2026년 가속기 빔 진단 협력 워크샵, 원자력연구원 양성자과학연구단

포항가속기연구소
POHANG ACCELERATOR LABORATORY
POSTECH

Generative 6-dimensional phase space reconstruction at the PAL-XFEL and its application for beam optimization

Seongyeol Kim
PAL-XFEL, Pohang Accelerator Laboratory

April 9, 2026

Contents

- **Motivation and Introduction to generative phase space reconstruction (GPSR)***
- **AI/ML applications to PAL-XFEL**
  - Beam phase space diagnostics using neural networks and differentiable simulations
- **Summary and future works**

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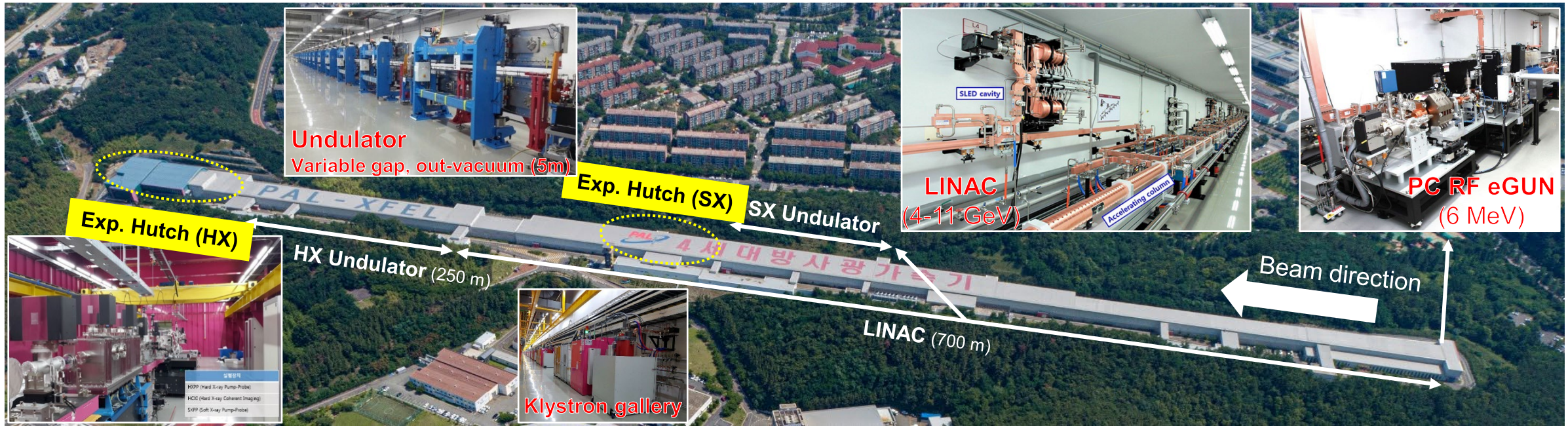
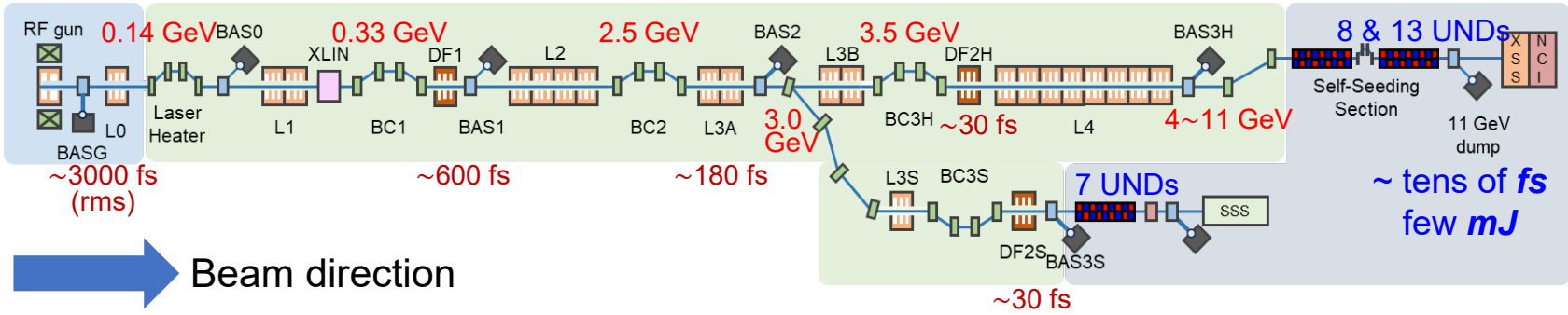
Brief introduction to PAL-XFEL

Pohang Accelerator Laboratory, X-ray Free Electron Laser



PAL-XFEL Layout



Undulator Line	HX	SX
Photon energy (keV)	2.0~20.0	0.25~1.25
Beam energy (GeV)	4~11	3.0
Beam charge (pC)	190/250	160/250
Peak current (kA)	~3	~2.5
E_{ph} tuning	Energy/Gap	Gap
Repetition rate (Hz)	60	60
FEL intensity	> 1 mJ	> 250 μJ

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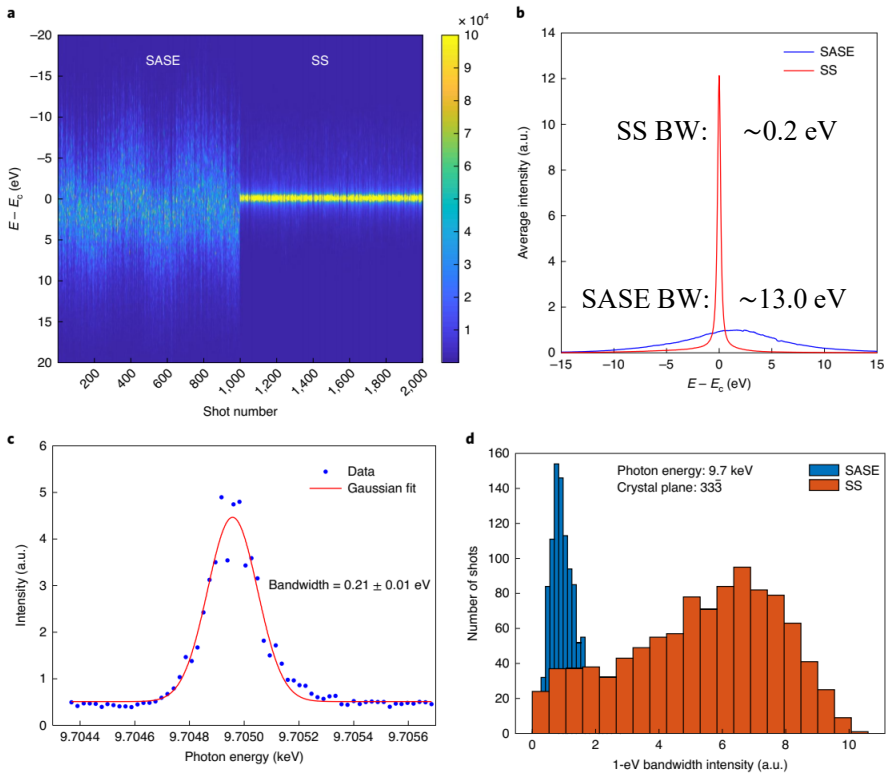
Novel XFEL modes @ PAL-XFEL

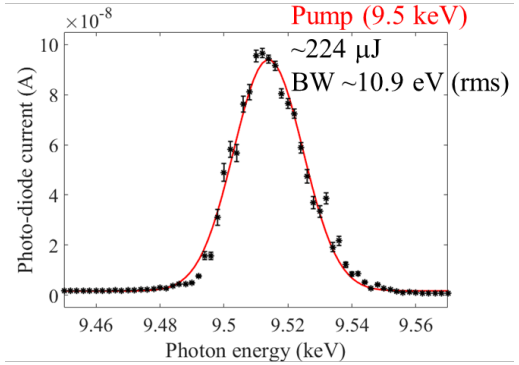
- C-K. Min *et al.*, *J. Synchrotron Radiation*, **26**, 110, 2019.
- I. Nam *et al.*, *Nat. Photonics* **15**, 2021.
- M. H. Cho *et al.*, *Sci. Rep.* **13**, 13786, 2023.
- C. H. Shim, Two-color FEL pulse generation at PAL-XFEL, IPAC24, 2024.
- Chang-Kyu Sung *et al.*, *Nucl. Inst. Meth. Phys. Res. A* **1076**, 170458, 2025.

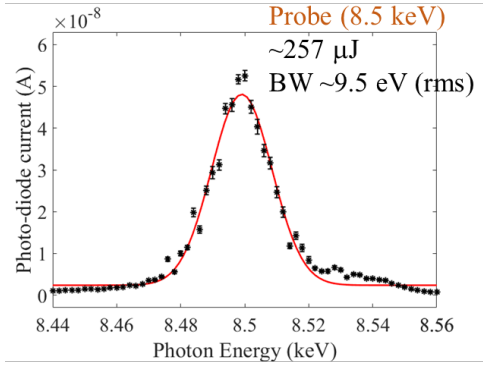
Self-seeding FEL mode



Spectral intensity: > 5 times larger than SASE

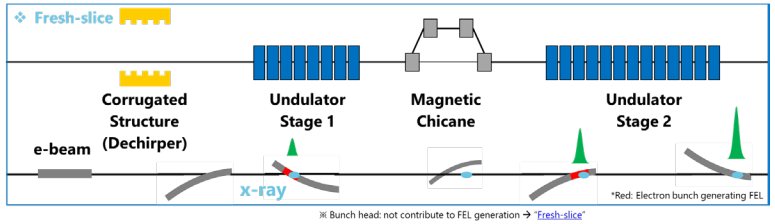
Two-color FEL

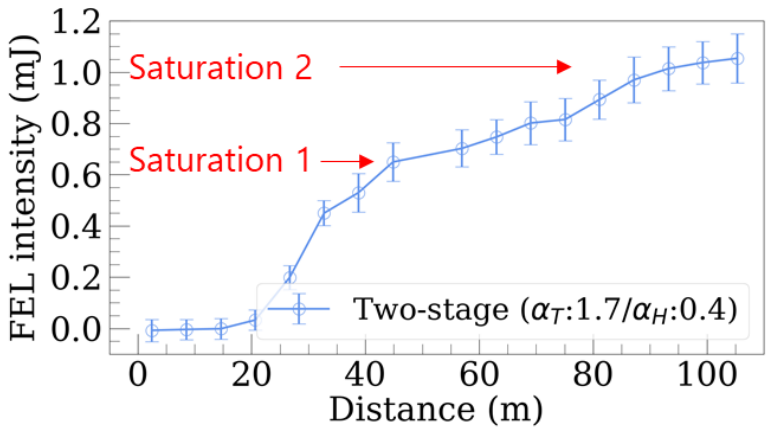




Pump + probe experiment using X-ray

Fresh-slice-based SASE





Enhance FEL performance (10 fs pulse length, bandwidth)

Novel FEL modes currently available / under development:

Support for a broader range of XFEL-based R&D programs

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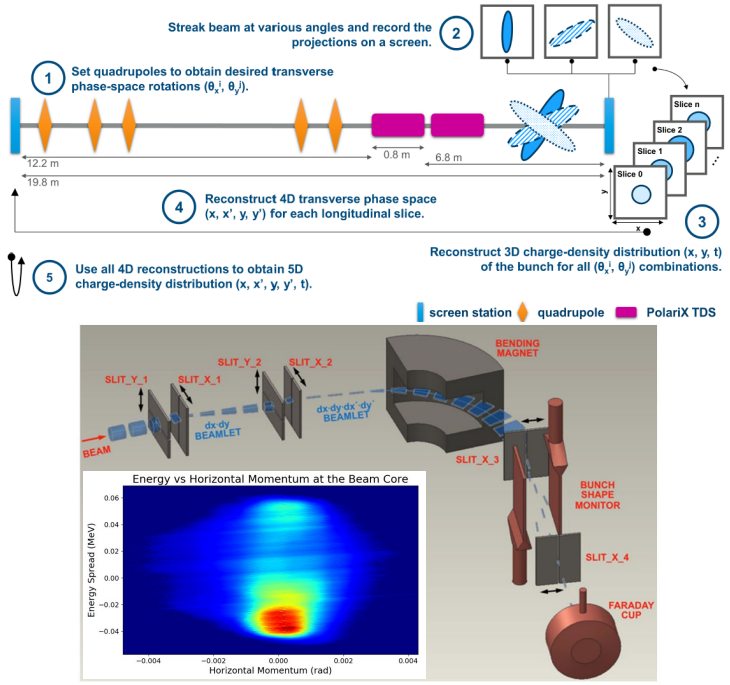
AI/ML applications to PAL-XFEL:

Machine learning-based 6D beam phase space diagnostics

* Accuracy, efficiency, and required time for diagnostics

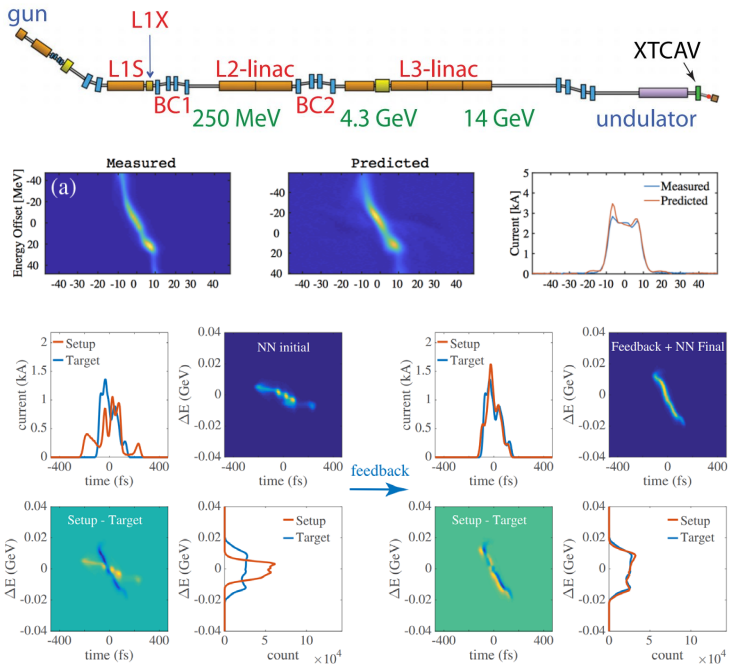
Introduction: 6-dimensional phase space diagnostics

Conventional diagnostics



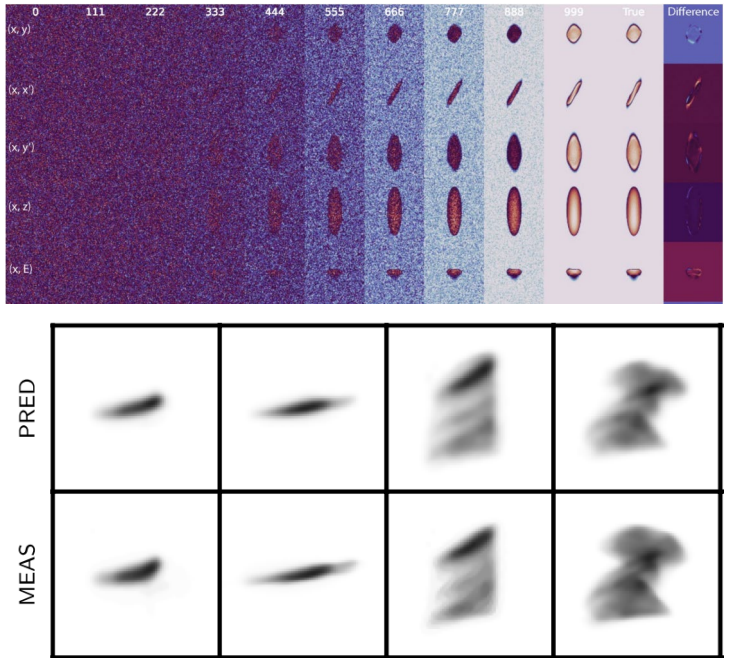
S. Jaster-Merz *et al.*, *PRAB* **27**, 072801, 2024.
B. Cathey *et al.*, *PRL* **121**, 064804, 2018.

Virtual diagnostics



C. Emma *et al.*, *PRAB* **21**, 112802, 2018.
A. Scheinker *et al.*, *PRL* **121**, 044801, 2018.

Generative learning



A. Scheinker, *Sci. Rep.* **14**, 29303, 2024.
A. Hoover, *PRAB* **28**, L084601, 2025.

Beam diagnostics from conventional approach to AI/ML technique-incorporated:

allows us to investigate phase space characterization in a robust way*

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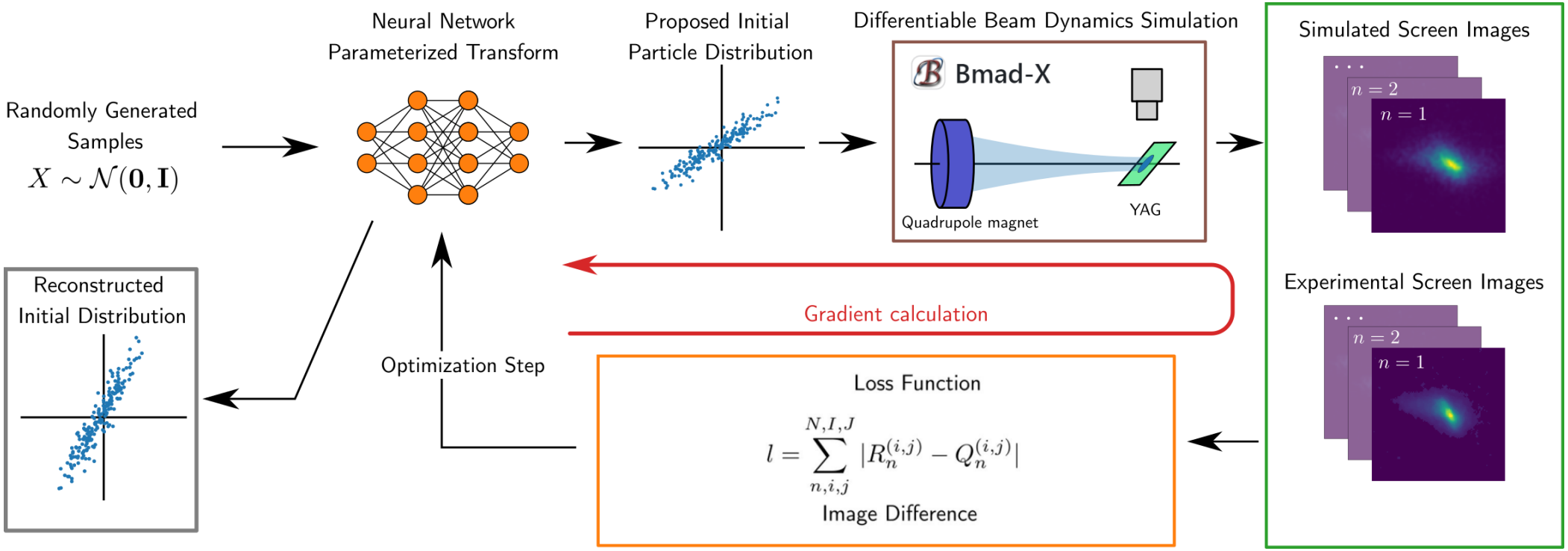
- R. Roussel *et al.*, *PRL* **130**, 145001, 2023.
- S. Kim *et al.*, *PRAB* **27**, 074601, 2024.
- R. Roussel *et al.*, *PRAB* **27**, 094601, 2024.
- J.P. Gonzalez-Aguilera *et al.*, *IPAC'24*, 2024.

Generative phase space reconstruction (GPSR)

Based on neural networks and differentiable simulations



Iteration process to update weights of neural networks:

To reconstruct beam phase space that successfully predicts experimental measurements

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Generative phase space reconstruction (GPSR)

- R. Roussel *et al.*, *PRL* **130**, 145001, 2023.
- S. Kim *et al.*, *PRAB* **27**, 074601, 2024.
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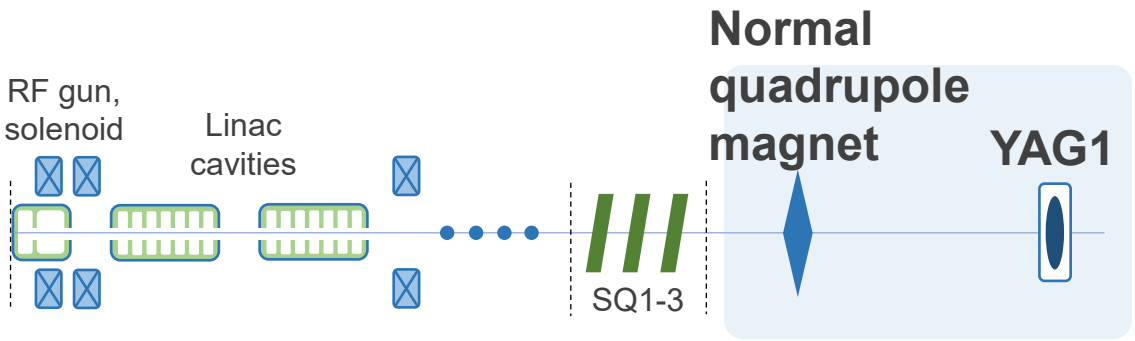
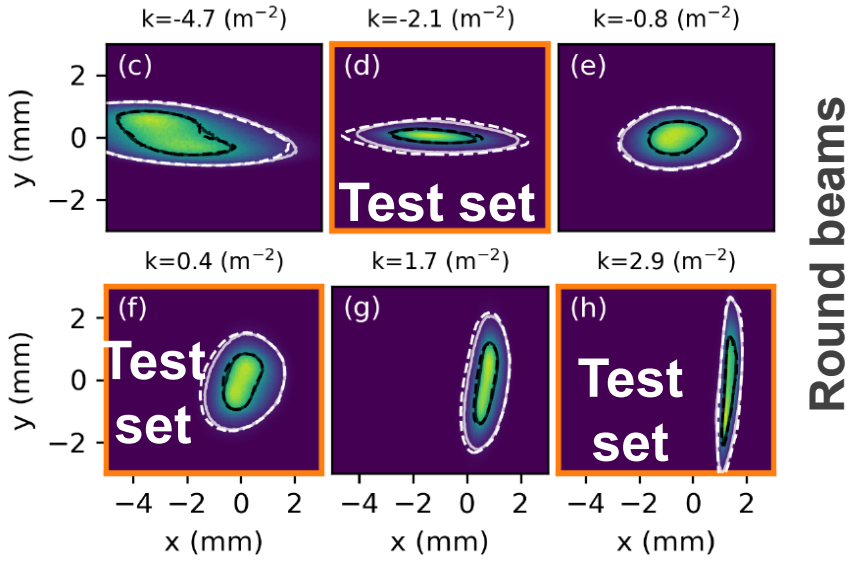
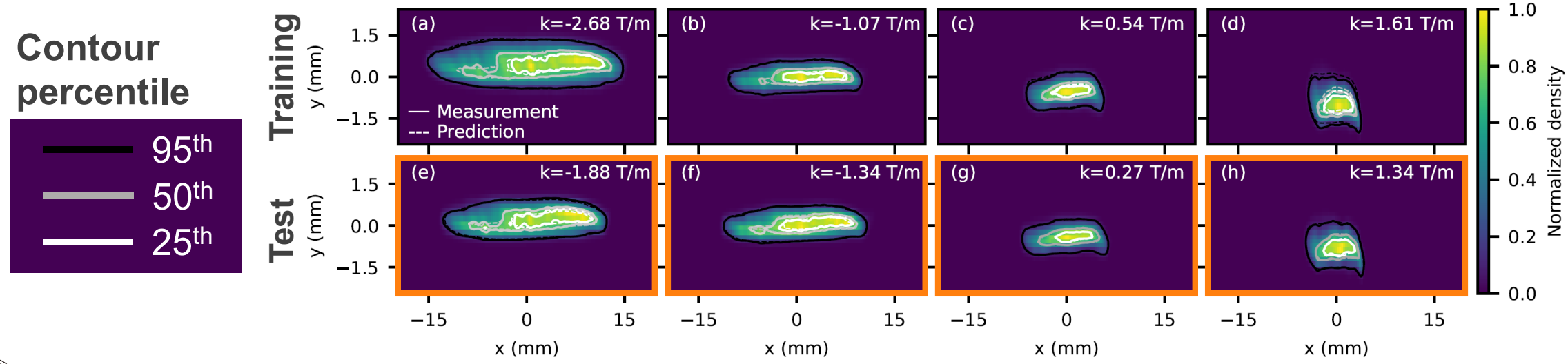




