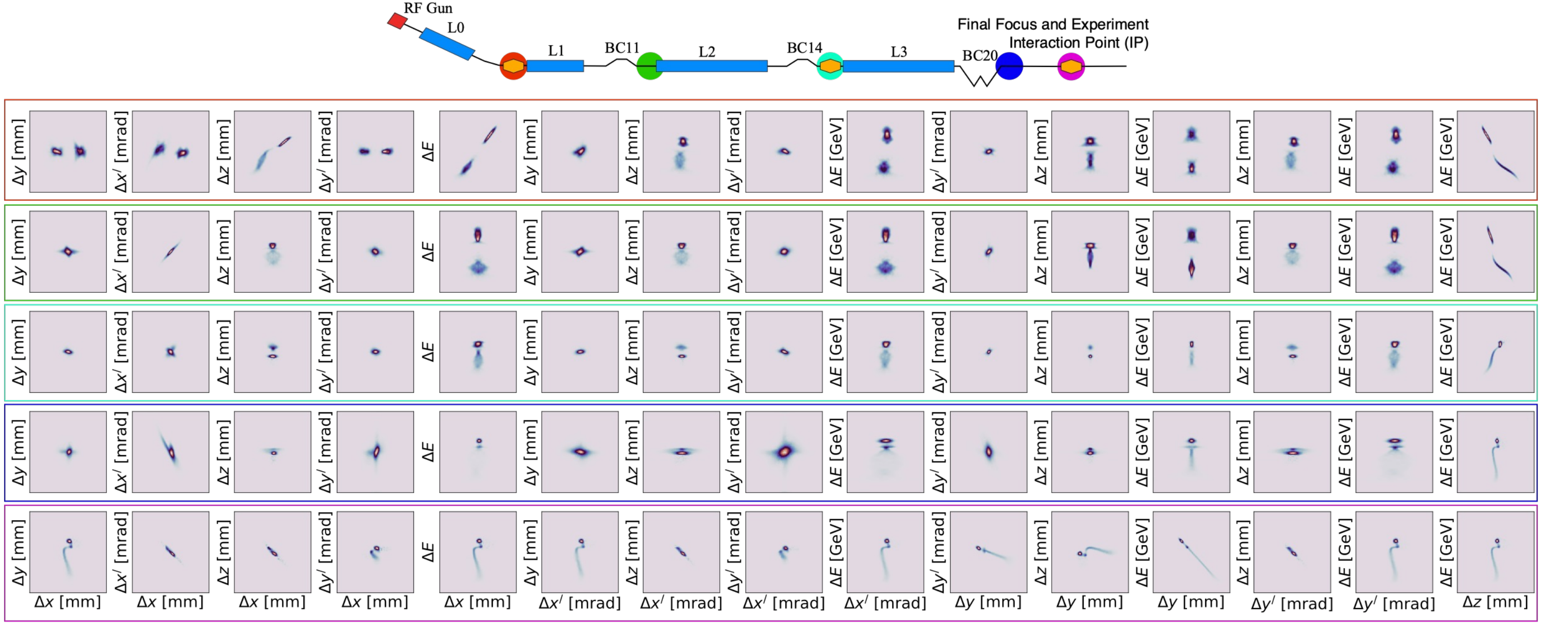
Mishra, Aashwin Ananda, et al. "Uncertainty quantification for deep learning in particle accelerator applications." *Physical Review Accelerators and Beams* 24.11 (2021): 114601.

Adaptive ML for time-varying systems: 6D phase space diagnostics. Encoder-decoder generative CNN for nonlinear data compression: Low-dimensional latent space tuning

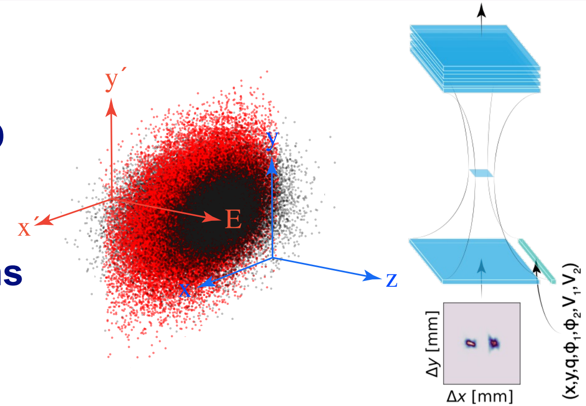


A. Scheinker. "Adaptive machine learning for time-varying systems: low dimensional latent space tuning." *Journal of Instrumentation* 16.10 (2021): P10008. https://doi.org/10.1088/1748-0221/16/10/P10008

A. Scheinker, et al. “An adaptive approach to machine learning for compact particle accelerators.” *Scientific Reports* **11,** 19187, 2021. https://doi.org/10.1038/s41598-021-98785-0



Predicting all 2D projections of 6D phase space at FACET-II at 5 different locations



6D (x, y, z, x', y', E)

2D projections

$(x, y), (x, z), (x, x'), (x, y'), (x, E)$

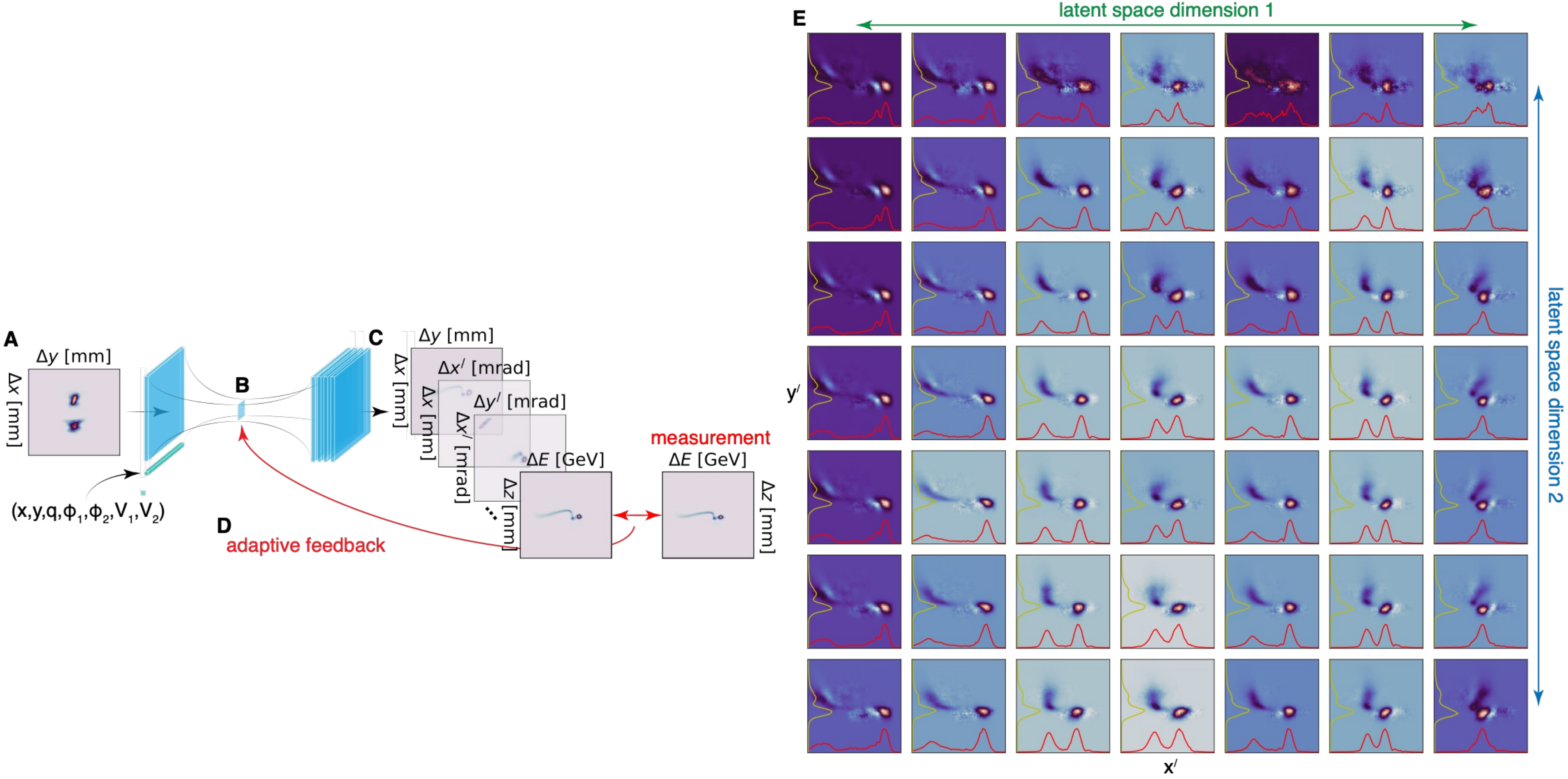
$(x', y), (x', z), (x', y'), (x', E)$

$(y, z), (y, y'), (y, E)$

$(y', z), (y', E)$

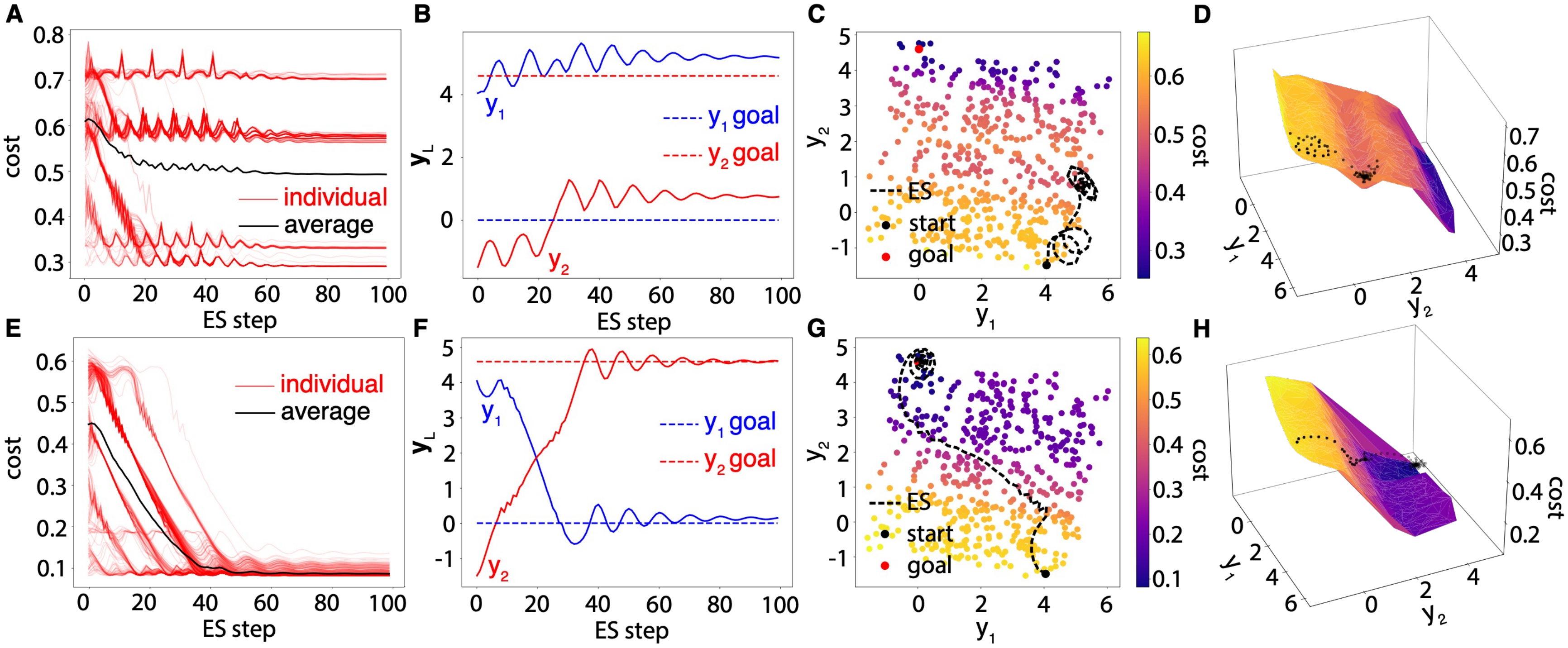
(z, E)

