

ICFA Mini-Workshop on AI/ML  
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**FRIB**



# Transverse 2D phase-space tomography using BPMs

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U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science

# Theoretical marginal profile estimation using turn-by-turn kicked beam centroid data



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# kicked beam centroid in normal form

- Time evolution of the 2D canonical variables in normal form read

$$x(t) - ip(t) = (x_0 - ip_0)e^{i\omega t} = \sqrt{2J_0}e^{i(\omega t - \theta)}$$

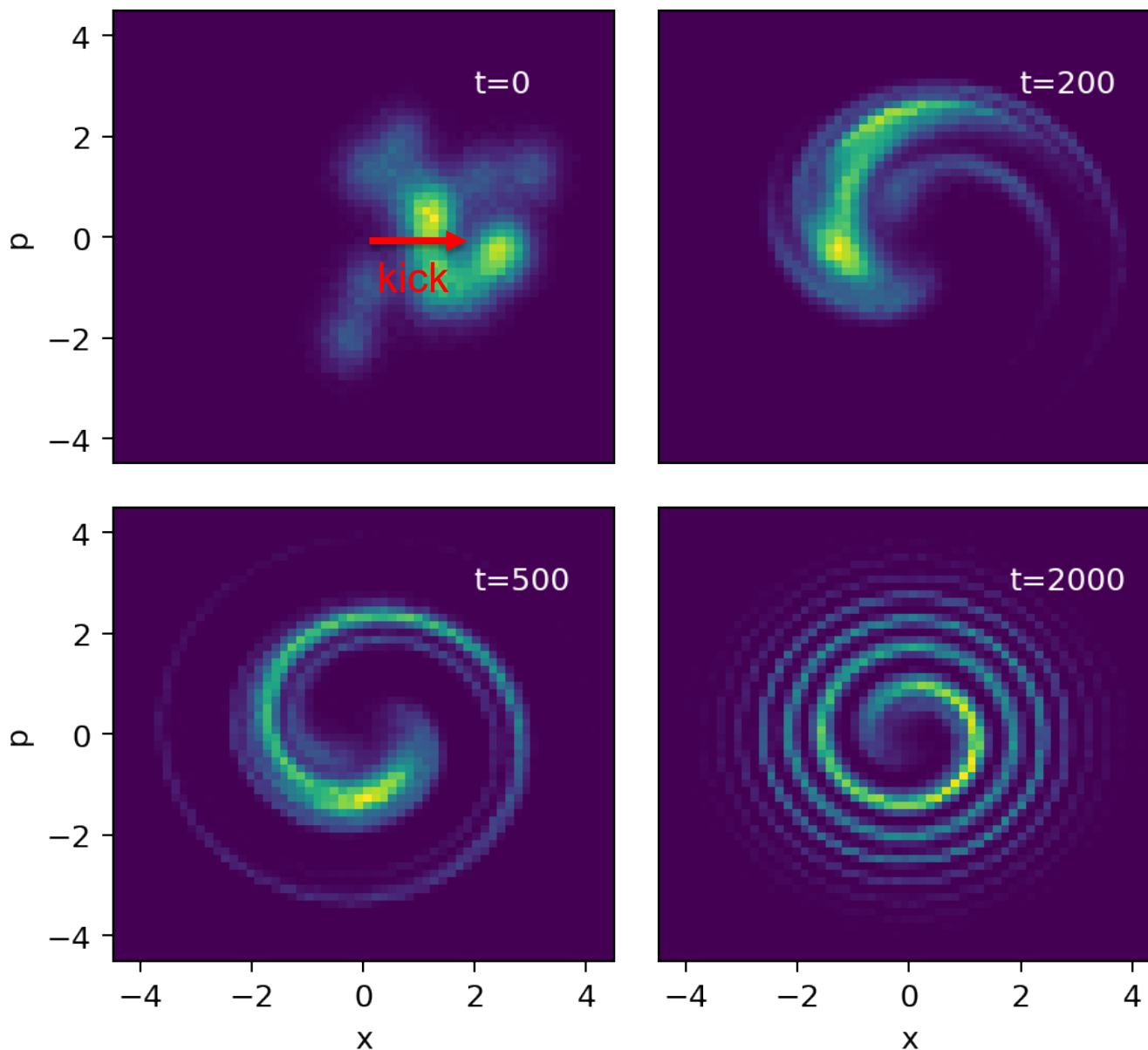
$$\omega(J_0), \quad J_0 = (x_0^2 + p_0^2)/2$$

- TBT(turn-by-turn) beam centroid data is function of initial (before kick) beam distribution

$$\langle x \rangle_t = \Re \int (x - ip)e^{i\omega t} \rho(x - x_0, p - p_0) dx dp$$

- We may be able to reconstruct beam phase-space using a BPM*

# illustration of nonlinear decoherence (due to phase mixing)



# Theoretical estimation of the marginal beam profile

- If assume

1. **slowly varying** betatron frequency over the beam area s.t.

$$\omega(\Delta J) = \mu_0 + \mu_1 \Delta J \dots \quad \Delta J \equiv J - J_0$$

2. **large kick strength** s.t.  $J_0/\epsilon \gg 1$

- Marginal beam profile (along the kick angle) can be analytically expressed

$$\lambda_\theta(x) = 2 \frac{|\mu_1|}{\pi} \Re \sum_{t=0}^T e^{i\theta} e^{-i(\mu_1 \sqrt{2J_0} x + \mu_0)t} \langle x \rangle_t$$

$$p_0 \cos \theta = x_0 \sin \theta$$

$$- \frac{|\mu_1|}{\pi} \sqrt{2J_0} \cos^2 \theta$$

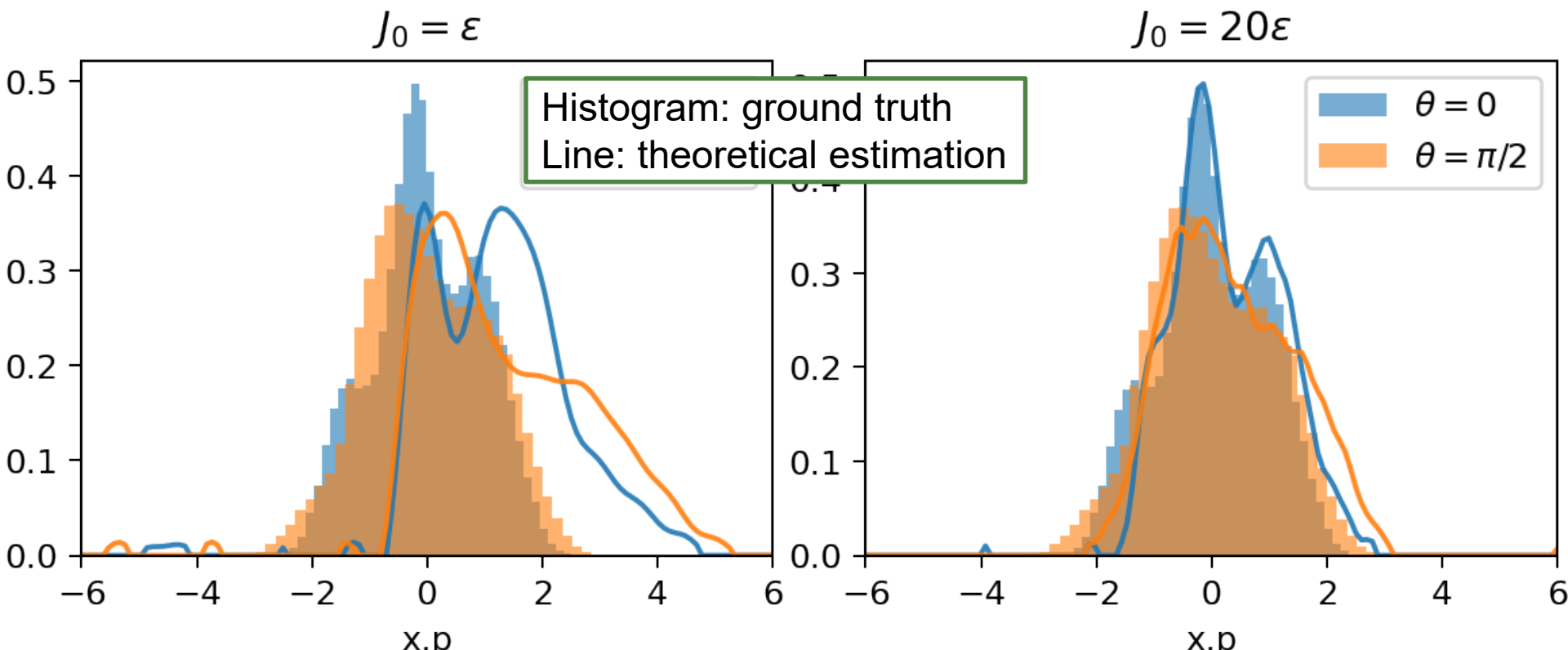
$$\lambda_\theta(x) \equiv \int \rho_\theta(x, p) dp$$

$$\rho_\theta(x, p) = \rho(x \cos \theta - p \sin \theta, p \cos \theta + x \sin \theta)$$

