HELMHOLTZ AI | ARTIFICIAL INTELLIGENCE COOPERATION UNIT

Towards a Data-driven Digital Twin of a Free Electron Laser

Anna Willmann

Hoffmann Lab
Institute of Radiation Physics
Helmholtz-Zentrum Dresden-Rossendorf

Hoffmann Lab: Helmholtz AI Young Investigator Group

AI for Photon Science

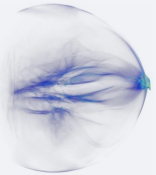
photon-ai-research.github.io

Digital twins of future laser-driven particle accelerators

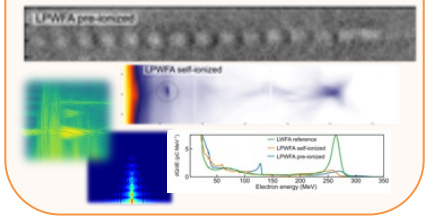
Surrogate modeling | ML-driven optimizer | Inverse Problems

Theory:
laser-plasma acceleration

$$\nabla \cdot \mathbf{D} = \rho$$
$$\nabla \cdot \mathbf{B} = 0$$
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$
$$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}$$



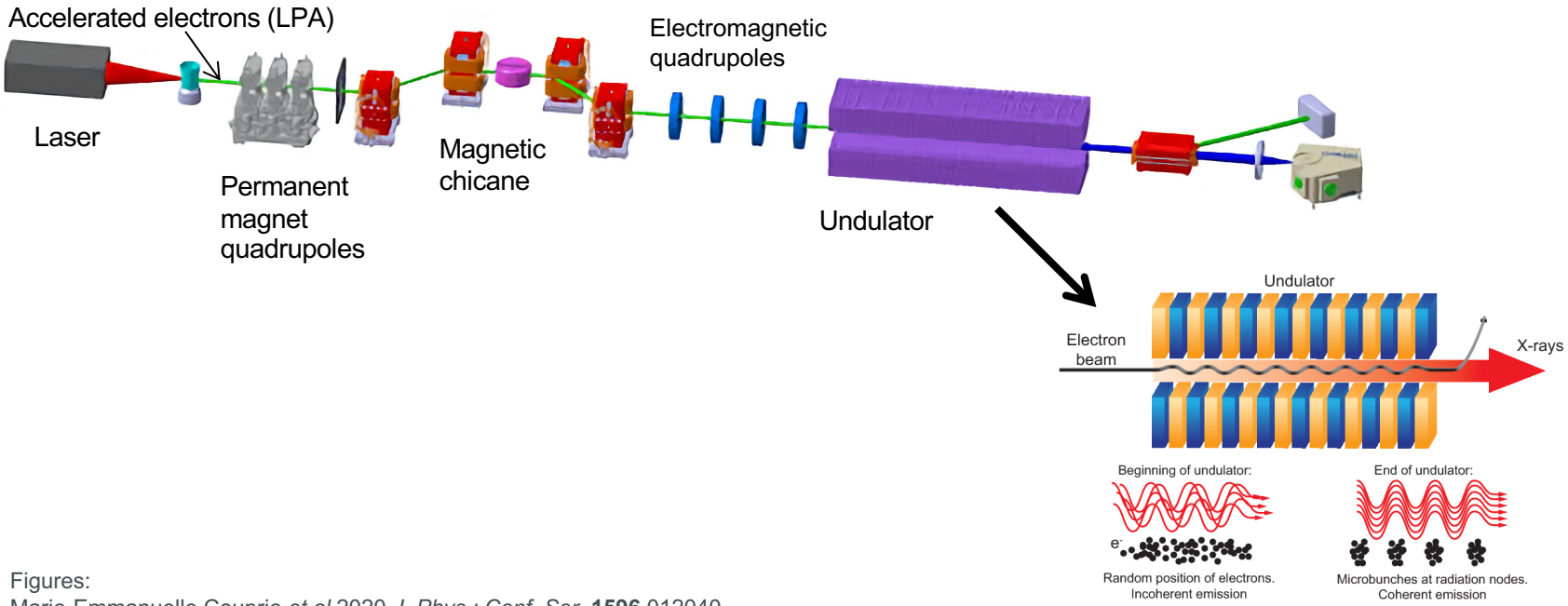
Experimental Data



Closing the loop between theory and experiment by researching data-driven digital twinning techniques

Free Electron Laser

Source of directional coherent X-rays with a short bandwidth and a high photon pulse.



Figures:
Marie-Emmanuelle Couprie *et al* 2020 *J. Phys.: Conf. Ser.* **1596** 012040
Nilsson, D. (2013). Zone Plates for Hard X-Ray Free-Electron Lasers.