Looking at only (z,E) to predict other phase space projections



A. Scheinker. "Adaptive machine learning for time-varying systems: low dimensional latent space tuning." *Journal of Instrumentation* 16.10 (2021): P10008.
https://doi.org/10.1088/1748-0221/16/10/P10008

Latent space-informed diagnostics choice can design convex cost functions for unique reconstructions



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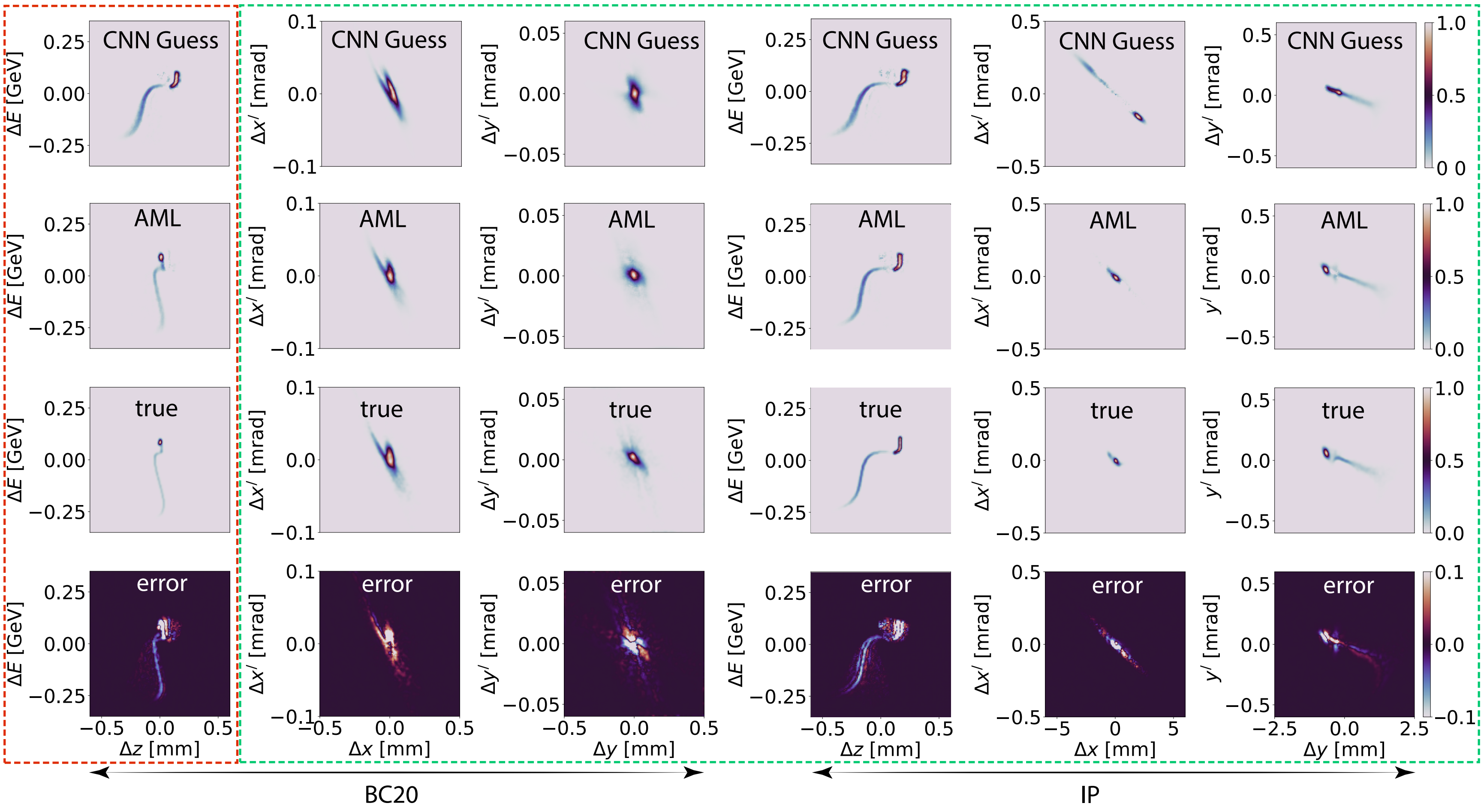
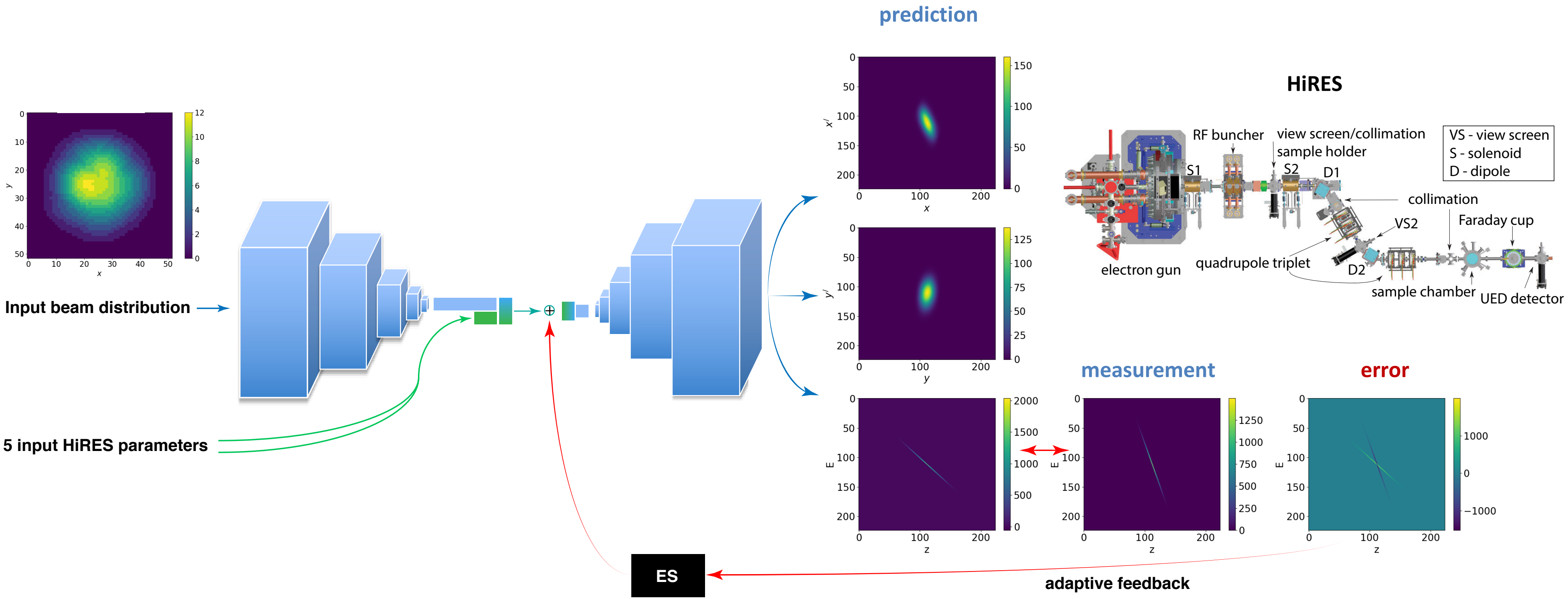
Looking at only (z,E) to predict other phase space projections



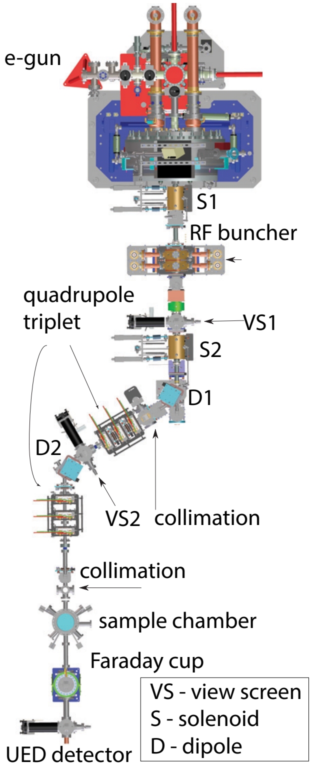
HiRES – Compact Ultra-fast Electron Diffraction (UED)

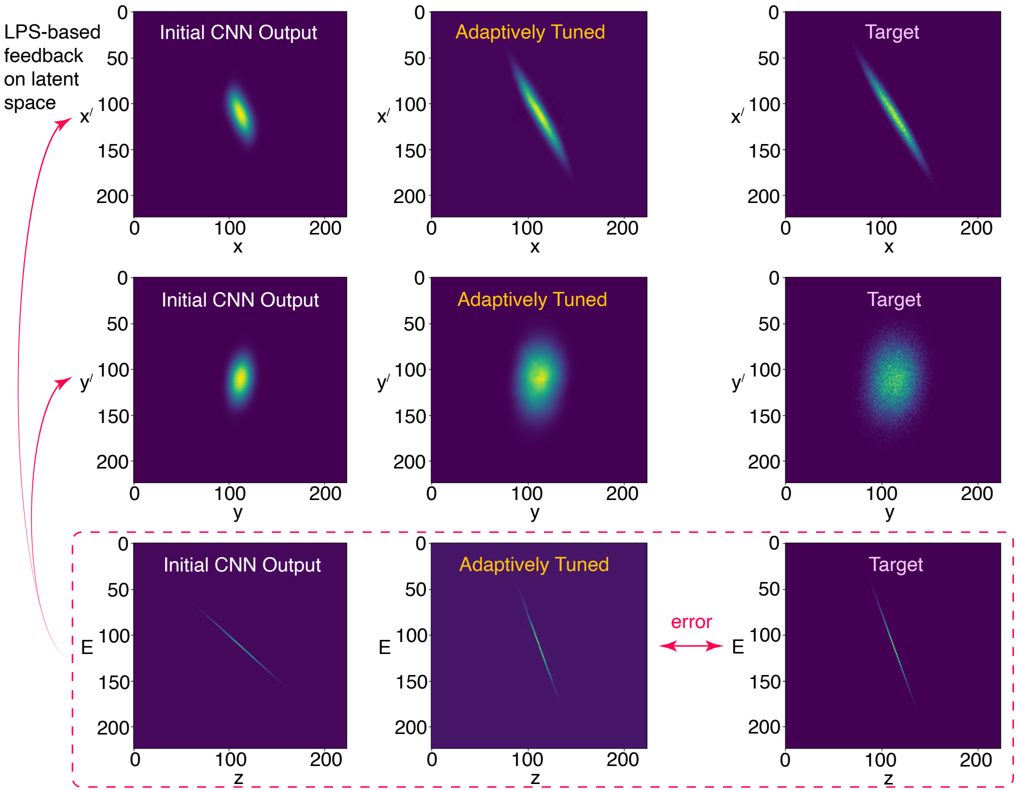


Scheinker, A., Cropp, F., Paiagua, S., & Filippetto, D. “An adaptive approach to machine learning for compact particle accelerators.” *Scientific Reports* **11,** 19187, 2021.
https://doi.org/10.1038/s41598-021-98785-0

