

Closing the Loop between Simulation and Experiment in Plasma and Photon Science

Jeffrey Kelling^{1,2}

Ritz Ann Aguilar¹, Ankush Checkervarty³, Hardik Ghoshal¹, Vedhas Pandit¹, Jeyhun Rustamov¹,
Jiaying Wang¹, Fong-Lin Wu¹, Michael Bussmann^{1,3}

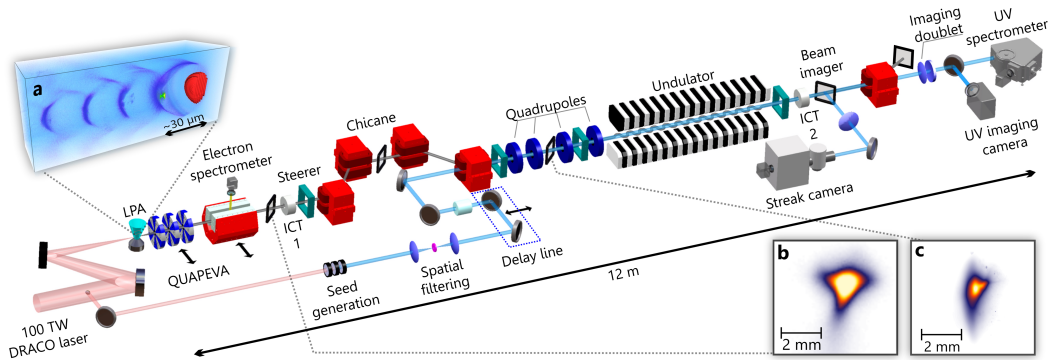
¹*Institute of Radiation Physics, Helmholtz-Zentrum Dresden - Rossendorf (HZDR)*

²*Faculty of Natural Sciences, Chemnitz University of Technology*

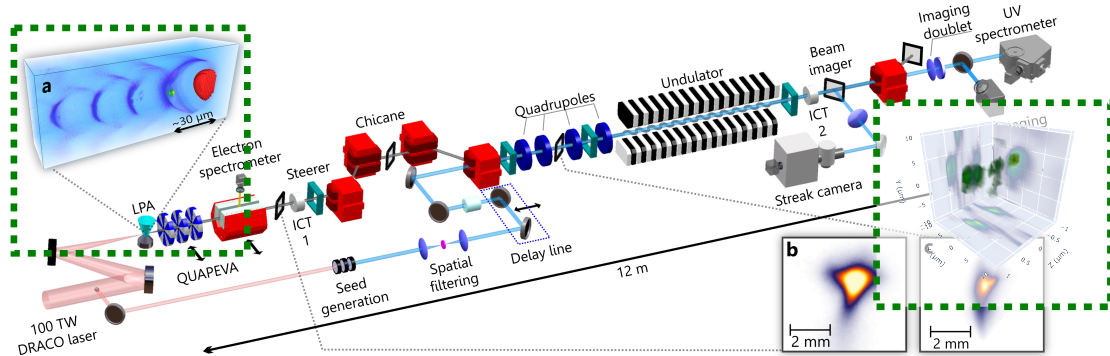
³*Center for Advanced Systems Understanding (CASUS)*

November 3, 2025

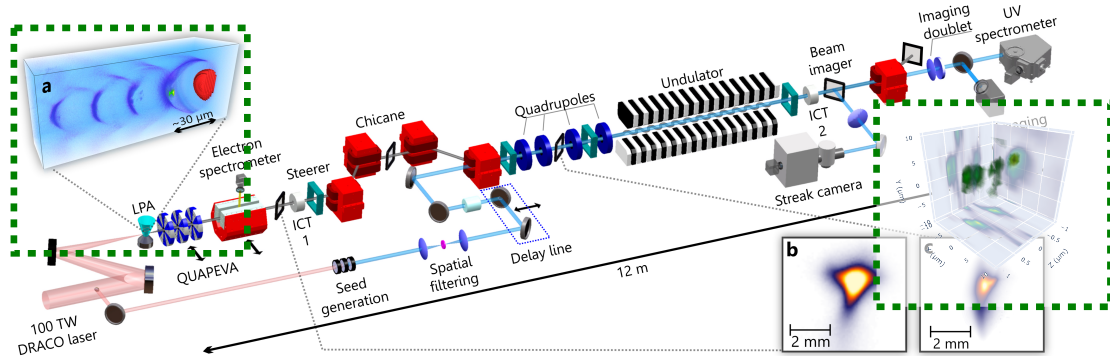
Laser-Plasma Accelerator-Driven Free Electron Laser @ HZDR