Flat / magnetized beams



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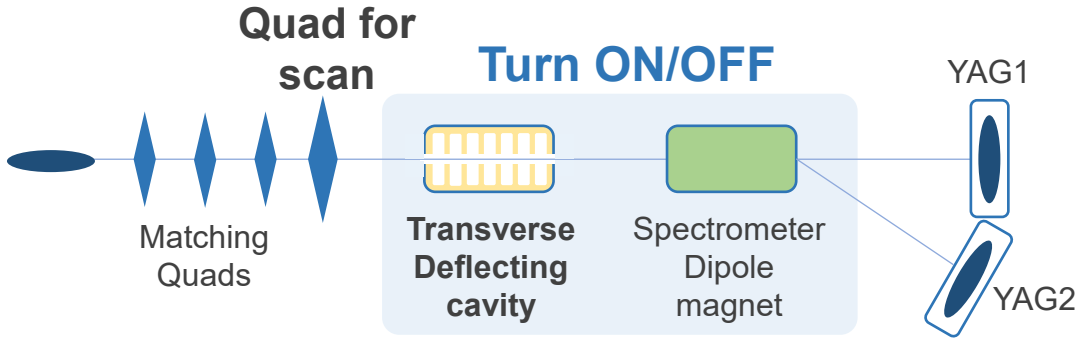
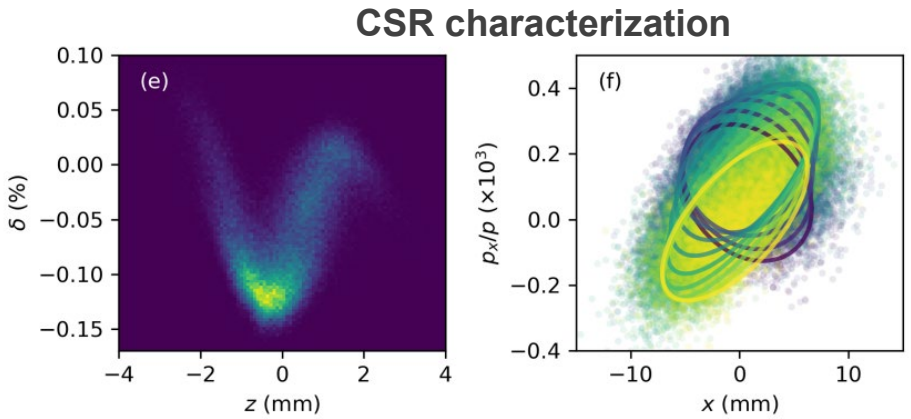
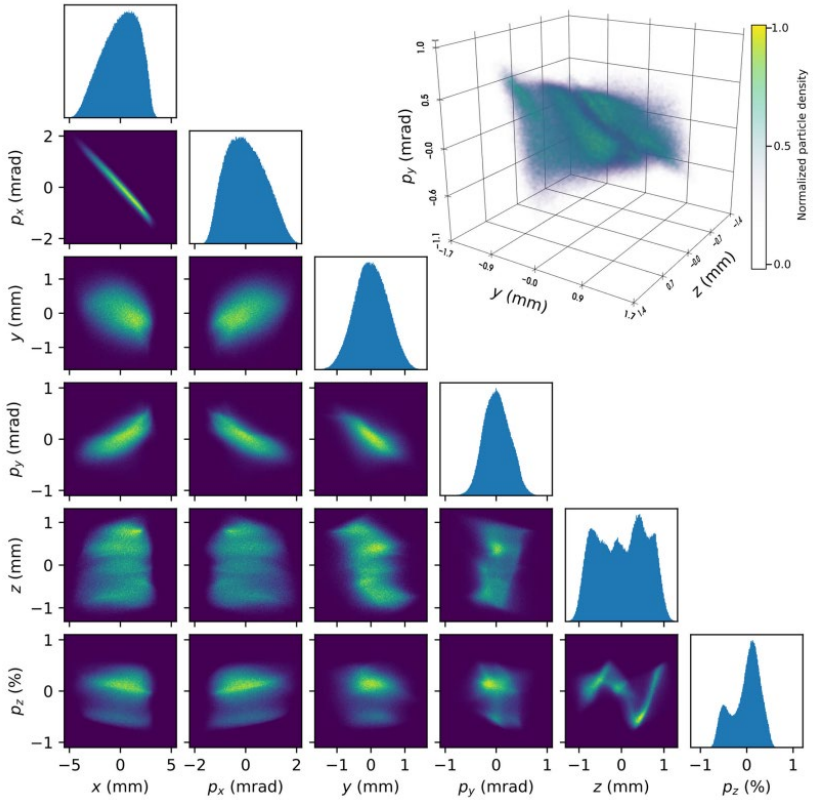
- R. Roussel *et al., PRL* **130**, 145001, 2023.
- S. Kim *et al., PRAB* **27**, 074601, 2024.
- R. Roussel *et al., PRAB* **27**, 094601, 2024.
- J.P. Gonzalez-Aguilera *et al., IPAC'24*, 2024.

Generative phase space reconstruction (GPSR)

R. Roussel *et al., Phys. Rev. Lett.* **130**, 145001, 2023.







➡ Complete 6-dimensional phase space reconstruction is made possible by introducing deflecting cavity + spectrometer

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AI/ML applications to PAL-XFEL:
Accelerating cavity-based 6D phase space reconstruction

Presentation based on:

- Seongyeol Kim *et al,* Scientific Reports, 10.1038/s41598-025-26954-6, 2025)

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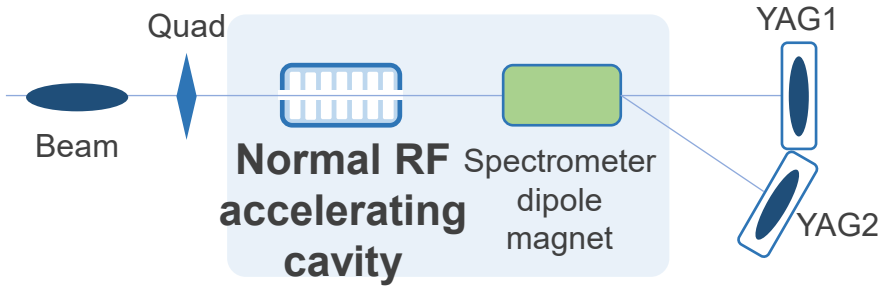
6D GPSR using RF accelerating cavity

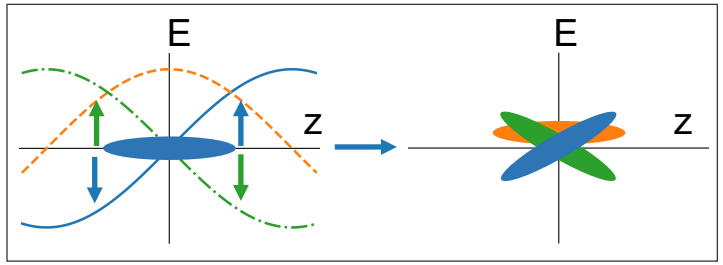
Inspired by conventional longitudinal emittance measurement*

*Longitudinal emittance:
- D. Dowell *et al., In. Proc. PAC'03,* 2003.
- D. Dowell *et al., Nucl. Inst. Meth. Phys. Res. A* **507**, 331, 2003.

Longitudinal phase space tomography:
- H. Loos *et al., Nucl. Inst. Meth. Phys. Res. A* **528**, 189-193, 2004.

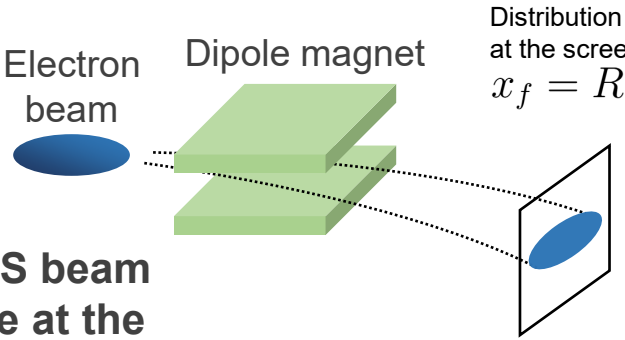


$$\Delta E(z) = eV\cos\left(k_{RF}z + \phi_{RF}\right)$$



For a given longitudinal distribution:

➡ **Energy changes induced by the cavity can be captured at the spectrometer screen**



Distribution at the screen

$$x_f = R_{11}x_0 + R_{12}x_0' + R_{16}\,\delta_0$$

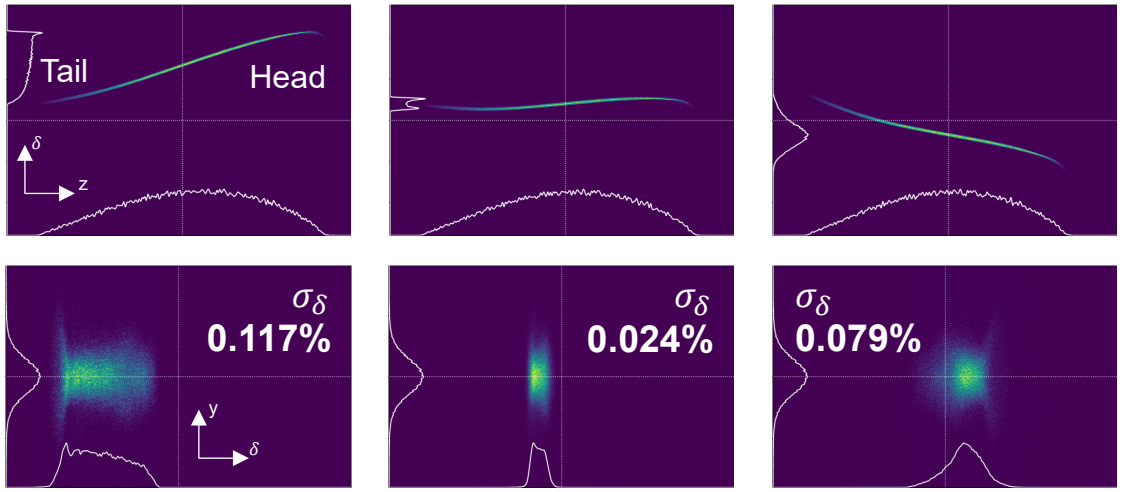
Dispersion of dipole magnet

Fractional energy spread $\delta = \dfrac{\Delta E}{E_{ref}}$

RMS beam size at the screen

$$\sigma_x = \sqrt{\beta_x\epsilon_x + \left(D_x\,\sigma_\delta\right)^2}$$ → **RMS energy spread**

Top: longitudinal phase space **Bottom: beam at spectrometer screen**



POHANG ACCELERATOR LABORATORY

6D GPSR using RF accelerating cavity

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- D. Dowell *et al., Nucl. Inst. Meth. Phys. Res. A* **507**, 331, 2003.

