XFEL Accelerator R&D Status
Virtual Diagnostics

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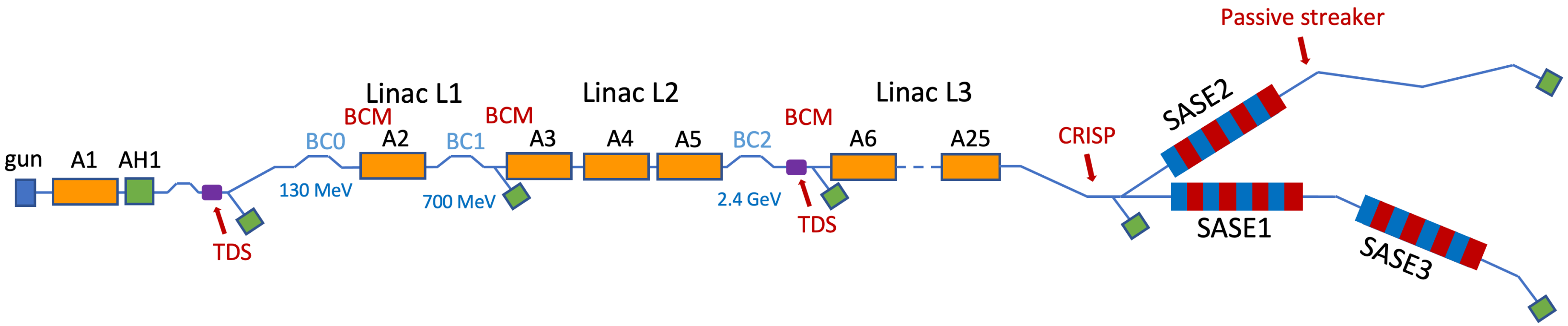
Scope of the R&D activity

- Longitudinal Phase Space (LPS) diagnostics are vital for operations and fundamental for advanced XFEL modes.
- Currently, 2 transverse deflecting structures (TDS) (destructive, low resolution). CRISP non-destructive but requires reconstruction, lacks phase information. Passive streaker also requires reconstruction and is destructive.
- Information about the properties of the beam can be obtained by combining non-invasive diagnostics with a theoretical accelerator model. Machine learning (ML) is a good technique for this.
- Virtual diagnostics tool in the control room is the final goal of this project, providing non-destructive predictions of the LPS.
- The development of surrogate ML models for the EuXFEL accelerator is a key component of virtual diagnostics.
  - Improvement of theoretical model through systematic beam dynamics studies.
  - Large scale start-to-end simulations (Ocelot).



Scope of the R&D activity

- Promised deliverables 2025:
  - Generation of Start-to-End Data on DESY Cluster for Surrogate Model Training (Q2 2025).
  - Development of the first prototype of the surrogate model for accelerator modelling (Q4 2025).

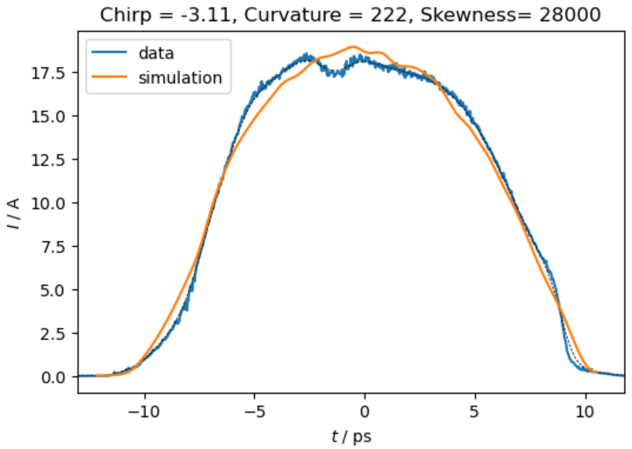
- Interfacing with “Mixed Longitudinal Diagnostic for EuXFEL” (Marc & Simon), collaboration with MSK, assistance from MCS high level controls will be required to implement the diagnostic tool for operations.