# however, the **large kick strength** assumption can be limited due to beam pipe aperture

- Illustration on a toy model:

$$\omega = \omega_0 + \omega_1 J + \omega_2 \frac{J^2}{2}$$



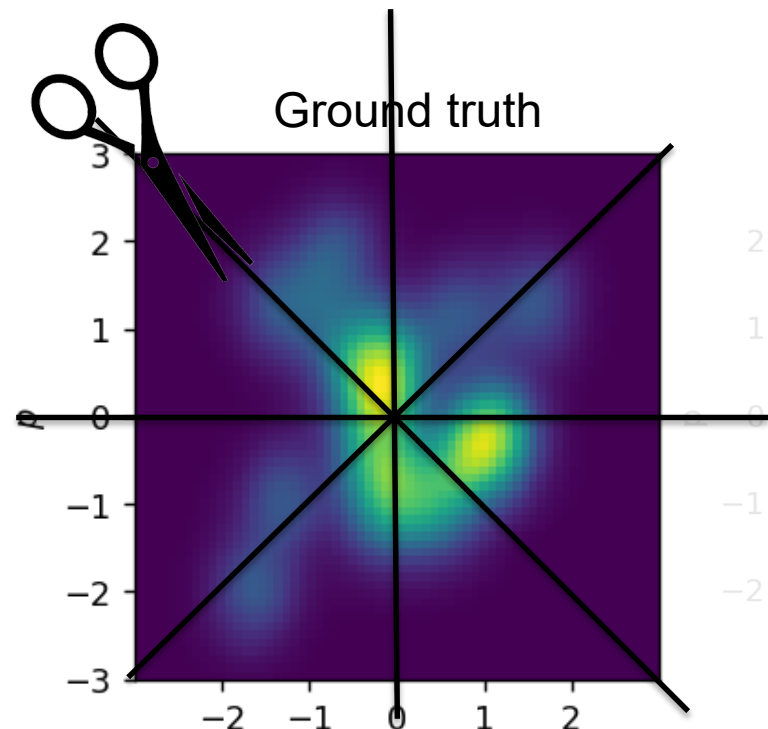
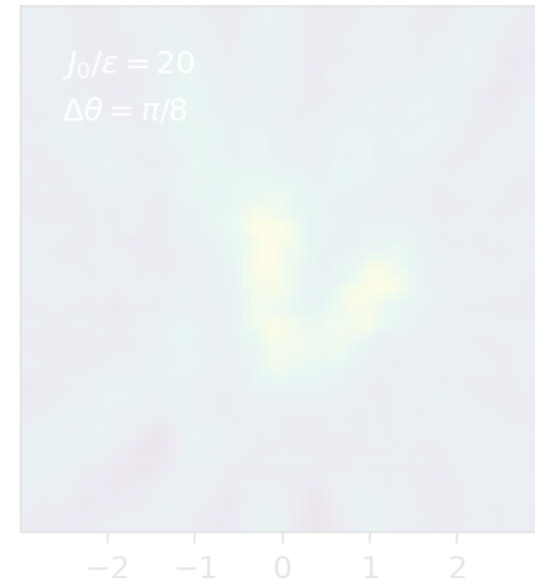
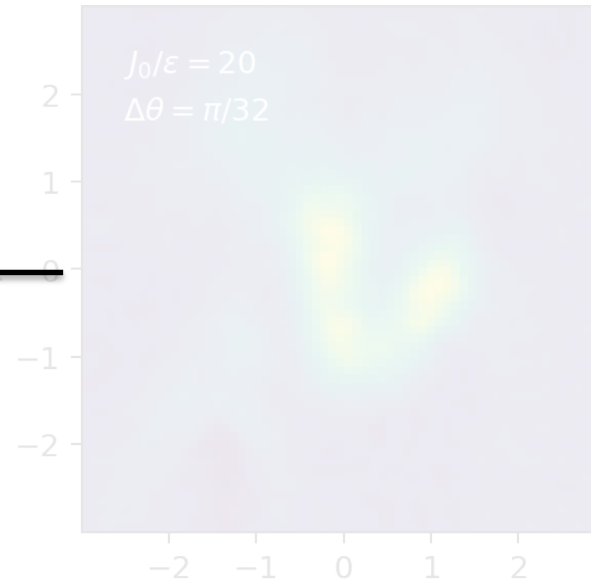
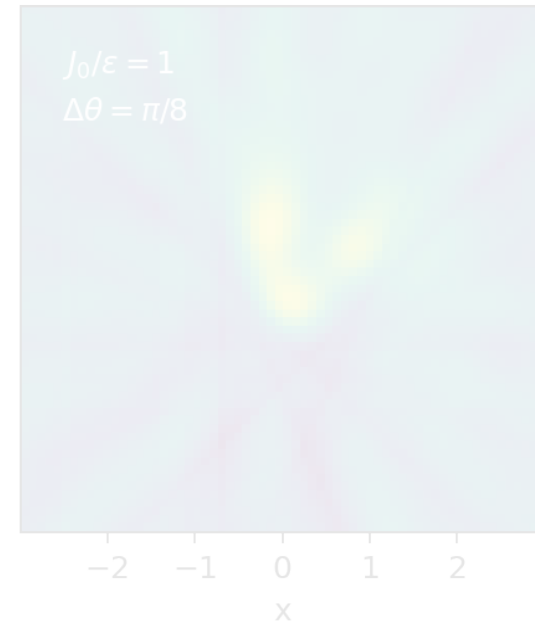
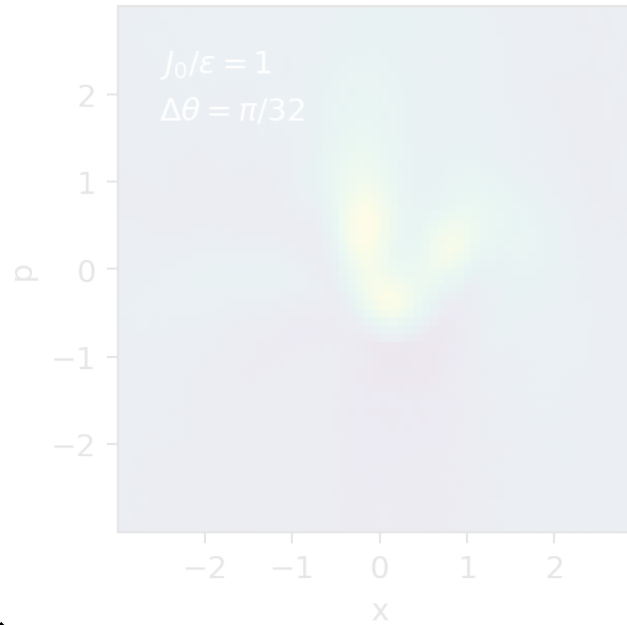
**Inverse Radon transformation (an algebraic tomography method) using theoretically estimated marginal profiles**



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# Inverse Radon transformation (an algebraic method) using theoretically estimated marginal profiles

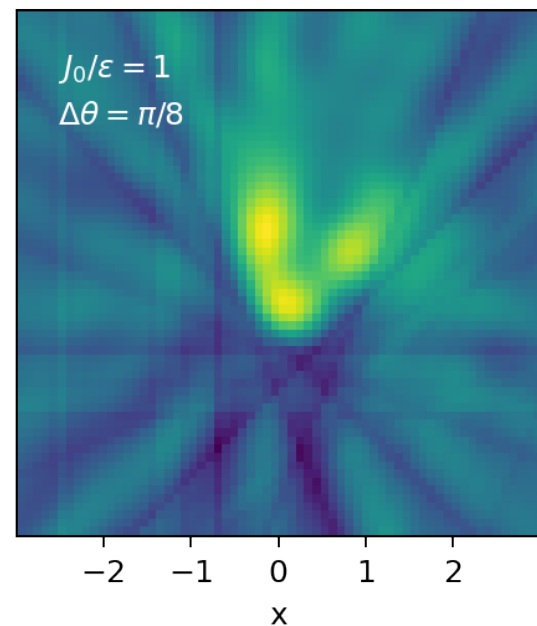
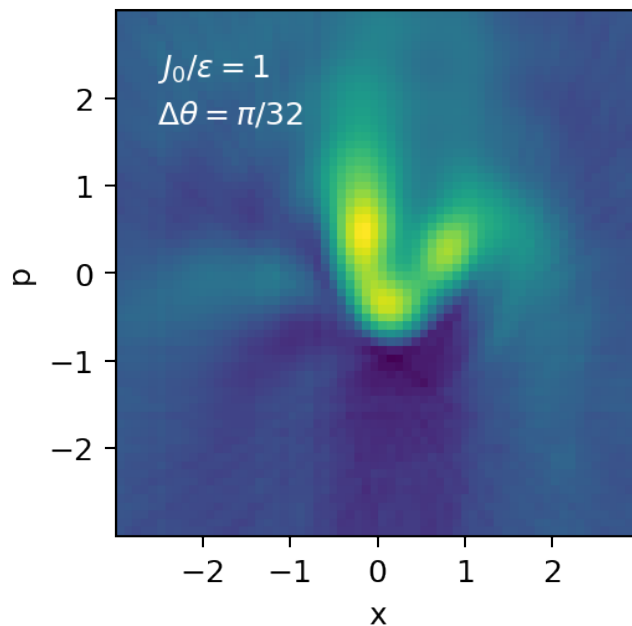
- Reconstruction of 2D phase-space via inverse Radon transform using beam profiles estimated theoretically on (virtual) BPM data of kicked beam at various kick angles