Digital Twin of a Free Electron Laser

Motivation

- Unveil correlation LPA-paremeters to FEL radiation

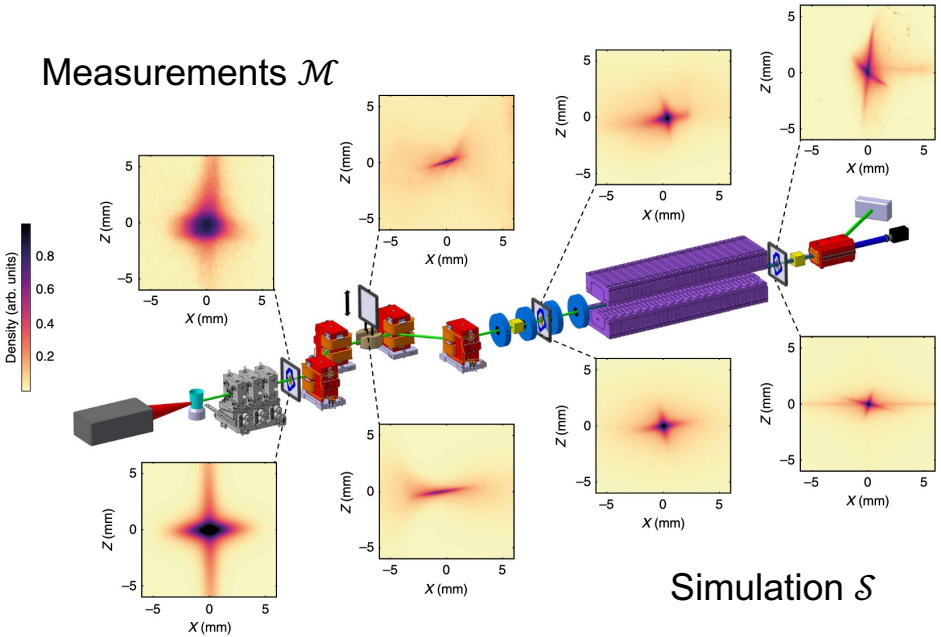


Figure:
André, T., et al. "Control of laser plasma accelerated electrons for light sources." *Nature communications* 9.1 (2018): 1-11.

Digital Twin of a Free Electron Laser

Motivation

- Unveil correlation LPA-paremeters to FEL radiation
- Fast and full inversion of the whole beamline from FEL radiation until LPA parameters

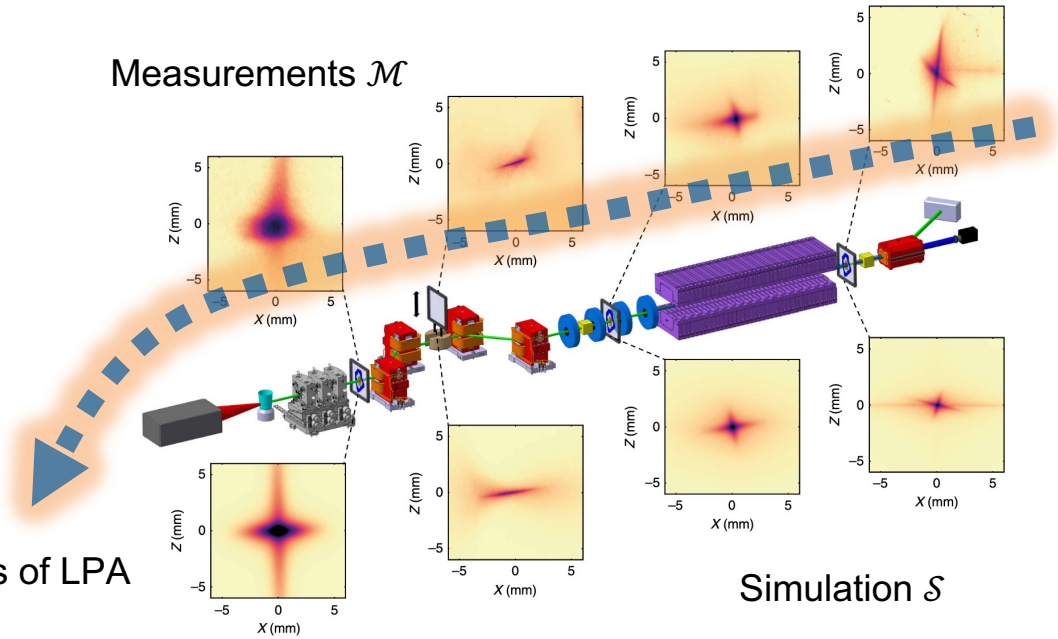


Figure:
André, T., et al. "Control of laser plasma accelerated electrons for light sources." *Nature communications* 9.1 (2018): 1-11.