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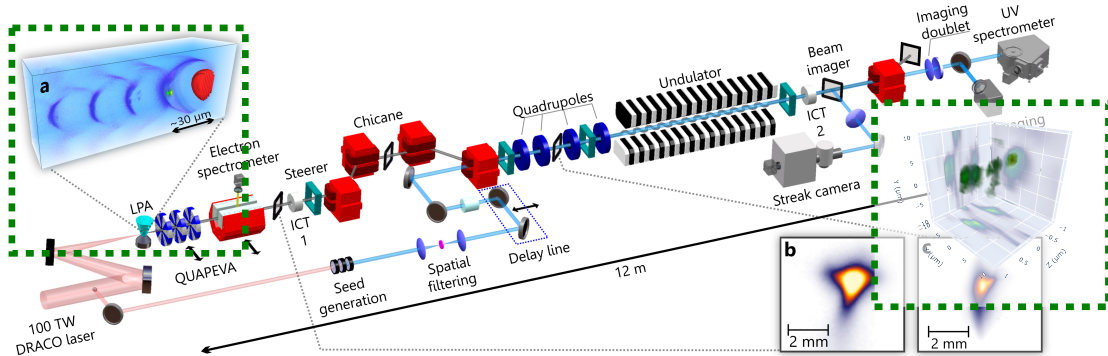


Experiments:

Inputs: Laser + plasma parameters

Outputs: Radiation + energy spectrum of bunch

Laser-Plasma Accelerator-Driven Free Electron Laser @ HZDR



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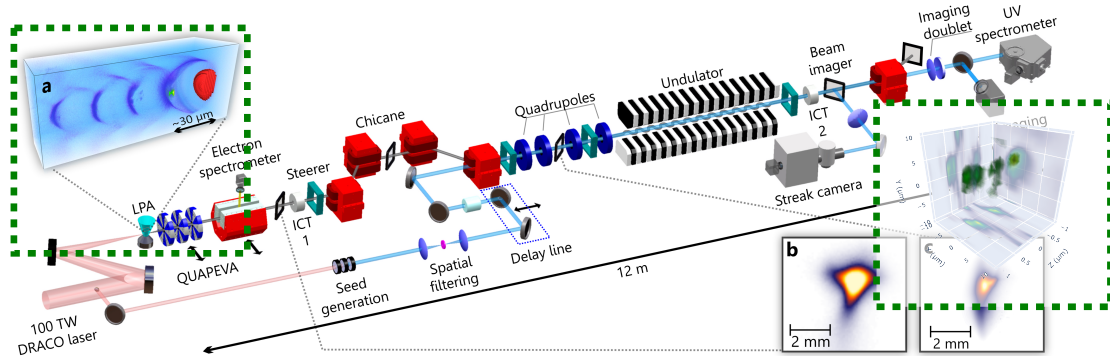
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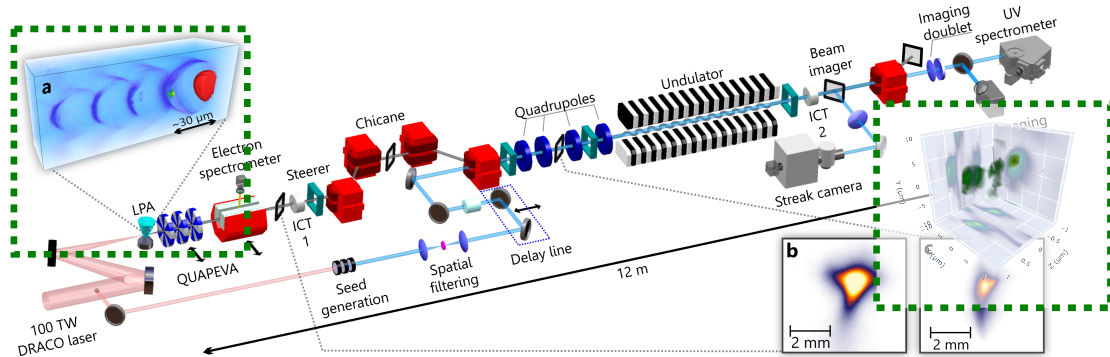
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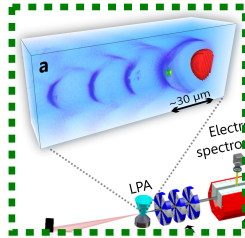
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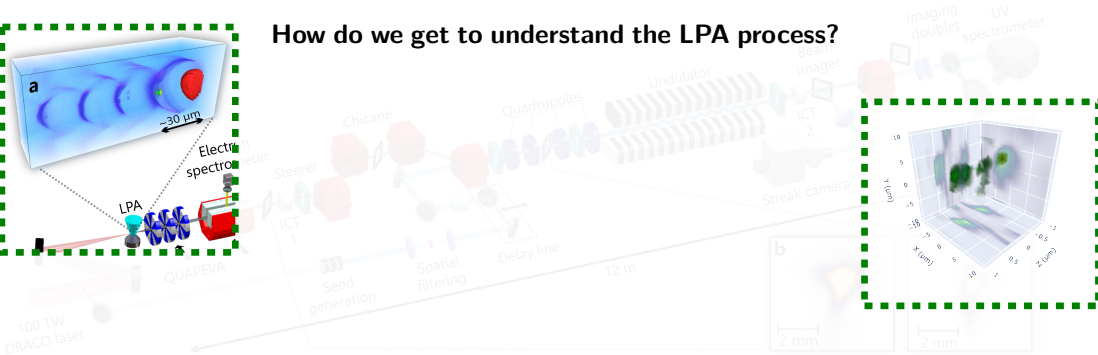
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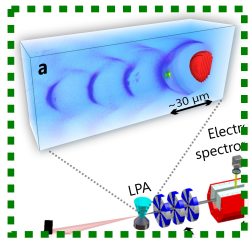
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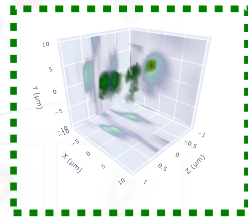


