15th International Beam Instrumentation Conference, Whistler, BC, Canada

Complete 6-dimensional phase space reconstruction based on neural networks and differentiable simulation with standard elements

Seongyeol Kim

Pohang Accelerator Laboratory, Republic of Korea

September 2, 2026

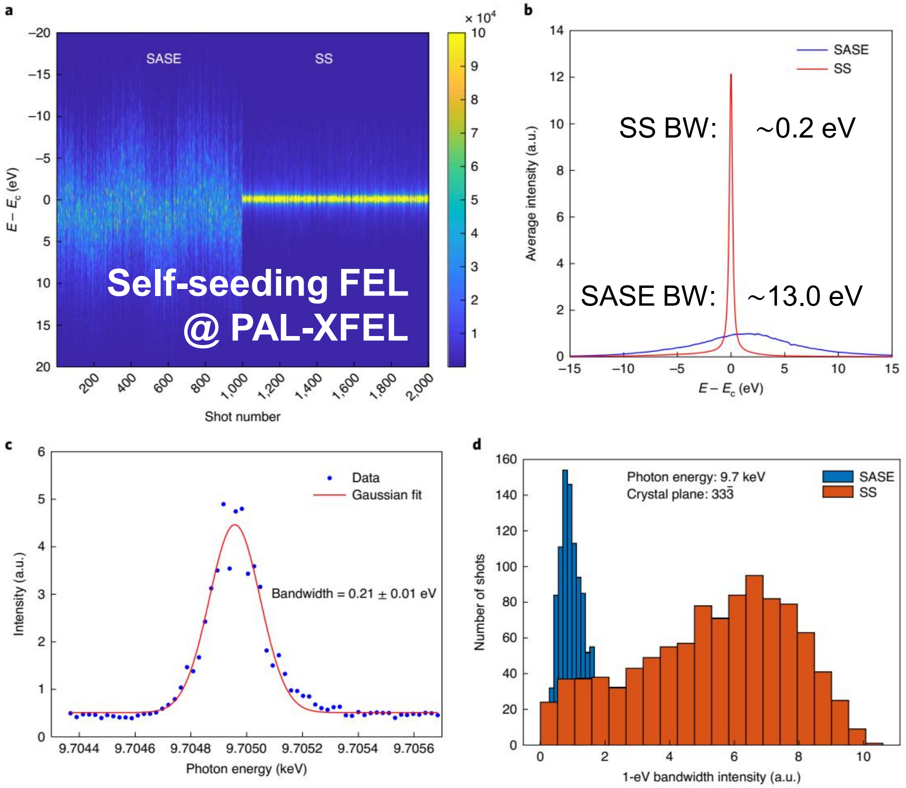
Email: sykim12@postech.ac.kr

Contents

- ❖ **Motivation of beam diagnostics**
  - ➢ Generative Phase Space Reconstruction technique (GPSR)
- ❖ **GPSR–based 6D phase space diagnostics**
  - ➢ Detailed 6D phase space reconstruction @ PAL-XFEL facility
  - ➢ Deployment + applications
- ❖ **Summary and future work**

Introduction

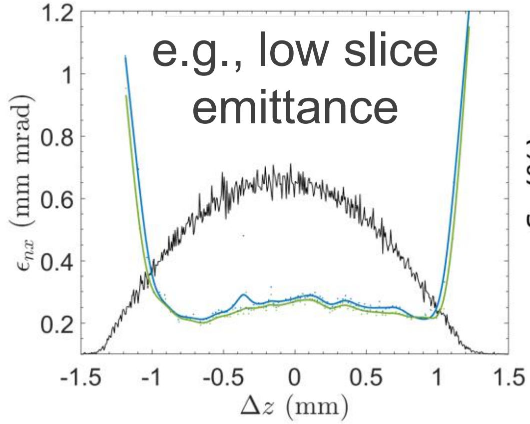
X-ray Free Electron Laser (XFEL)

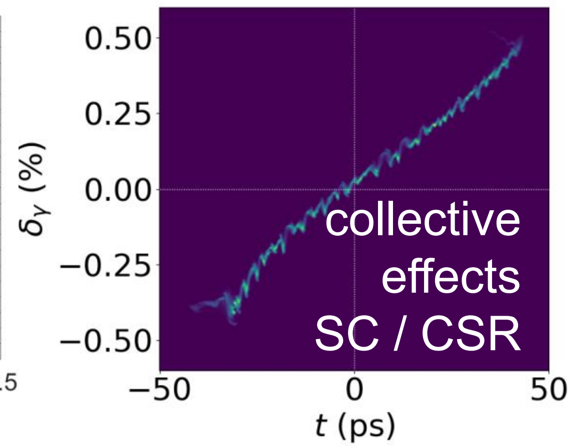


- H.-S. Kang et al., Nat. Photonics **11**, 2017.
- I. Nam *et al., Nat. Photonics* **15**, 2021.

Desired beam conditions for high-quality XFEL:

- ➢ Low transverse/longitudinal emittances
- ➢ Low slice energy spread
- ➢ Flat slice emittance
- ➢ Suppression of nonlinear distortions on 6D phase space





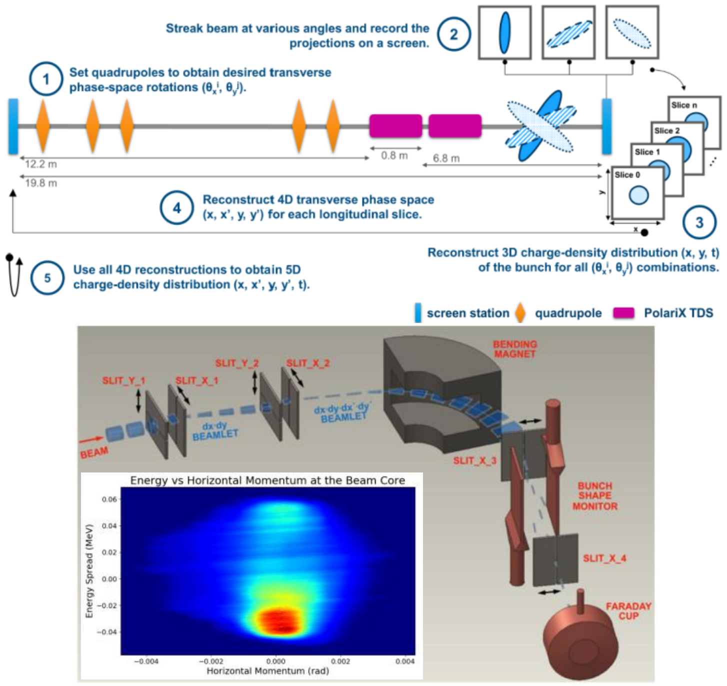
For ultra short, high-brightness X-ray free electron laser:

Precise 6D phase space diagnostics are essential

* Accuracy, efficiency, and required time for diagnostics

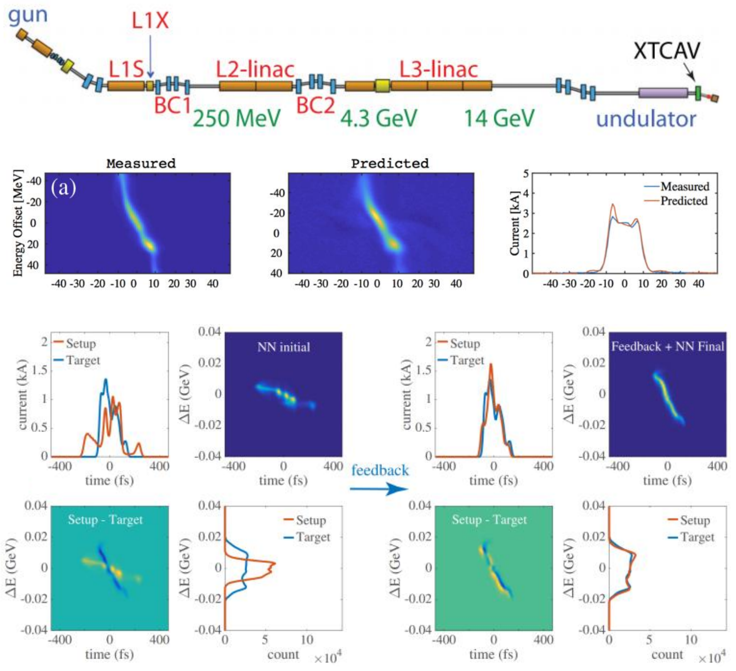
Introduction: phase space diagnostics

Conventional diagnostics



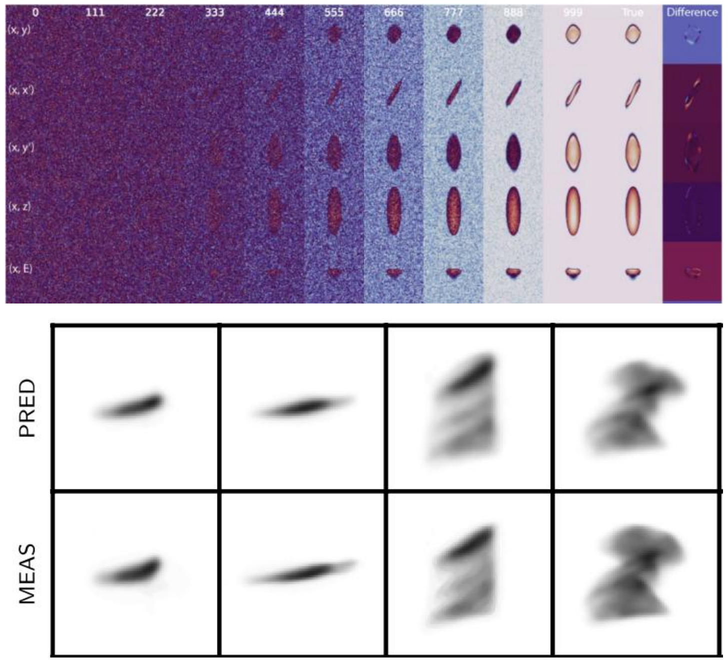
S. Jaster-Merz *et al.*, *PRAB* **27**, 072801, 2024.
B. Cathey *et al.*, *PRL* **121**, 064804, 2018.

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:

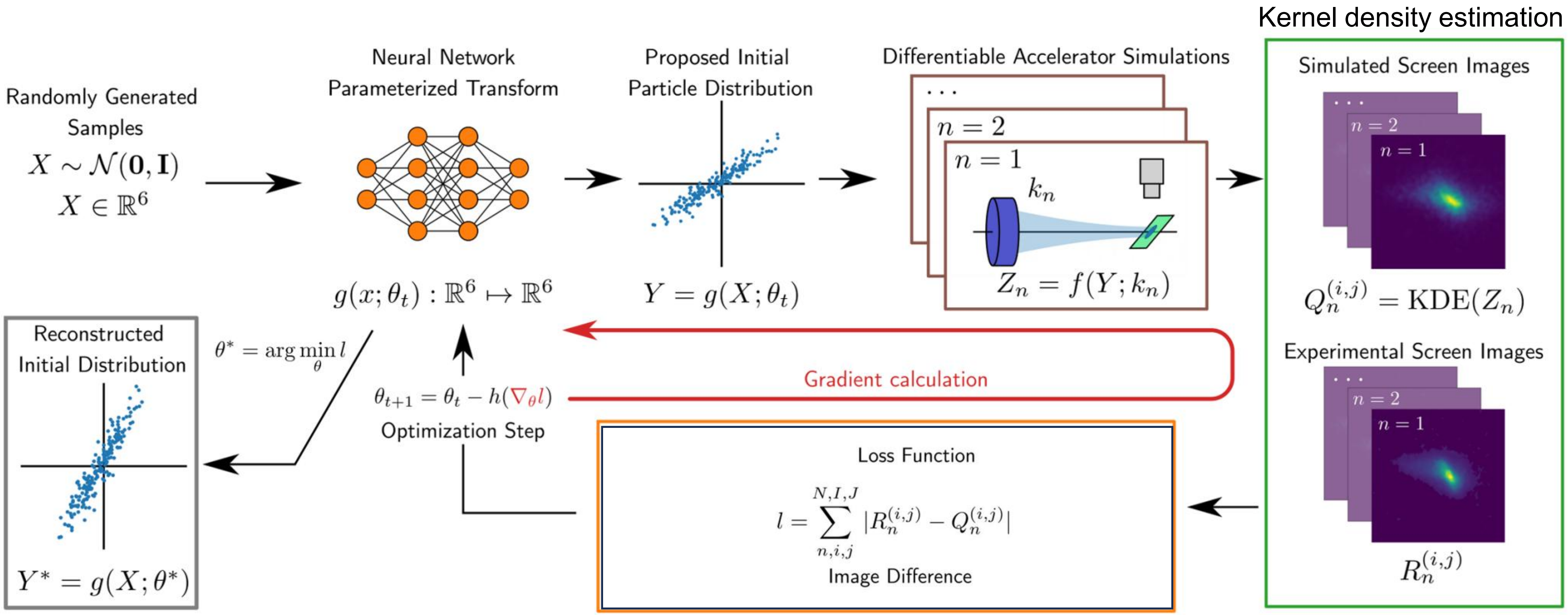
allows us to investigate phase space characterization in a robust way*

POHANG ACCELERATOR LABORATORY

- 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.
- R. Roussel *et al.,* arXiv:2604.20125, 2026.