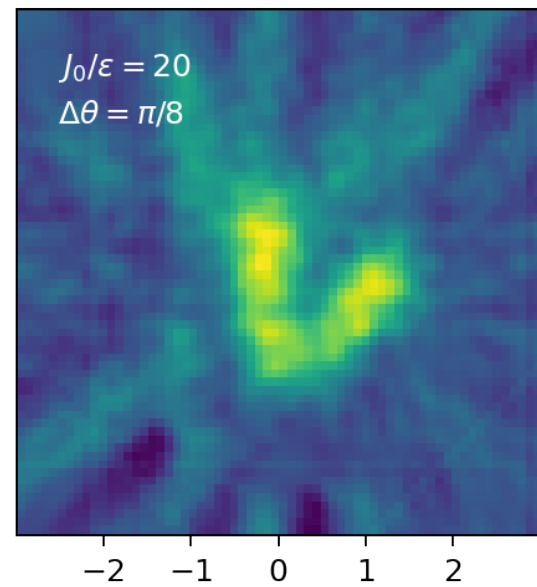
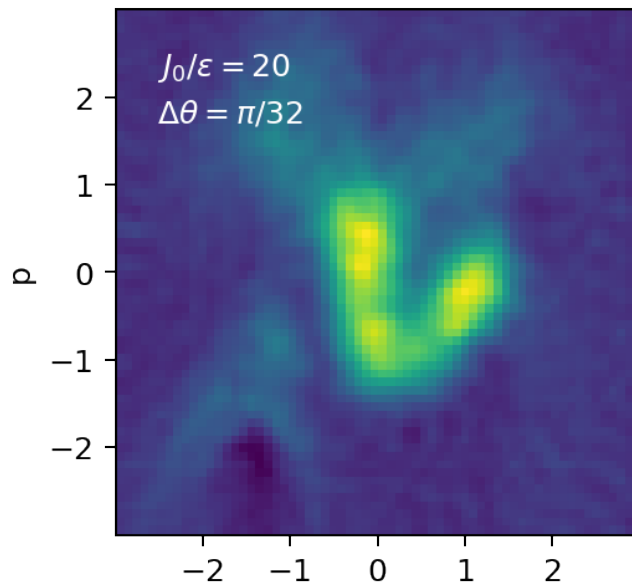
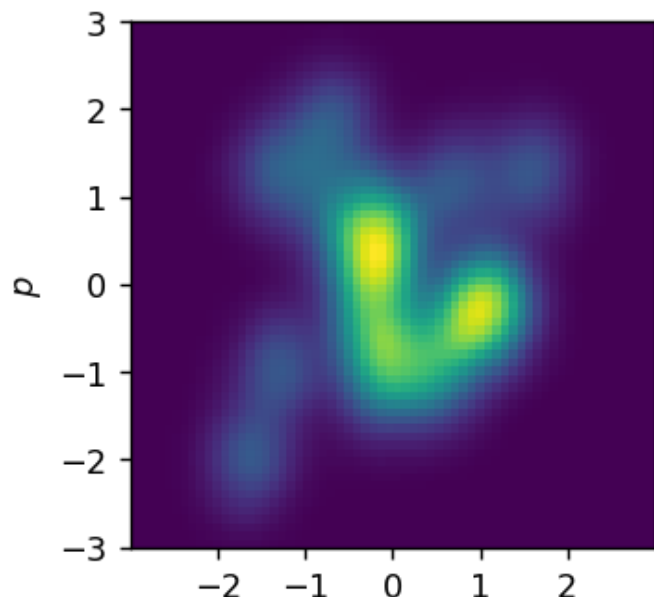


# Inverse Radon transformation (an algebraic method) using theoretically estimated marginal profiles

- Reconstruction of 2D phase-space via inverse Radon transform using beam profiles estimated theoretically on (virtual) BPM data of kicked beam at various kick angles



Ground truth



# Summary of inverse Radon with theoretical profile estimation

- Requires **knowledge of optics parameters**
  - transformation from physics to normal coordinate
  - oscillation frequency at kick action
  - nonlinear frequency detuning at kick action
  - kick action and angle in normal coordinate
- Requires **strong kicks**
  - generally not possible in presence of tight physical aperture
- Requires **enough angular resolution**
  - needs many kicks of different angles

# Gaussian Mixture Model (GMM)



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# use Gaussian Mixture Model (GMM)

- TBT beam centroid is analytically integrable for isotropic Gaussian

$$\begin{aligned} \langle x \rangle_{\mathcal{N},t} &= \Re \int (x - ip) e^{i\omega t} \mathcal{N}(\mathbf{x} - \mathbf{x}_0, \sigma \mathbf{I}) dx dp \\ &= \frac{x_0(1 - \tau^2) + 2p_0\tau}{(1 + \tau^2)^2} \exp\left(-\frac{J_0}{\epsilon} \frac{\tau^2}{1 + \tau^2}\right) \cos \Psi \\ &\quad - \frac{2x_0\tau - p_0(1 - \tau^2)}{(1 + \tau^2)^2} \exp\left(-\frac{J_0}{\epsilon} \frac{\tau^2}{1 + \tau^2}\right) \sin \Psi \end{aligned}$$

$$\begin{aligned} \omega(\Delta J) &= \mu_0 + \mu_1 \Delta J \dots \\ \Psi &\equiv \mu_0 t - \frac{(J_0/\epsilon)\tau^3}{1 + \tau^2} \\ \tau &\equiv \epsilon \mu_1 t \end{aligned}$$

- Therefore, one can model the beam density by GMM

$$\rho_{GMM}(x, p) = \frac{1}{G} \sum_{g=1}^G \mathcal{N}(\mathbf{x} - \mathbf{m}_g, \sigma_g \mathbf{I})$$

$$\langle x \rangle_{GMM,t} = \Re \int (x - ip) e^{i\omega t} \rho_{GMM}(x - x_0, p - p_0) dx dp$$

# use Gaussian Mixture Model (GMM)

- Virtual BPM data  $\langle x \rangle_{BPM,k,t}$  is generated from the toy model

$$\omega = \omega_0 + \omega_1 J + \omega_2 \frac{J^2}{2}$$

- Fit parameters by minimizing

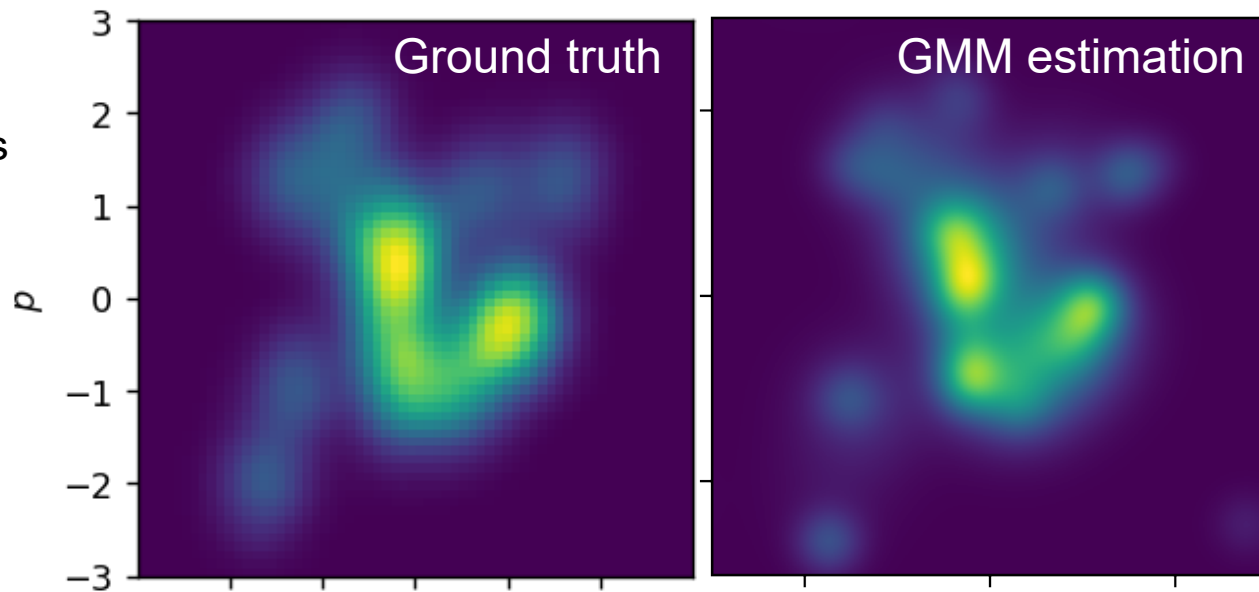
$$\sum_{k=1}^K \sum_{t=0}^T \left( \langle x \rangle_{BPM,k,t} - \langle x \rangle_{GMM,k,t} \right)^2 + \alpha$$