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Full 3D Simulations: 

+ provide full information about studied process

- full laser pulse shapes
- full output particle phase-space



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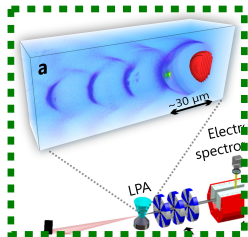
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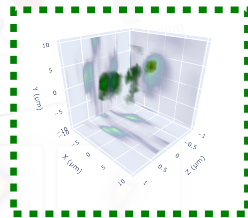
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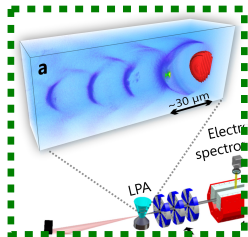
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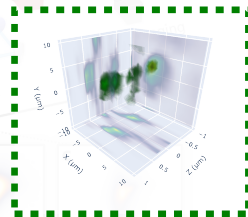
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How can we connect observations from simulation and experiment?

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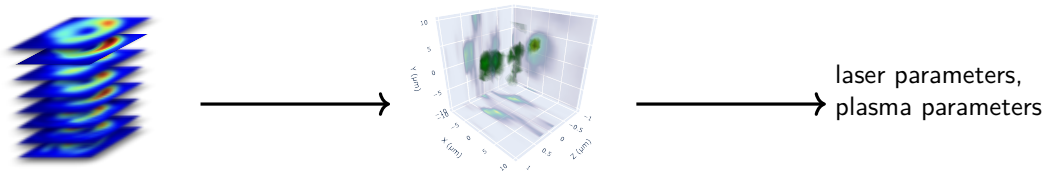
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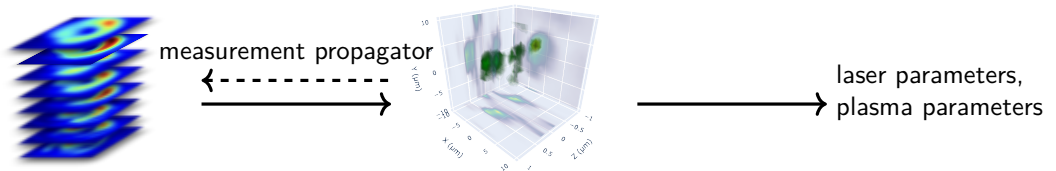
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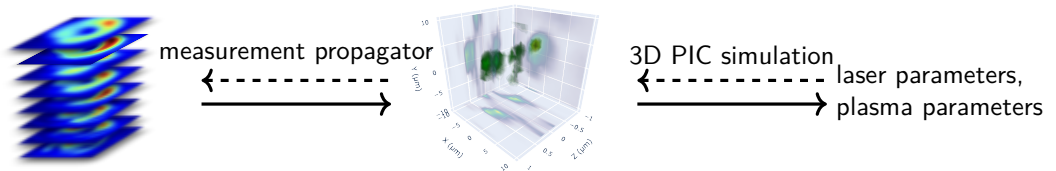
Two inverse Problems