Longitudinal phase space tomography:
- H. Loos *et al., Nucl. Inst. Meth. Phys. Res. A* **528**, 189-193, 2004.

Transfer matrix for cavity and drift

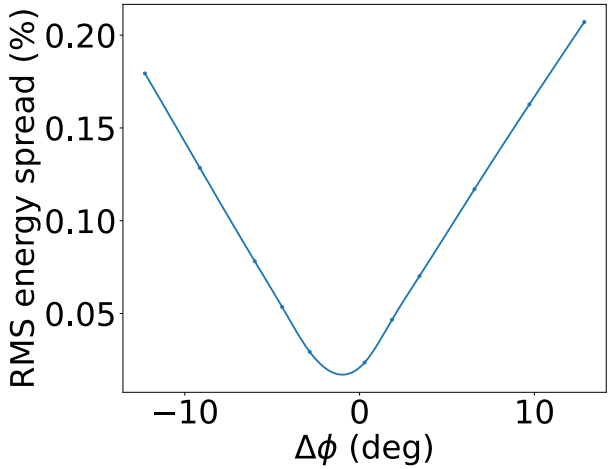
$$M = \begin{pmatrix} 1 & l \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -V\sin(\phi_{RF}) & 1 \end{pmatrix} \quad \text{where} \quad \Sigma_i = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix} = \begin{pmatrix} < z^2 > & < z\delta > \\ < z\delta > & < \delta^2 > \end{pmatrix}$$

$$\sigma_{22}^{YAG} = \sigma_\delta^2 = V^2\sigma_{11}\,\phi^2 - 2V\sigma_{12}\,\phi + \sigma_{22}$$

RMS energy spread at the screen $= A\phi^2 + B\phi + C$ ➡ Similar to normal quadscan: Estimation of second-order moments

$$\epsilon_z = \sqrt{\sigma_{11}\sigma_{12} - \sigma_{12}^2}$$ ➡ **Emittance**

Example: Quadratic behavior of energy spread



By combining quadrupole field and cavity phase scans, **and GPSR**:

We can obtain complete 6-dimensional coupled phase space of the beam

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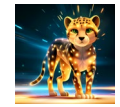
- Bmad-X: https://github.com/bmad-sim/Bmad-X
- Transition in progress from Bmad-X to Cheetah simulation: https://github.com/desy-ml/cheetah

Experimental setup for the GPSR @ PAL-XFEL



GPSR demo section

Parameters	# of samples
Quad strength	16
XLIN phase	5
BC condition	2
Total samples	160(80 for train)

Quadrupole Magnet **Q1**

Q2

Q3-4

11.424 GHz X-band RF Linearizer **(XLIN)**

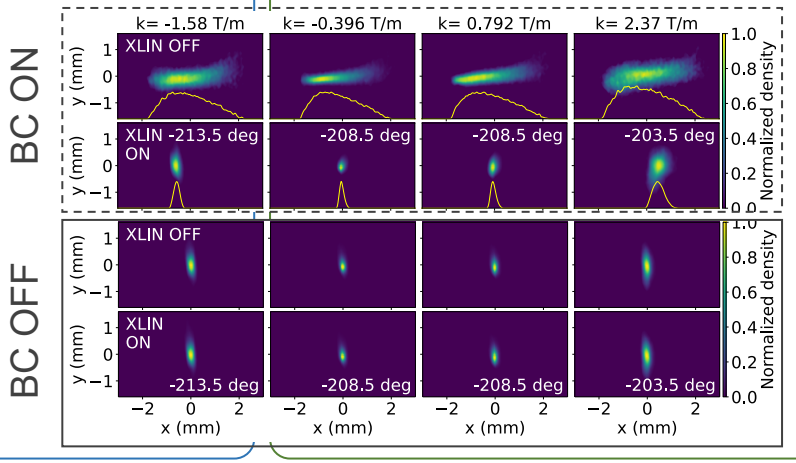
Electron beam
250 pC
260.5 MeV

Bunch compressor dipole (BC)

Camera

YAG1

YAG1 (x-y) image



GPSR validation section

elegant

2.856 GHz S-band transverse deflecting cavity (TCAV)

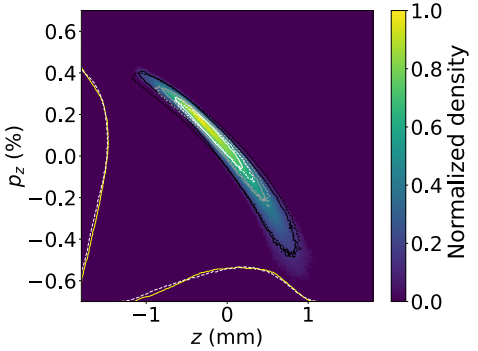
Q5

Q6-7

Dipole spectrometer

YAG2 ~25 m

(z-p_z) image @ YAG2

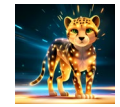


Not included in the GPSR training!

POHANG ACCELERATOR LABORATORY

- Bmad-X: https://github.com/bmad-sim/Bmad-X
- Transition in progress from Bmad-X to Cheetah simulation: https://github.com/desy-ml/cheetah

Experimental setup for the GPSR @ PAL-XFEL



GPSR demo section

GPSR setup	Values
# of particles	100,000
# of iterations	1,000
Training time	~30 mins (Nvidia A100)

Quadrupole Magnet **Q1**

Q2

Q3-4

11.424 GHz X-band RF Linearizer **(XLIN)**

Electron beam
250 pC
260.5 MeV

Bunch compressor dipole (BC)

Camera

YAG1

GPSR validation section

elegant

2.856 GHz S-band transverse deflecting cavity (TCAV)

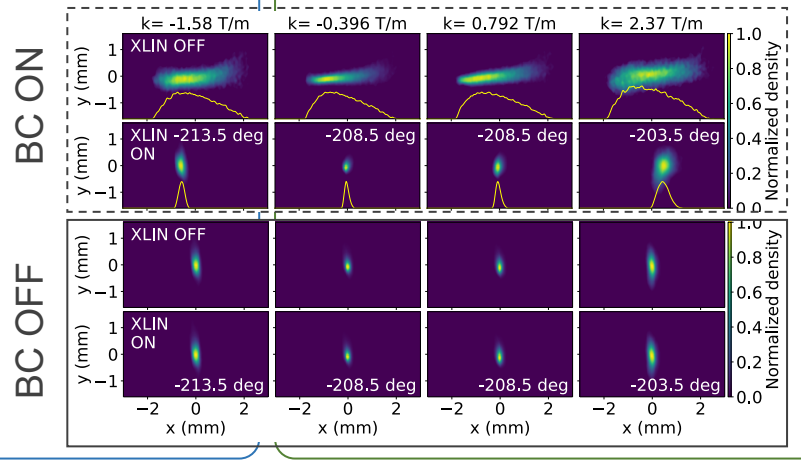
Q5

Q6-7

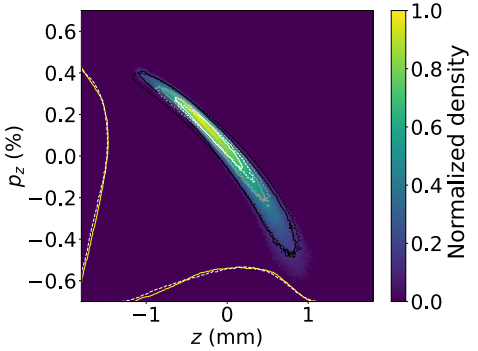
Dipole spectrometer

YAG2 ~25 m

YAG1 (x-y) image



(z-p_z) image @ YAG2



Not included in the GPSR training!

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Predictions using reconstructed phase space: YAG1