*some regularization loss*

- $K(= 8)$  kick actions from  $[2\epsilon, 4\epsilon]$  and kick angles equally spaced in  $[0, \pi]$

In order to reduce computational complexity of optimization, optics parameters are first optimized using single Gaussian kernel model and global optimization (differential evolution method).

Then, all parameters are optimized through Nelder-Mead method.



# Summary of GMM

- **Computational complexity**
  - There are too many parameters to fit :
    - » multiple Gaussian kernels (used 100),
    - » optics parameters (e.g.  $\mu_0$ ,  $\mu_1$ ),
    - » kick strengths and angles
  - Using a black-box optimization tool took **12 hours using single core**
  - hard to estimate model uncertainty due to computational complexity
  - Maybe relieved with GPU and differentiable implementation.
- Resolution is limited by number of Gaussian kernels.
- **May have better fit for optics parameter** (compared to single Gaussian beam model )

# Differentiable Particle simulation Model (DPM)



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# use Differentiable Particle Model

- Use particle model and simple differentiable simulation model
  - Motivated by [1] to reduce computational complexity with
  - Simple betatron frequency model:

$$\omega = \mu_{0,k} + \mu_1 \Delta J$$

- Particle locations, optics parameters are updated through gradient decent of the objective minimizing difference between prediction and true BPM TBT data with 8 different kicks *~corresponds to negative log likelihood*

$$\sum_{k=1}^K \sum_{t=0}^T \left( \langle x \rangle_{BPM,k,t} - \langle x \rangle_{PM,k,t} \right)^2 + \alpha \quad \text{some regularization loss}$$

- Approximate Bayesian ensemble by anchoring (with L2 regularization) [2,3] model parameters to the randomized particle locations and prior optics parameter estimations using single Gaussian model. *~corresponds to negative log prior*

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[1] Ryan Roussel et al, "Phase Space Reconstruction from Accelerator Beam Measurements Using Neural Networks and Differentiable Simulations"

[2] Ian Osband et al, "Randomized Prior Functions for Deep Reinforcement Learning", NeurIPS 2018

[3] Tim Pearce et al, "Bayesian Inference with Anchored Ensembles of Neural Networks, and Application to Exploration in Reinforcement Learning", ICML2018



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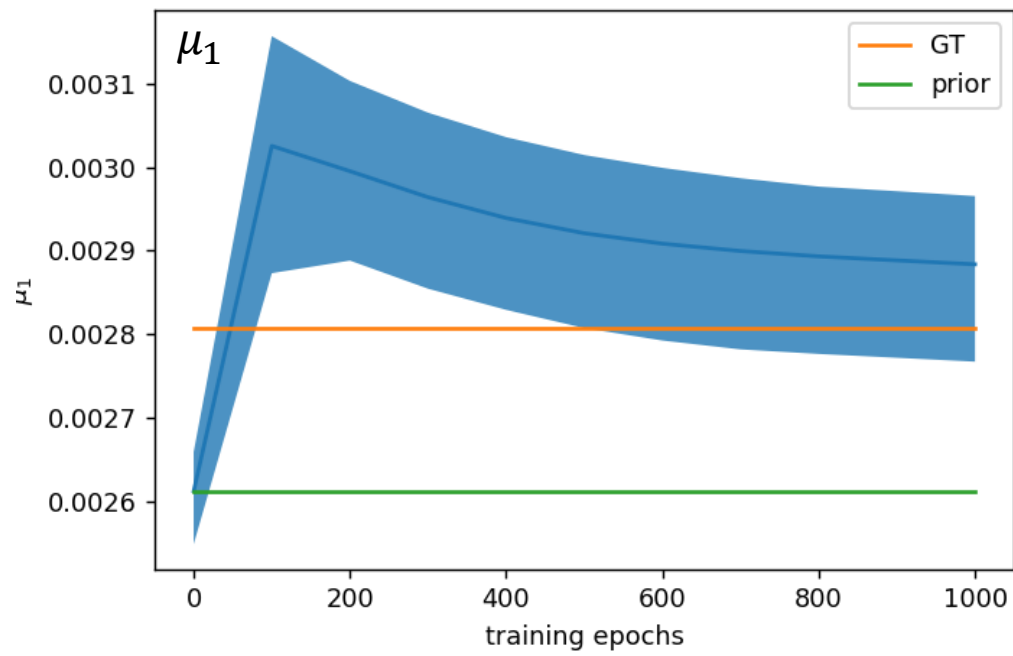
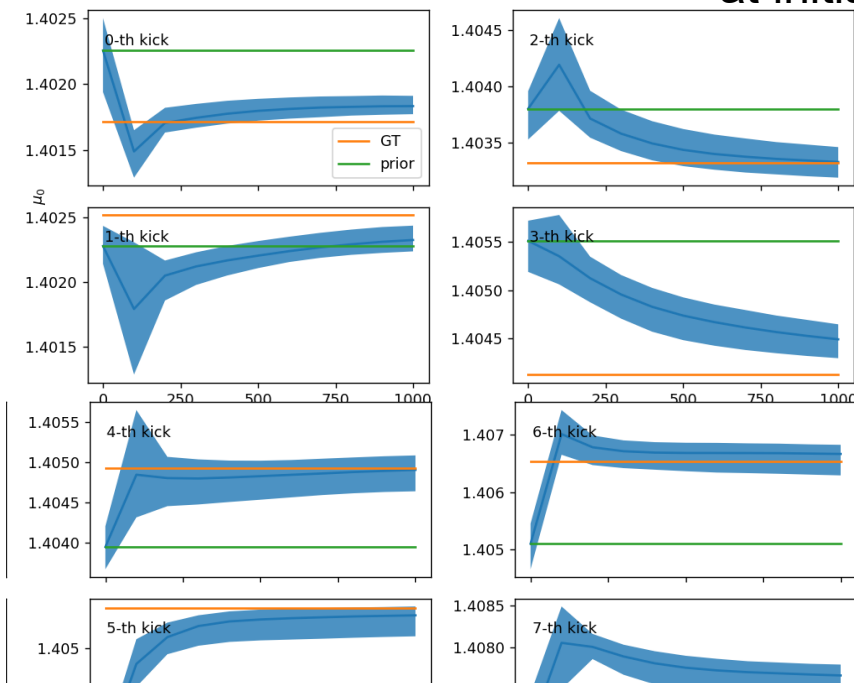
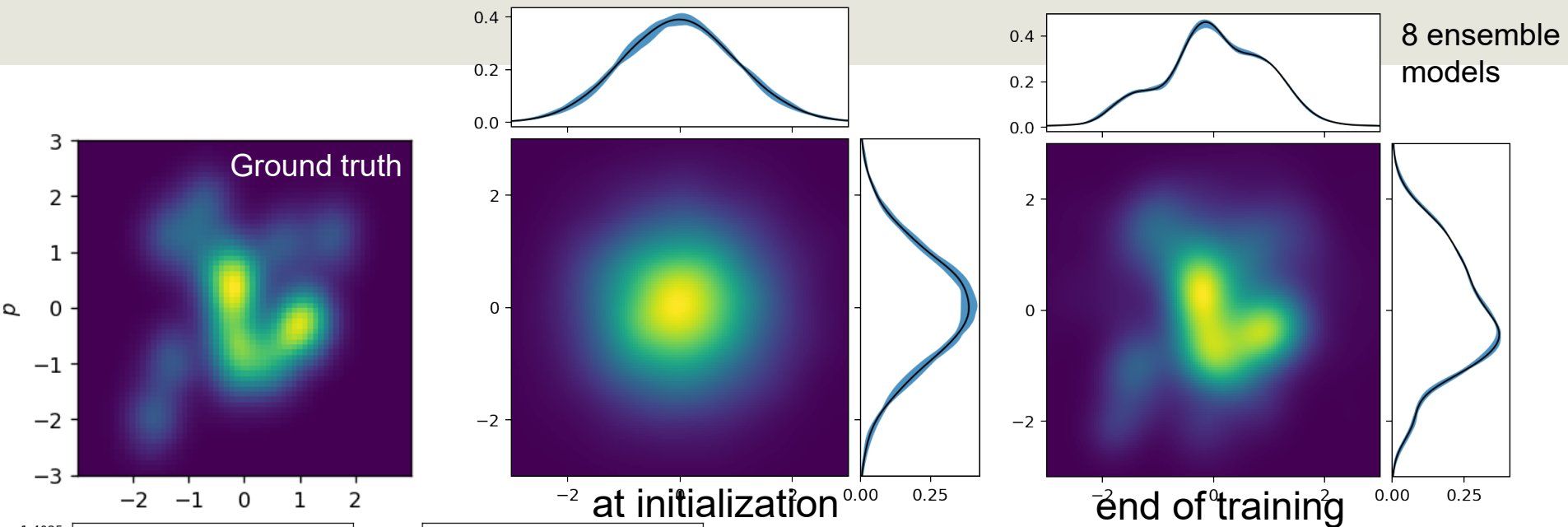
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# use Particle Model