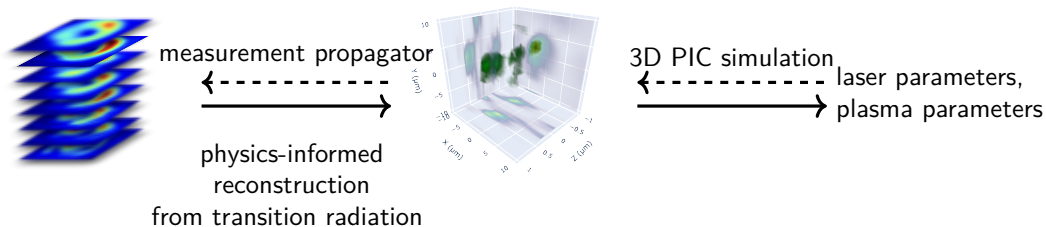
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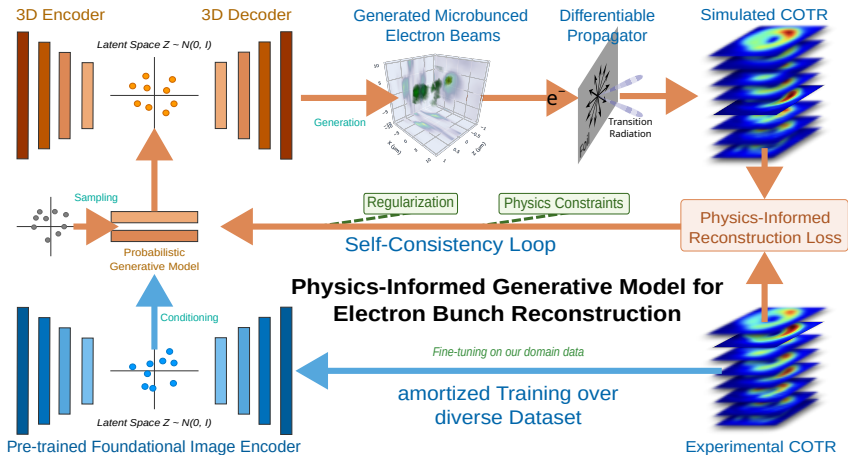
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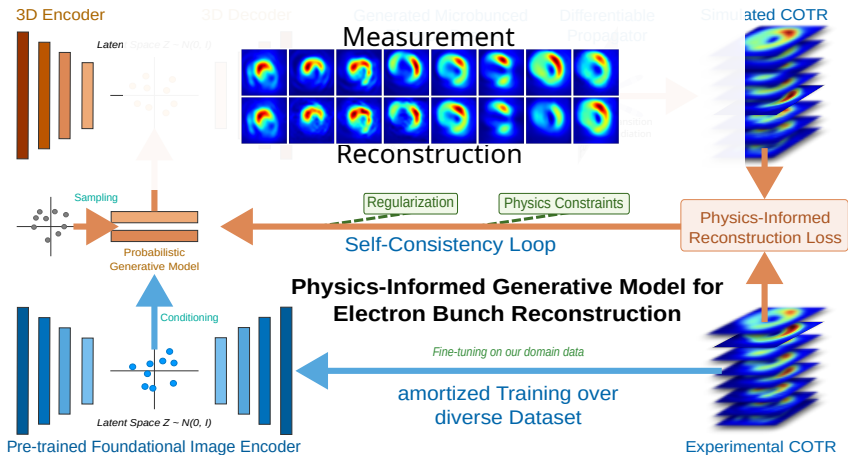
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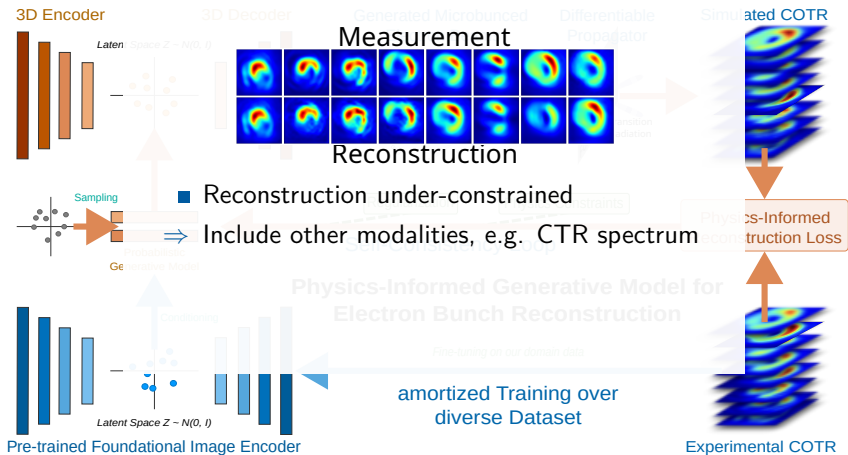
Electron-Bunch Recontrauction from Coherent Optical Transition Radiation (COTR)