Generative phase space reconstruction (GPSR)

Based on neural networks and differentiable simulations

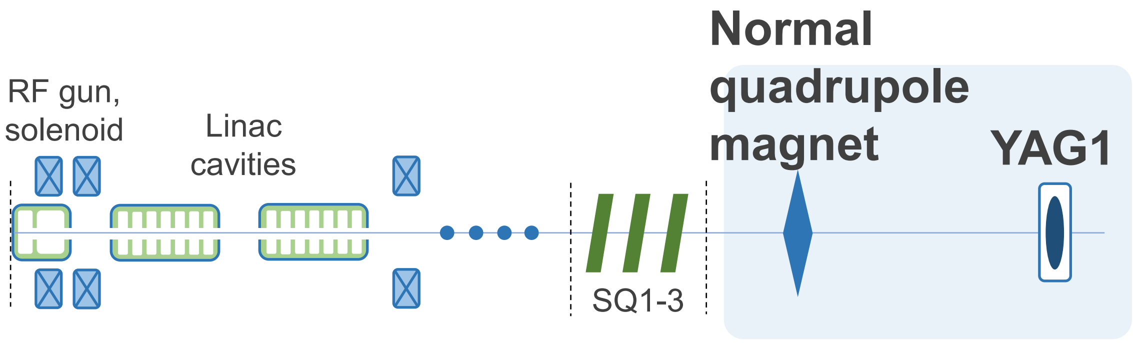


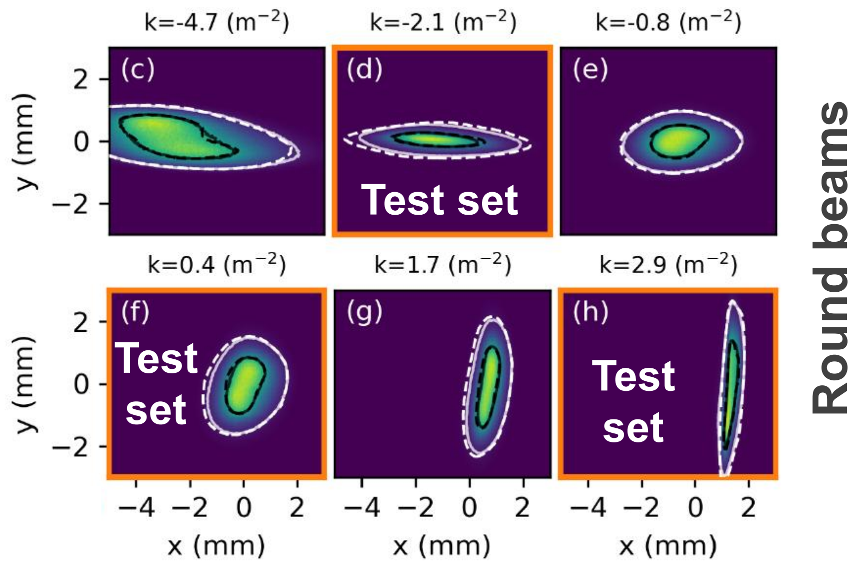
Iteration process to optimize ~1k neural network parameters using gradient calculation:

Possible to reconstruct beam phase space that successfully predicts experimental measurements

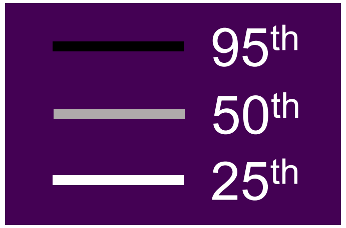
Generative phase space reconstruction (GPSR):

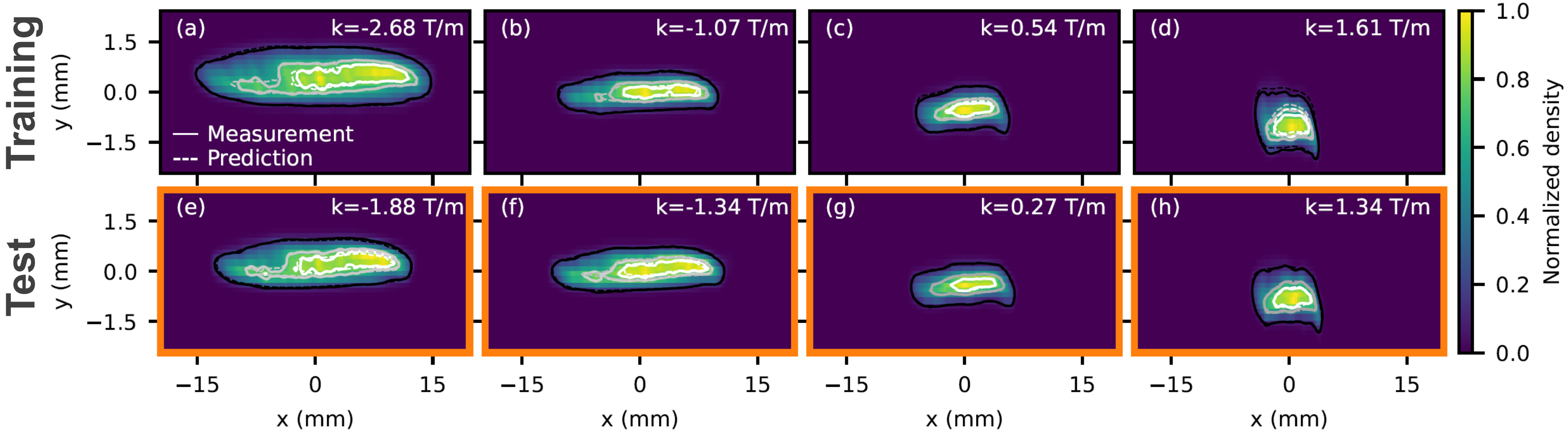
- R. Roussel *et al., PRL* **130**, 145001, 2023.
- S. Kim *et al., PRAB* **27**, 074601, 2024.
- R. Roussel *et al., PRAB* **27**, 094601, 2024.
- J.P. Gonzalez-Aguilera *et al., IPAC'24*, 2024.
- R. Roussel *et al.,* arXiv:2604.20125, 2026.





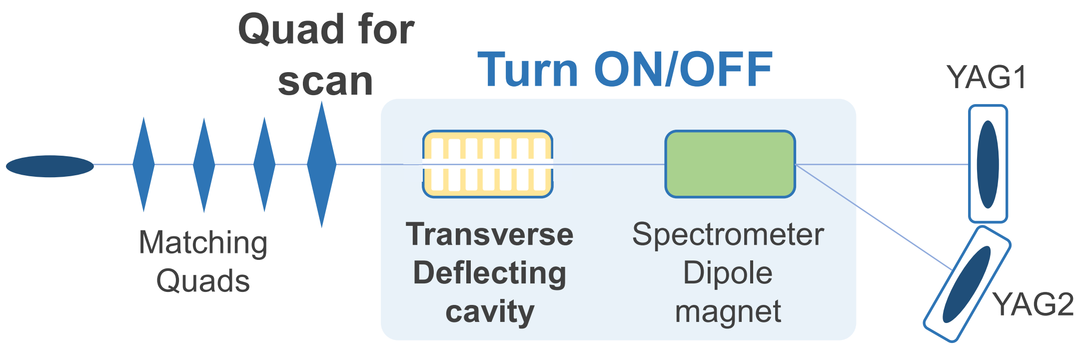
Flat / magnetized beams



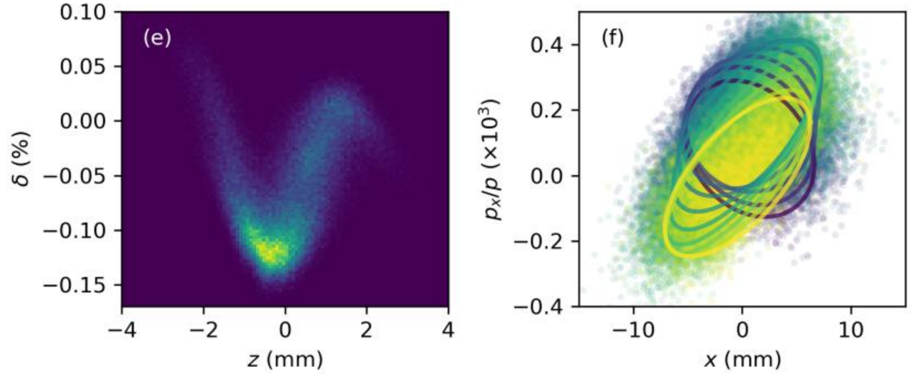


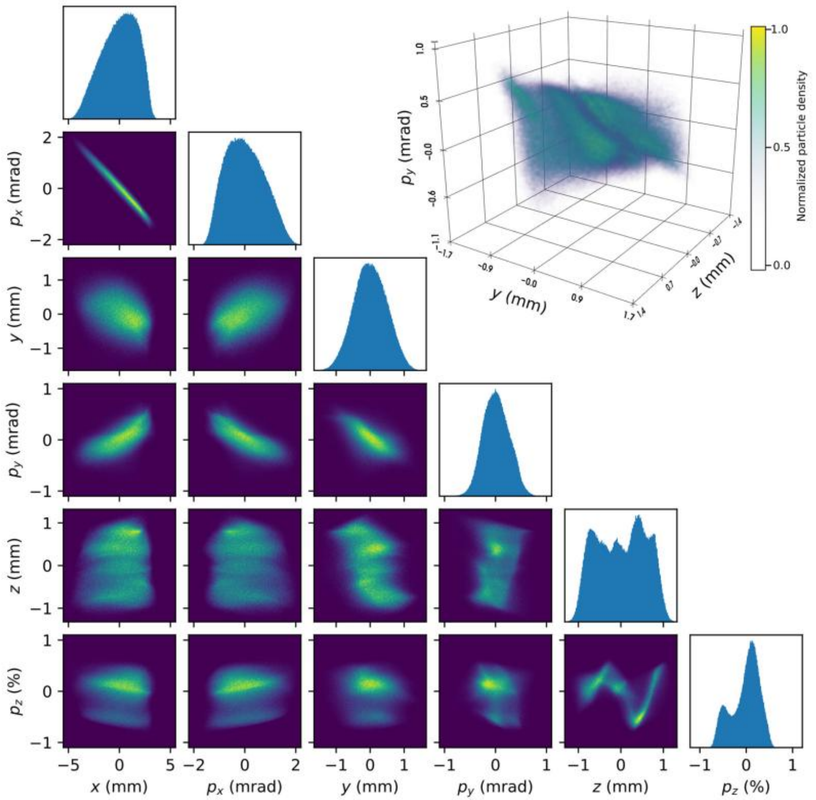
- R. Roussel *et al.*, *PRL* **130**, 145001, 2023.
- S. Kim *et al.*, *PRAB* **27**, 074601, 2024.
- R. Roussel *et al.*, *PRAB* **27**, 094601, 2024.
- J.P. Gonzalez-Aguilera *et al.*, *IPAC'24*, 2024.
- *R. Roussel *et al.*, arXiv:2604.20125, 2026.

Generative phase space reconstruction (GPSR):



CSR characterization





➡ **6-dimensional phase space reconstruction is also successfully performed and currently deployed @ LCLS-II, SLAC***

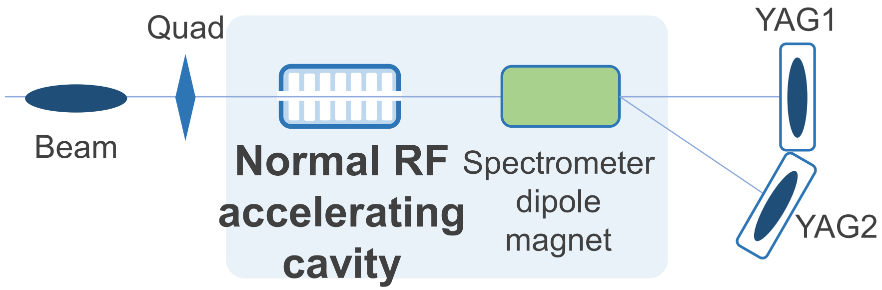
POHANG ACCELERATOR LABORATORY

6D GPSR using RF accelerating cavity

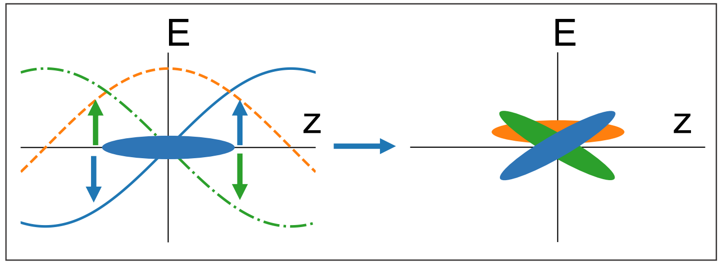
Inspired by conventional longitudinal emittance measurement*

*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.

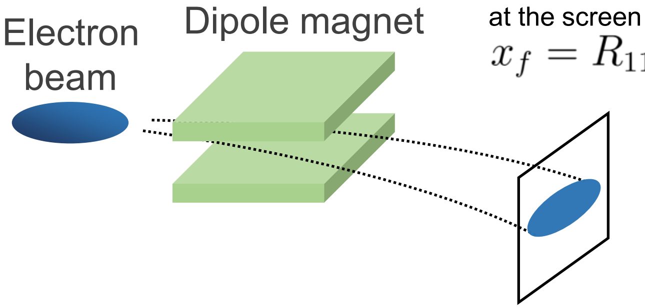


$$\Delta E(z) = eV\cos\left(k_{RF}z + \phi_{RF}\right)$$



For a given longitudinal distribution:

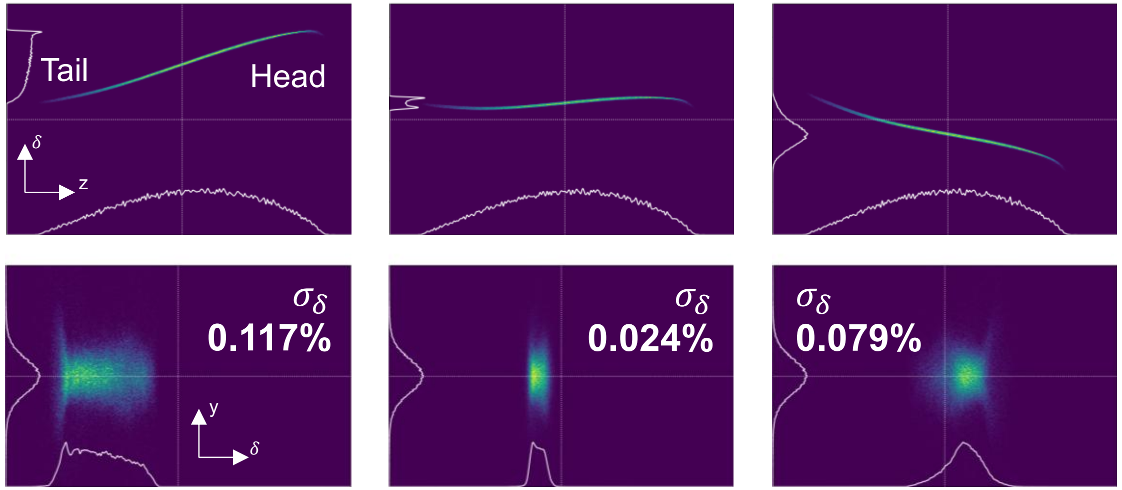
➡ **Energy changes induced by the cavity can be captured at the spectrometer screen**



$$x_f = R_{11}x_0 + R_{12}x'_0 + R_{16}\,\delta_0$$

$$\delta = \frac{\Delta E}{E_{ref}}$$

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



POHANG ACCELERATOR LABORATORY

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.