# Summary of PM

- **Computational complexity**
  - With gradient decent (ADAM) optimization, it still took 10 hours (using one CPU core) for 8 models ( ~ 1h for each model)
  - Maybe relieved with implementation.
- **UQ may be feasible due to faster training** (compared to GMM without differentiable model)
- **Better fit for optics parameter** (compared to single Gaussian beam model )

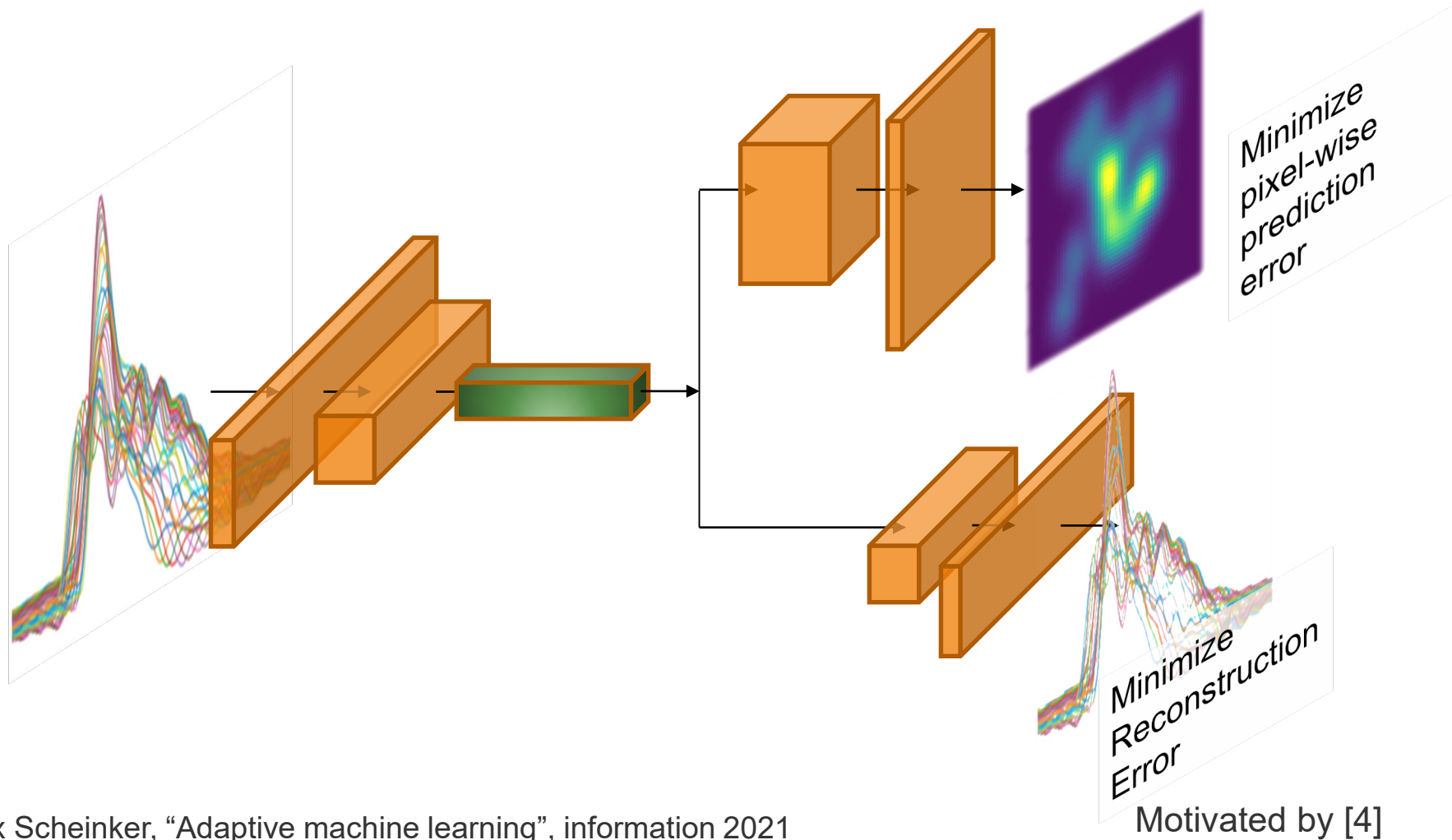
# Neural Network (NN) Model with supervised learning and model uncertainty



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# Use NN

- Input: theoretically estimated marginal profiles
- Output: beam density plot and reconstructed marginal profiles