Achievements in the past year

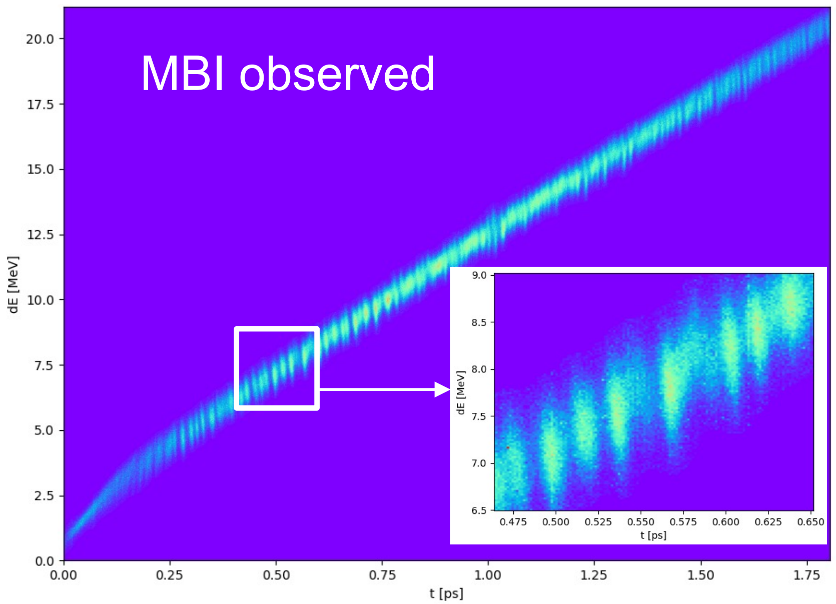
- **Infrastructure for Start-to-End Simulations:** EuXFEL lattice repository https://github.com/ocelot-collab/EuXFEL-Lattice
  - *Single source of truth* for EuXFEL lattice. Tested against MAD8, includes different optics variants.
  - Validation of s2e simulations with collective effects against reference simulations from 2019.

- **Validation of the Accelerator Model with Measurements:**
  - First measurement campaign in March before shutdown.
  - Benchmarked injector measurements with simulations.
  - Laser Heater off, scan of L1 chirp, collected BC2 data with CRISP and TDS.
  - Observed strong microbunching instability (MBI)—requires update of the Ocelot model to include this effect.
  - We measured LPS at 9 different compression points for analysis.