Adaptive ML-Based Diagnostics @ HiRES

Work with: Eric Cropp and Daniele Filippetto





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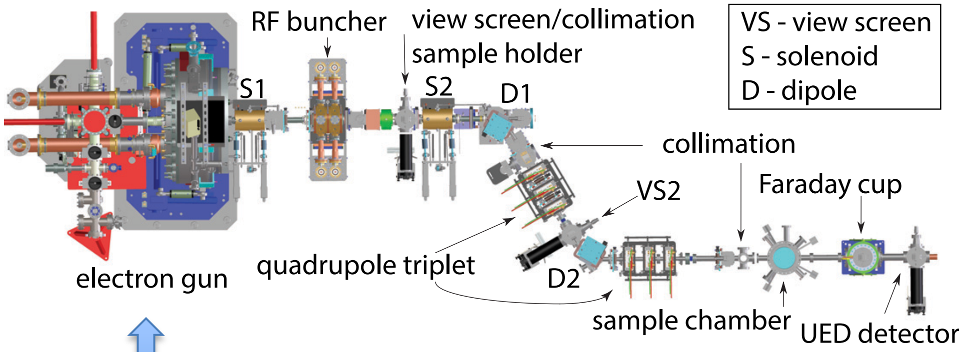
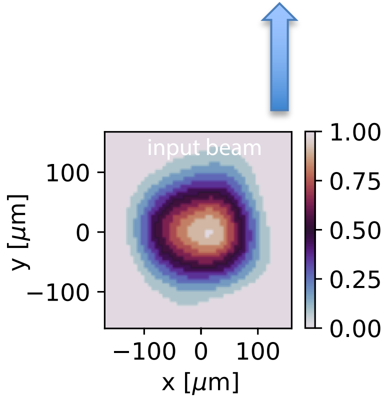
https://doi.org/10.1088/1748-0221/16/10/P10008

Adaptive ML-Based Diagnostics @ HiRES

Inverse Model Determines Unknown/Time-Varying Input Beam Distribution





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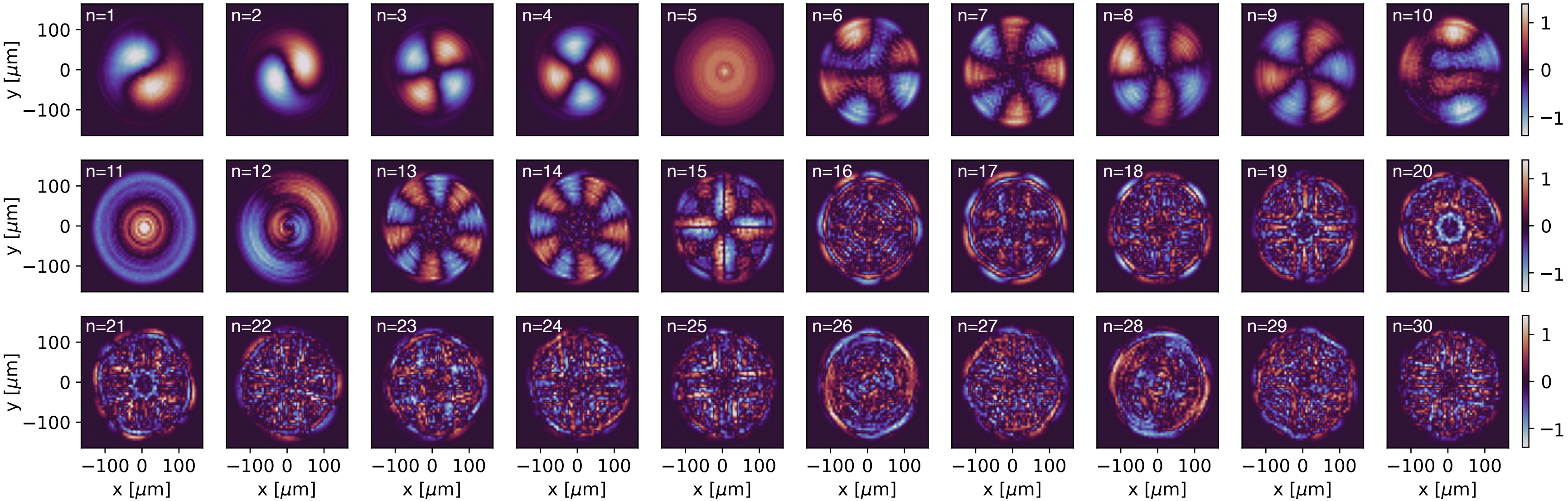
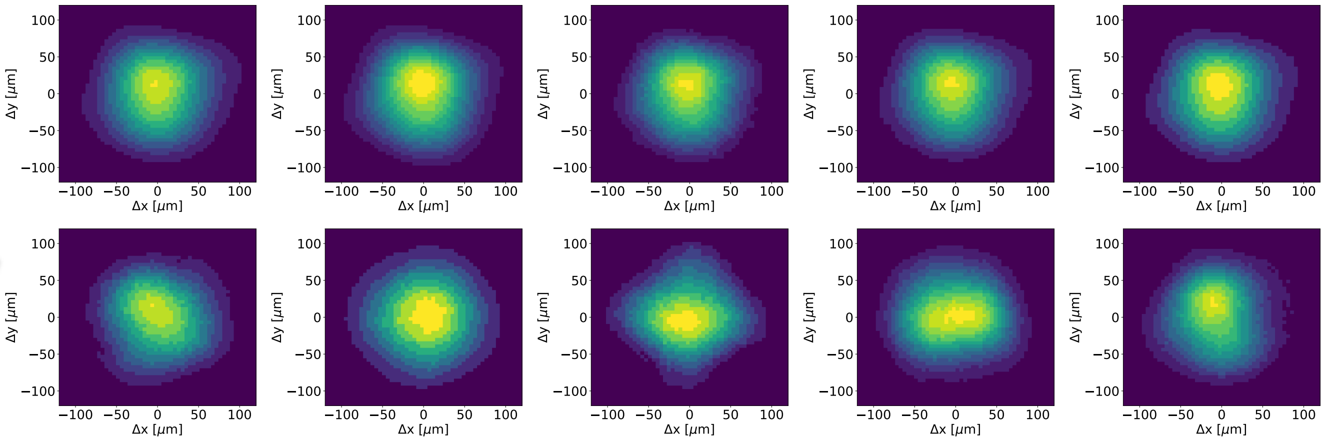
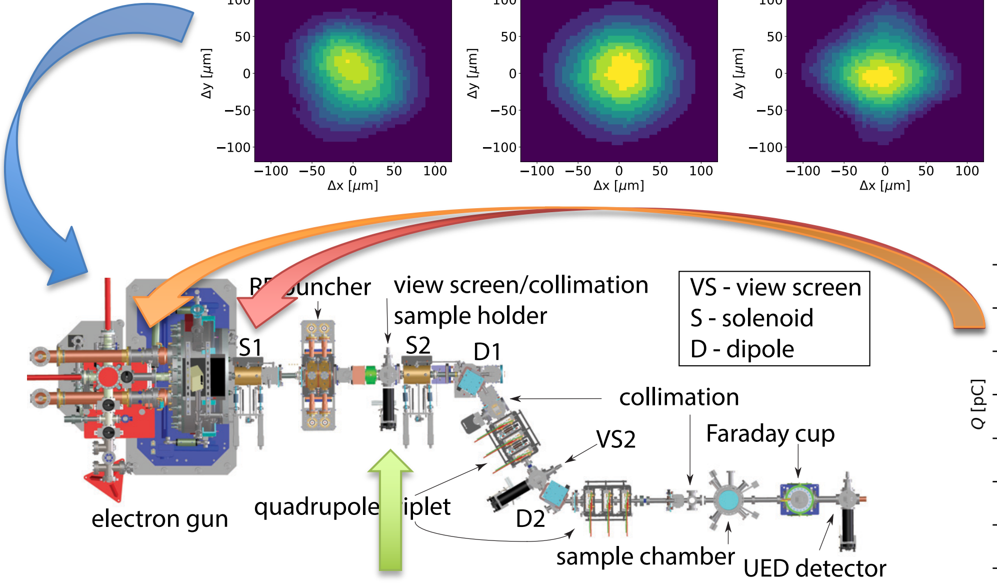
PCA Used to Find Basis for Electron Beam