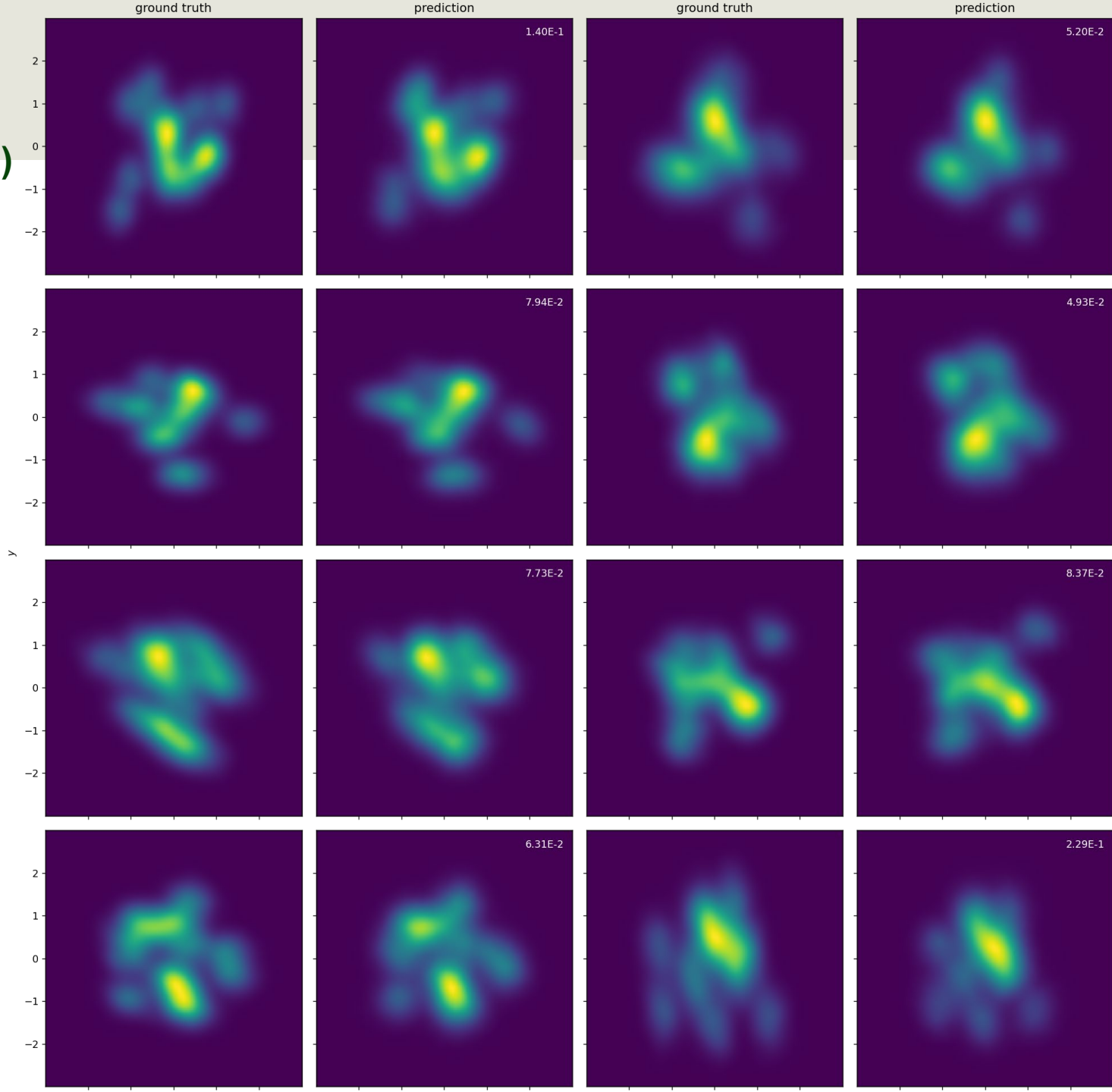
# How training data generated

- Virtual BPM TBT data from toy-simulation-model

$$\omega = \omega_0 + \omega_1 J + \omega_2 \frac{J^2}{2}$$

- Each data is generated using randomly sampled model parameters of simulation (“*domain randomization*” for “*sim-to-real*” )
  - randomized model parameters need to cover the expected real machine behavior
    - » beam emittance  $\epsilon \sim \mathcal{N}(1, \sigma_\epsilon)$
    - » frequency parameters  $\omega_i \sim \mathcal{N}(\bar{\omega}_i, \sigma_{\omega_i}), \quad i \in [0 - 2]$
    - » kick strengths and angles  $J_{0,k} \sim \mathcal{N}(\bar{J}_{0,k}, \sigma_{J_0}), \quad \theta_k \sim \mathcal{N}(\bar{\theta}_k, \sigma_\theta), \quad k \in [1,8]$

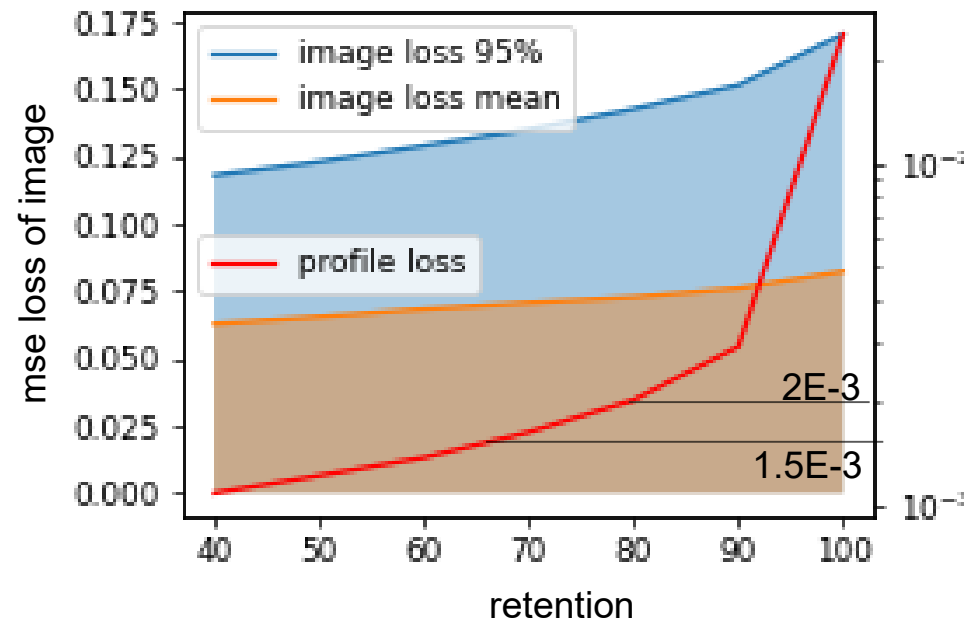
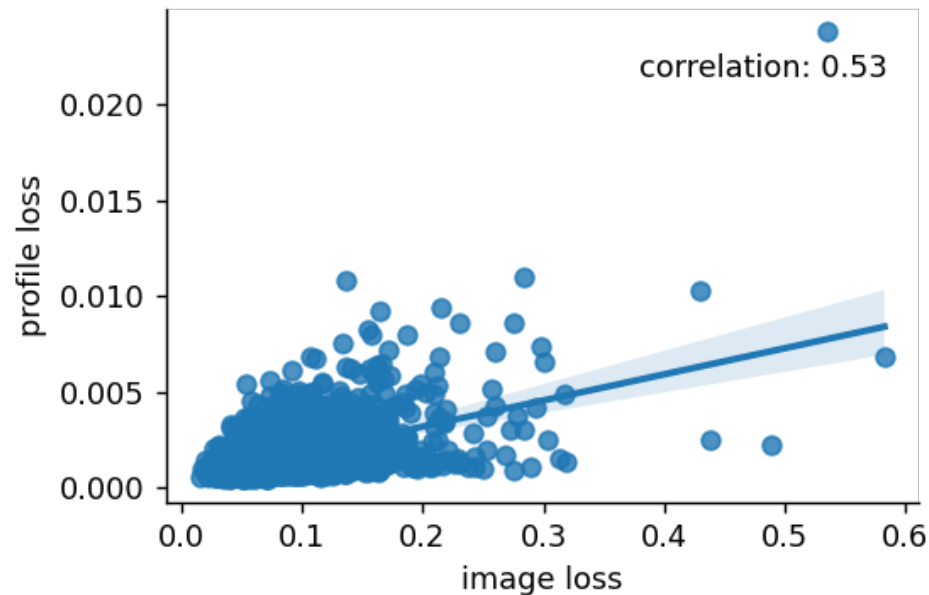
**Some of  
random  
(except the 1<sup>st</sup> one)  
prediction  
samples**





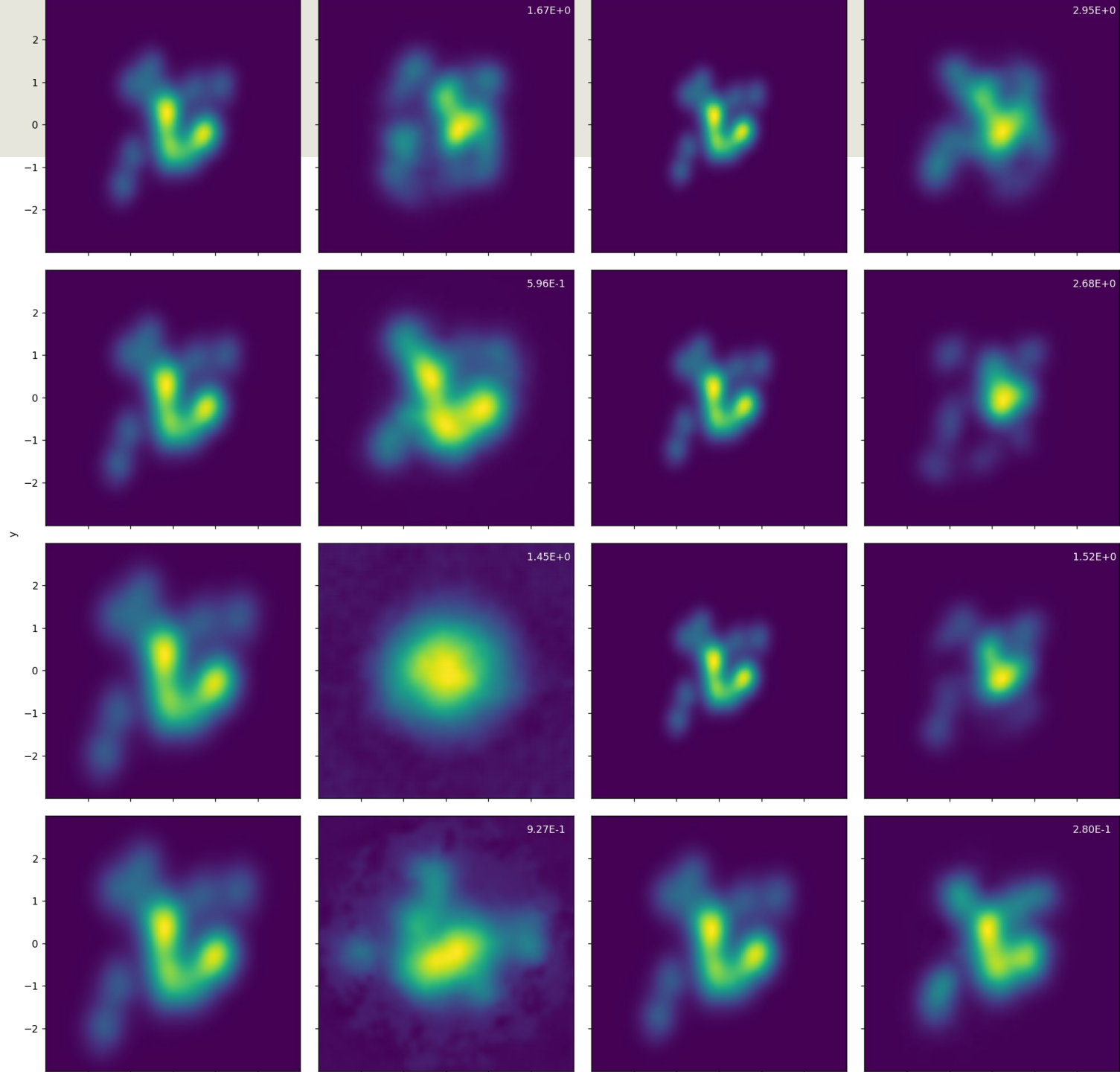
# UQ using reconstruction loss of input profile