Test dataset

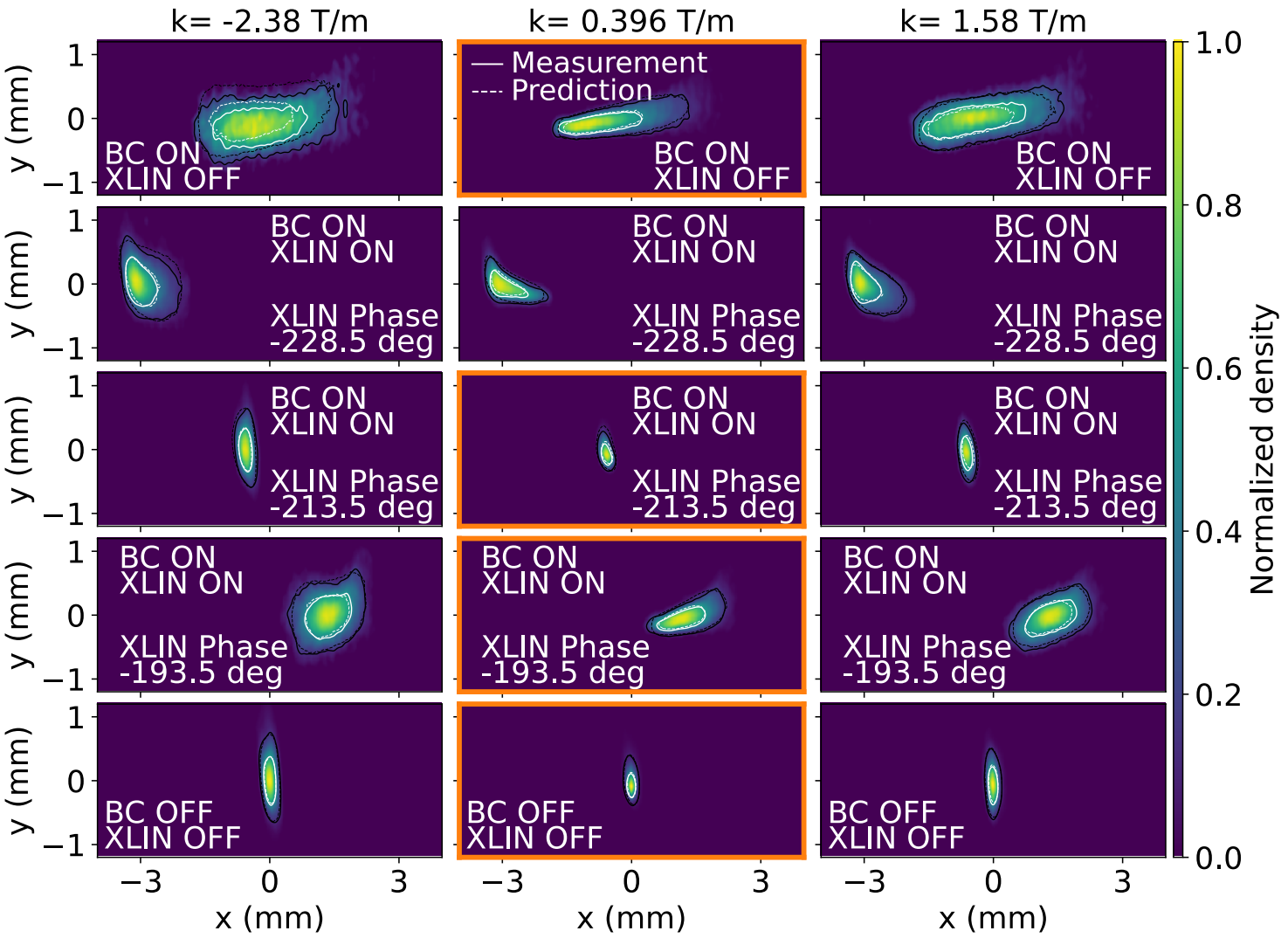
Training dataset

Background:
Measurement

90th
50th
Contour percentile

Measurements
Predictions

Reconstructed initial beam phase space successfully predicts YAG1 images



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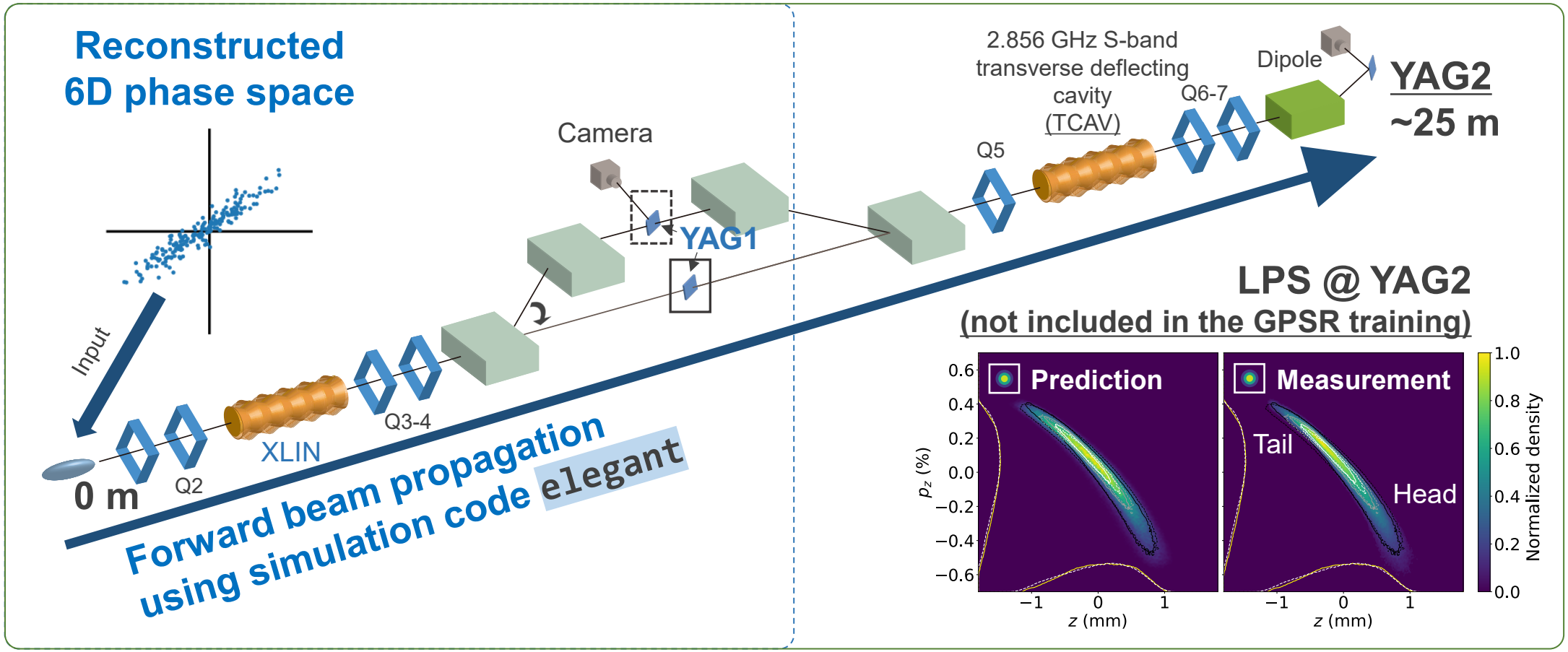
GPSR validation using downstream measurements



6D reconstructed phase space of the beam:

➡ **Can be used to predict the phase space at multiple locations**

Predictions using reconstructed phase space: YAG2

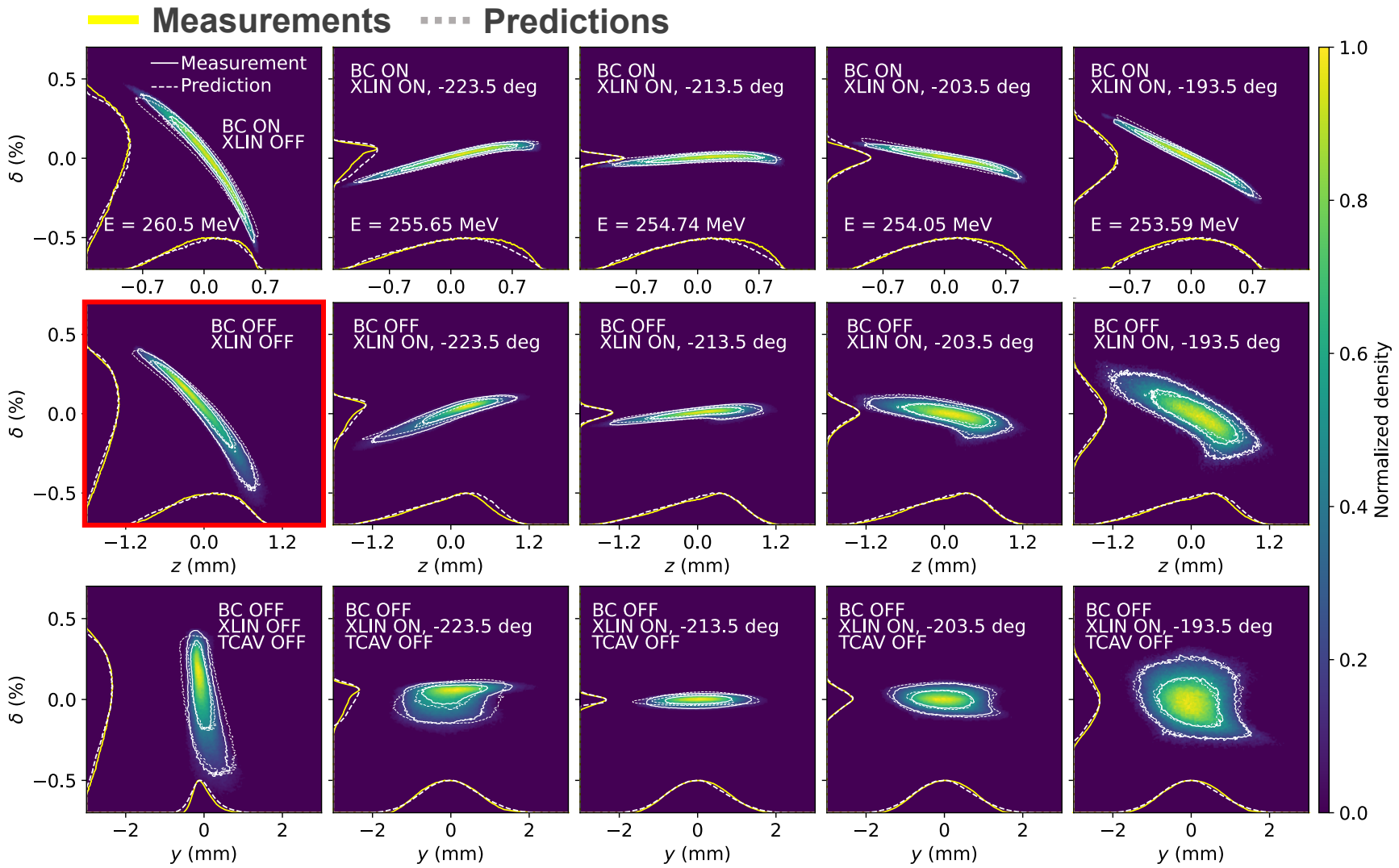
Independent downstream measurements

Background: **Measurement**

Measurements

Predictions

GPSR also successfully predicts independent downstream measurements!



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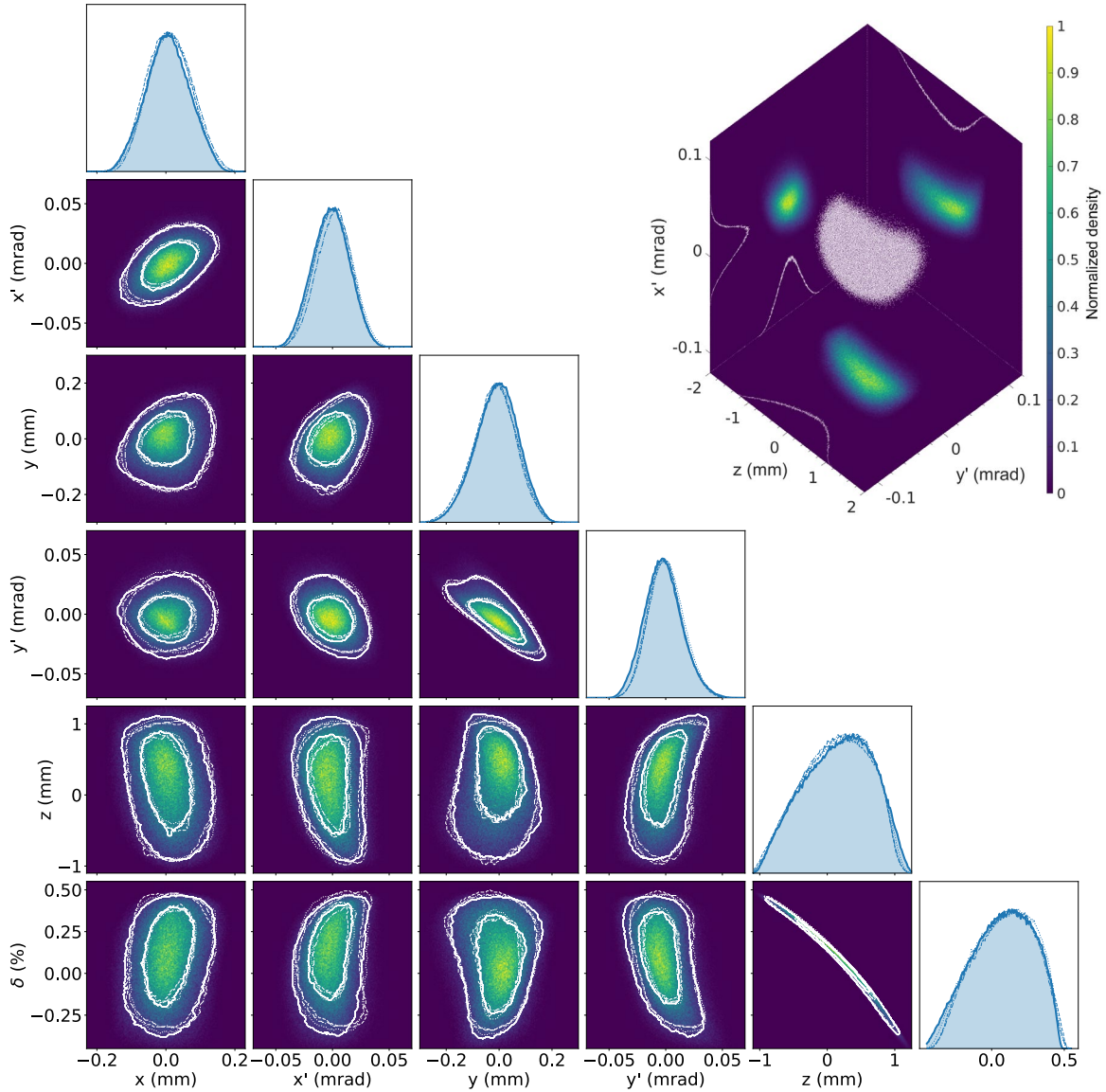
Reconstructed phase space @ Q1 entrance



Parameters	4D Reconstruction	6D reconstruction
β_x (m)	4.59±0.08	4.51±0.07
β_y (m)	7.65±0.11	7.81±0.10
α_x (rad)	−0.55±0.02	−0.52±0.05
α_y (rad)	1.18±0.02	1.15±0.06
ε_{nx} (mm mrad)	0.43±0.01	0.43±0.01
ε_{ny} (mm mrad)	0.41±0.01	0.41±0.02

Parameters	Measurement	6D reconstruction
ε_{nz} (mm mrad)	137.34±17.240	143.36±3.87
σ_z (mm)	0.45±0.01	0.46±0.00
σ_{pz} (%)	0.24±0.01	0.22±0.00
Slice σ_{pz} (%)		0.01 (typical)

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AI/ML applications to PAL-XFEL:
Optimization of the beamline based on diagnostics

Presentation based on:

- Seongyeol Kim *et al., In. Proc. ICALEPCS 2025*, 2025 (10.18429/JACoW-ICALEPCS2025-MOCG004)

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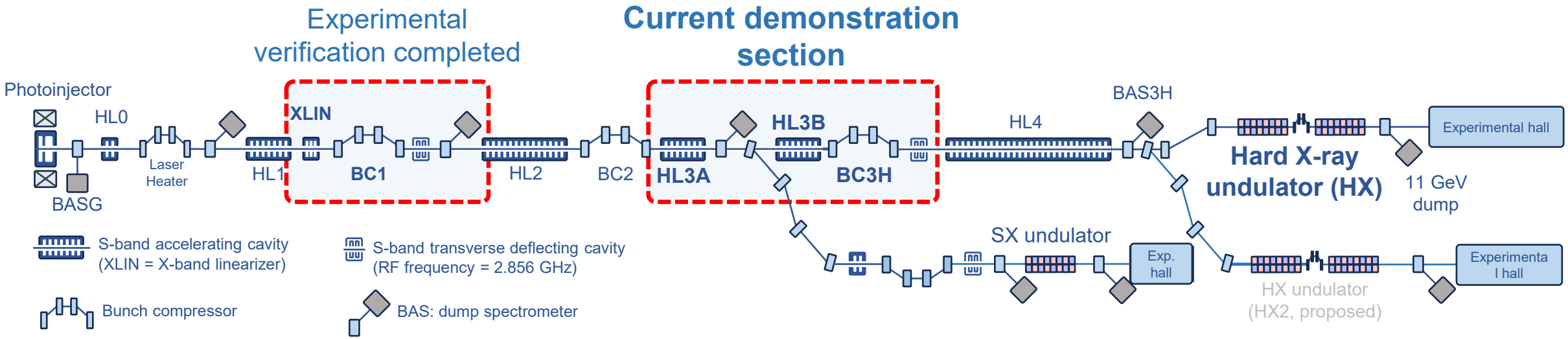
➢ PAL-XFEL figure adapted from: S. Kim *et al., In. Proc. IPAC'25*, 2025 (MOPB098).

GPSR setup @ PAL-XFEL beamline

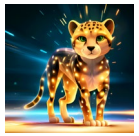


Goal of the demonstration :

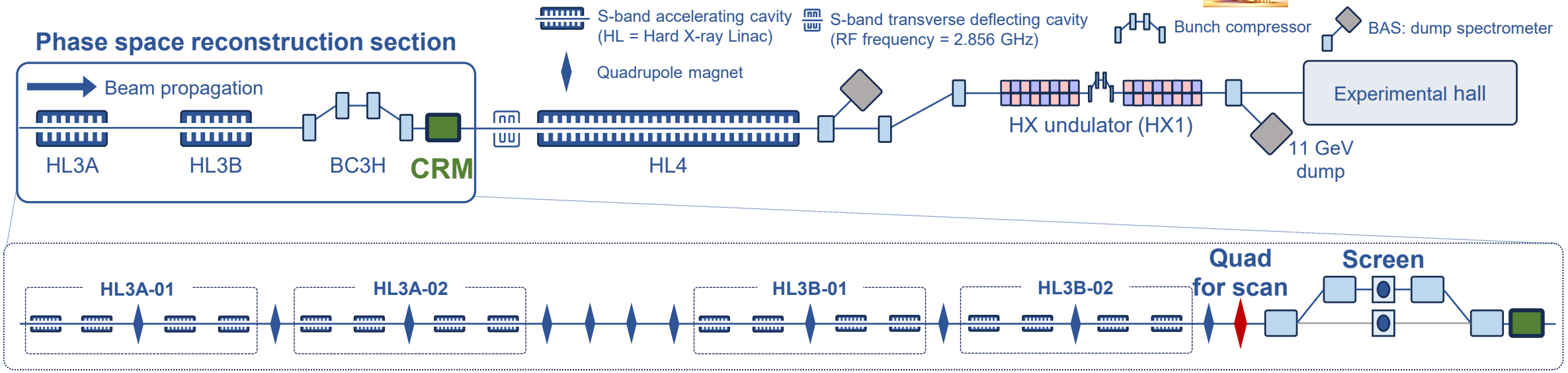
- **Accurate 6-dimensional phase space reconstruction before BC3H bunch compressor**
- **Beamline optimization using non-differentiable simulation (elegant) for emittance preservation against CSR**

POHANG ACCELERATOR LABORATORY

- PAL-XFEL figure adapted from: S. Kim *et al., In. Proc. IPAC'25*, 2025 (MOPB098).
- Differentiable simulation used for this demonstration: Cheetah https://github.com/desy-ml/cheetah



GPSR setup @ PAL-XFEL beamline

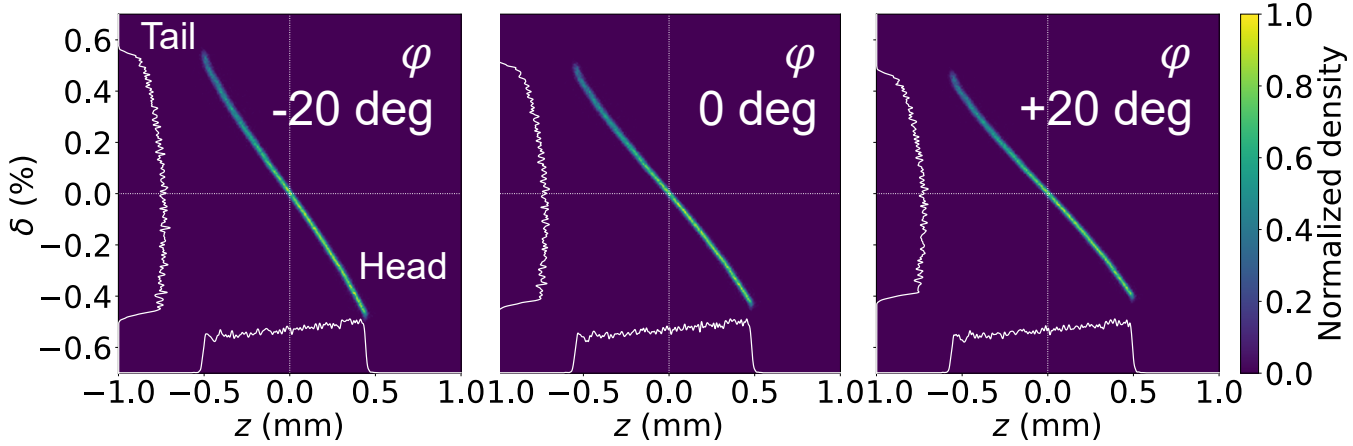


Initial beam energy: 2.45 GeV
16 accelerating cavities (~56 MV/m each)

For successful reconstruction:

➡ **RMS bunch length was considered as an additional physical constraint for loss evaluation**

Longitudinal phase space after HL3



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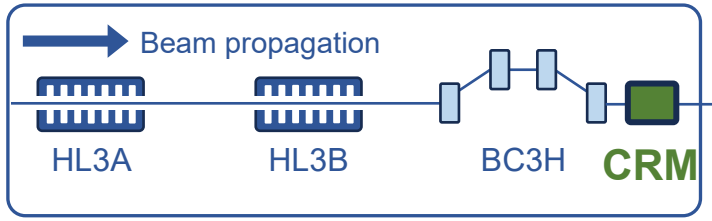
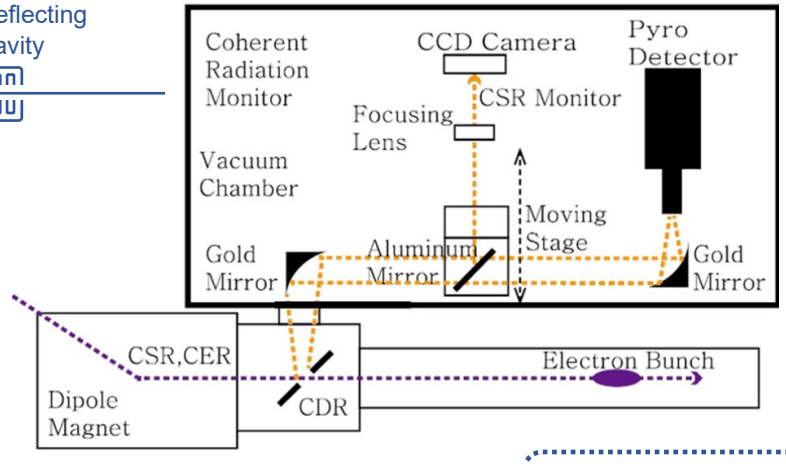
➢ CRM monitor: J. Ko *et al., Rev. Sci. Instrum.* **89**, 063302 (2018)

Physics constraint for GPSR

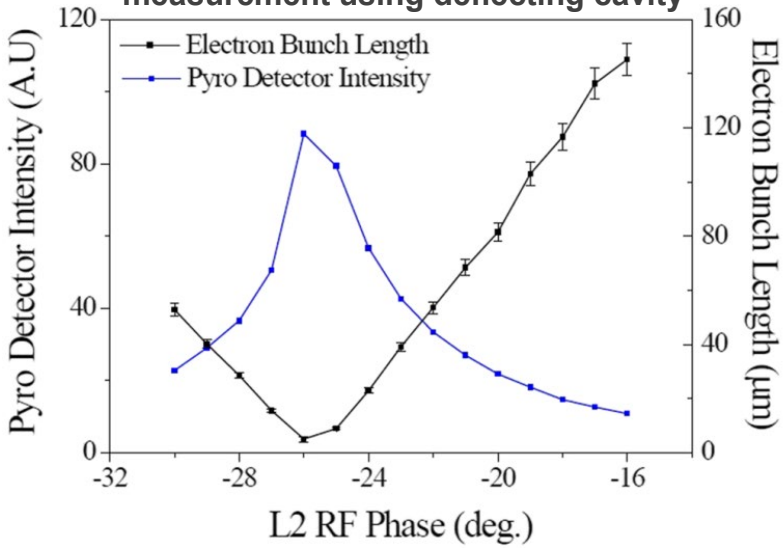
Phase space reconstruction section



Coherent radiation monitor (CRM) device for on-line bunch length monitoring



Calibration with bunch length measurement using deflecting cavity



Total loss for NN weight update

$$l = \sum_{n,i,j}^{N,I,J} \left| R_n^{(i,j)} - Q_n^{(i,j)} \right| + \lambda \sum_{n}^{N} \left| \Delta\sigma_{n,i} + \Delta\sigma_{n,f} \right|$$

Beam image @ screen

RMS bunch length **before** compression

Weight

RMS bunch length **after** compression

Physics – constraint

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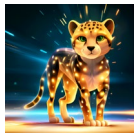
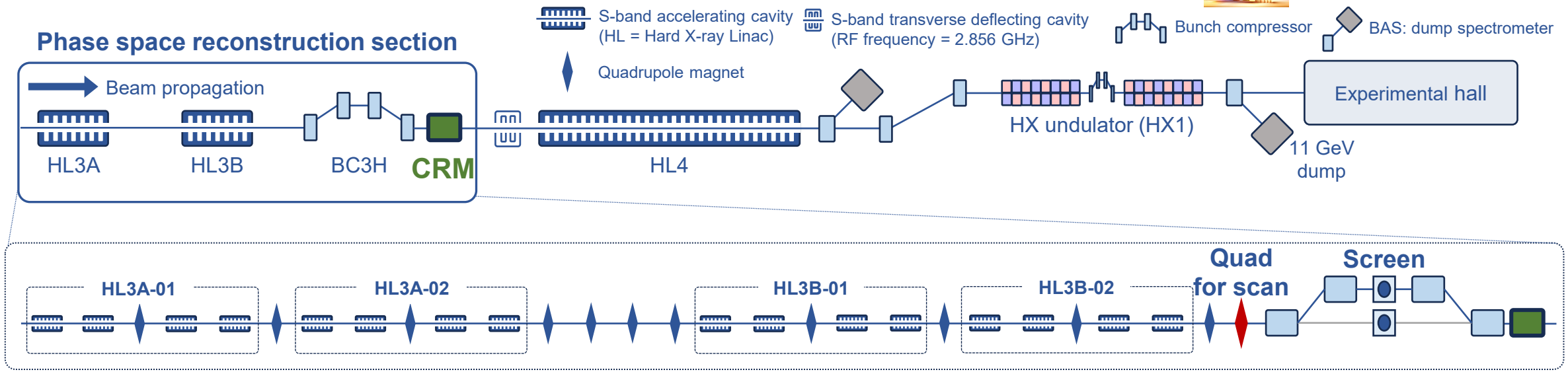
- PAL-XFEL figure adapted from: S. Kim *et al., In. Proc. IPAC'25*, 2025 (MOPB098).
- Differentiable simulation used for this demonstration: Cheetah https://github.com/desy-ml/cheetah