Digital Twin of a Free Electron Laser

Inverse Problem

Surrogate Modeling | ML-driven optimizer | Inverse Problem

Inverse problem
extract the simulation parameters from diagnostic measurements

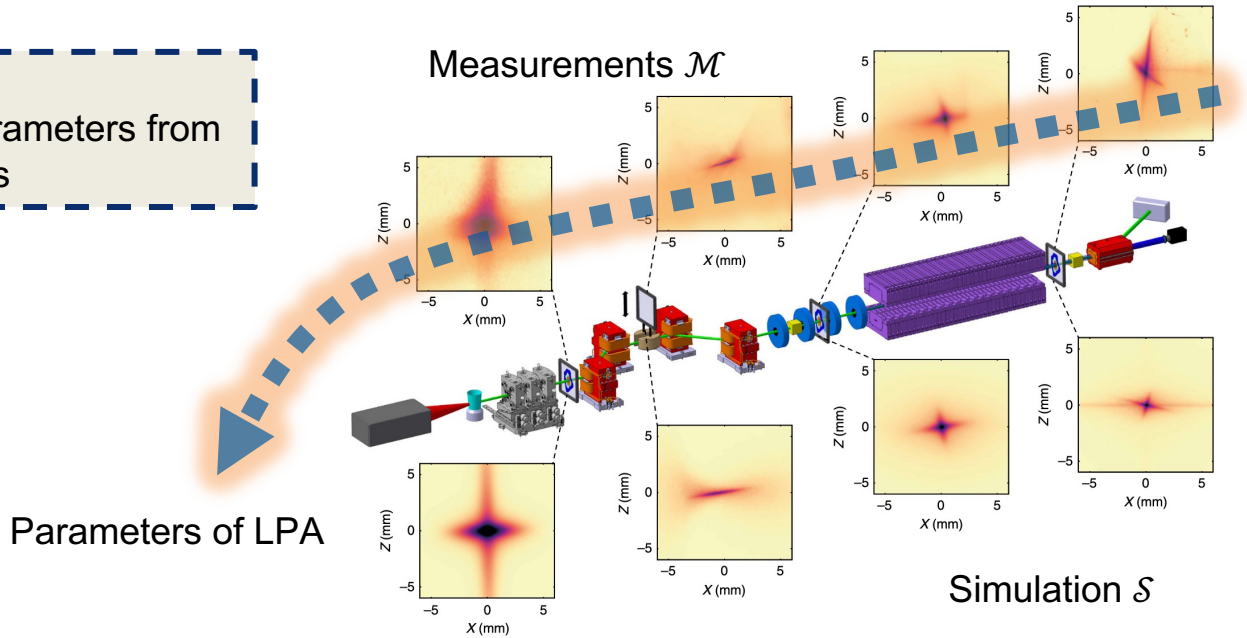


Figure:
André, T., et al. "Control of laser plasma accelerated electrons for light sources." *Nature communications* 9.1 (2018): 1-11.

Digital Twin of a Free Electron Laser

Inverse Problem

Inverse problem
extract the simulation parameters from diagnostic measurements

$$\boldsymbol{p}^*_{LPA} = argmin_{\boldsymbol{p}_{LPA}}\, dist(\mathcal{M}, \mathcal{S}(\boldsymbol{p}_{LPA}))$$

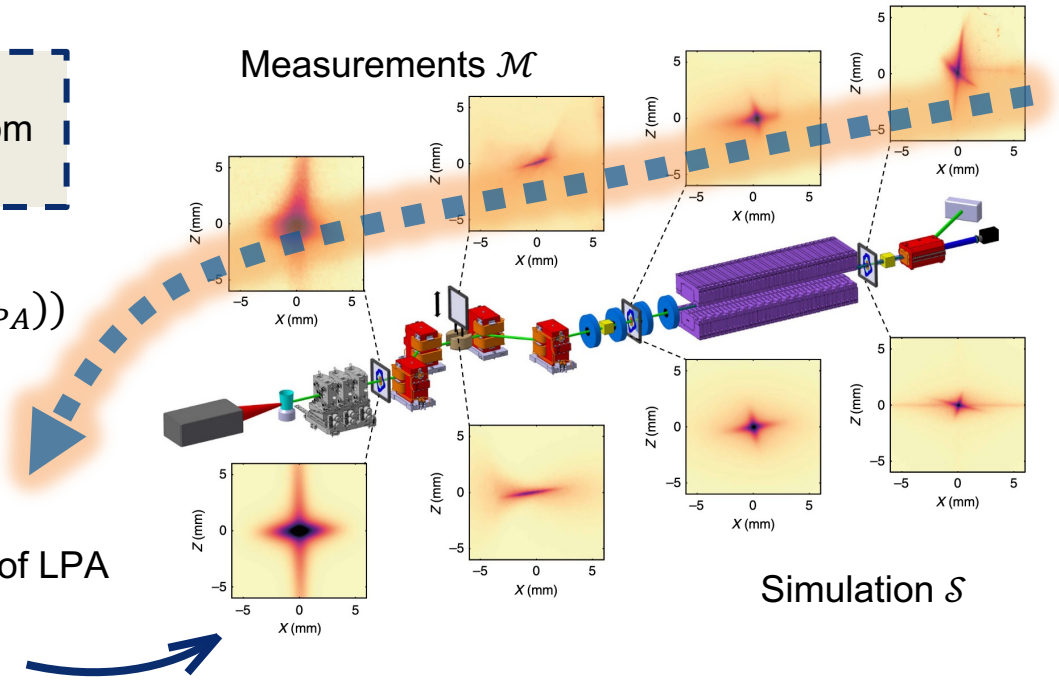


Figure:
André, T., et al. "Control of laser plasma accelerated electrons for light sources." *Nature communications* 9.1 (2018): 1-11.