- UQ using ensemble
  - As it is expected that the model predictions in the training distribution are close each other while predictions in out-of-distribution show large variance for each model
- The reconstruction loss can also be used for UQ
  - As it is also expected to be small in the training distribution while large in out-of-distribution

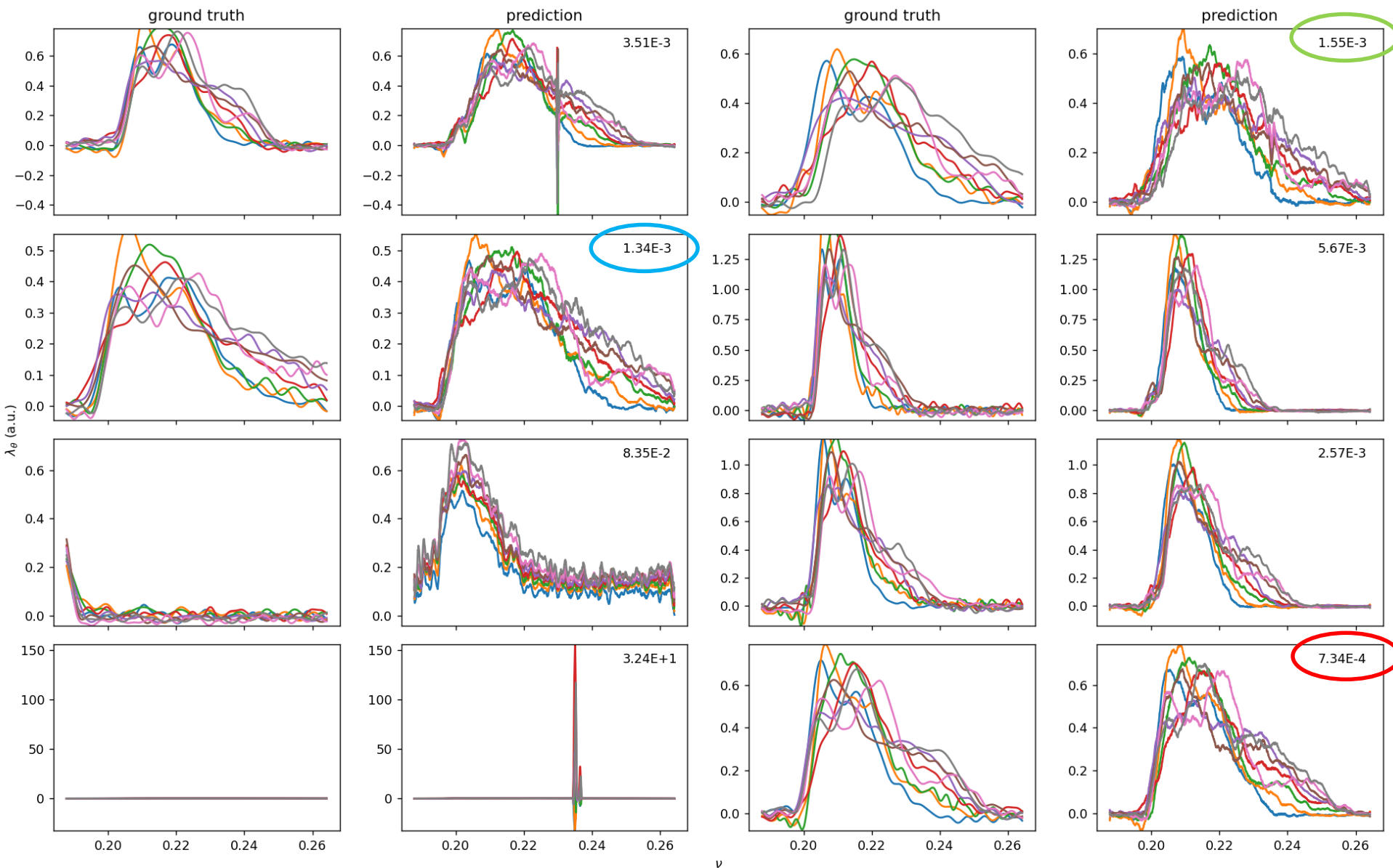


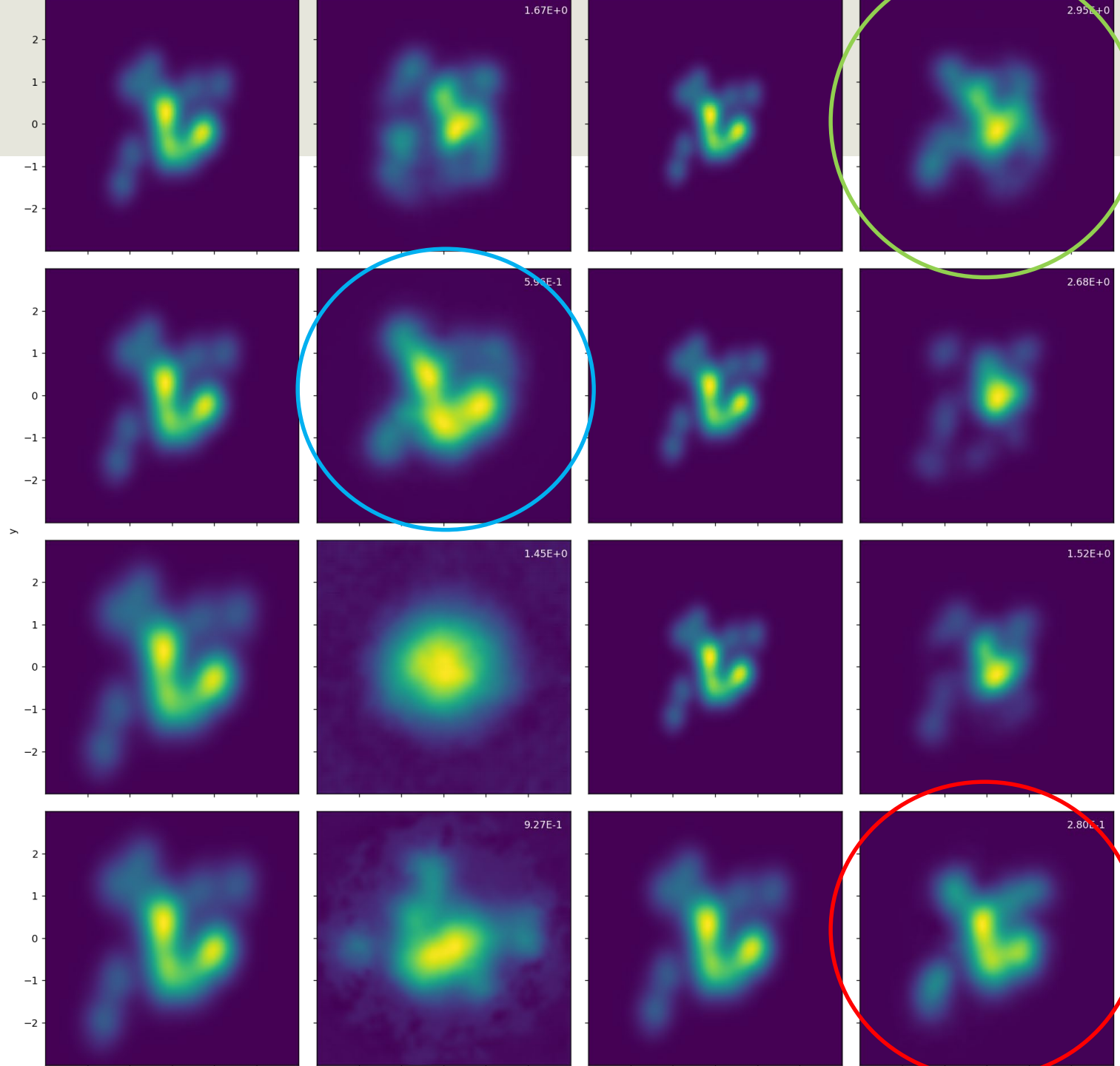
# Out of distribution samples

- OOD samples are generated by sampling from 4 times larger parameter variances (than the variance used for the training data generation)
  - » beam emittance  $\epsilon \sim \mathcal{N}(1, 4\sigma_\epsilon)$
  - » frequency parameters  $\omega_i \sim \mathcal{N}(\bar{\omega}_i, 4\sigma_{\omega_i}), \quad i \in [0 - 2]$
  - » kick strengths and angles  $J_{0,k} \sim \mathcal{N}(\bar{J}_{0,k}, 4\sigma_{J_0}), \quad \theta_k \sim \mathcal{N}(\bar{\theta}_k, 4\sigma_\theta), \quad k \in [1,8]$