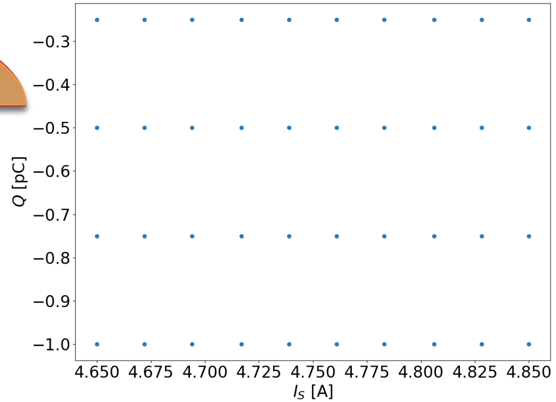


$$I_{i,N_{pca}} = \sum_{n=1}^{N_{pca}} \alpha_{i,n} \times \mathrm{PC}_n.$$

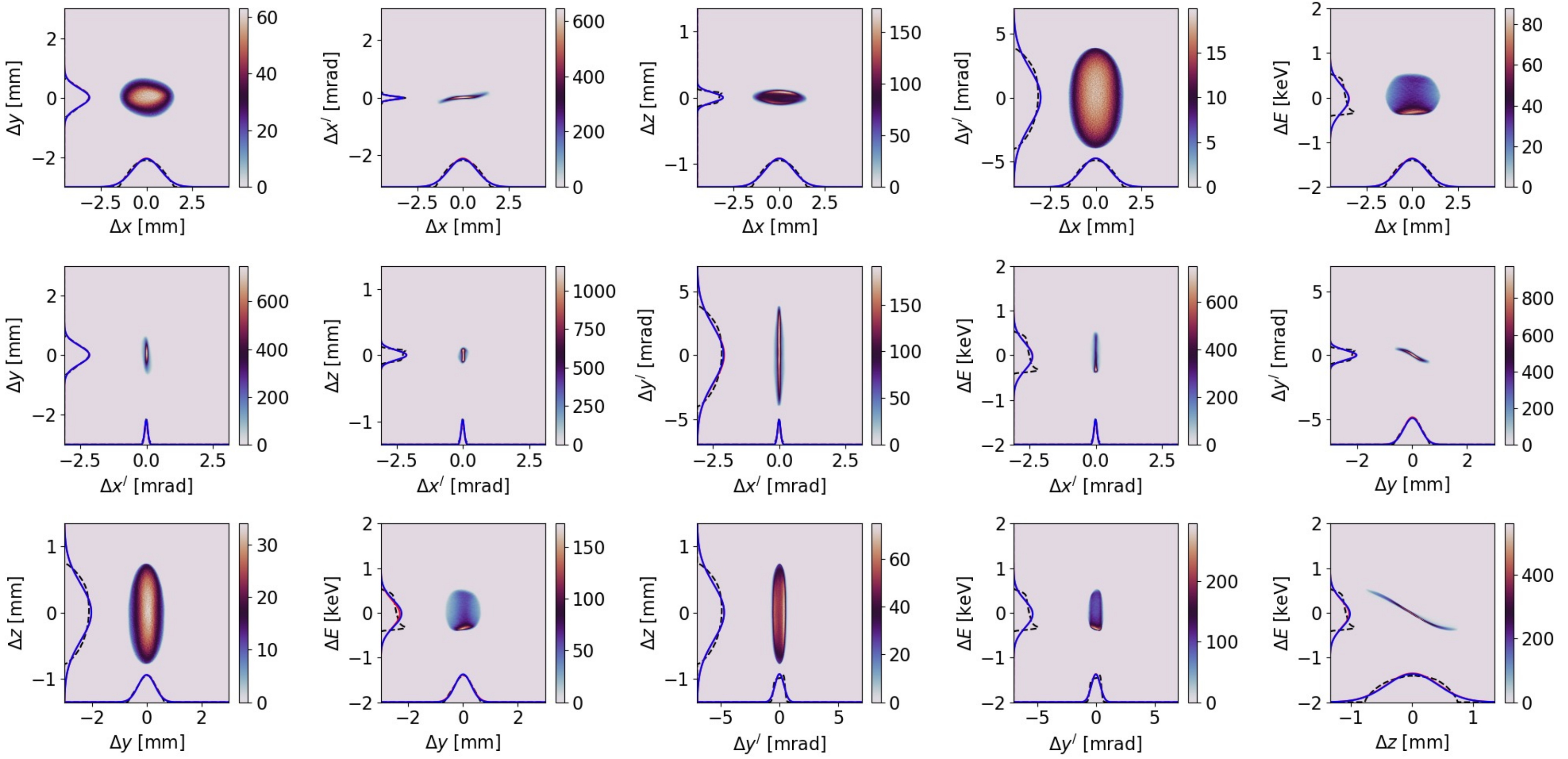
HiRES – AML for 6D Phase Space Trained with Measured and Synthetic Input Images over a Range of Bunch Charge and Solenoid Current





