Machine-learning Driven Beamline Alignment at EuXFEL

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Abstract

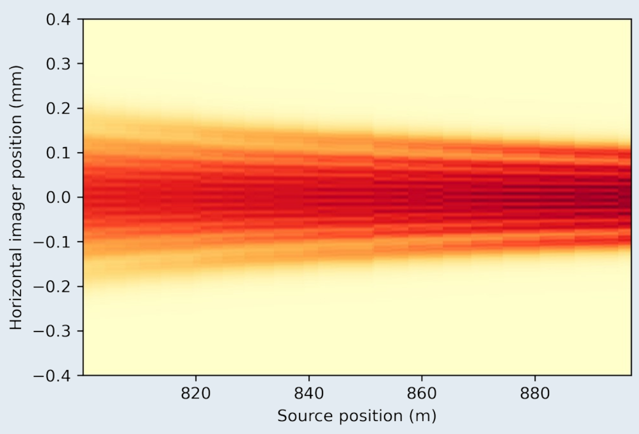
EuXFEL is a large scale laser facility which operates seven different instruments and the eighth is coming into operation now. All the instruments have a few hundred meters multi-component optical setups, which includes grazing incidence offset mirrors and focusing elements, such as CRL or KB mirrors. To increase efficiency of operation, automation of the beamline alignment procedure has a great importance to deliver the XFEL radiation with its unique properties to the experiment.
At EuXFEL the SiMEX platform [1] for simulating FEL experiments was developed and operated. Here we present an extended approach, in which a Convolutional Neural Network (CNN) model is trained with beam-profile simulations extracted from FEL simulations [2] in combination with the wave-front propagation package (WPG) [3]. The CNN model is used to estimate the beamline parameters, which we demonstrate here with a proof-of-principle application varying the source position in the simulations. Furthermore, we show that data taken at a newly commissioned soft x-ray beamline at EuXFEL agrees well with the WPG predictions.

Motivation

* State-of-the art simulation codes for the beam propagation through hard and soft x-ray beamlines can make accurate prediction of the wave front and intensity profile, but for a direct feedback to the instrument alignment, these calculations are too expensive
* Machine-learning tools might be suited to perform highly non-linear regression on image data training sets to reconstruct the alignment parameters of a measured image on an imager screen and subsequently identify the parameters that need to be optimized

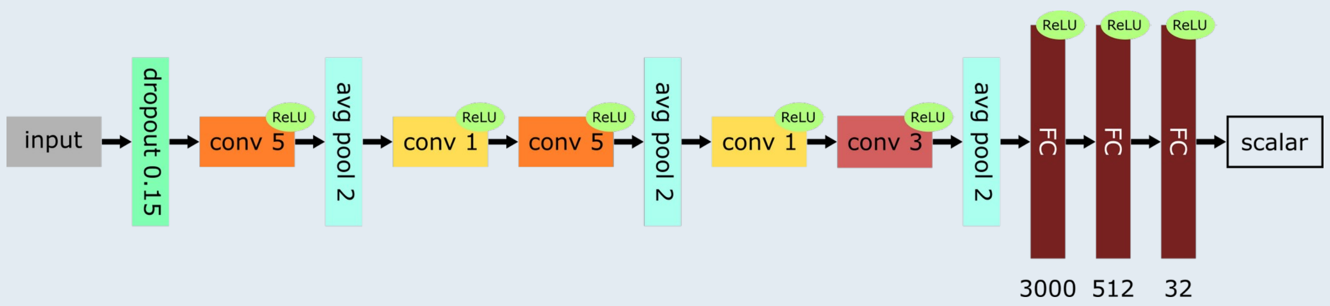
WPG Simulations

* First set of simulations with minimal optical setup: one horizontal offset mirror, one aperture, and one imager screen
* Source position in the undulator section is varied between 800 and 900 m
* Photon energy: 8.5 keV
* The x projections of the simulated beam profiles show a clear change in size and diffraction pattern from clipping on the aperture



Machine-learning Model

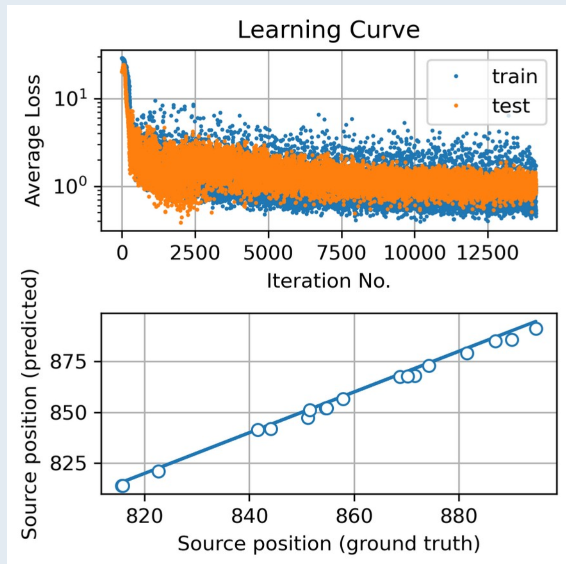
* Standard convolutional architecture, similar to the famous LeNet net [4], with a total of 5 convolutional layers and three fully connected layers
* At the moment x projections are used as one-dimensional input, but extension to 2D image data is straightforward
* Dropout is used for regularization, together with data augmentation, which involve spatially shifting the input data, intensity scaling, and additive Poissonian noise