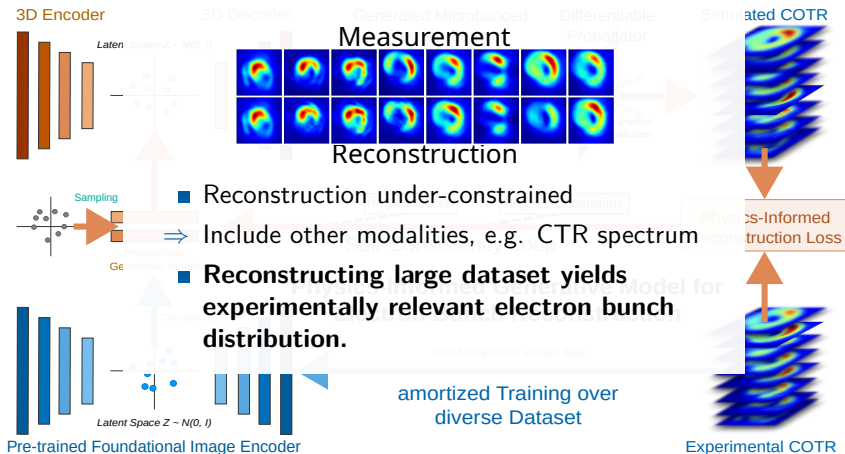
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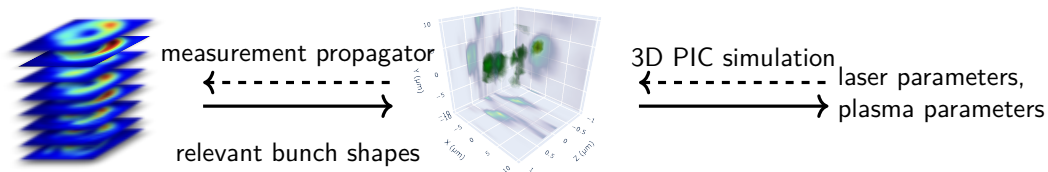
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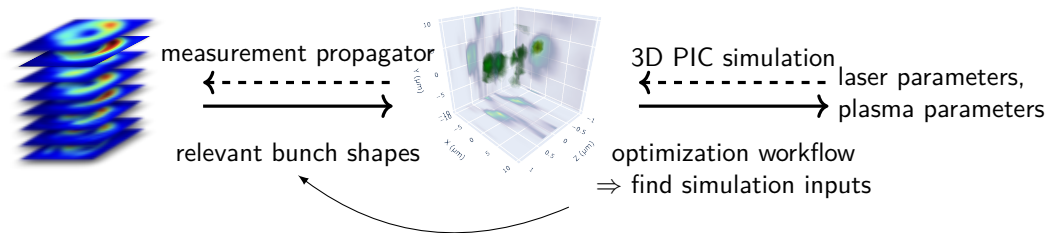
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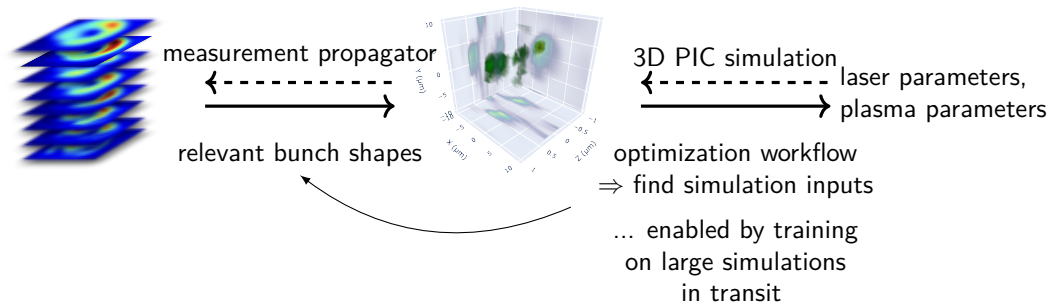
Towards Understanding the Experimental Regime