GPSR setup @ PAL-XFEL beamline



Parameters	Value
# of cavity phases	10 (including all cavities off)
# of quad strengths	7
BC3H status	2 (ON / OFF)
Total # of training samples	140
Other quadrupole magnets	Set with certain strengths

Parameters	Value
Initial beam energy	2.45 GeV
Beam charge	182 pC
# of x,y bins (resolution)	(800, 100) (20 um/pixel)
# of reconstructed particles	100,000
# of iterations	2000

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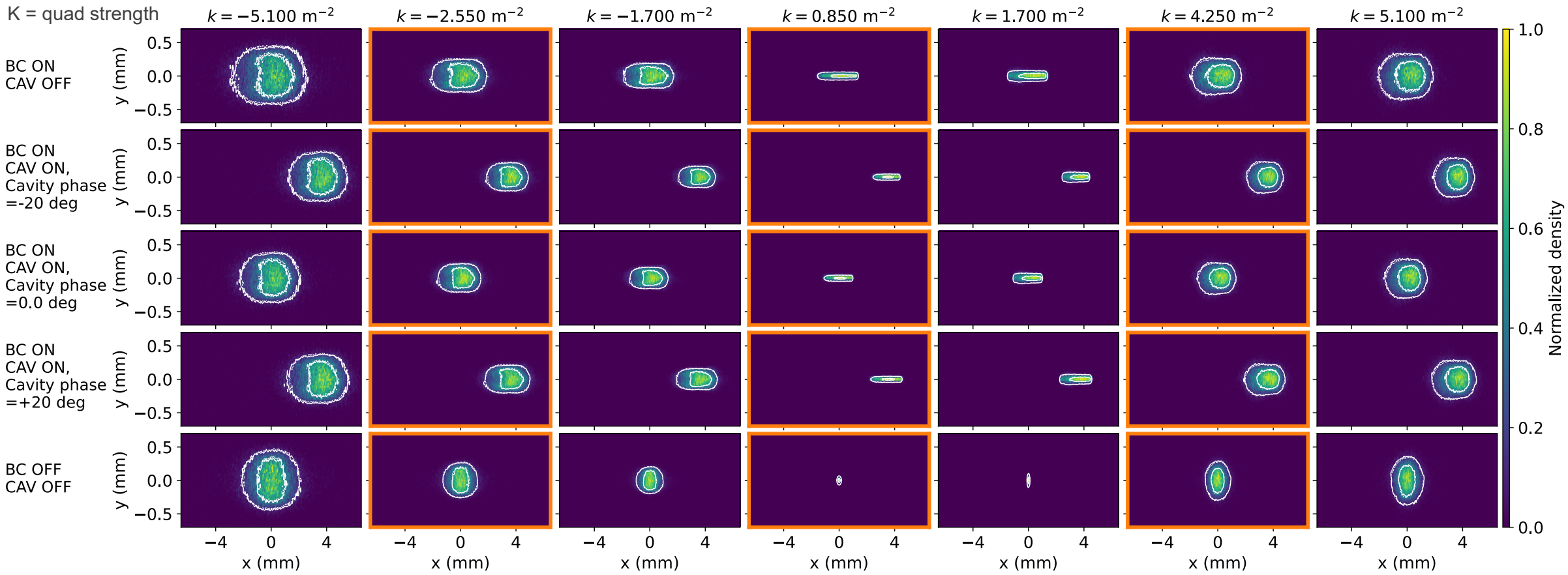
Predictions using reconstructed phase space

Test dataset Training dataset Colormap image: Ground truth

Contour lines (90th, 50th)
Measurements
Predictions



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Predictions using reconstructed phase space

Test dataset

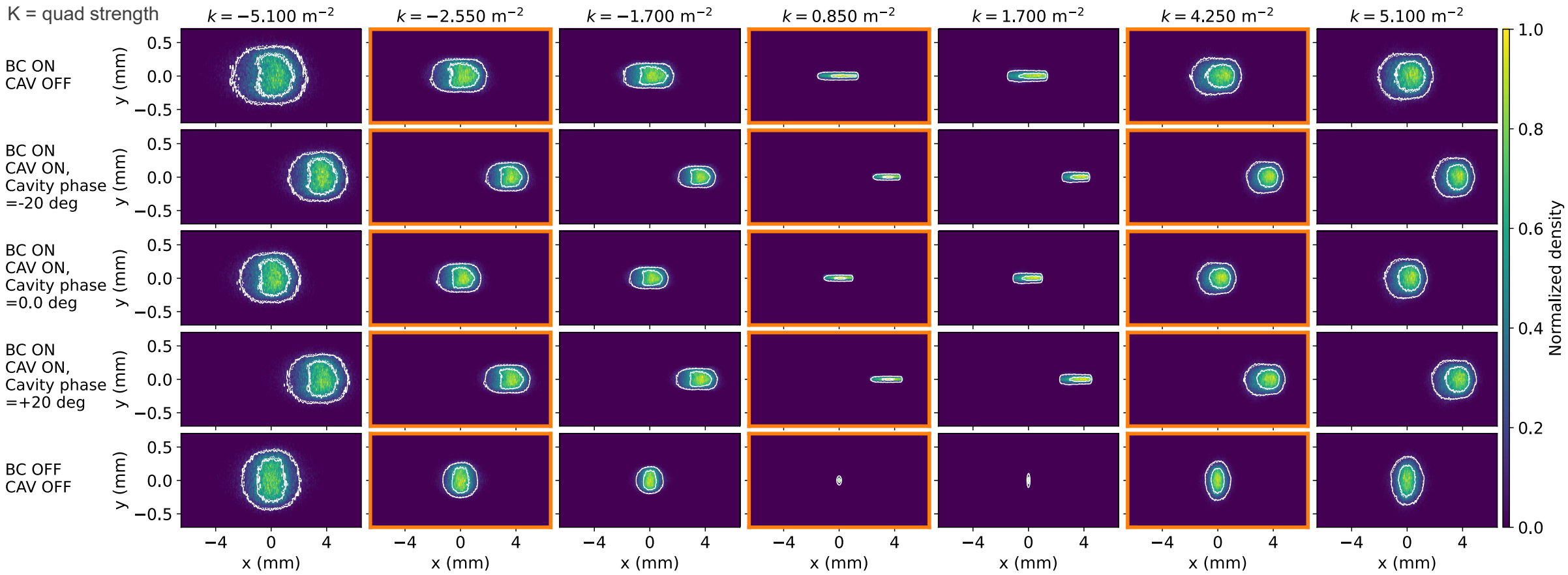
Training dataset

Colormap image: Prediction

Contour lines (90th, 50th)

Measurements

Predictions



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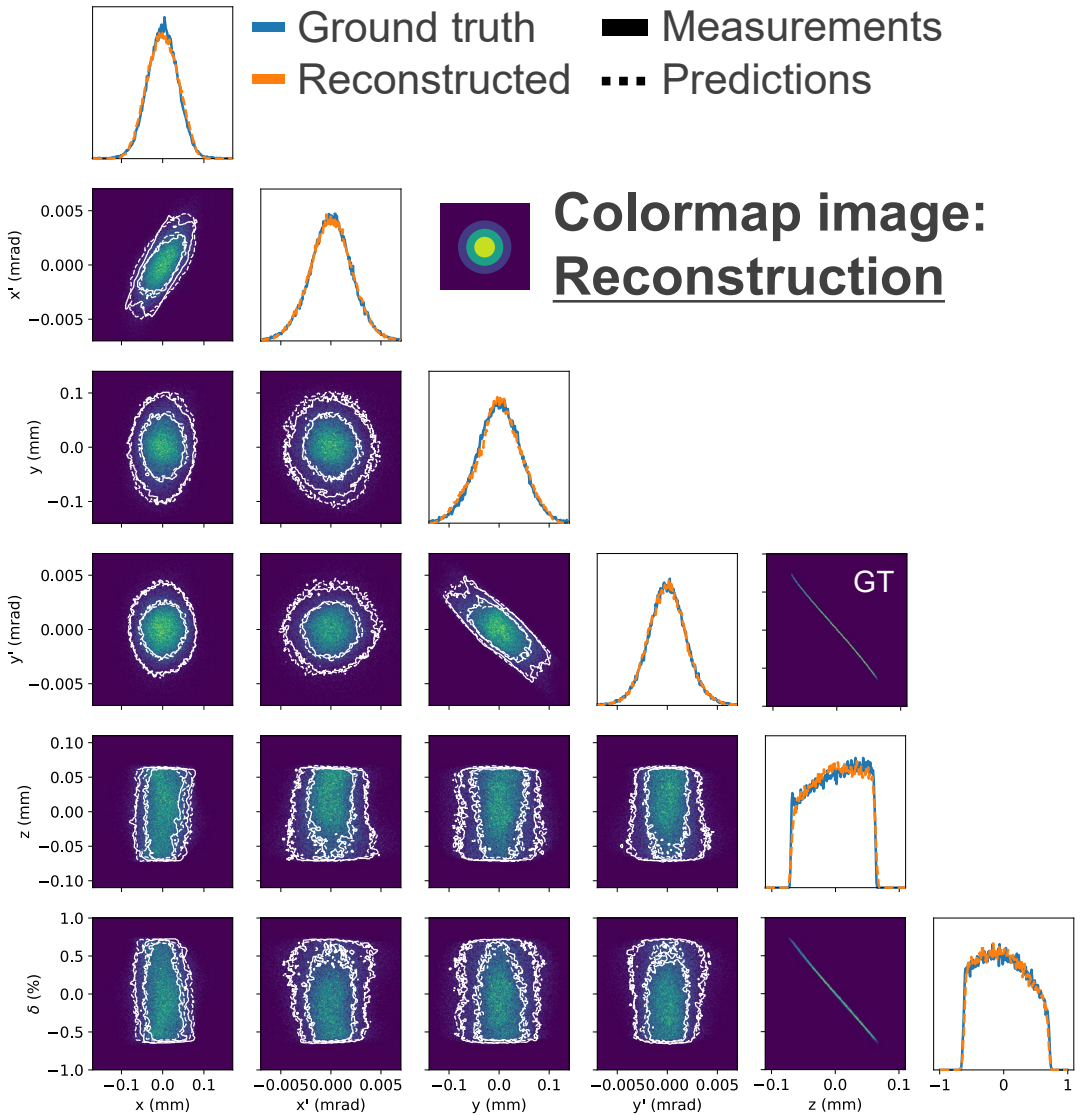
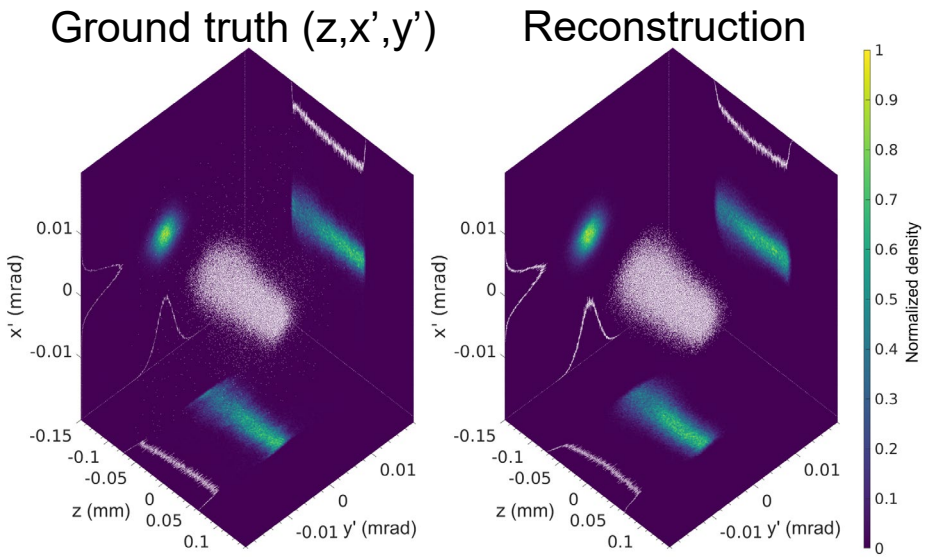
elegant: https://www.aps.anl.gov/Accelerator-Operations-Physics/Software