* We observe that for regression, batch normalization layers should be avoided and that average pooling is superior to max pooling

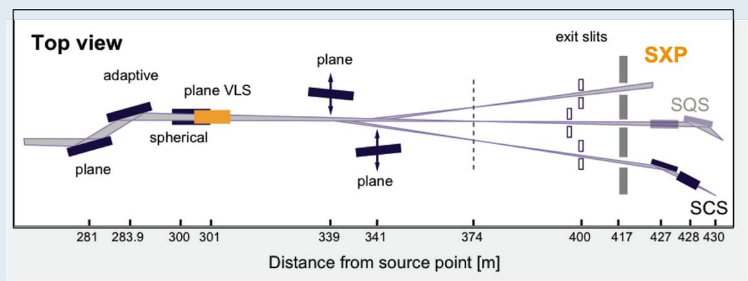
Numerical Results: Fitting of Source Position

* Training with Adam optimizer and a learning rate of 1E-4 results in good convergence
* Average absolute error in source position is ~1m
* First training data set had 70 images, training will be repeated with 100 images and in 2D

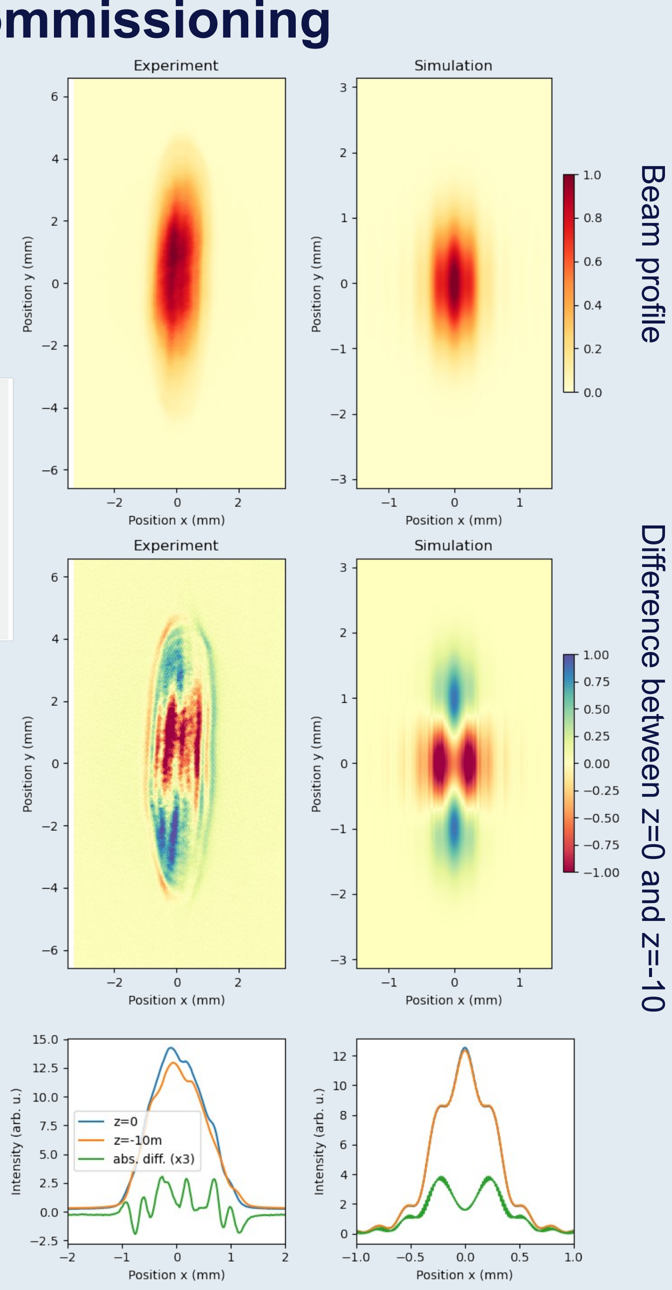


First Measurements: SXP Commissioning

* New soft x-ray beamline SXP was recently commissioned at EuXFEL
* Source position was varied in the undulator by ~10m through opening two downstream undulator segments



* Optical components: three steering mirrors, one imager at exit slit
* Photon energy: 900 eV
* Qualitatively, the change in beam profile for increased source position is reproduced by the WPG simulations
* Simulations indicate that the sensitivity of the beam profile to the source position is less pronounced for longer wavelengths; therefore we expect more pronounced effects at the hard x-ray beamlines of EuXFEL and/or at alignment of focusing KB mirrors.



Summary / Outlook

* Successful prediction of source positions from set of imager data simulated with WPG using a CNN
* Promising imager data collected at beamline; with a more complete data set, the CNN can be trained on the experimental data directly

References

1. https://github.com/PaNOSC-ViNYL/SimEx
2. AIP Conference Proceedings 2054, 030019 (2019)
3. Journal of Applied Crystallography 08/2016; 49(4) pp.1347-1355. doi:10.1107/S160057671600995X, https://github.com/samoylv/WPG
4. Lecun, Y.; Bottou, L.; Bengio, Y.; Haffner, P. (1998). Proc. IEEE. 86 (11): 2278–2324. doi:10.1109/5.726791.

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