Transfer matrix for cavity and drift

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

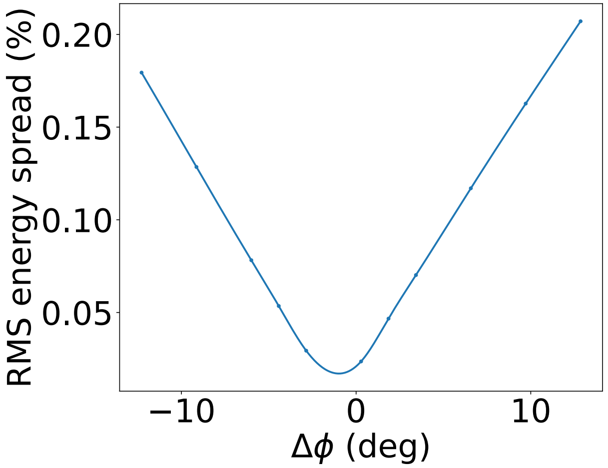
$$\sigma_{22}^{YAG} = \sigma_\delta^2 = V^2\sigma_{11}\,\phi^2 - 2V\sigma_{12}\,\phi + \sigma_{22}$$

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

POHANG ACCELERATOR LABORATORY

*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.

6D GPSR using RF accelerating cavity

Inspired by conventional longitudinal emittance measurement*

1. Dominated by quadscan

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

Screen measurement

2. determined @ dispersive section under transverse constraints

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

3. Constrained by energy spread under given RF parameters

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

4. (z, δ) **Correlation by cavity phase scan: Complete 6D phase space**

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

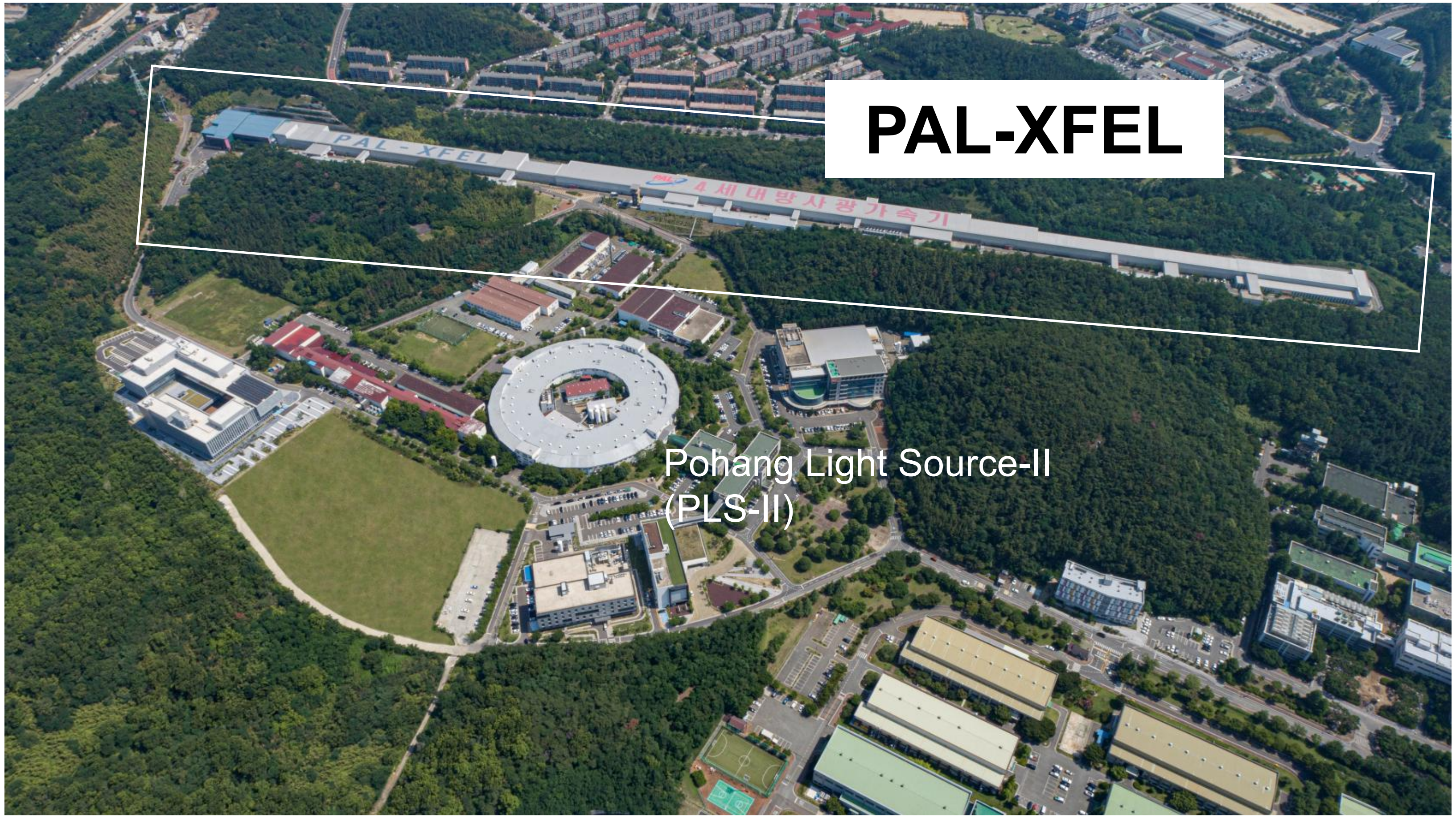
We can obtain complete 6-dimensional coupled phase space of the beam

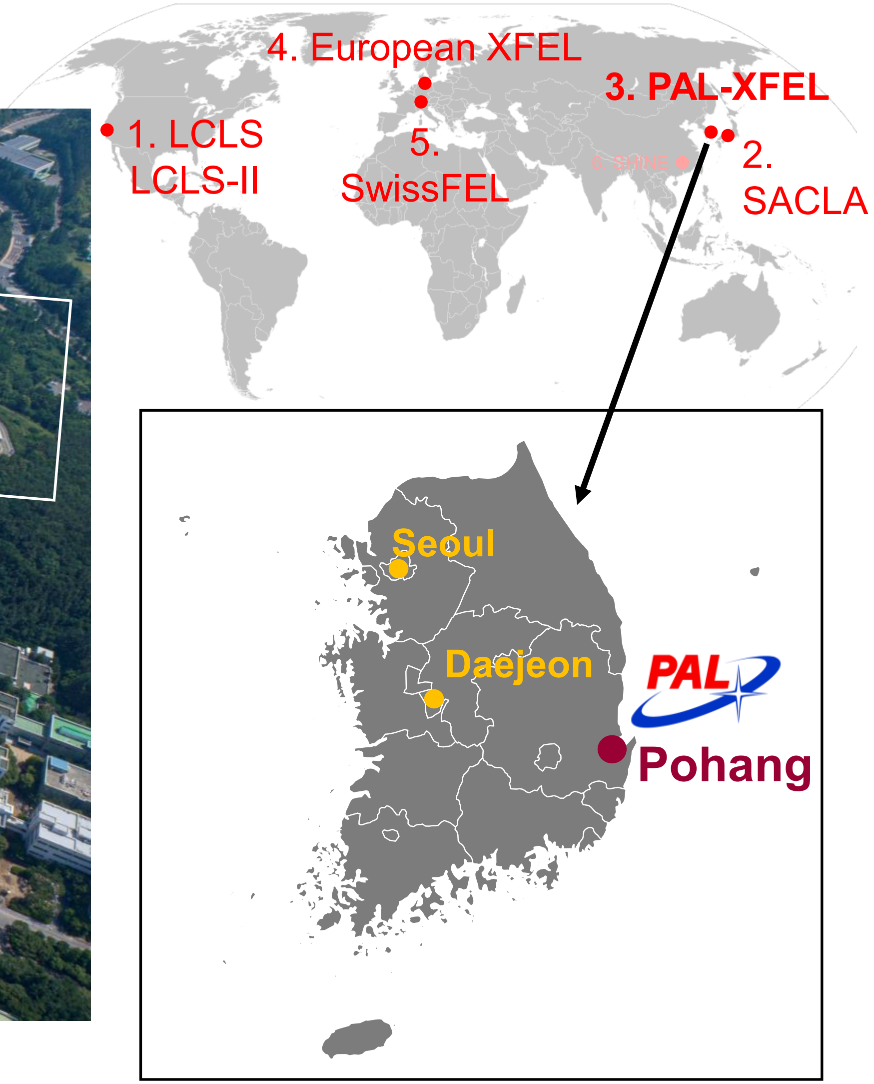
6D phase space reconstruction @ PAL-XFEL, Korea

Based on:

- Seongyeol Kim *et al., Sci. Rep.* **15**, 43049, 2025.

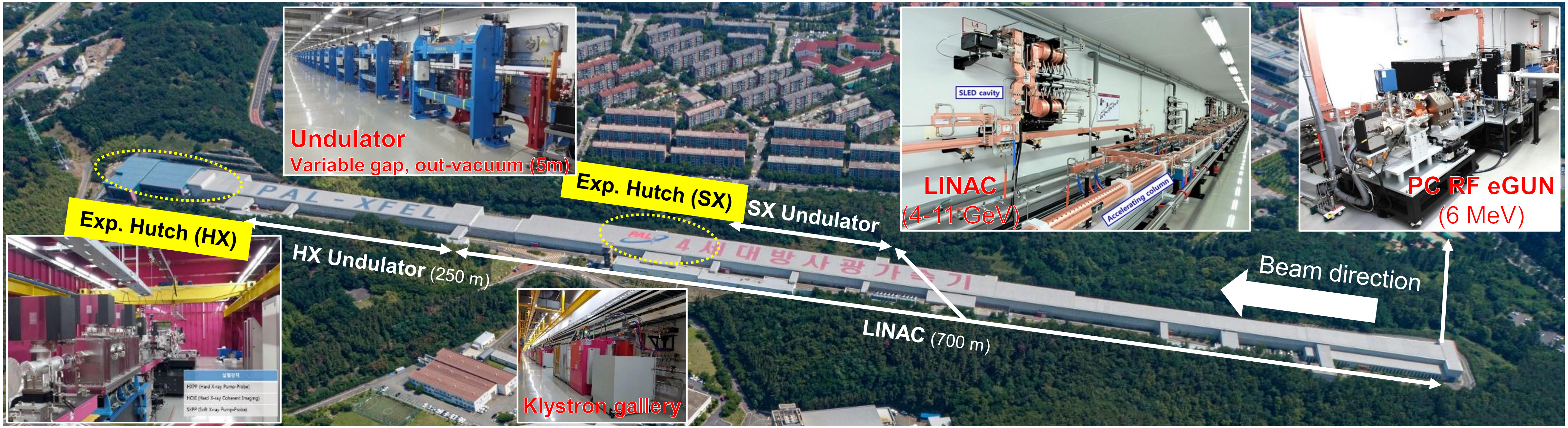
Pohang Accelerator Laboratory, X-ray Free Electron Laser