Solution to Inverse Problem

Optimizer

Surrogate modeling | ML-driven optimizer | Inverse Problem

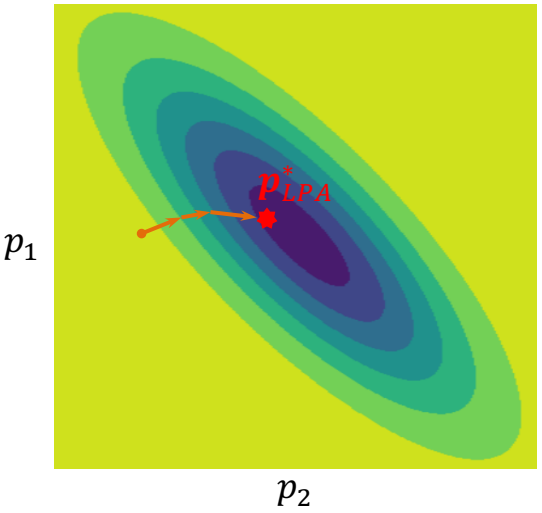
Optimization problem:

$$\boldsymbol{p}^*_{LPA} = argmin_{\boldsymbol{p}_{LPA}}\, dist(\mathcal{M}, \mathcal{S}(\boldsymbol{p}_{LPA}))$$

Each step of optimizer requires computation of $\mathcal{S}(\boldsymbol{p}_{LPA})$

⇒ ML-based Surrogate Model $\tilde{\mathcal{S}}$ for fast forward pass

Gradient Descend



Surrogate Modeling

Surrogate modeling | ML-driven optimizer | Inverse Problem

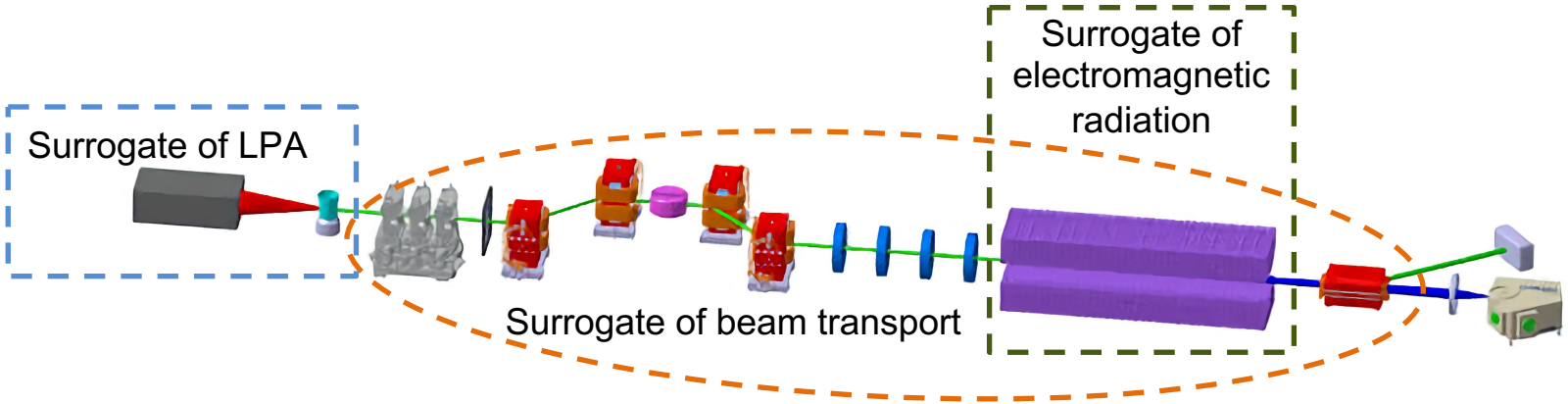


Figure:
Marie-Emmanuelle Couprie *et al* 2020 *J. Phys.: Conf. Ser.* **1596** 012040