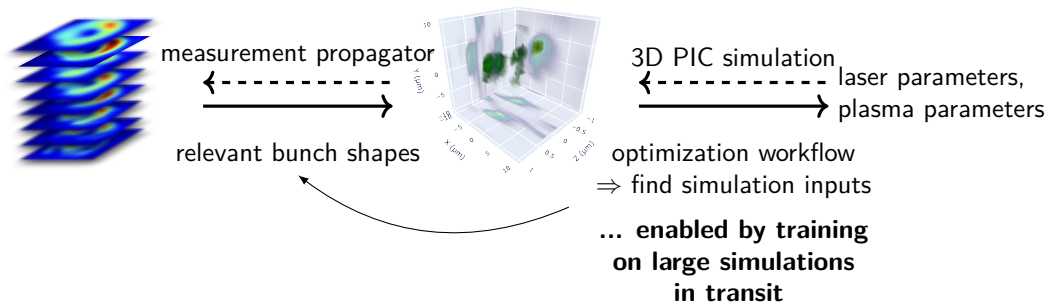
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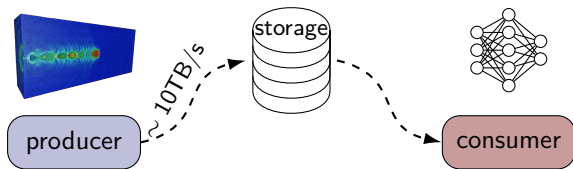
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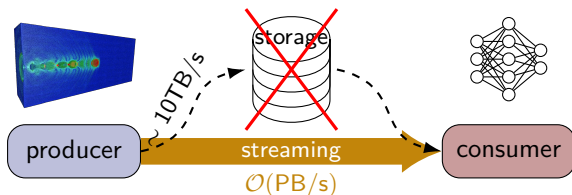
Training Surrogate Models from Large-Scale Simulations¹



- Storage capacity or bandwidth may limit the amount of high-fidelity data that can be stored for training.

¹Kelling et al. 2025, <https://arxiv.org/abs/2501.03383>

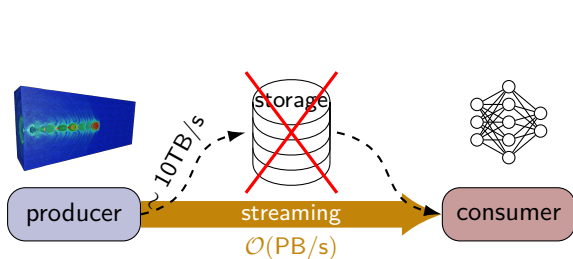
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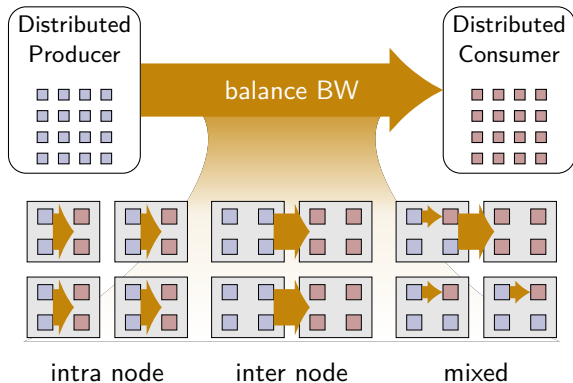
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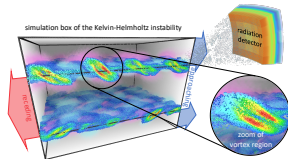
- Storage capacity or bandwidth may limit the amount of high-fidelity data that can be stored for training.
- Direct streaming workflow bypassing storage.
- Parallel training to maximize throughput. →



(c) producer and consumer are distributed across nodes (gray boxes), arranged to balance bandwidth requirements with availability

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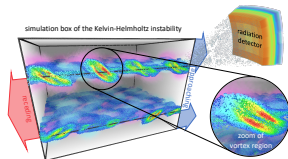
Learning Representations in-Transit²



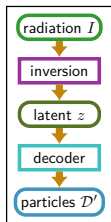
Kelvin-Helmholtz instability

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Learning Representations in-Transit²