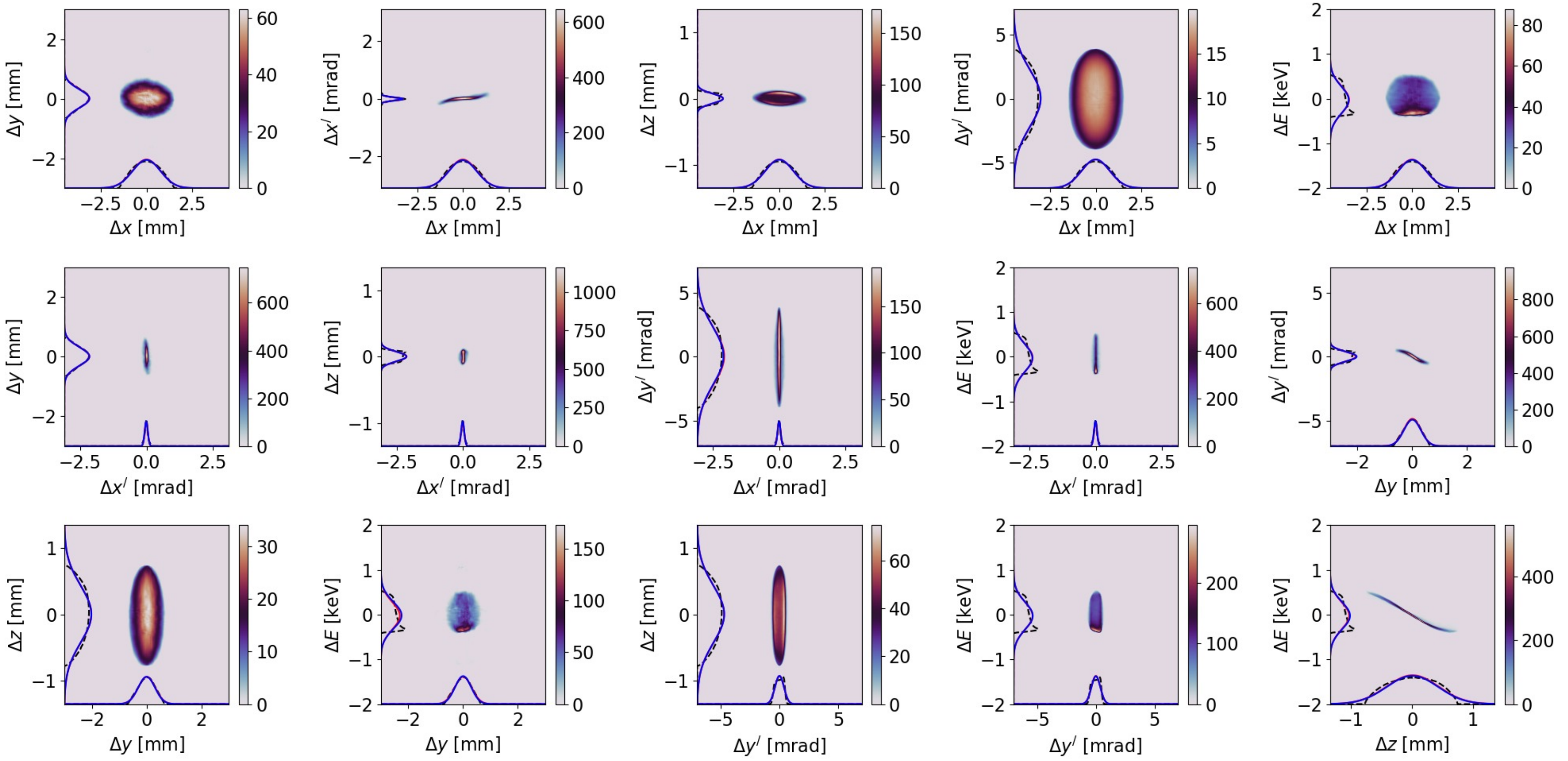


True

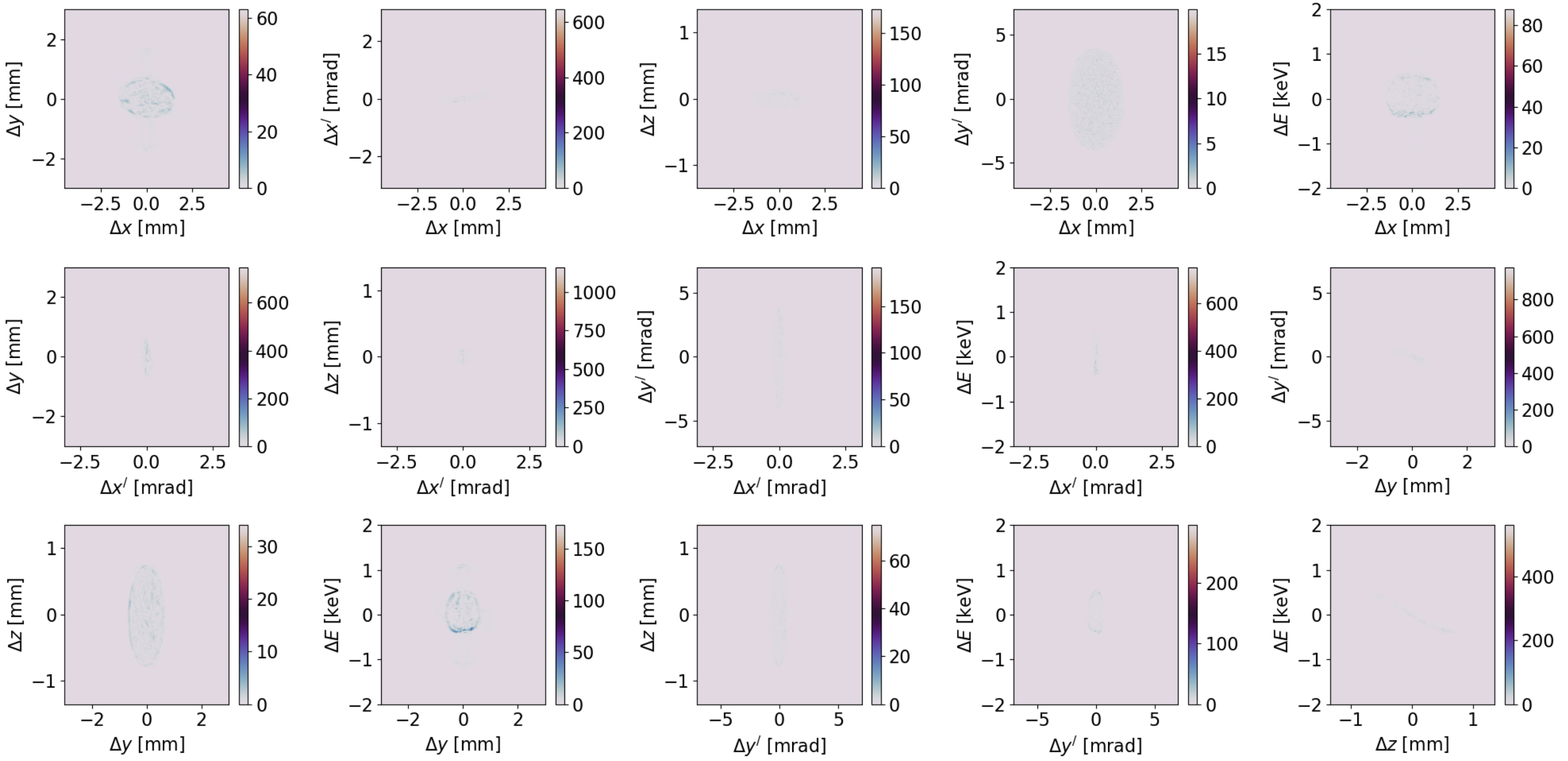


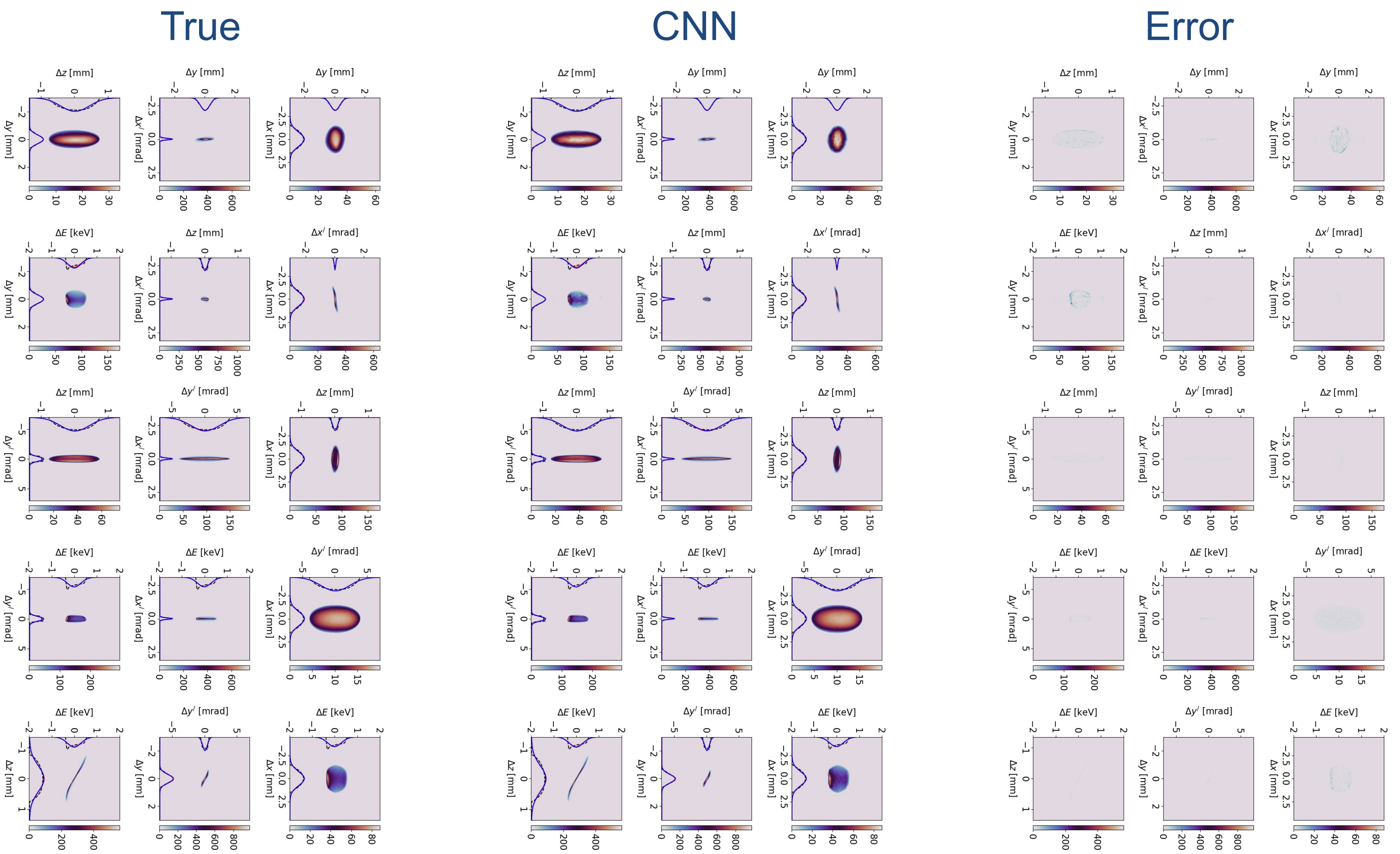
Δy [mm]
Δx [mm]
Δx′ [mrad]
Δx [mm]
Δz [mm]
Δx [mm]
Δy′ [mrad]
Δx [mm]
ΔE [keV]
Δx [mm]
Δy [mm]
Δx′ [mrad]
Δz [mm]
Δx′ [mrad]
Δy′ [mrad]
Δx′ [mrad]
ΔE [keV]
Δx′ [mrad]
Δy′ [mrad]
Δy [mm]
Δz [mm]
Δy [mm]
ΔE [keV]
Δy [mm]
Δz [mm]
Δy′ [mrad]
ΔE [keV]
Δy′ [mrad]
ΔE [keV]
Δz [mm]