Surrogate Modeling

Surrogate modeling | ML-driven optimizer | Inverse Problem

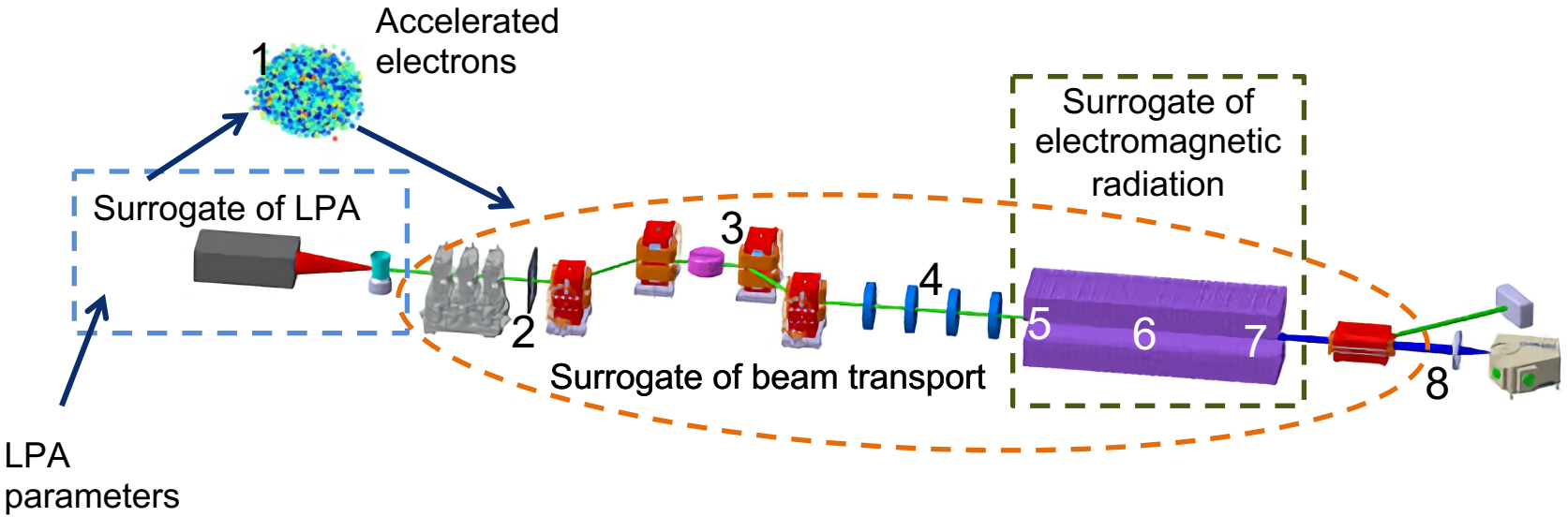


Figure:
Marie-Emmanuelle Couprie *et al* 2020 *J. Phys.: Conf. Ser.* **1596** 012040

Surrogate Model of Electron Beam Transport

Surrogate modeling | ML-driven optimizer | Inverse Problem

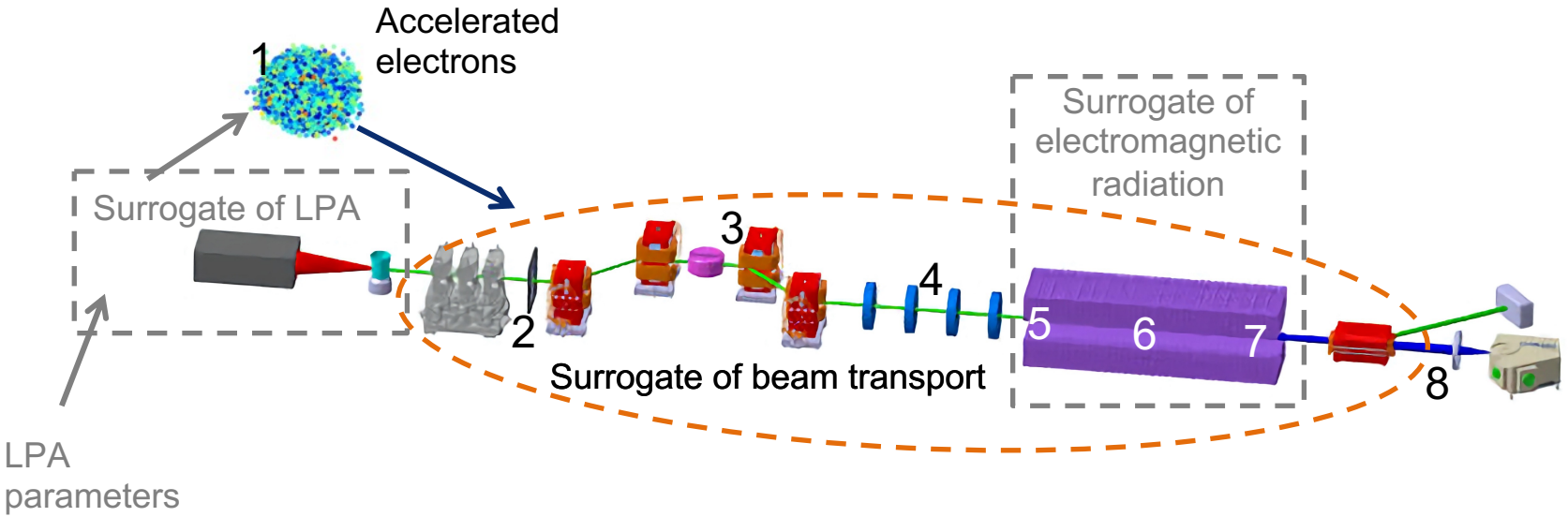


Figure:
Marie-Emmanuelle Couprie *et al* 2020 *J. Phys.: Conf. Ser.* **1596** 012040