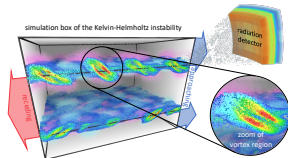
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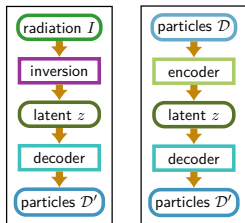
(a) inversion
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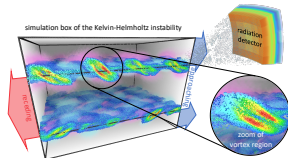


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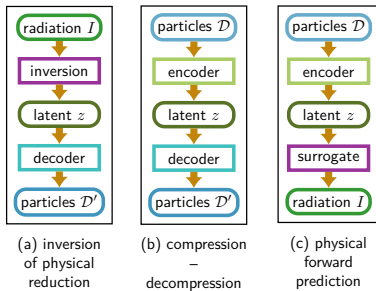
(b) compression
–
decompression

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Learning Representations in-Transit²

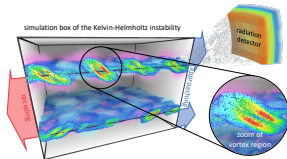


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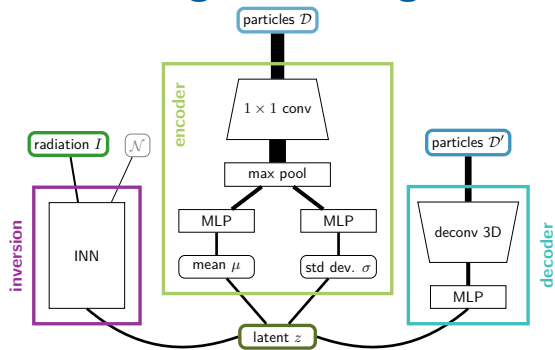
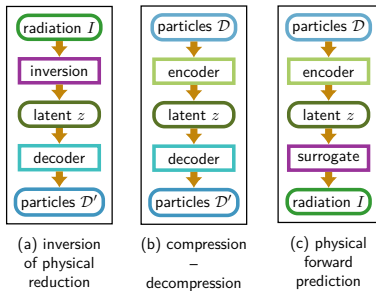


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Learning Representations in-Transit... among other things²

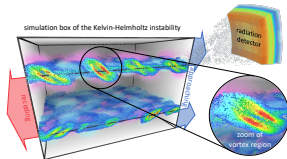


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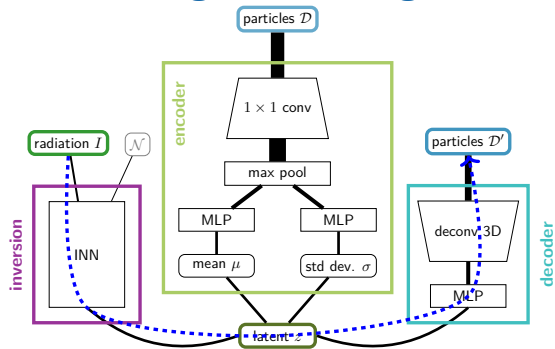
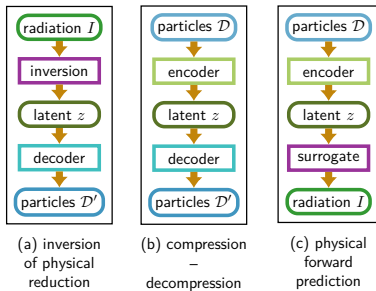


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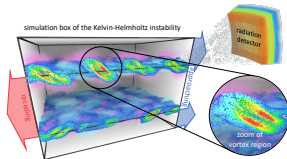
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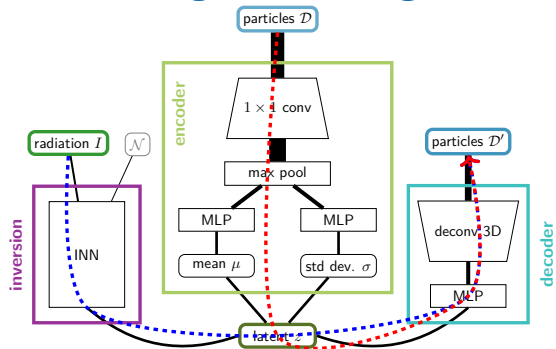
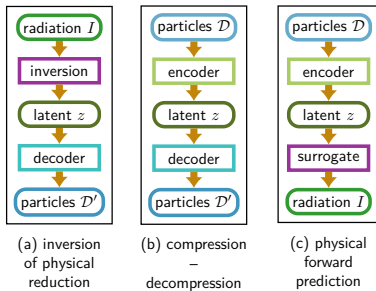
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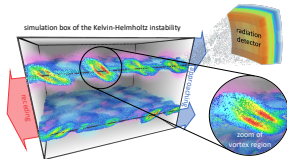