CNN

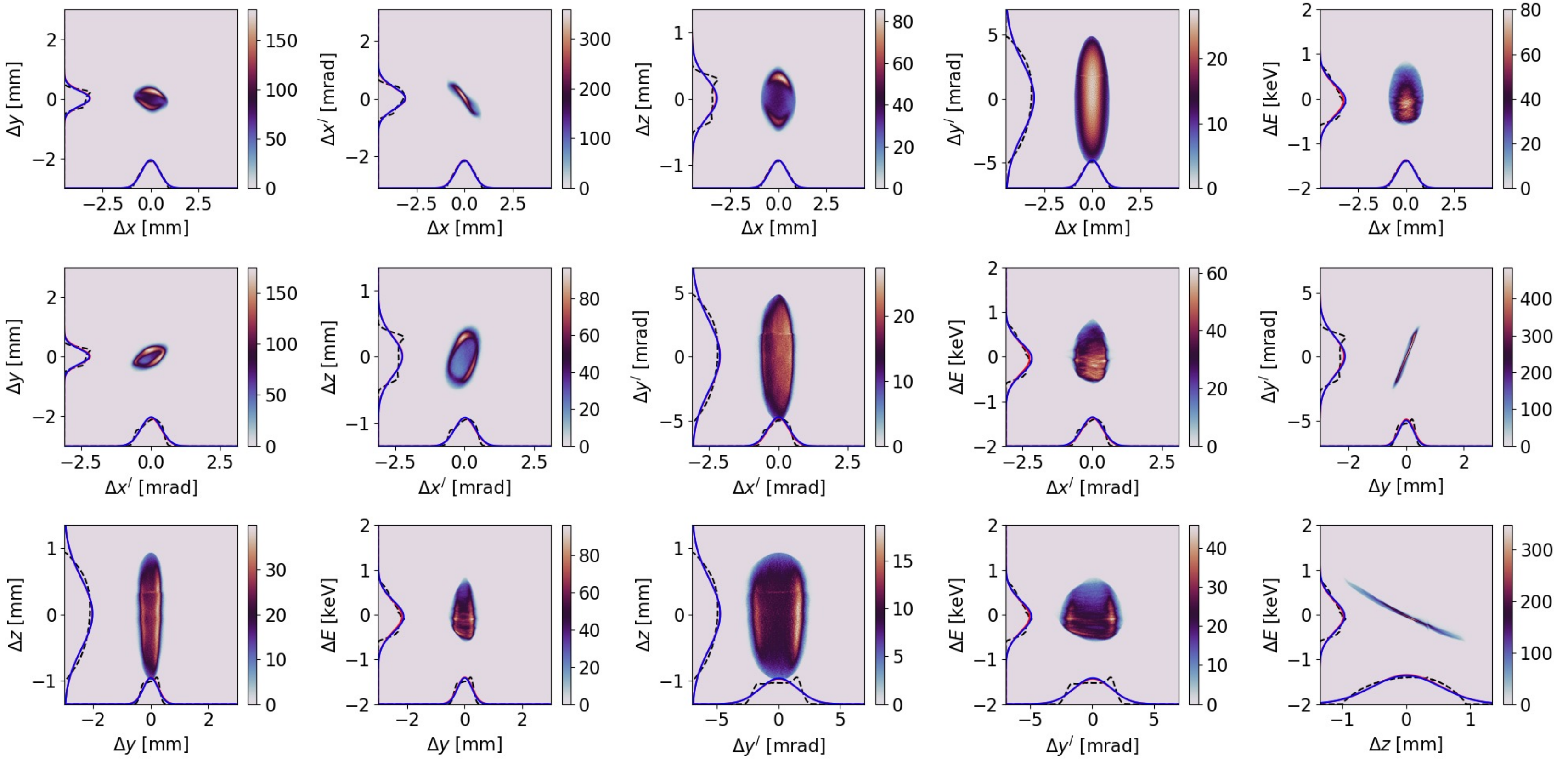


Difference

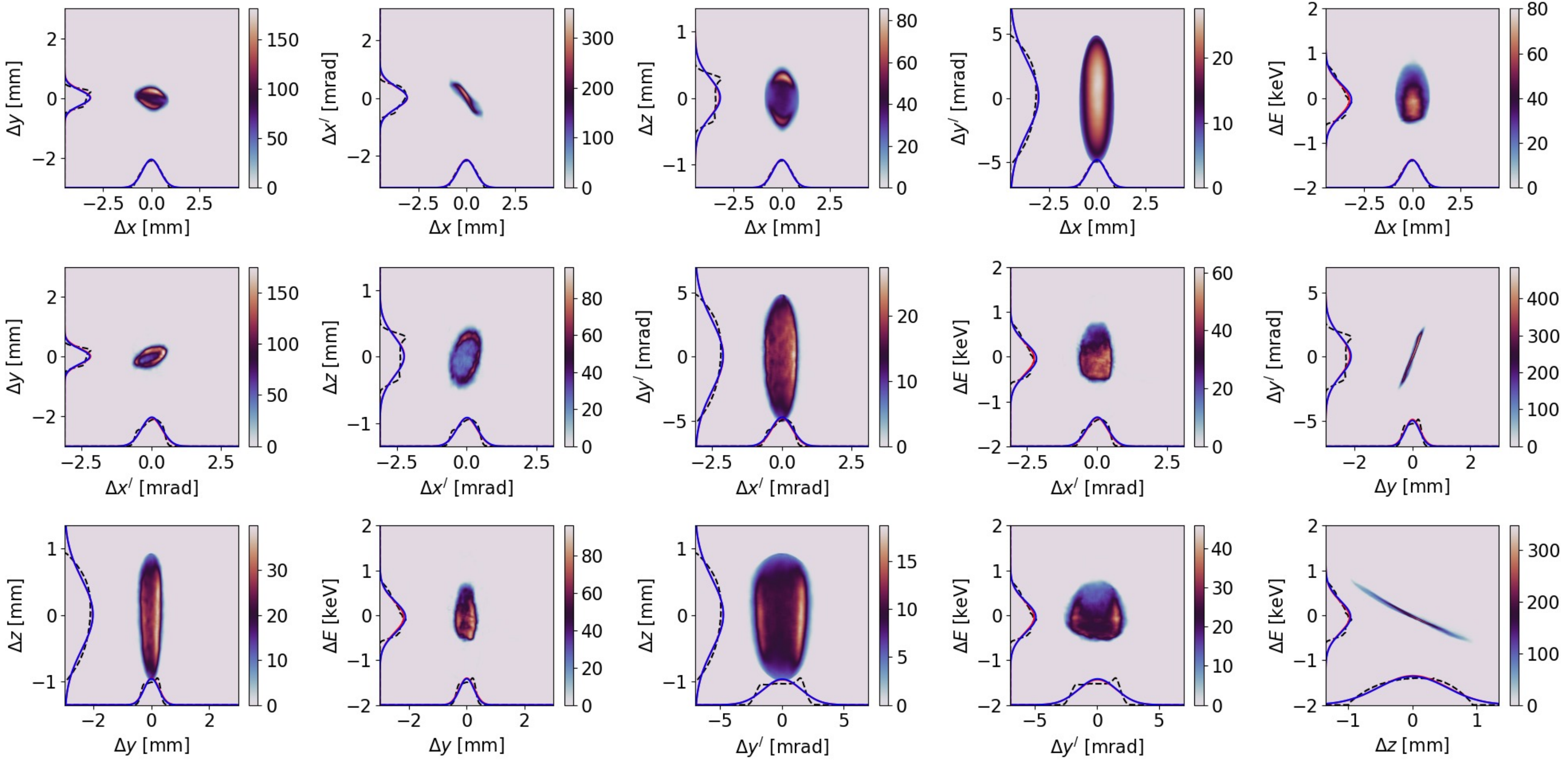



True
CNN
Error

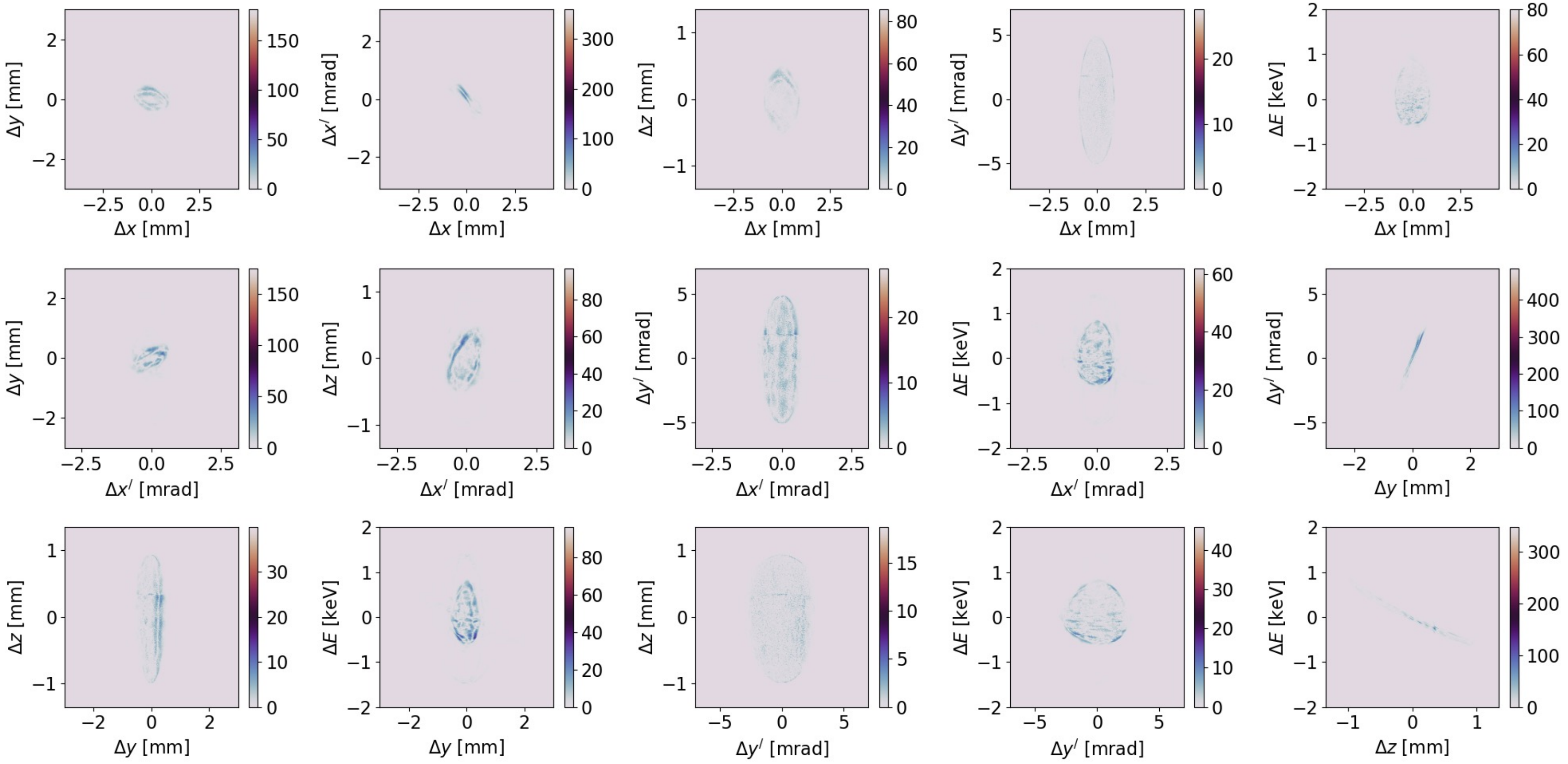
True

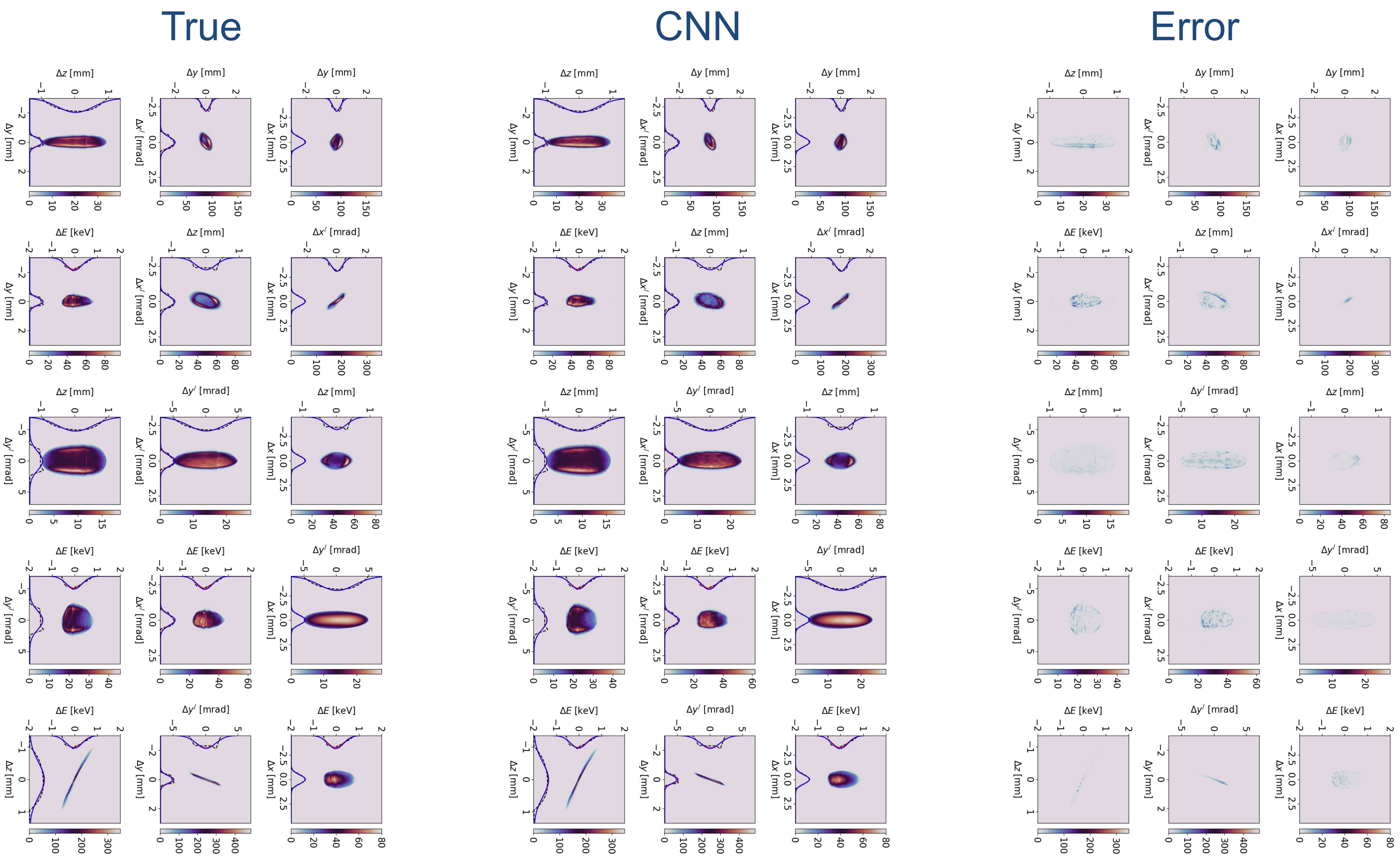

Δy [mm]
Δx [mm]
Δx′ [mrad]
Δx [mm]
Δz [mm]
Δx [mm]
Δy′ [mrad]
Δx [mm]
ΔE [keV]
Δx [mm]
Δy [mm]
Δx′ [mrad]
Δz [mm]
Δx′ [mrad]
Δy′ [mrad]
Δx′ [mrad]
ΔE [keV]
Δx′ [mrad]
Δy′ [mrad]
Δy [mm]
Δz [mm]
Δy [mm]
ΔE [keV]
Δy [mm]
Δz [mm]
Δy′ [mrad]
ΔE [keV]
Δy′ [mrad]
ΔE [keV]
Δz [mm]