Injector TDS measurements vs simulations



B2 TDS, L1 chirp = -3.4

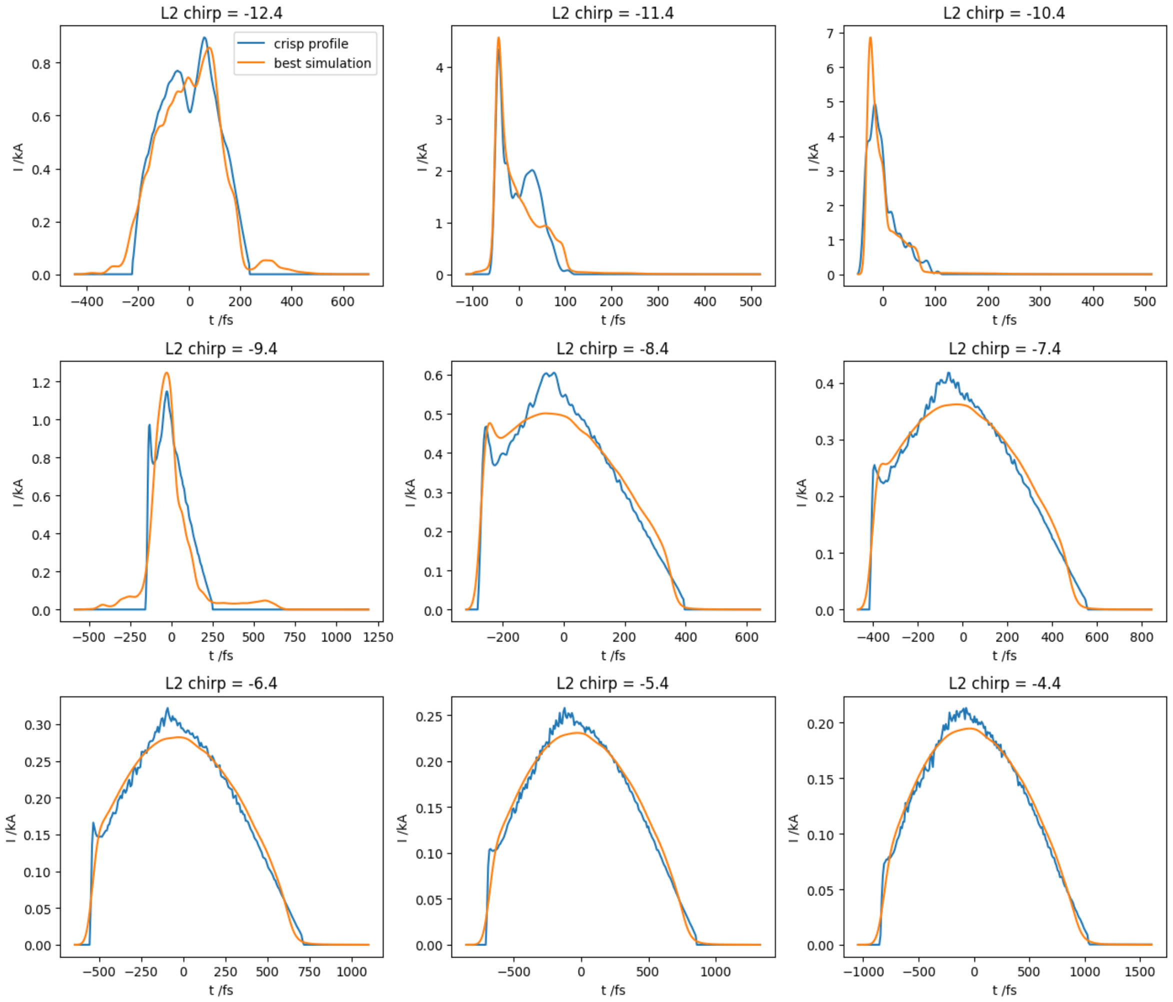


Achievements in the past year

- Matching simulation with measurements.
  - Adjusting RF parameters to match measured current profiles.
  - MBI effect was strong in these measurements (and Ocelot simulation model currently does not include it).

- Set-up in place for cross-checking and matching of simulations with measurements.
  - Systematic validation of the model is planned for next year.
  - Bayesian Optimization leverages parallelisation and can be used efficiently on the cluster.

- Ongoing effort on improving the agreement between simulations and measurements (e.g., selecting the optimal parameters to reproduce the measured beam characteristics, identify a common RF-offset).



Maximal parameter variation in BO optimizations

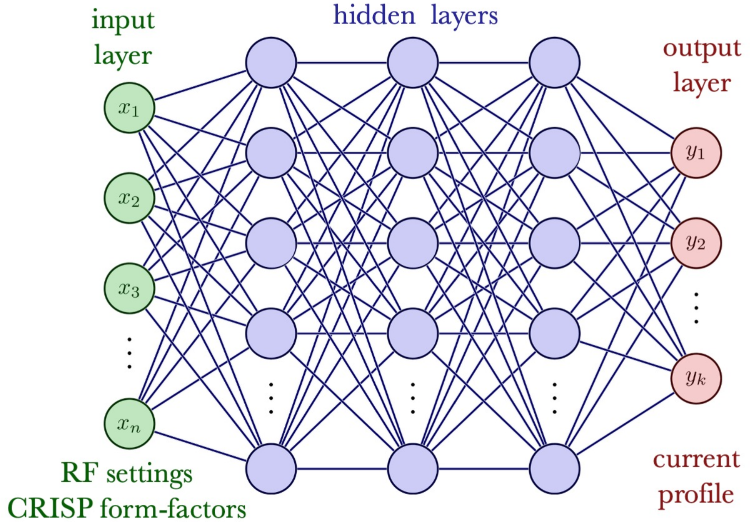
voltage of the first harmonic cavity (inj.)	±2.5 MeV	phase of the first harmonic cavity (inj.)	±0.3 deg
voltage of the high harmonic cavity (inj.)	±2 MeV	phase of the high harmonic cavity (inj.)	±0.3 deg
voltage in L1	±5 MeV	phase in L1	±0.3 deg
voltage in L2	±15 MeV	phase in L2	±0.5 deg

Parameter	Base value	Range
Injector chirp (1/m)	-9.11	±0.5
Injector curvature ($1/m^2$)	222	±100
Injector cubic coefficient ($1/m^3$)	28000	±2000
L1 chirp (1/m)	10.4	±1
L1 sum voltage (GeV)	0.57	±0.01
L2 chirp (1/m)	-5.4	±1
L2 sum voltage (GeV)	1.7	±0.01