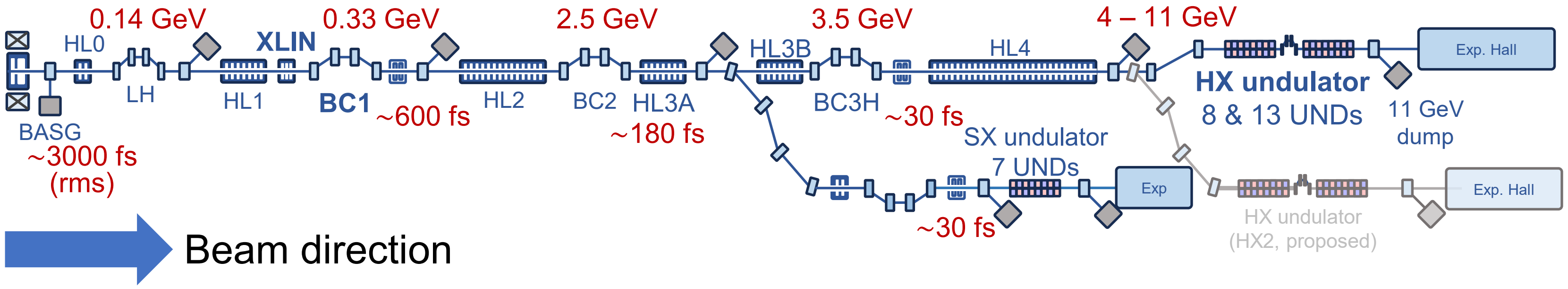


POHANG ACCELERATOR LABORATORY

Pohang Accelerator Laboratory, X-ray Free Electron Laser

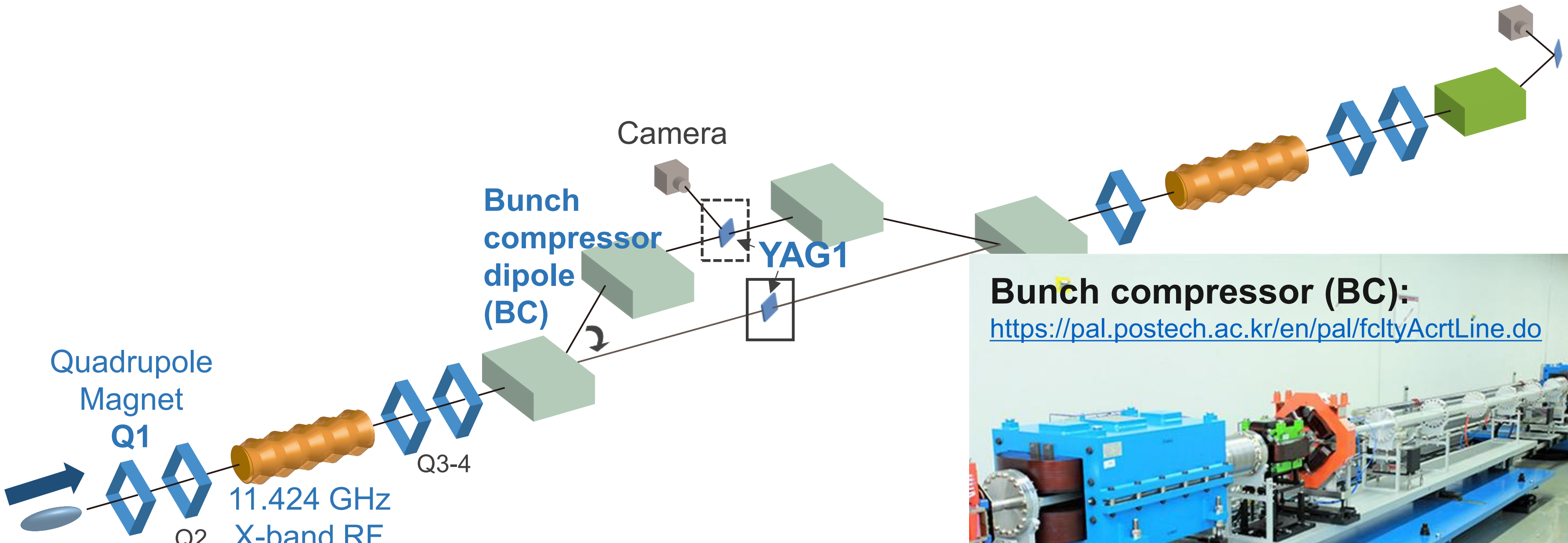


PAL-XFEL Layout



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

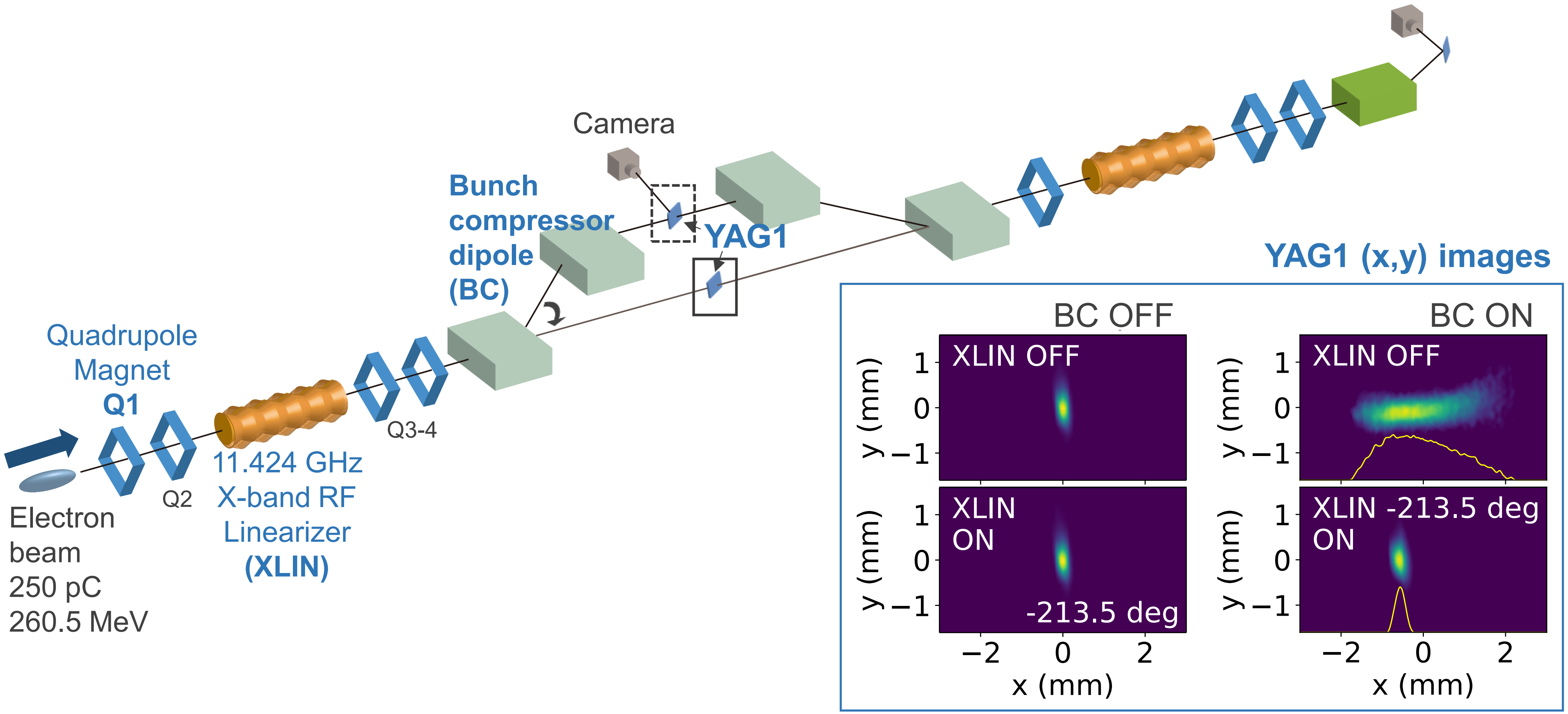
Experimental setup for the GPSR @ PAL-XFEL



Bunch compressor (BC):
https://pal.postech.ac.kr/en/pal/fcltyAcrtLine.do

POHANG ACCELERATOR LABORATORY

Experimental setup for the GPSR @ PAL-XFEL

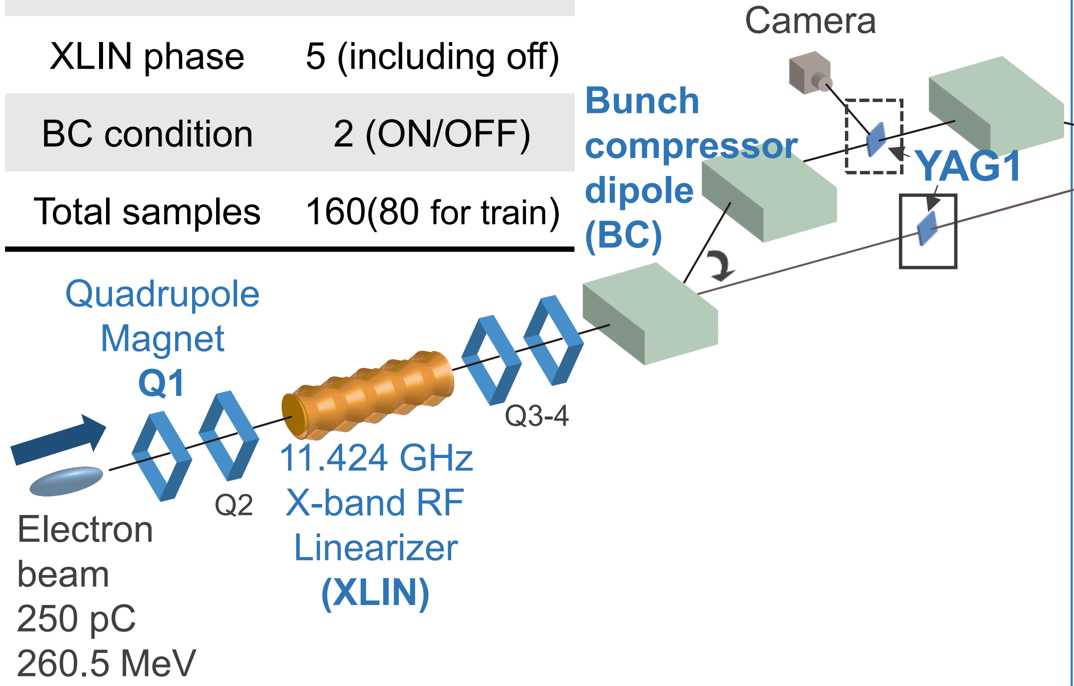


- Bmad-X: https://github.com/bmad-sim/Bmad-X
- Transition in progress from Bmad-X to Cheetah simulation @ PAL-XFEL: https://github.com/desy-ml/cheetah

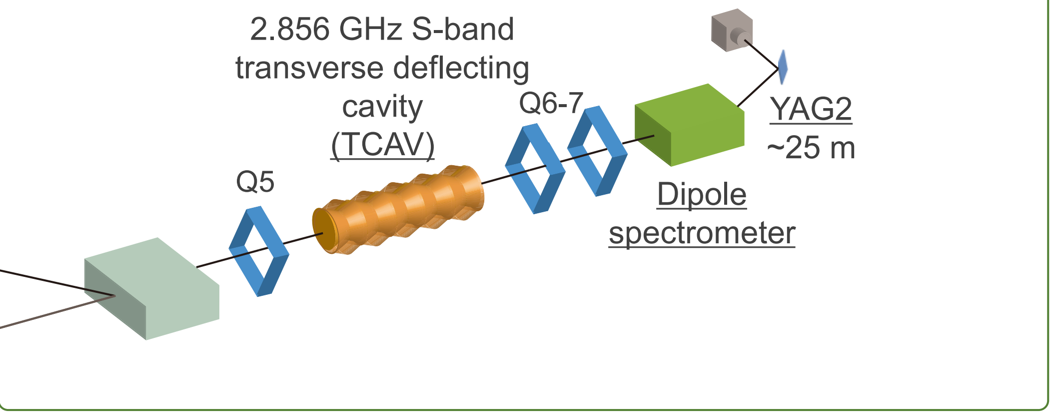
Experimental setup for the GPSR @ PAL-XFEL