CNN

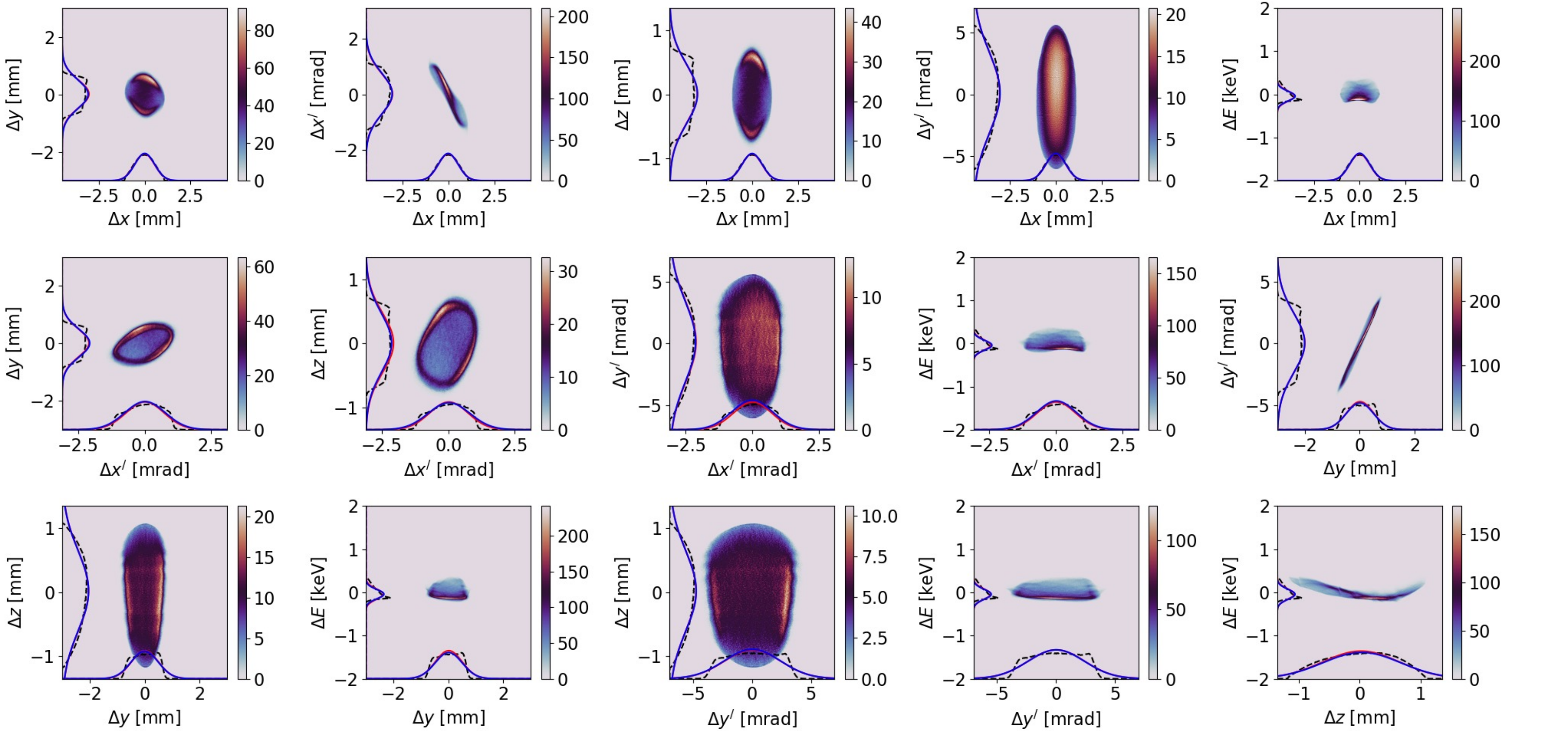


Difference

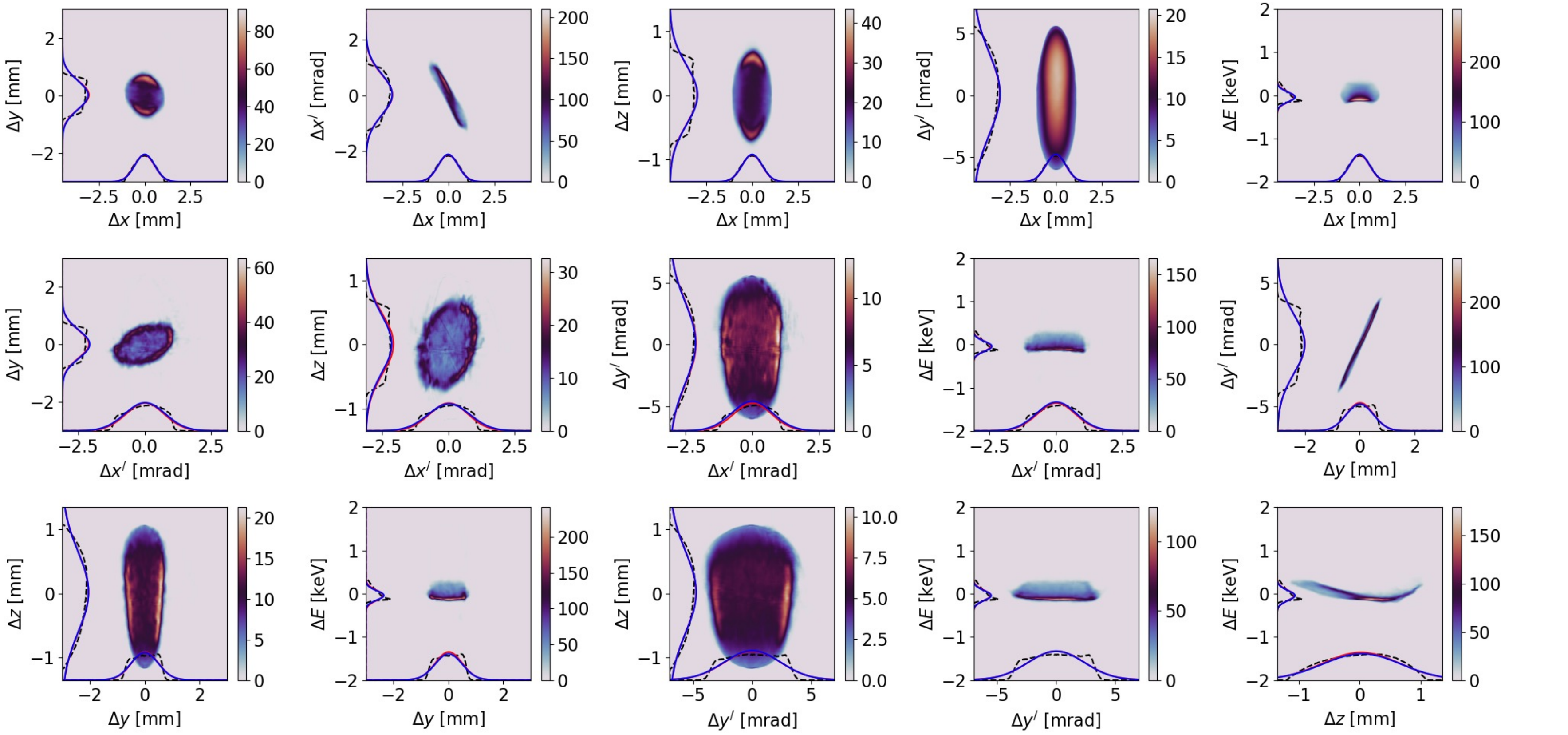



True
CNN
Error

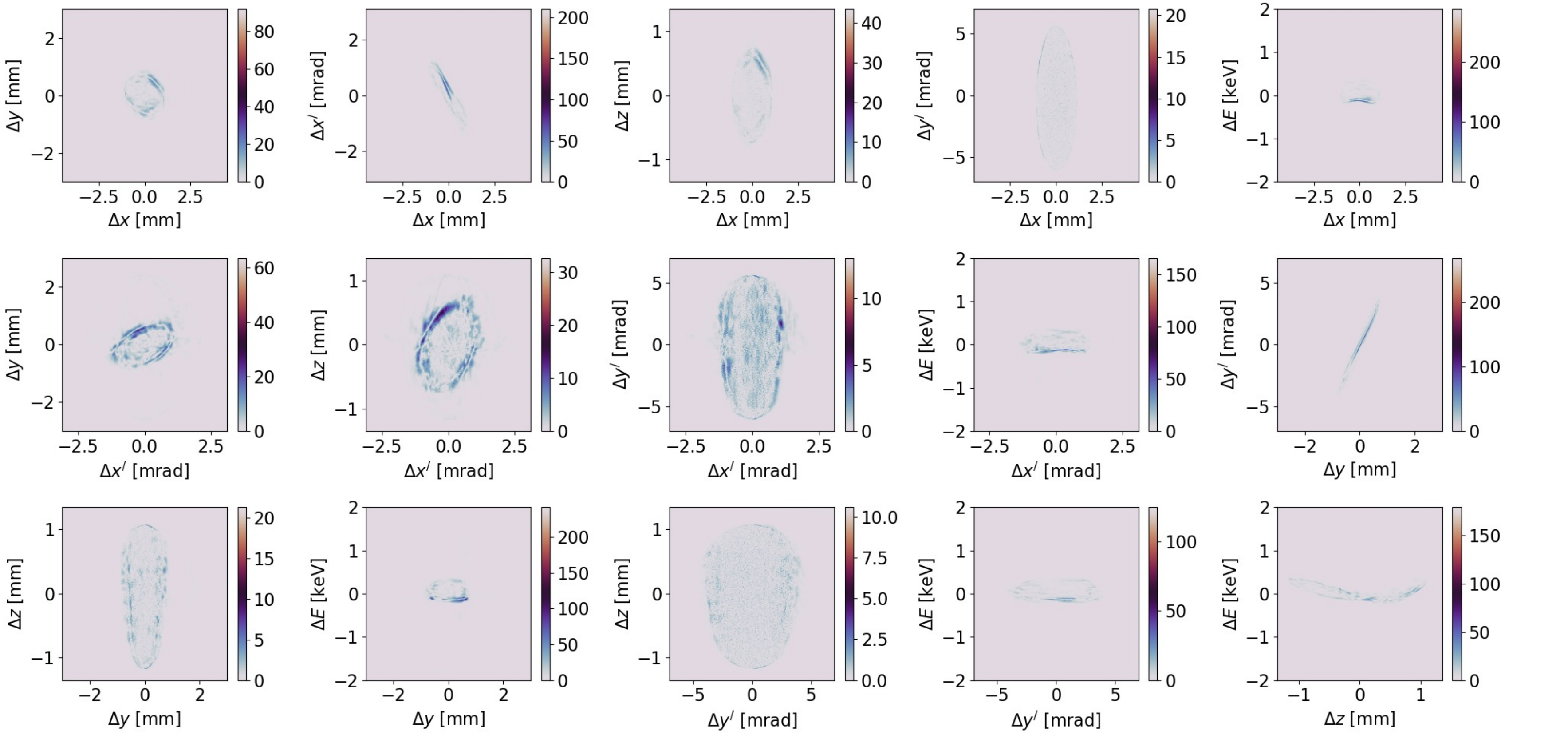
True

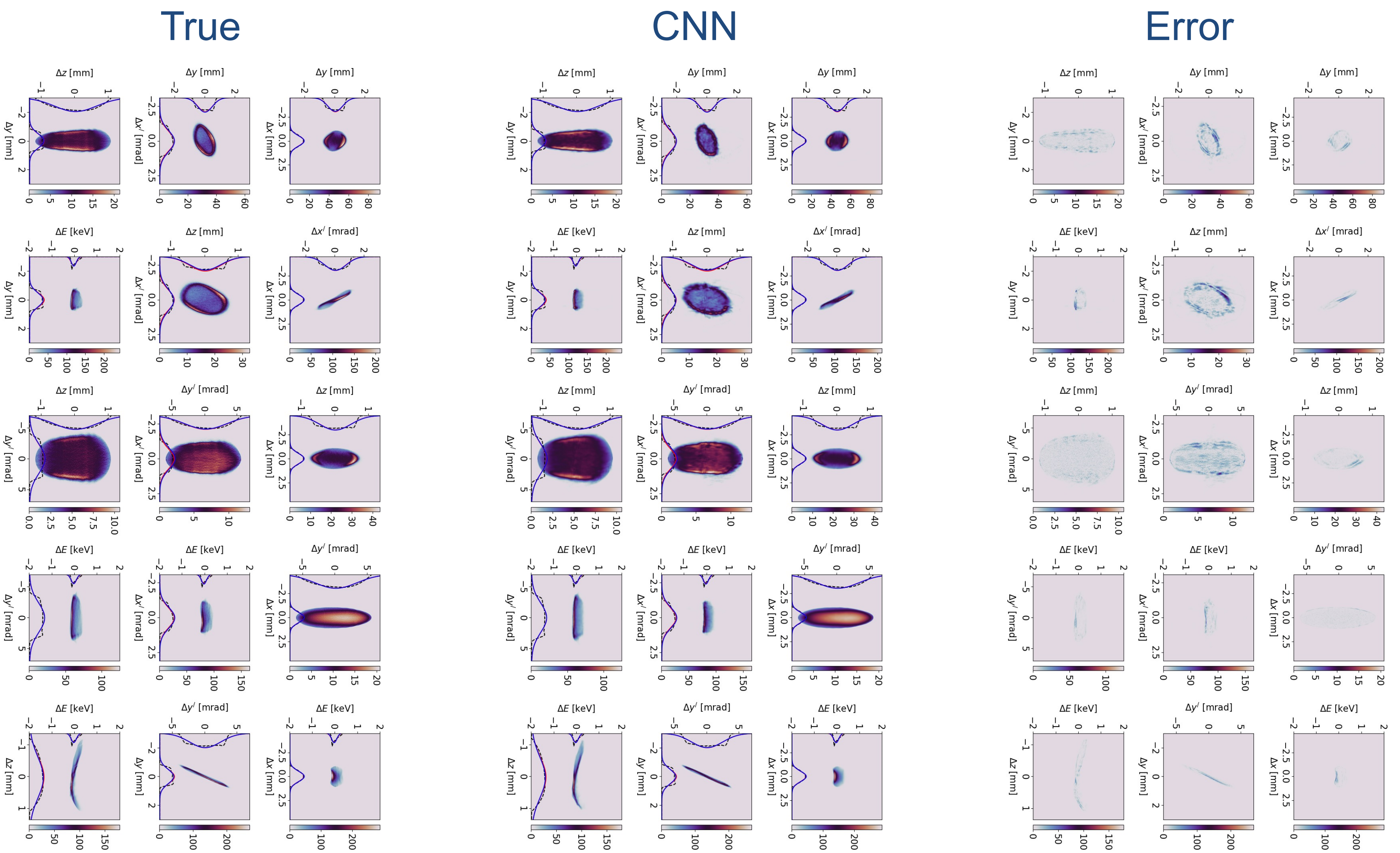


CNN

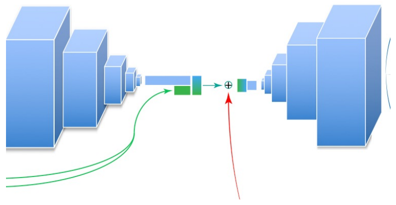


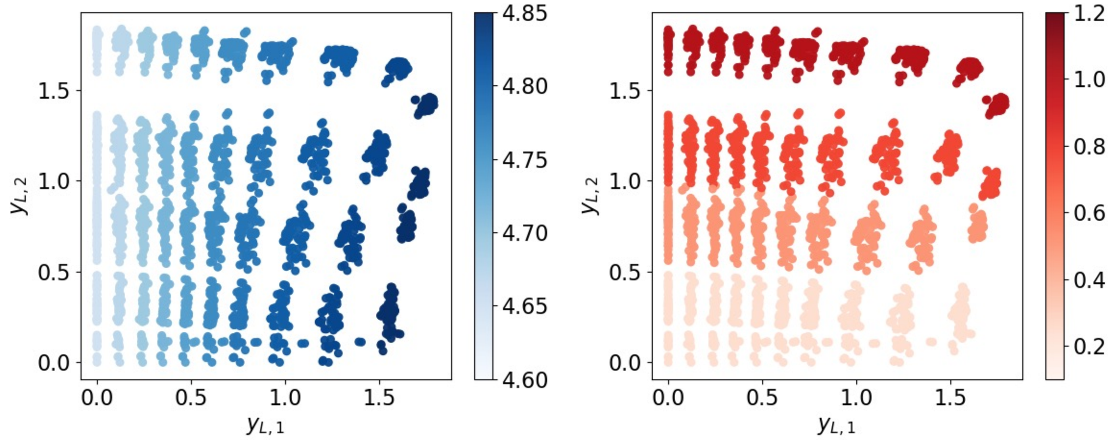
Difference

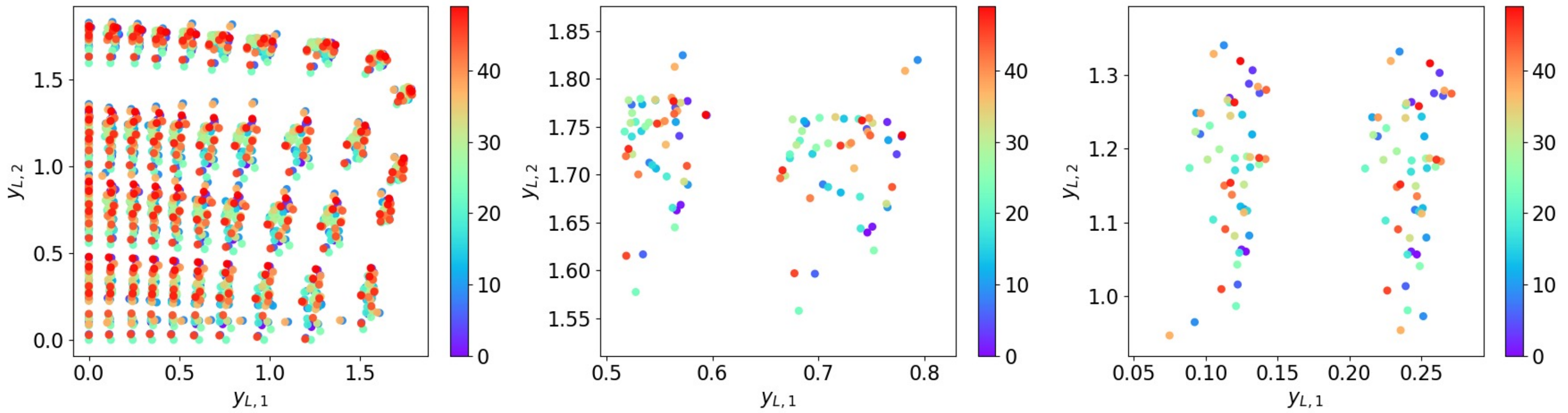



True
CNN
Error

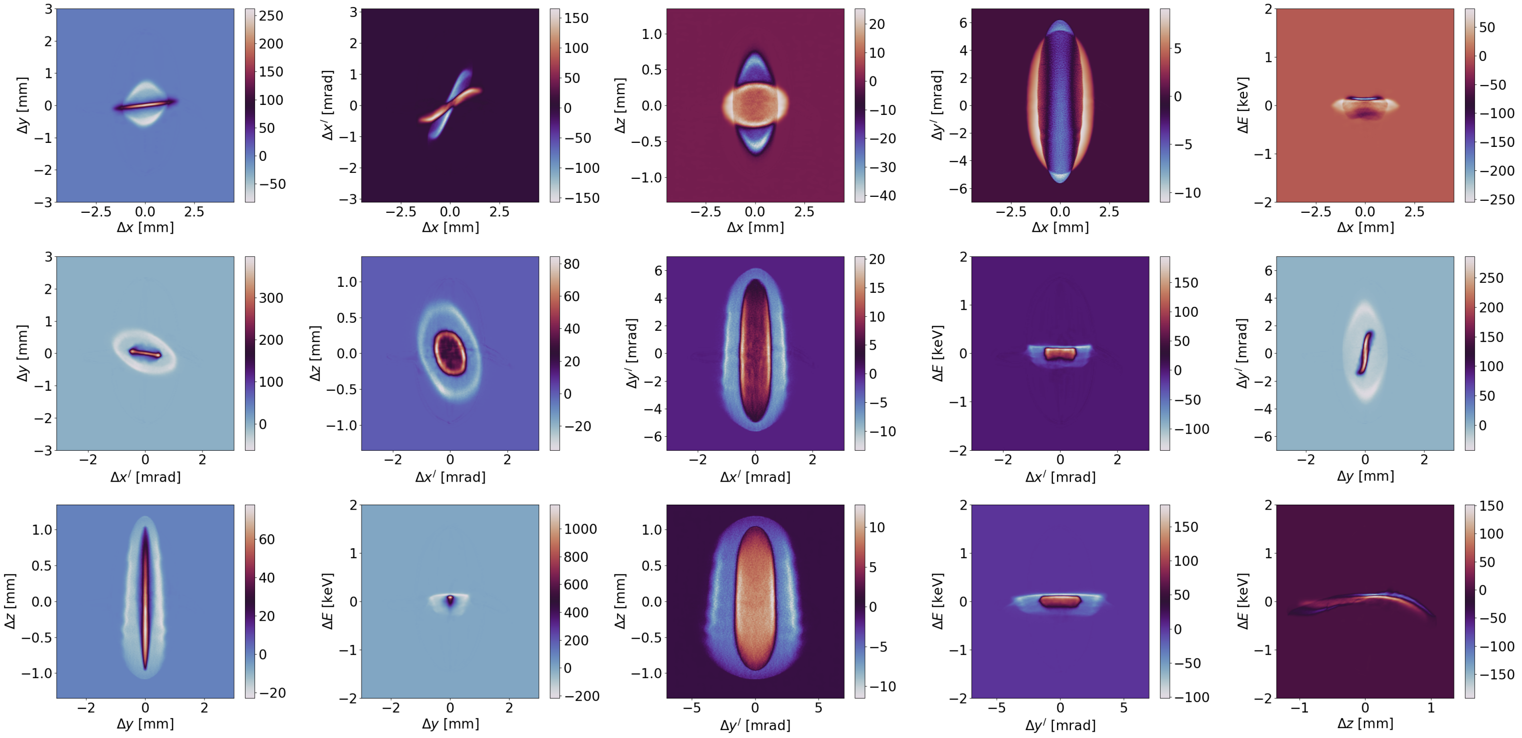
HiRES – Latent space representation



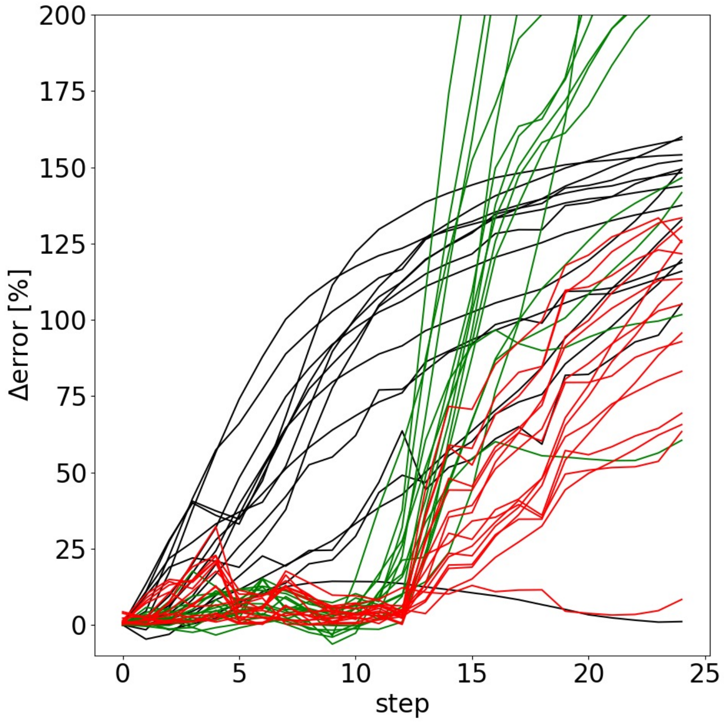




Phase space projection differences for beam far outside of the span of training data.



Errors [%] of 15 projections of the 6D phase space as the input beam distribution leaves the span of the training set and so do the solenoid current and bunch charge.



A measure of the % difference of the 15 projections relative to initial input and parameter settings as the beam changes.

A measure of the % error of the 15 projections if the input beam and parameter settings are known. The error remains small within the span of the training set and then the CNN catastrophically fails as the training set is left behind (it is actually worse than doing nothing), as expected.

A measure of the % error of the 15 projections if the input beam and parameter settings are unknown, but adaptive ML is used for active feedback based on (z,E) measurements. No catastrophic failure in this robust approach.

Adaptive ML phase space projection errors for point far outside of training set span.