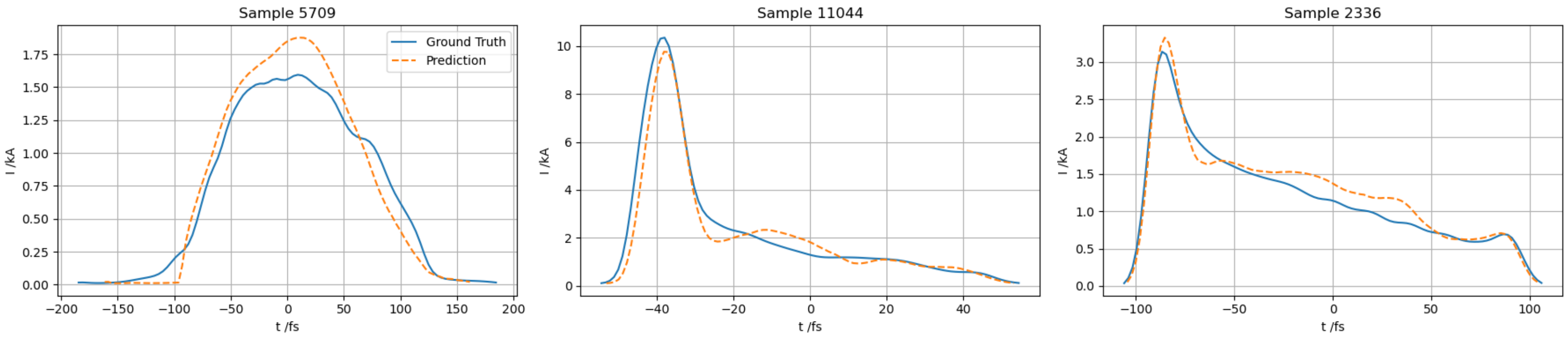
Achievements in the past year

- **Data generation for surrogate model training.**
  - s2e simulations from the gun to the end of collimation section.
  - RF parameters around operational working point, current profile and CRISP spectrum recorded for each.

- **Neural network architecture trained** and tested reconstructing current profiles from RF settings and THz spectrum formfactors.
  - Starting with a simplified problem (only current profile prediction).



Random Test Samples



HELMHOLTZ
DESY.

Deviations from plan

- Currently none

Timeline of this R&D activity

Date / Period	Milestone Description	New Date/ Period
Q4/2023	PostDoc hired	1.12.2024
Q2/2025	Generation of Start-to-End Data on DESY Cluster for Surrogate Model Training. This data will include various parameters and features related to the electron beam dynamics and will serve as a basis for developing and refining the ML surrogate model for the EuXFEL accelerator. The PostDoc should have familiarity with the beam dynamics simulation software used in the MXL group.	Q2/2025
Q4/2025	Development of the first prototype of the surrogate model for accelerator modeling The postdoc will develop a first prototype of the surrogate model for the accelerator, using the improved theoretical models and generated start-to-end (s2e) data. This initial prototype will serve as a foundation for further development, testing, and refinement of the ML surrogate model for the EuXFEL accelerator.	Q4/2025
Q2/2026	Cross-Checking the ML Surrogate Model (Theoretical Model) with Electron Beam Property Measurements The postdoc will carry out beam studies on the accelerator to cross-check the developed ML surrogate model (theoretical model) against the measurements of the electron beam properties.	Q2/2026
Q4/2026	Integration of Surrogate Models with Non-Invasive Diagnostics The postdoc will integrate the developed ML surrogate models with non-invasive diagnostics, such as BCM, CRISP, and RF parameters. This integration will enable real-time monitoring of electron beam properties, which is essential for tuning the accelerator to non-standard operation modes.	Q4/2026
Q2/2027	Publish the results.	Q2/2027

Risks to R&D Project

- The EuXFEL accelerator compression scheme is rather complicated, with 3 bunch compressors and only two TDS with limited resolution (B2 TDS after final compressor). The lack of LPS diagnostics may limit our knowledge of the machine, resulting in a less accurate model.
- B2 TDS hardware has had reliability issues.

Outlook / Summary

- Machine learning pipeline framework in place, needs to be up-scaled, extended to full LPS images.
  - More simulations to cover wider range of RF parameters.
- More measurements for validation of Ocelot model (suppress MBI).
- Test surrogate model against measurements.
- Introduce virtual diagnostics tool into the control room.

Thank you