GPSR demo section

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



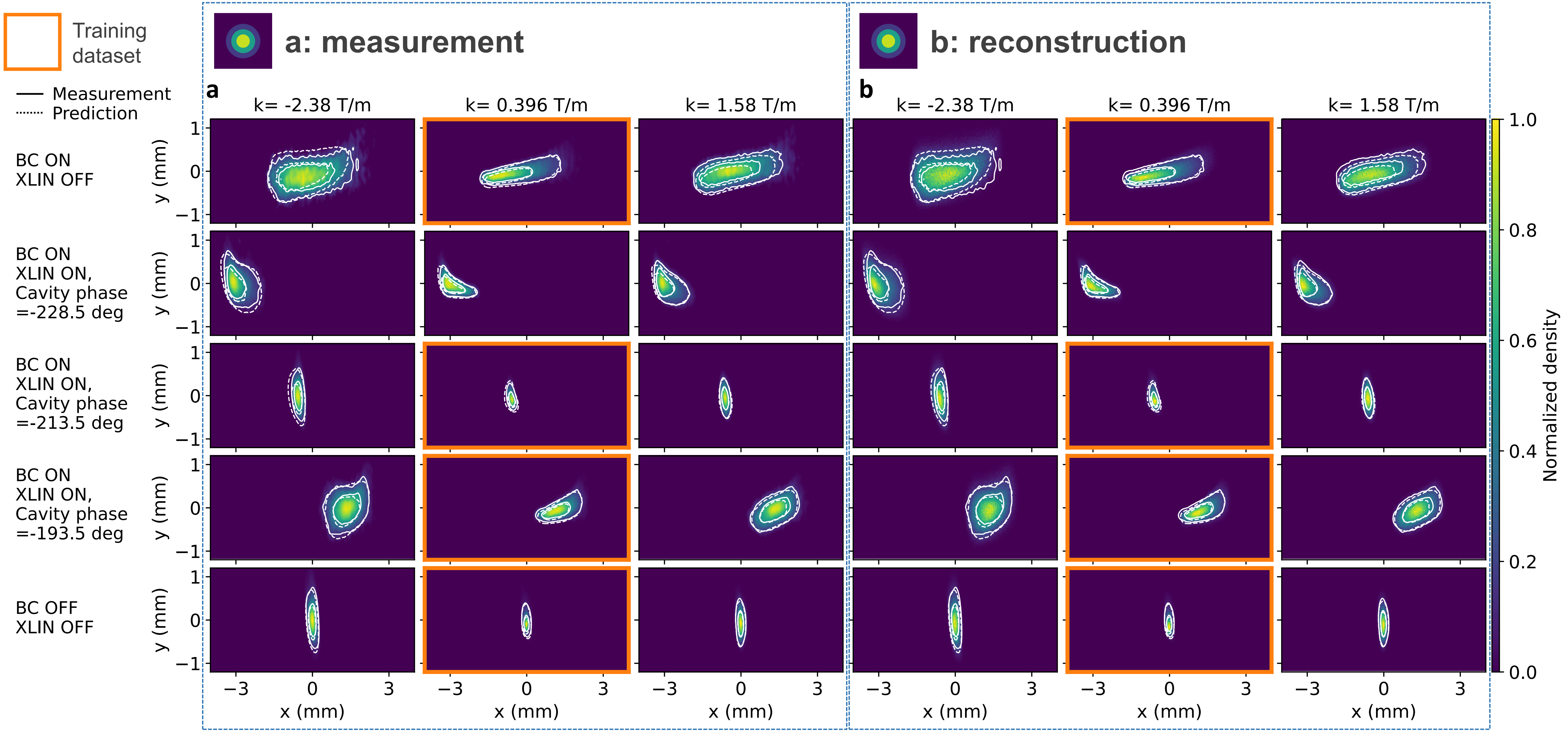
GPSR validation section



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

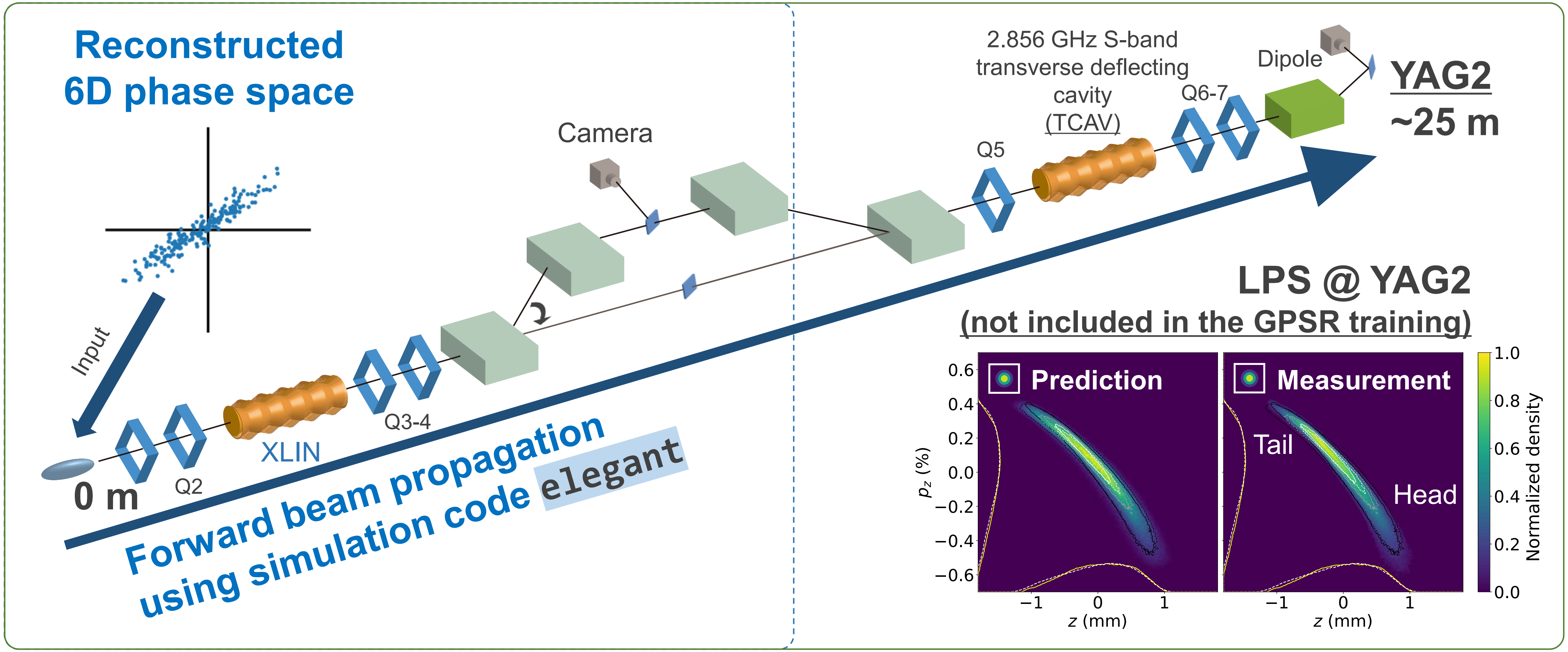
POHANG ACCELERATOR LABORATORY

Comparison of training and test datasets @ YAG1



POHANG ACCELERATOR LABORATORY

GPSR validation using downstream measurements



6D reconstructed phase space of the beam:

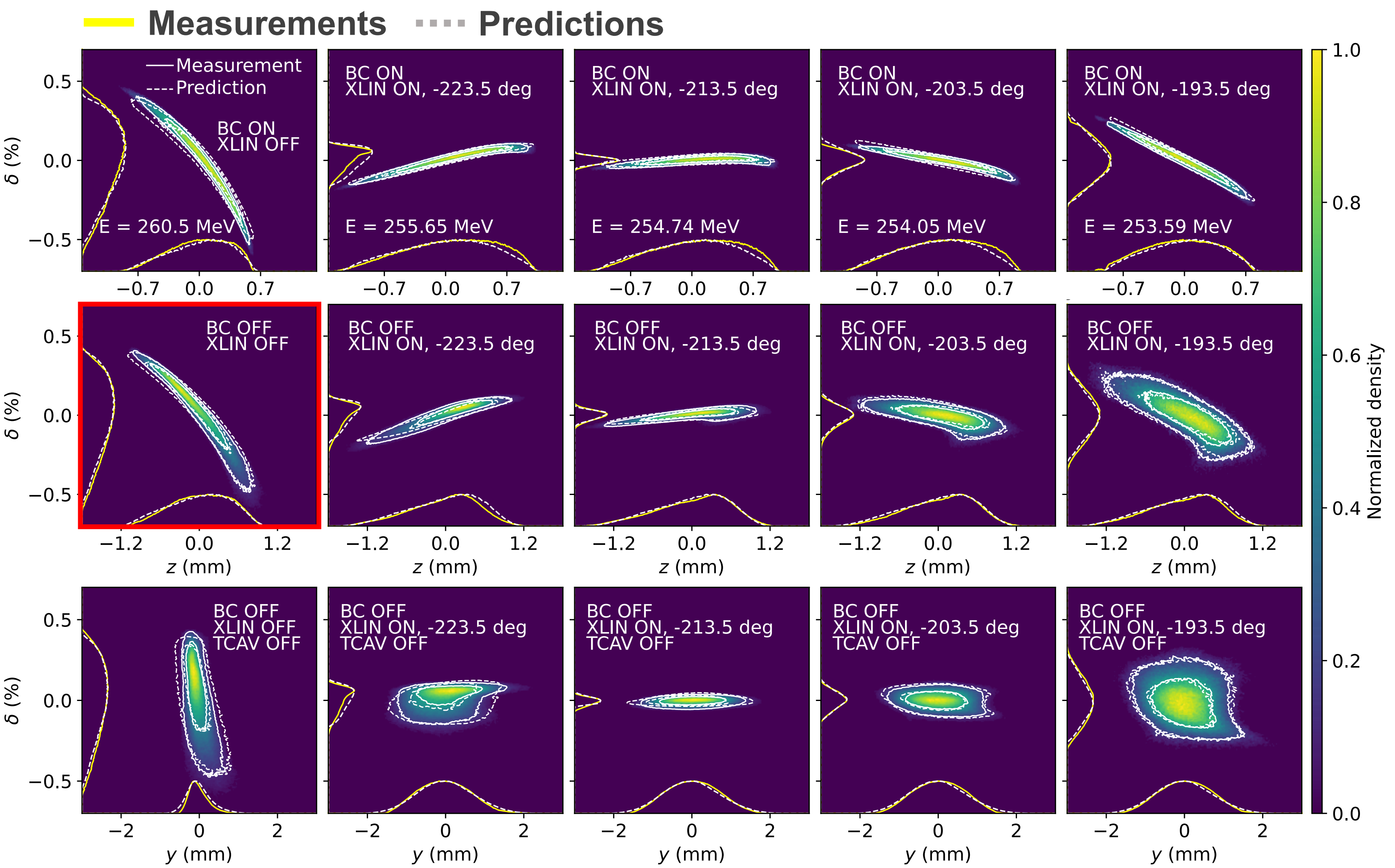
Can be used to predict the phase space at downstream beamline

POHANG ACCELERATOR LABORATORY

Predictions using reconstructed phase space @ YAG2

Beam image:
Measurement

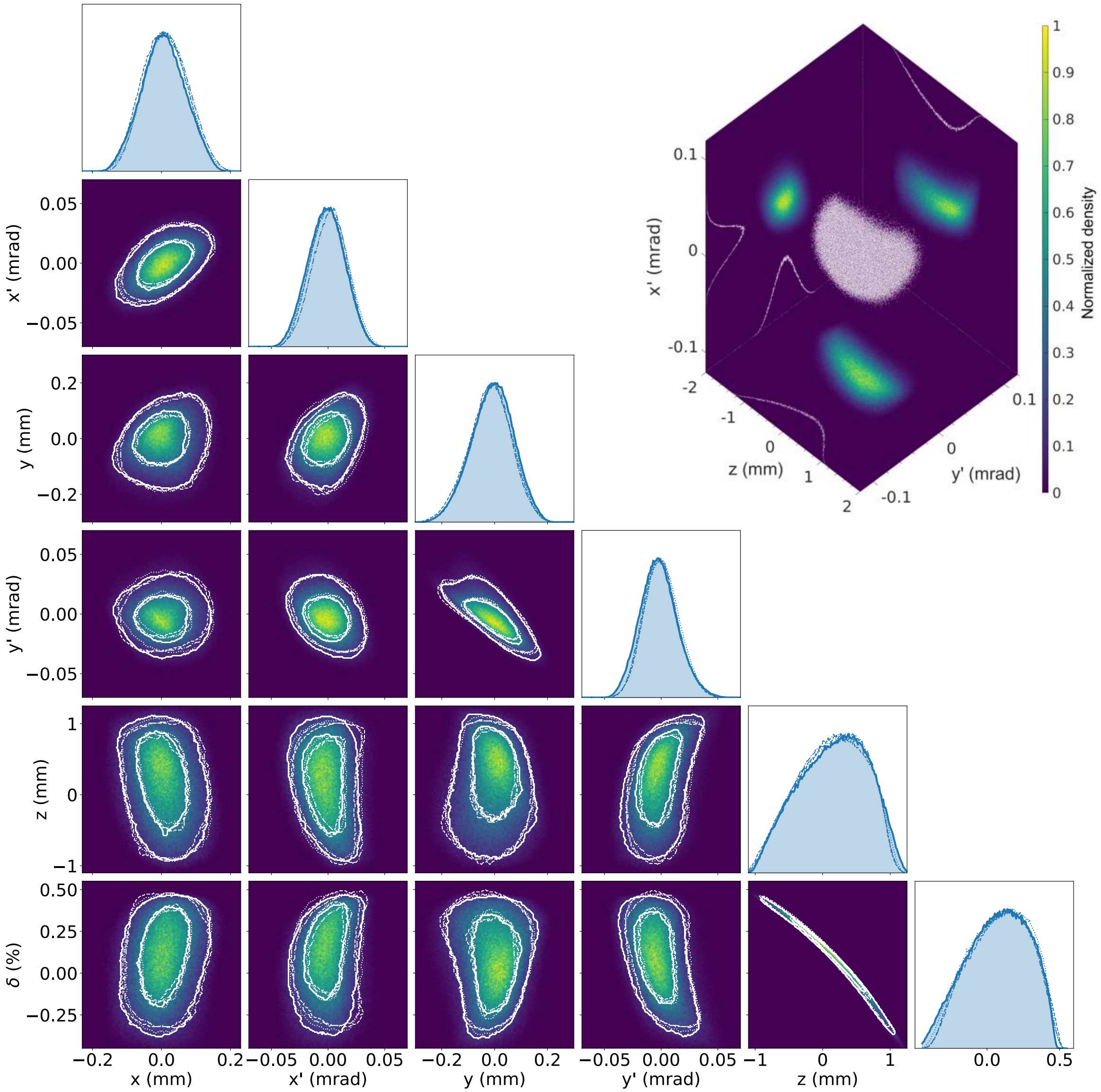
Measurements
Predictions



GPSR also successfully predicts independent downstream measurements!

Reconstructed phase space closely resembles true physical distribution

Reconstructed phase space @ Q1 entrance

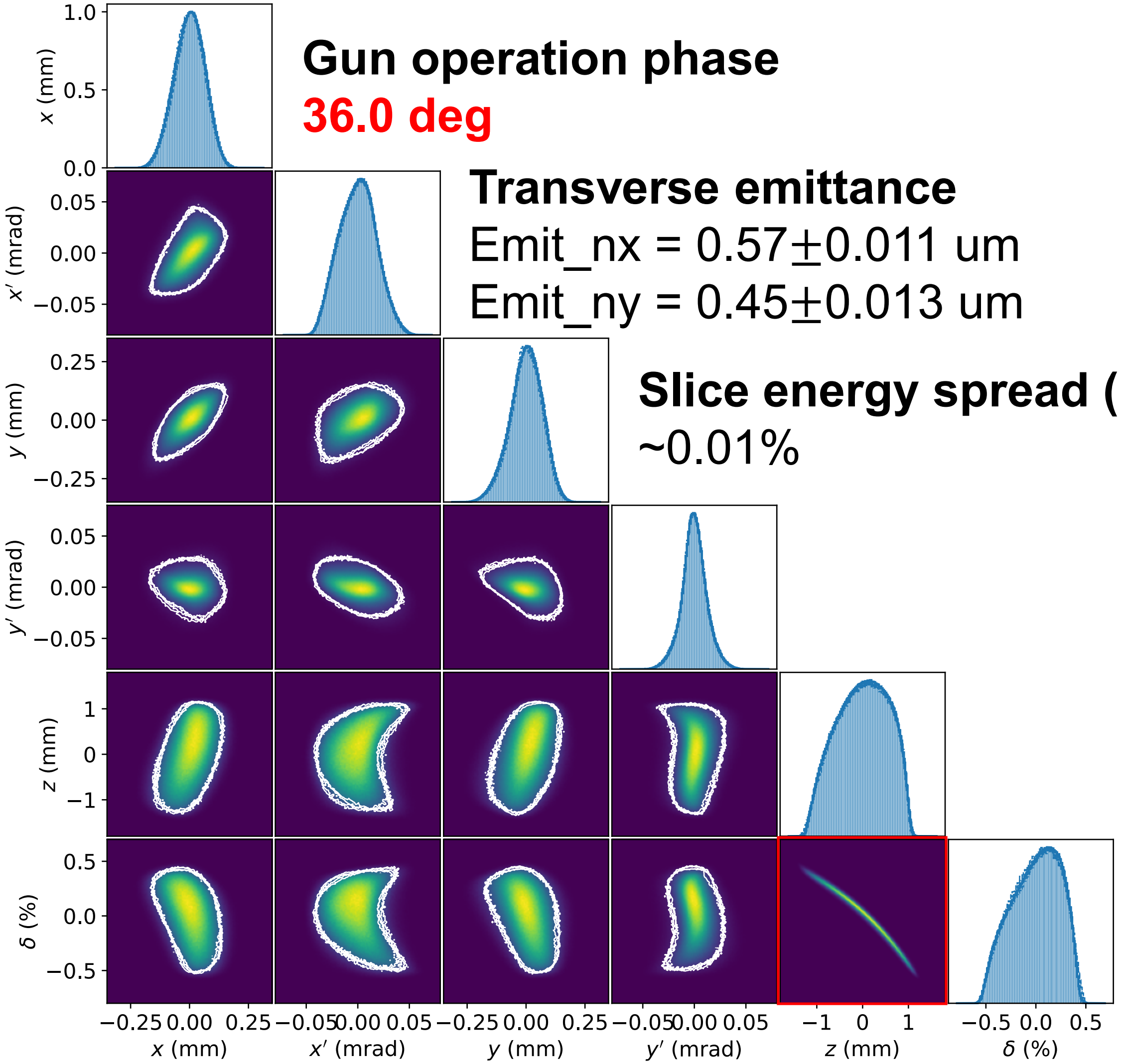


Parameters	4D Reconstruction	6D reconstruction
β_x (m)	4.59±0.08	4.51±0.07
β_y (m)	7.65±0.11	7.81±0.10
α_x (rad)	−0.55±0.02	−0.52±0.05
α_y (rad)	1.18±0.02	1.15±0.06
ε_{nx} (mm mrad)	0.43±0.01	0.43±0.01
ε_{ny} (mm mrad)	0.41±0.01	0.41±0.02