Reconstructed 6-dimensional phase space



Colormap image: Reconstruction



Successful reconstruction using physics-constrained GPSR:

can be used for downstream optimization using non-differentiable simulation "elegant"

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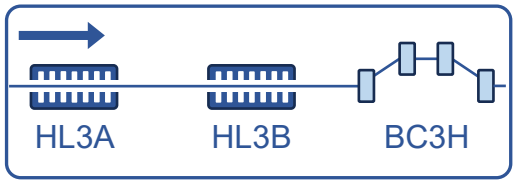
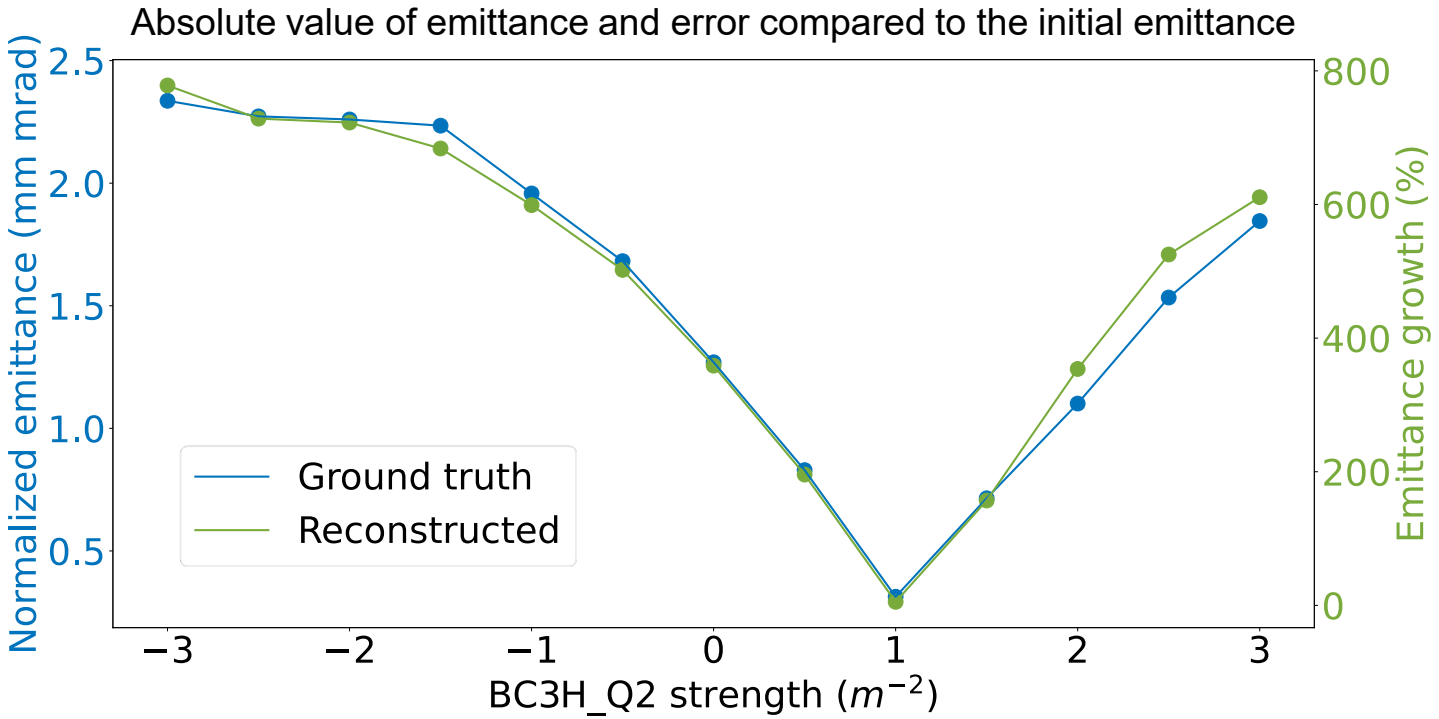
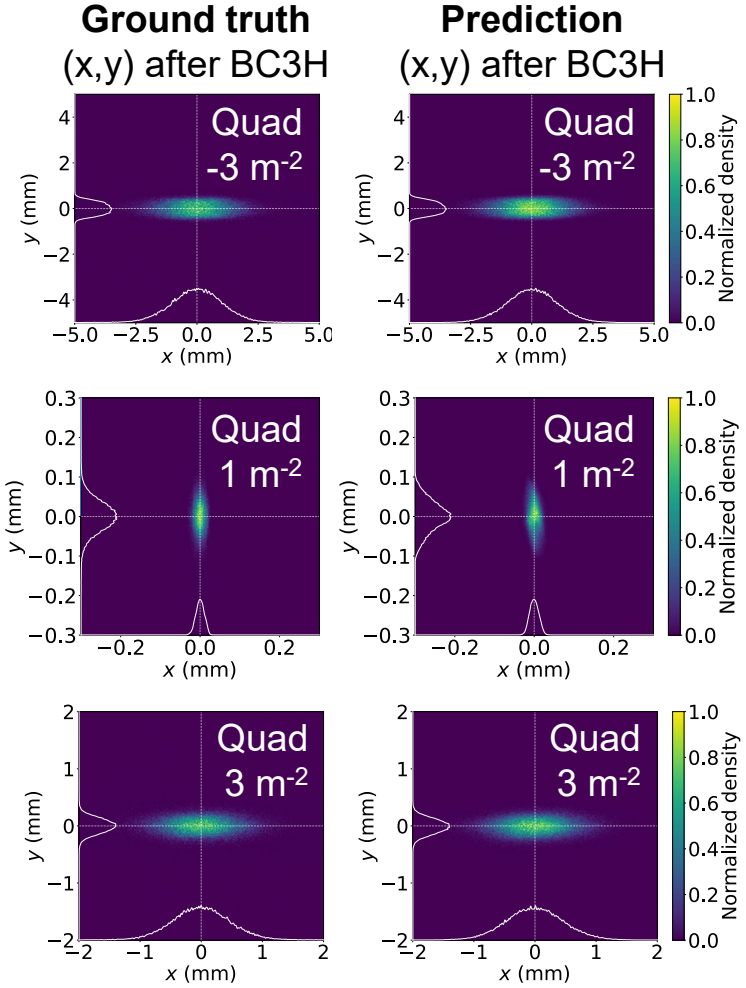
elegant: https://www.aps.anl.gov/Accelerator-Operations-Physics/Software

Comparison of CSR-induced emittance trend

Simulation code: elegant (APS)







Robust GPSR-based beam diagnostics:

can be applied for optimization against collective effects using non-differentiable simulations

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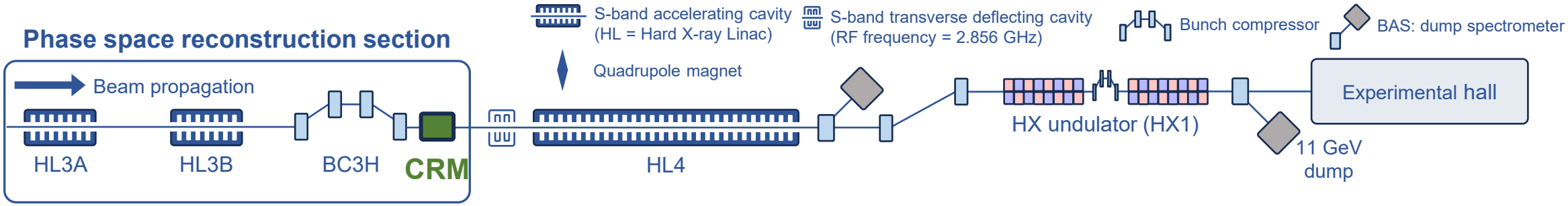
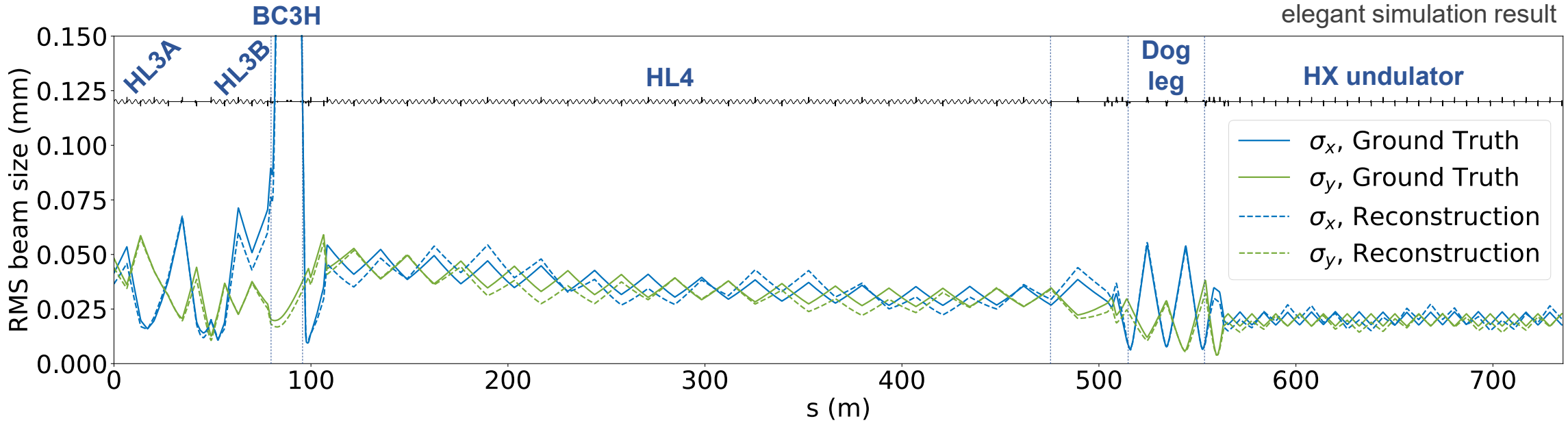
*elegant simulation code used

Further downstream prediction* (up to HX beamline end)





Robust GPSR-based beam diagnostics:

also enables entire beamline optimization for maximizing XFEL quality

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Summary and future work

Summary and future work

- **6-dimensional phase space reconstruction using accelerating cavity was successfully demonstrated at the user facility**
  - All the coupled phase spaces can be successfully predicted
  - Specialized diagnostic elements are no longer required > readily applicable using common elements such as accelerating cavity, quad, dipole, and screen
- **GPSR-based phase space can be used for further applications**
  - Near unique solution: can represent the physical ground truth > prediction against CSR
  - Emittance preservation against collective effects can be effectively predicted
- **PAL-XFEL enhancement will be carried out**
  - Beam diagnostics using the GPSR technique will be performed @ PAL-XFEL to investigate the machine condition: measurement-based model calibration can be performed
  - Therefore, measurement-based optimization using calibrated model can be performed to maximize the FEL quality and on-line virtual diagnostics

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