Surrogate Model of Electron Beam Transport

Given:
parameters of accelerated electron beam after LPA – emmitance and beta

Approximate:
phase space representation of electron beam at defined positions in the transport line

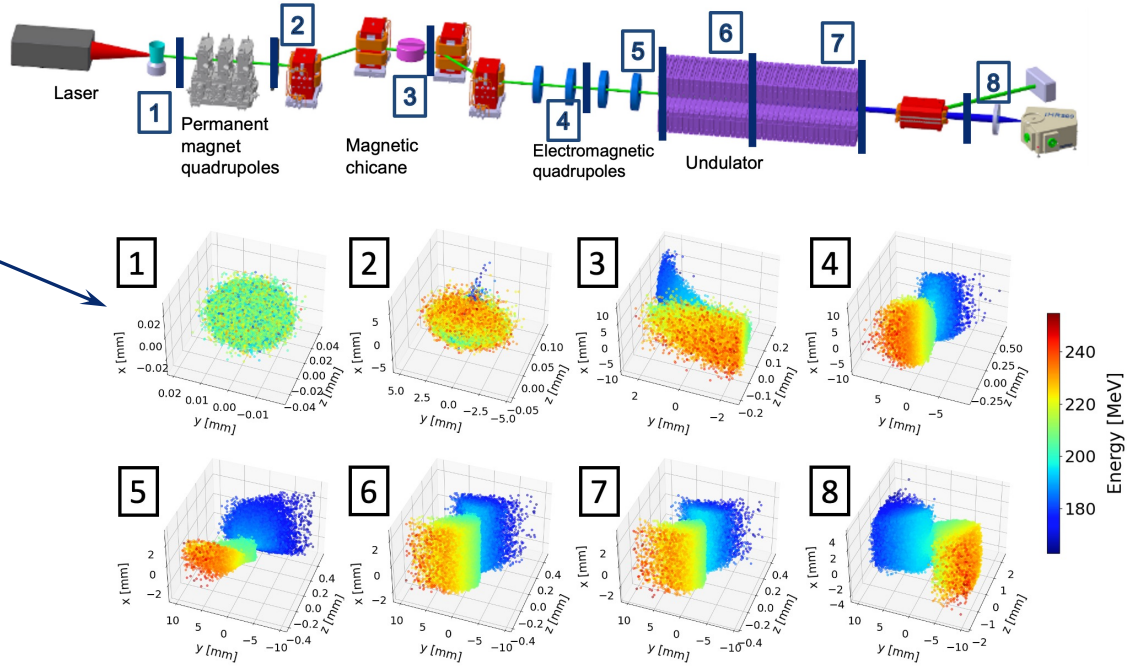


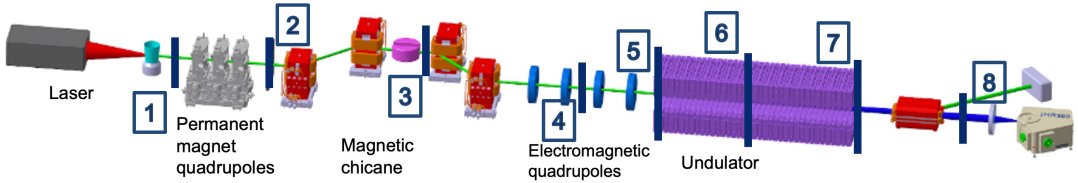
Figure:
Marie-Emmanuelle Couprie *et al* 2020 *J. Phys.: Conf. Ser.* **1596** 012040

Surrogate Model of Electron Beam Transport

Challenge

- Tracking of each particle is not required
- Electron cloud is given by a distribution of electrons