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_δ (%)	**0.24±0.01**	**0.22±0.00**
Slice σ_δ(%)		**0.01 (typical)**

POHANG ACCELERATOR LABORATORY

6D GPSR: 2026. 03 measurement*

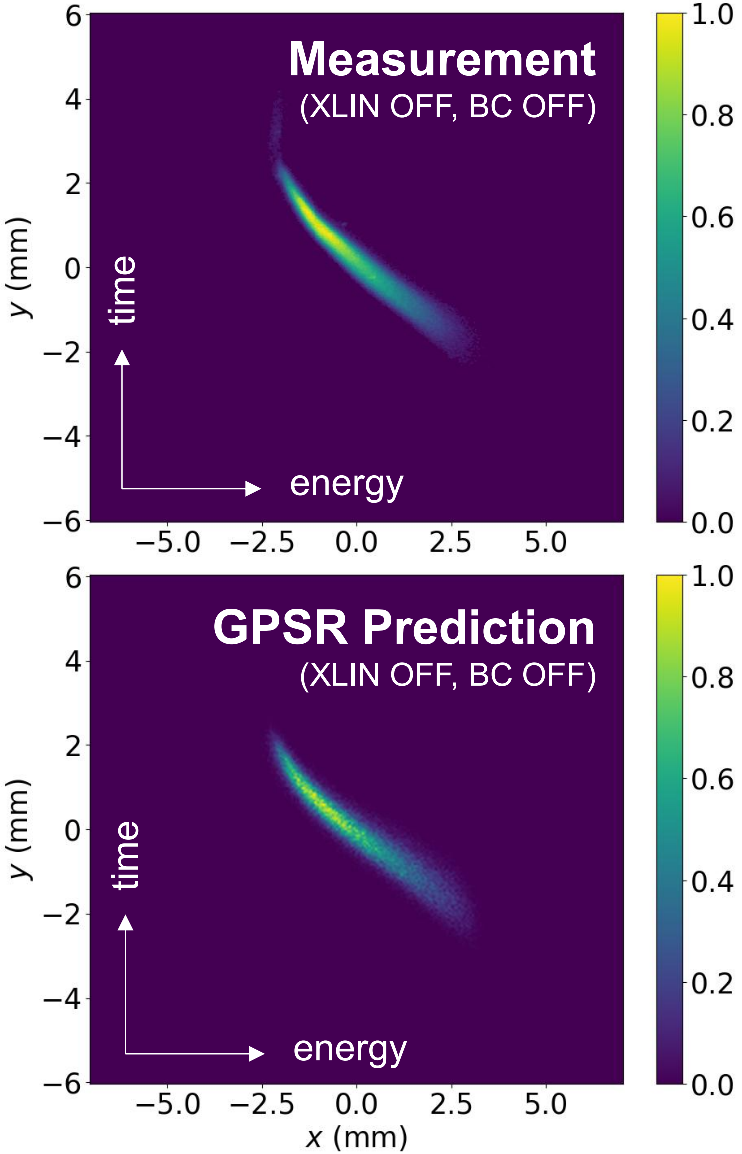


Gun operation phase
36.0 deg

Transverse emittance
Emit_nx = 0.57±0.011 um
Emit_ny = 0.45±0.013 um

Slice energy spread (RMS)
~0.01%

Longitudinal phase space: **(x,y) projection**

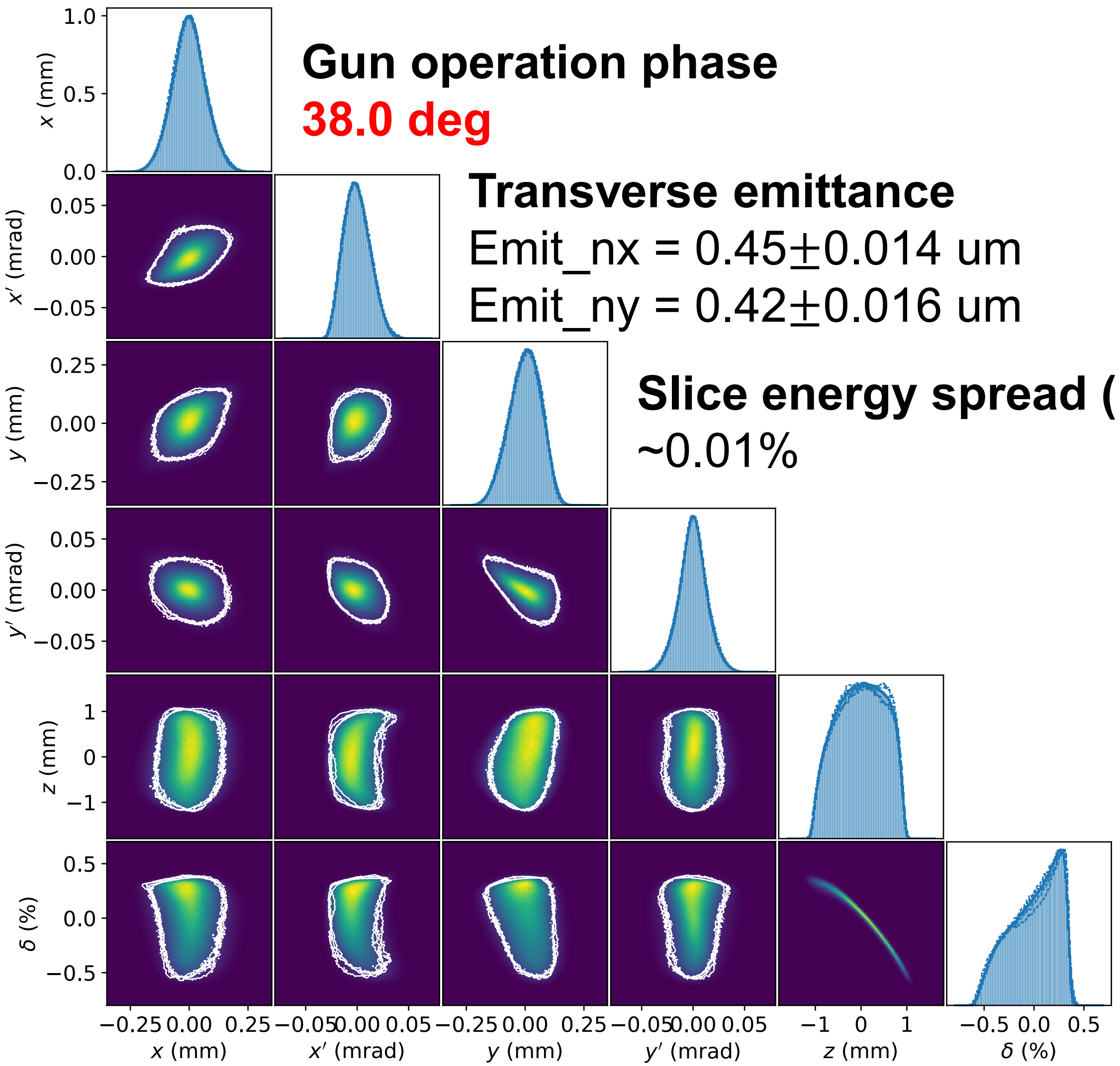


6D GPSR: 2026. 08 measurement*

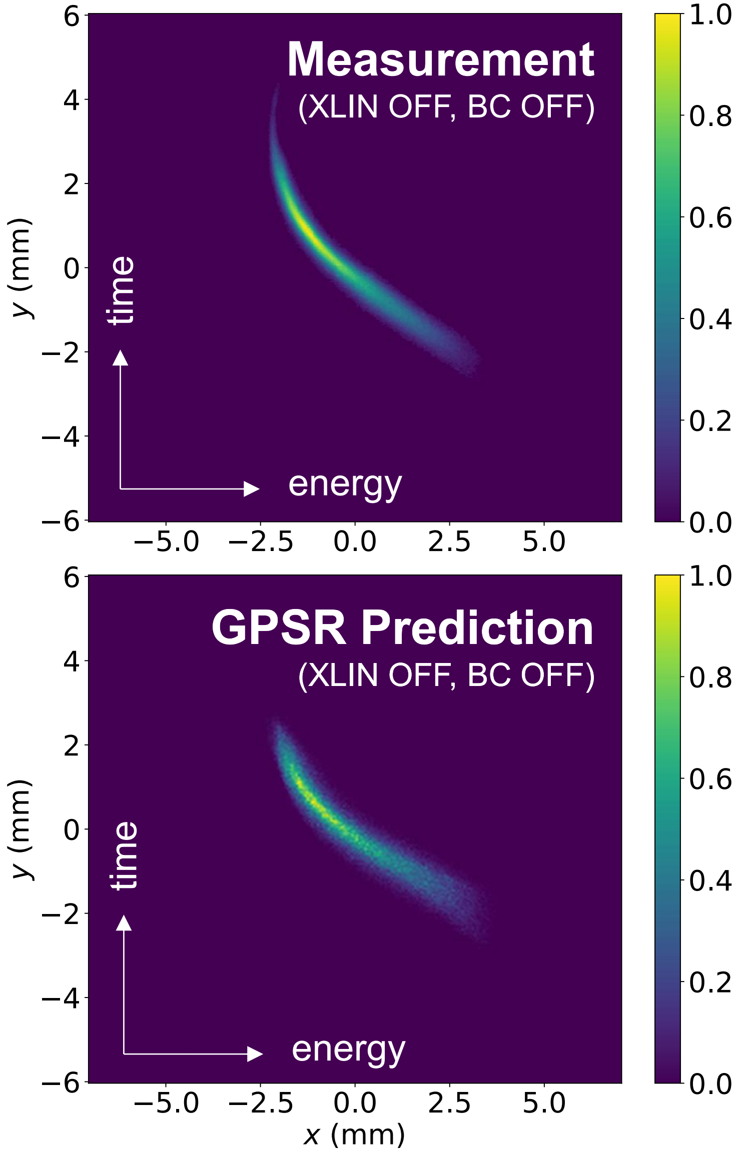
Gun operation phase
38.0 deg

Transverse emittance
Emit_nx = 0.45±0.014 um
Emit_ny = 0.42±0.016 um

Slice energy spread (RMS)
~0.01%



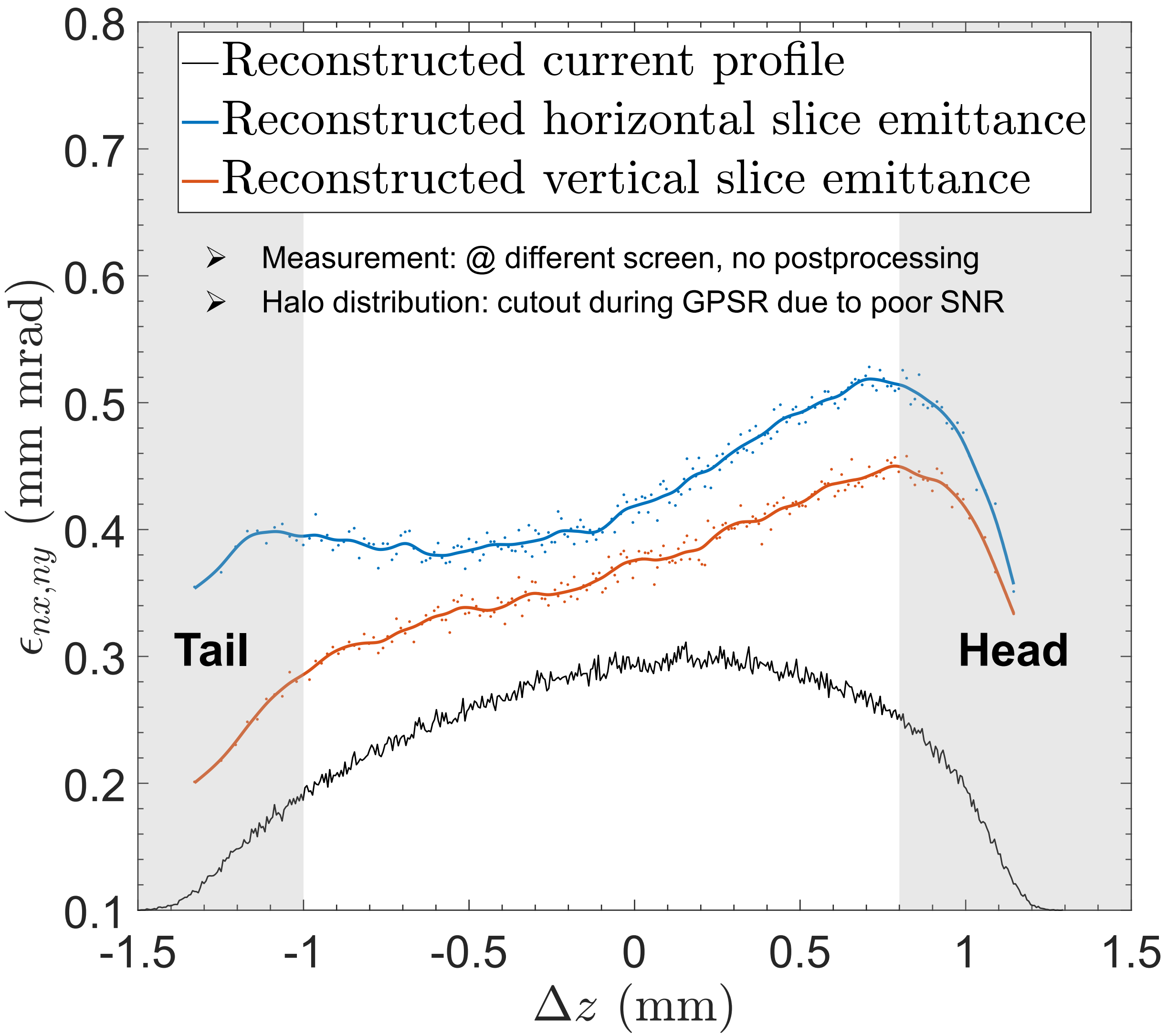
Longitudinal phase space: **(x,y) projection**