# profile reconstruction losses





# Summary of NN

- Computational complexity is no longer a problem but the collection of training data and training time can be problematic
- The reconstruction loss looks promising alternative method for UQ
- Domain randomization is used for “sim-to-real” adaption.
  - However, (as is the case of GMM or PM) the simulation model may not enough for real machine

# Conclusion



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# Conclusion

- TBT(turn-by-turn) beam centroid data is function of initial (before kick) beam distribution
  - Beam profile can be theoretically estimated when  $J_0/\epsilon \gg 1$ 
    - » ML methods does not require large kick
- We investigated various method for 2D phase-space tomography using kicked beam turn-by-turn (virtual) BPM data
- GMM, PM methods are promising as long as
  - Computational complexity problem can be improved through differentiable simulation model and GPU implementation
- NN method is promising as long as
  - Enough (simulational) training data that can represent the real machine can be collected
- In all cases, simple but well-representative simulational model plays important role





# Acknowledgements

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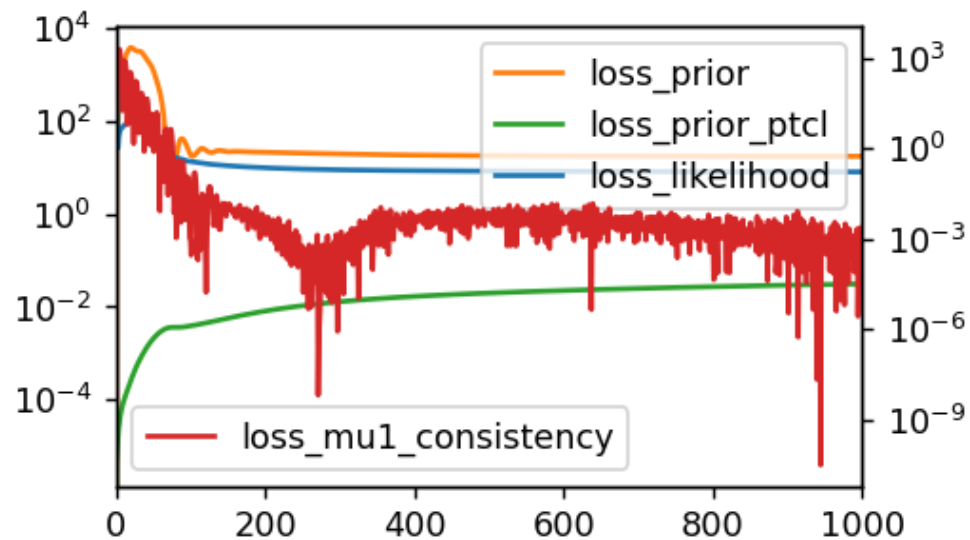
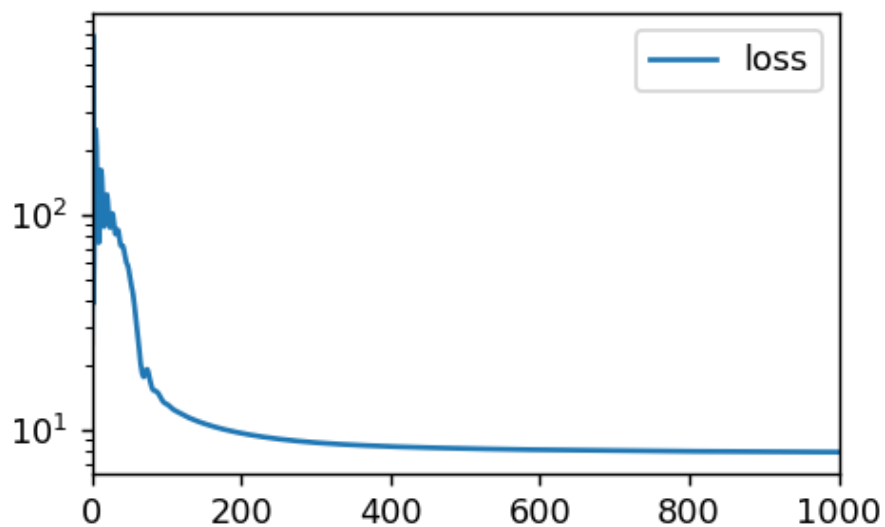
**Backup slide**



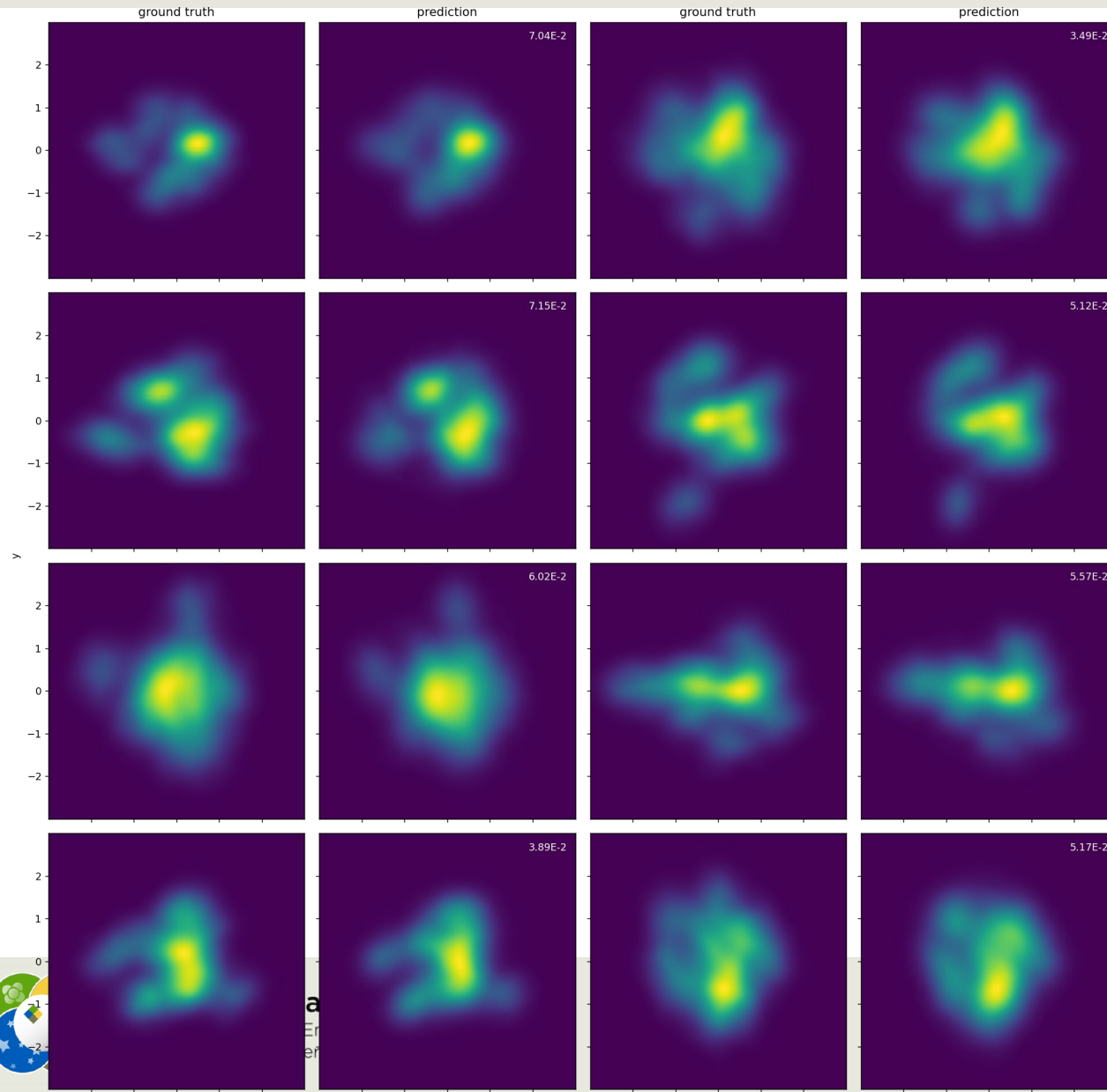
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# PM training loss



# NN test samples of best profile loss



# NN test samples of worst profile loss