=> Flexible sampling from any electron cloud



Phase space representation is processed as point cloud

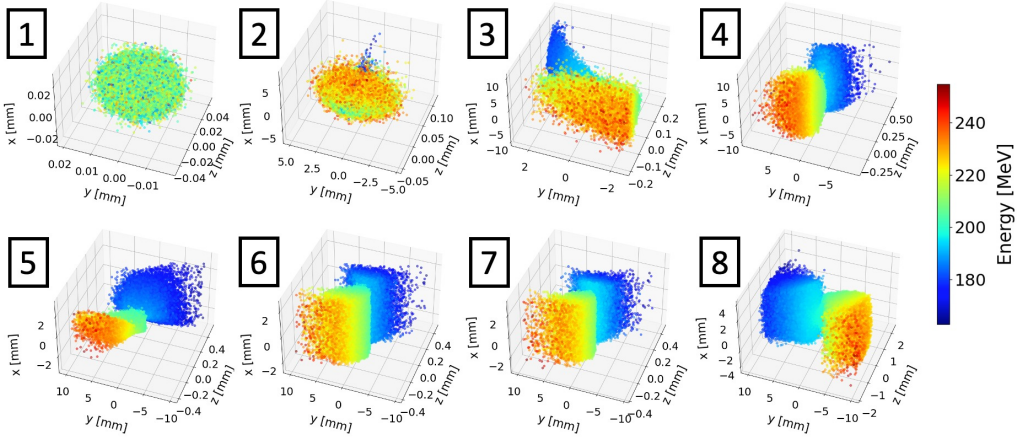


Figure:
Marie-Emmanuelle Couprie *et al* 2020 *J. Phys.: Conf. Ser.* **1596** 012040

Surrogate Model of Electron Beam Transport

Generative Model: Normalizing Flows

Goal

Take samples from **a normal distribution** and transform them into **distribution of electrons**

Approach

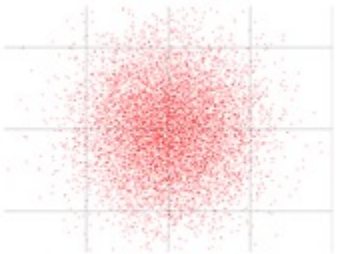
f is **invertible neural network**

$g = f^{-1}$ is differentiable

Change of variable formula

$$p_X(x) = p_Z(f(x)) \left| det \frac{\partial f(x)}{\partial x^T} \right|$$

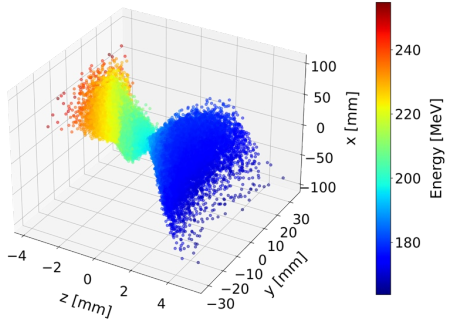
$p_Z(z)$



$x = g(z, \boldsymbol{p})$

$z = f(x, \boldsymbol{p})$

$p_X(x)$

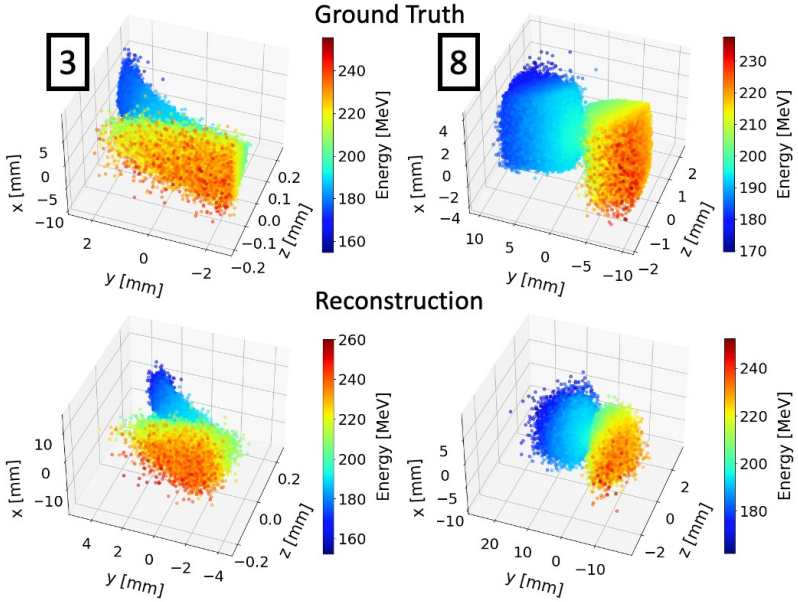


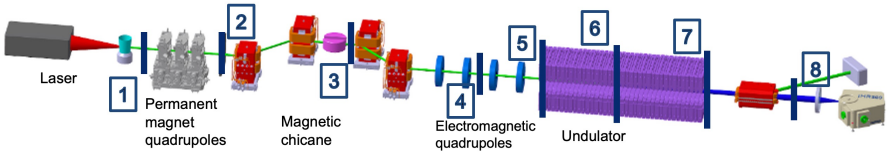
$\boldsymbol{p}$ – parameters of an initial electron bunch

Ardizzone, Lynton, et al. "Guided image generation with conditional invertible neural networks." *arXiv preprint arXiv:1907.02392* (2019).