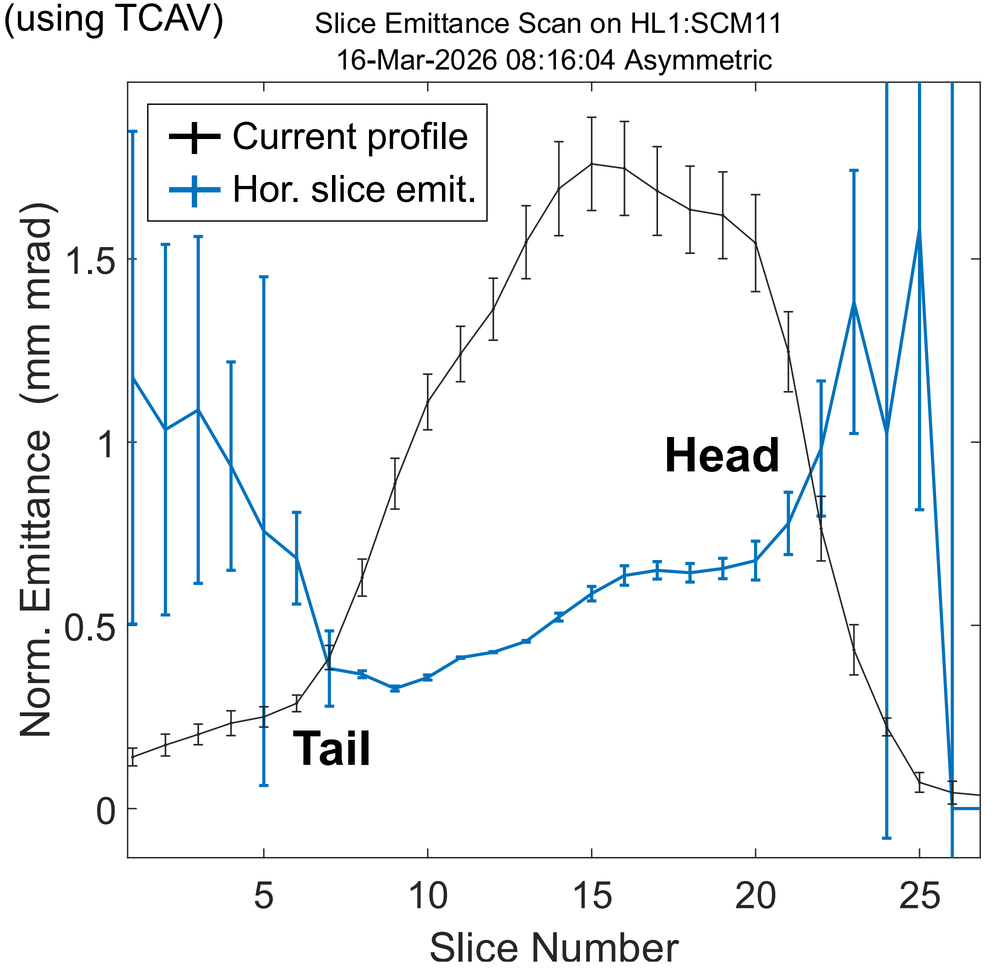
POHANG ACCELERATOR LABORATORY

6D GPSR: 2026. 03 measurement*

- Slice emittance

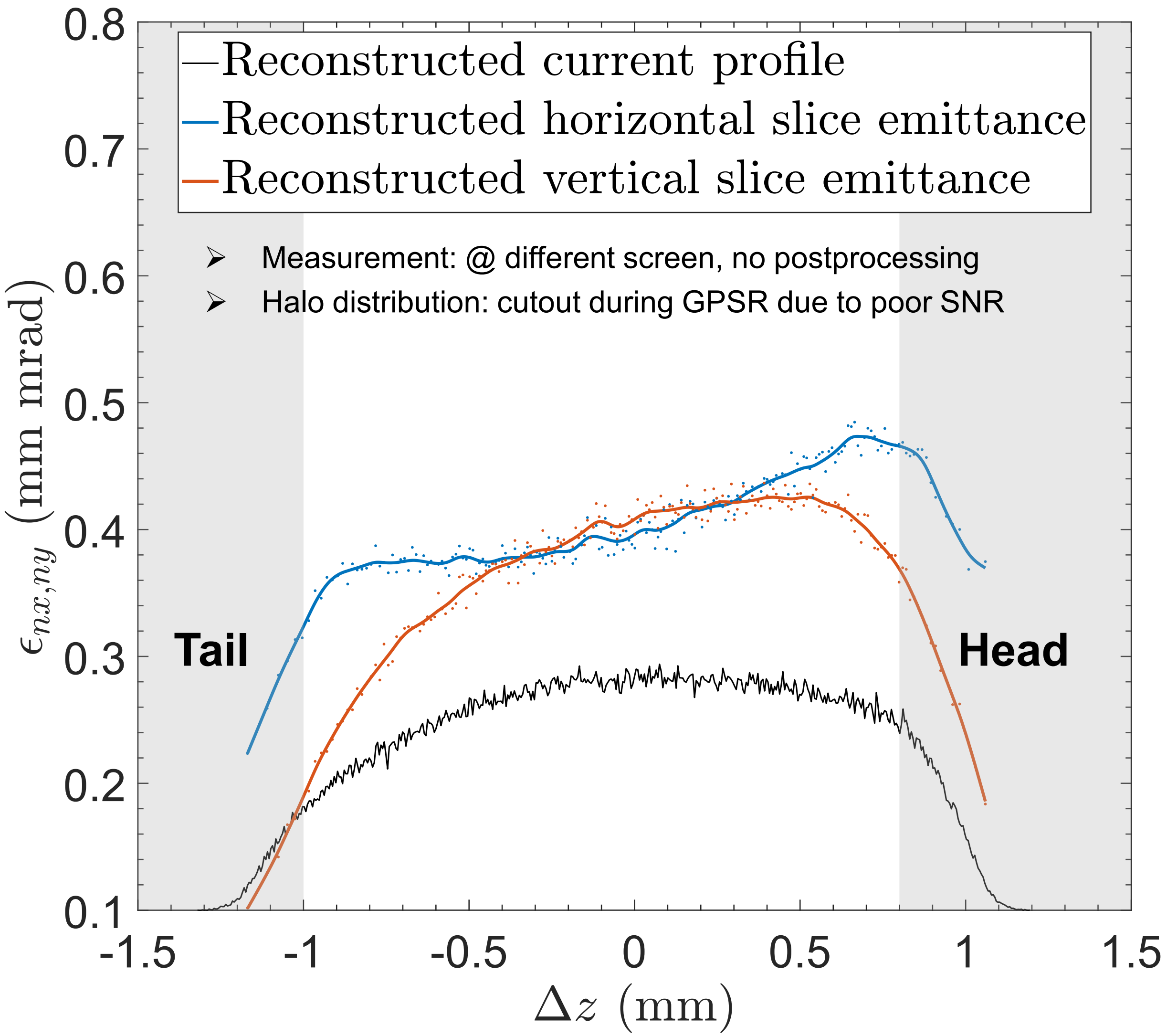


Conventional slice emittance measurement @ different screen (using TCAV)



6D GPSR: 2026. 08 measurement*

- Slice emittance

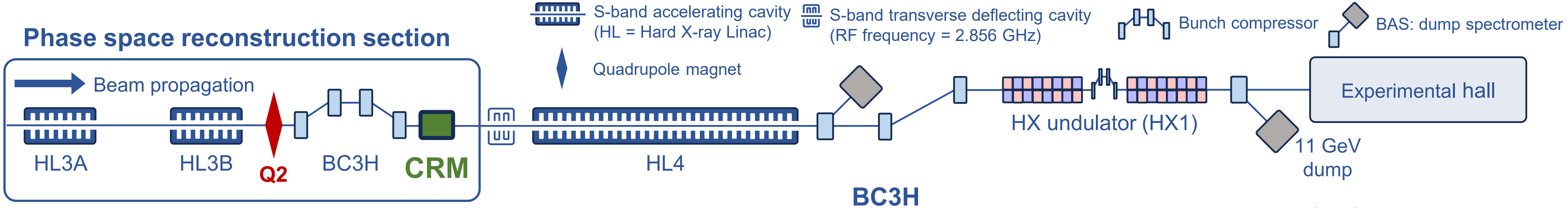


Detailed 6D phase space diagnostics to investigate current beam condition:

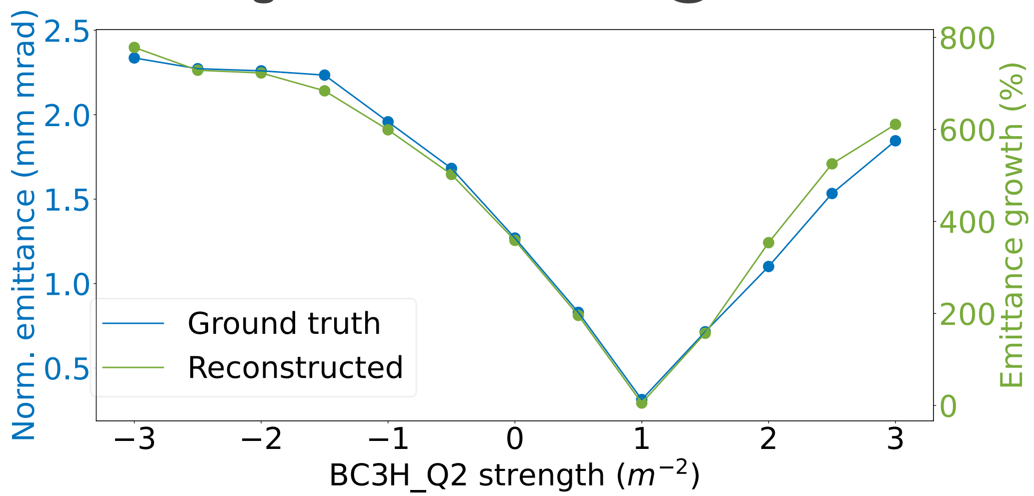
Routinely perform every March and August, before starting half-year user service @ PAL-XFEL

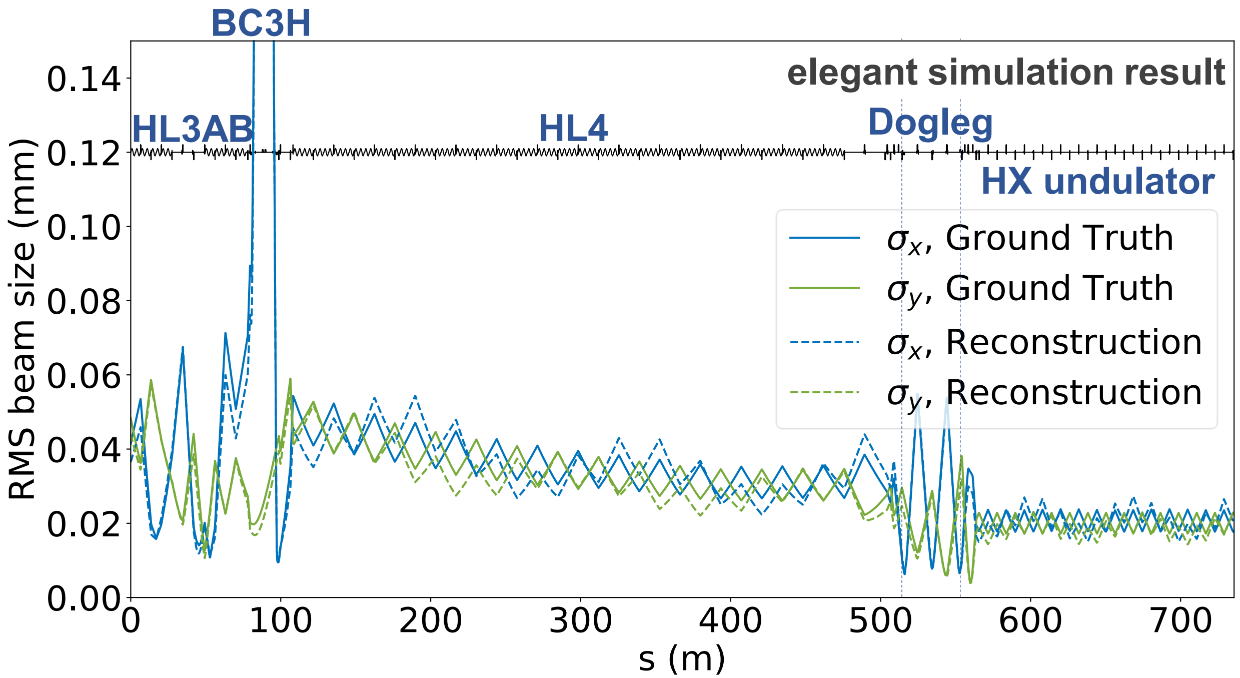
*For more information on the GPSR-based optimization:
S. Kim *et al.*, *In. Proc. ICALEPCS 2025*, Chicago, IL, USA, **MOCG004** (2025)

6D GPSR applications: optimizations*



GPSR + elegant: CSR effects @ BC3H chicane



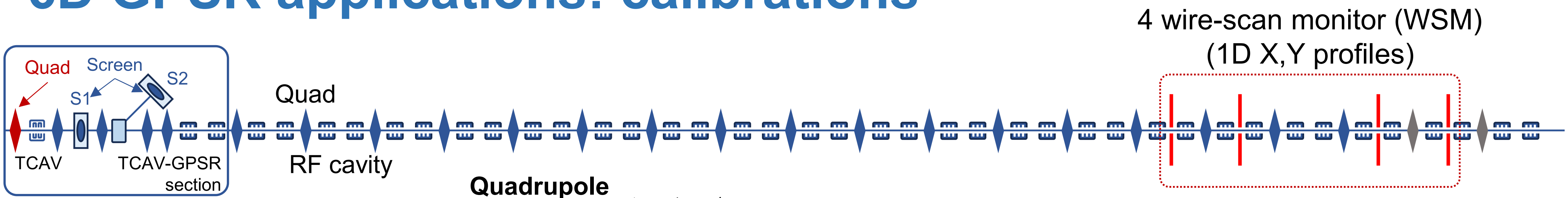


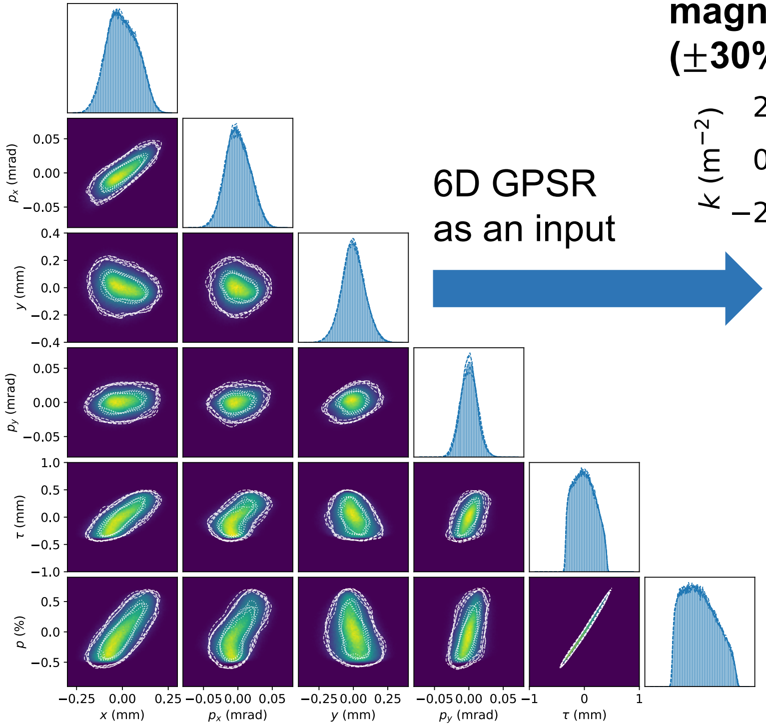
With the reconstructed phase space that resembles true physical distribution:

We can perform beamline optimization with high-fidelity simulations

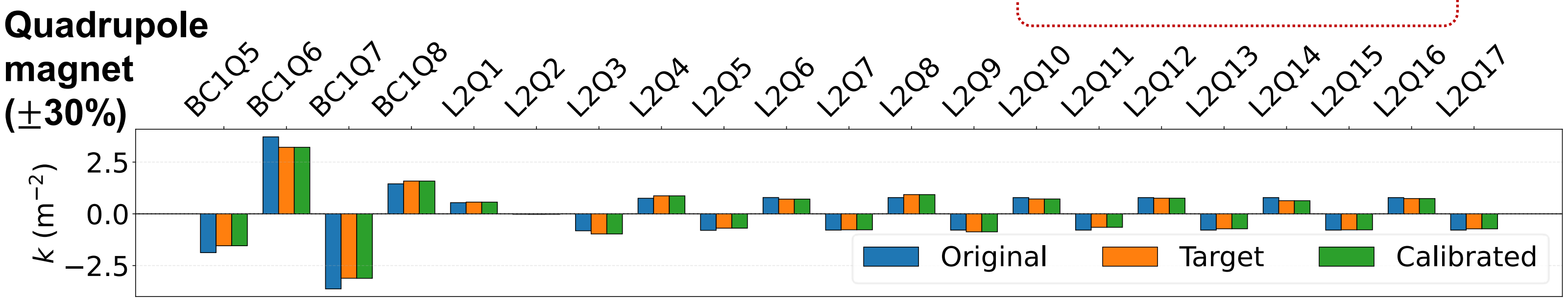
POHANG ACCELERATOR LABORATORY

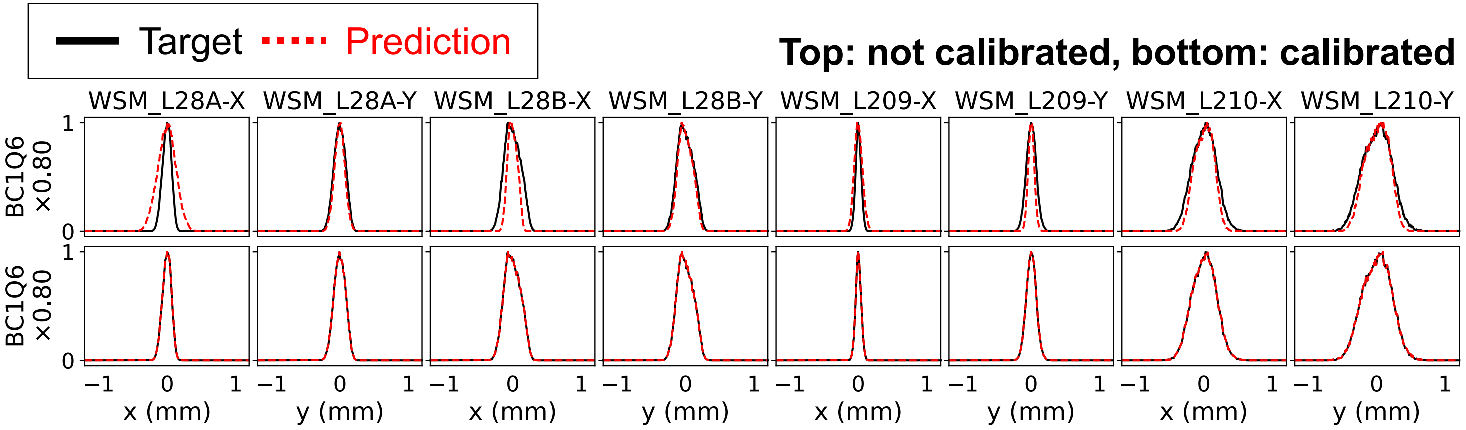
6D GPSR applications: calibrations





6D GPSR as an input



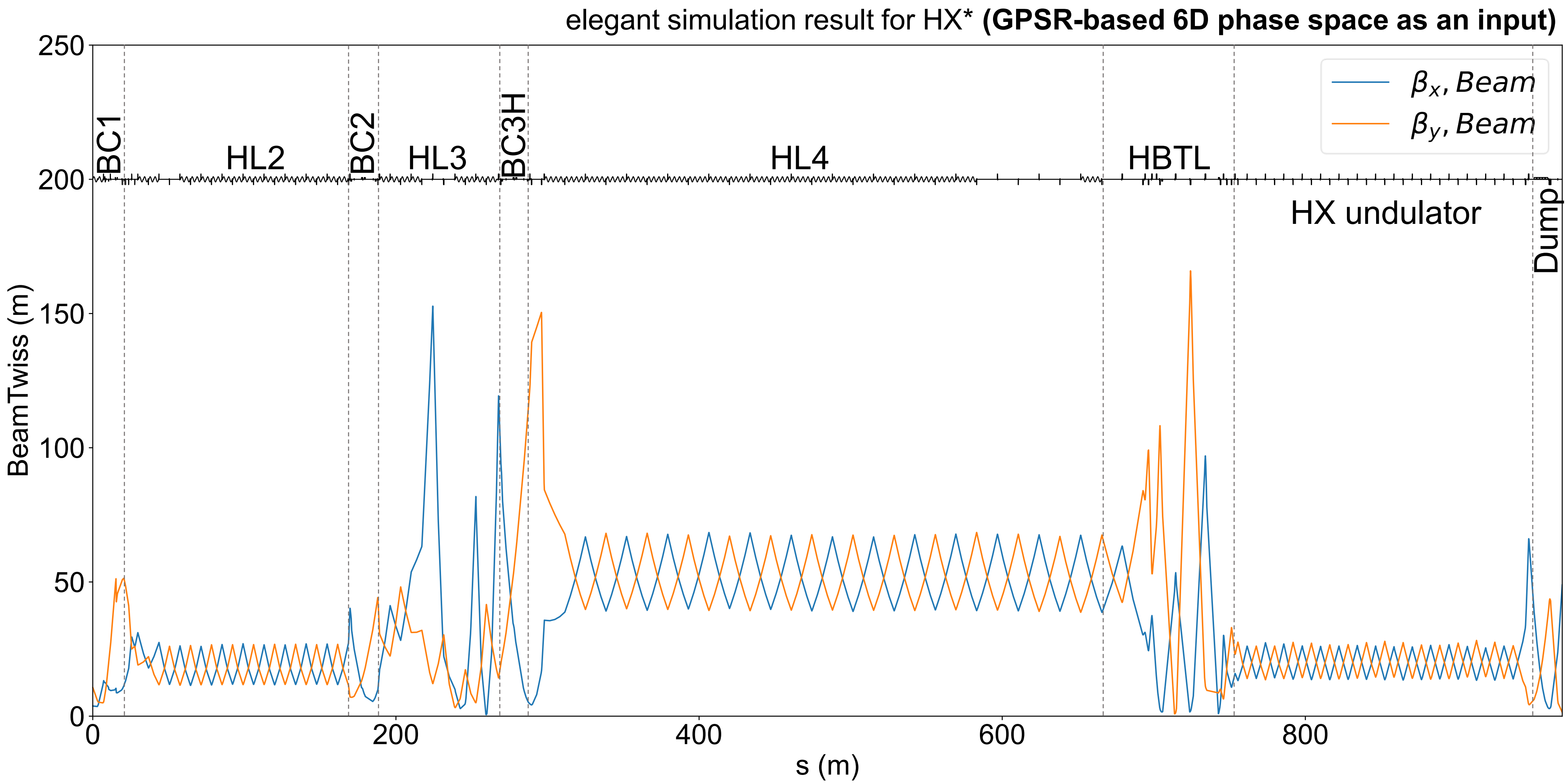


With the reconstructed phase space that resembles true physical distribution:

Model calibration is feasible (WEP037, today's poster session)

*PAL-XFEL hard X-ray (HX) beamline

Future direction: AI/ML-based accelerator operation



Detailed phase space diagnostics, calibration, and model-based optimization:

AI/ML-based operations will be feasible (pre-optimization, on-line virtual diagnostics, etc…)

POHANG ACCELERATOR LABORATORY

Summary and future works

- **GPSR-based phase space reconstruction was successfully demonstrated both at test and user facilities**
  - All the coupled phase spaces can be successfully predicted also for special beams
  - readily applicable using common elements such as RF cavity, quad, dipole, and screen
  - **Highlight: Reconstructed phase space closely resembles the true physical distribution**
  - Optimization of the beamline using 6D GPSR results, incorporated into physics simulations

- **On-going work and and near/long-term plans**
  - We are now conducting experimental demonstration of GPSR-based simulation model calibration (and integration of differentiable simulation + high-fidelity simulation)
  - Using the calibrated simulation model, we will perform beamline optimization to investigate optimal condition that maximizes FEL quality
  - Once we confirm that the GPSR-based calibrated model provides primary beam parameters within acceptable error range, it would be useful to develop a digital twin in a robust way (Also it would be useful as virtual diagnostics right next to the machine status monitors!)

Acknowledgements

포항가속기연구소 POHANG ACCELERATOR LABORATORY
POSTECH

Haeryong Yang
Myung-Hoon Cho
Kookjin Moon

Seongyeol Kim
Chi Hyun Shim
Hoon Heo

Gyujin Kim
Chang-Kyu Sung

SLAC NATIONAL ACCELERATOR LABORATORY

Auralee Edelen
Ryan Roussel

We also thank the PAL-XFEL accelerator control team members and Prof. Moses Chung of POSTECH

THE UNIVERSITY OF CHICAGO

Juan Pablo Gonzalez-Aguilera (now @ SLAC)
Young-Kee Kim

- This work was supported by the National Research Foundation of Korea (NRF) grant (2019R1I1A1A01041573, RS-2024-00347026, RS-2024-00455499), funded by the Korea government (MSIT).
- This work was also supported by the U.S. Department of Energy, Office of Science under Contract No. DE-AC02-06CH11357 and No. DE-AC02-76SF00515 and the Center for Bright Beams, NSF award PHY-1549132.
- This research used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility located at Lawrence Berkeley National Laboratory, operated under Contract No. DE-AC02-05CH11231 using NERSC award BES-ERCAP0020725.

Pohang Accelerator Laboratory

80 Jigokro-127-beongil,
Nam-gu, Pohang,
Gyeongbuk 37673, Republic of Korea

Email: sykim12@postech.ac.kr