Surrogate Model of Electron Beam Transport

Results: Testing Data



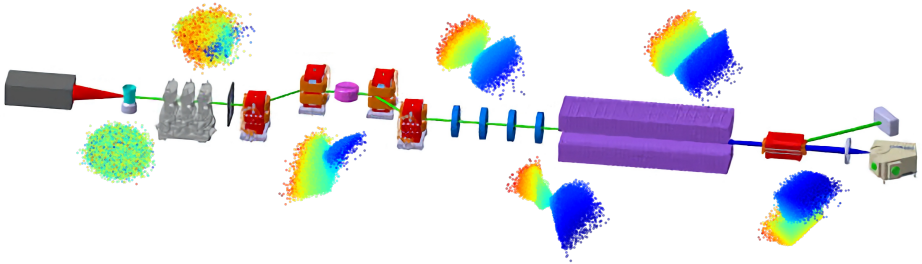


- Model is able to recognize different screens and reconstruct a shape of distribution
- Flexible inference w.r.t. number of electrons
- Easy to adjust to another setting of a beamline (only new training data required)

Figure:
Marie-Emmanuelle Couprie *et al* 2020 *J. Phys.: Conf. Ser.* **1596** 012040

Summary

Digital Twin is foundation for autonomous operation/tuning of accelerators and beamlines

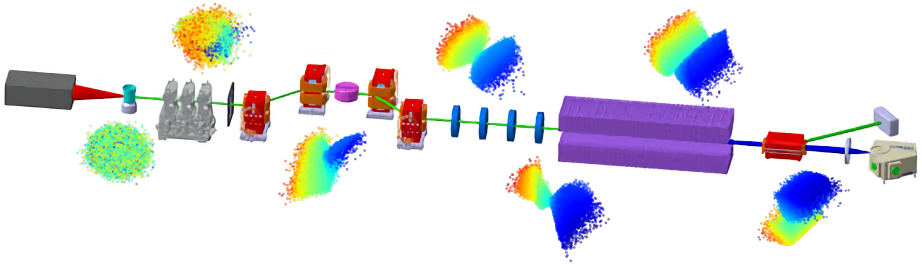


Surrogate model is able to produce electron clouds along a beamline

Summary

Digital Twin is foundation for autonomous operation/tuning of accelerators and beamlines

Surrogate modeling | ML-driven optimizer | Inverse Problems



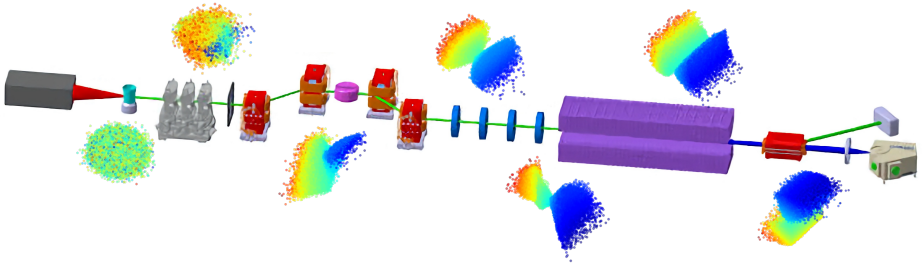
Surrogate model is able to produce electron clouds along a beamline

Electron clouds can be mapped to experimental data by integration of another surrogate models and an optimizer

Summary

Digital Twin is foundation for autonomous operation/tuning of accelerators and beamlines

Surrogate modeling | ML-driven optimizer | Inverse Problems



Surrogate model is able to produce electron clouds along a beamline

Electron clouds can be mapped to experimental data by integration of another surrogate models and an optimizer

Simple development of further surrogate models based on normalizing flows to solve inverse problems:

library NF4IP

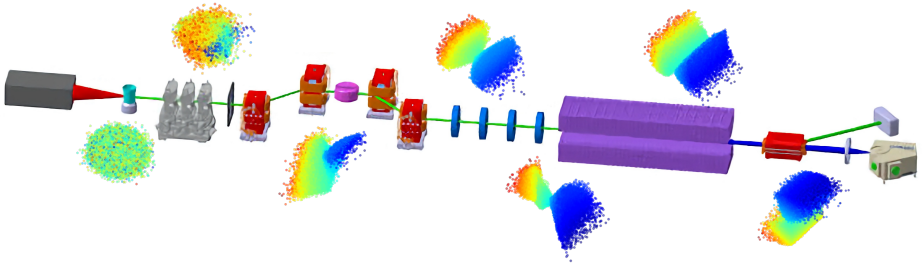
https://github.com/Photon-AI-Research/NF4IP

Summary

Thank you for your attention!

Digital Twin is foundation for autonomous operation/tuning of accelerators and beamlines

Surrogate modeling | ML-driven optimizer | Inverse Problems



Surrogate model is able to produce electron clouds along a beamline

Electron clouds can be mapped to experimental data by integration of another surrogate models and an optimizer

Simple development of further surrogate models based on normalizing flows to solve inverse problems:

library NF4IP

https://github.com/Photon-AI-Research/NF4IP