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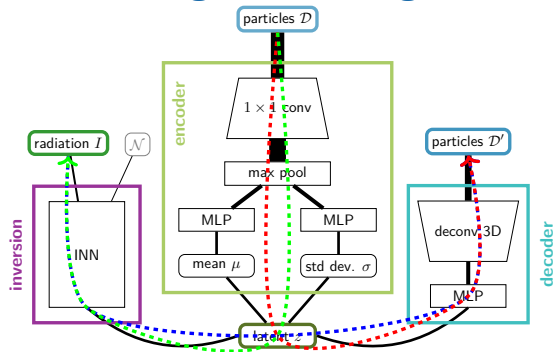
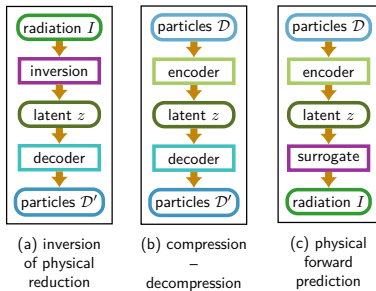
(b) - $\rightarrow$ point cloud variational autoencoder

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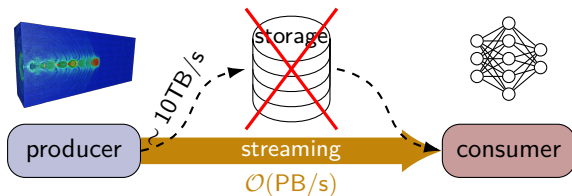
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- (a) - → inverse problem
- (b) - → point cloud variational autoencoder
- (c) - → radiation surrogate

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Proof of Concept: In-Transit Learning⁴

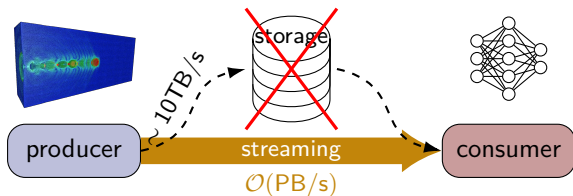


- Data is not stored, so not repeated in time.
- ⇒ Variant of Experience-replay³ to avoid forgetting.
- Statistics from ensemble of simulation domains.

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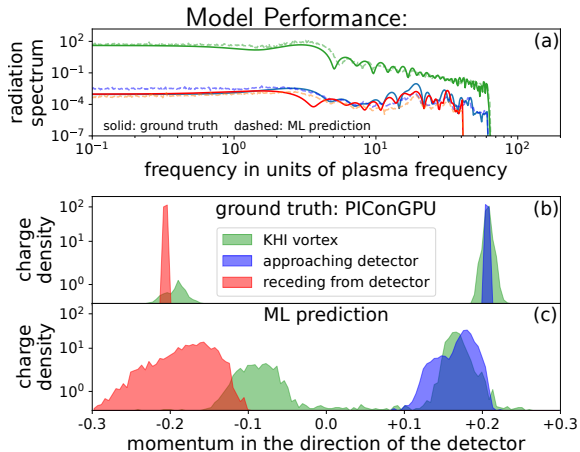
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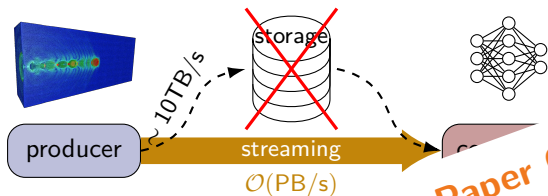
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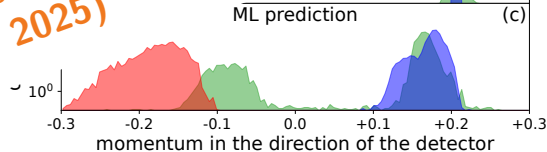
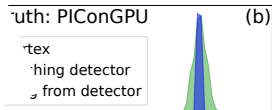
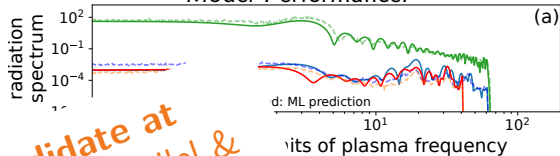
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**Best Paper Candidate at
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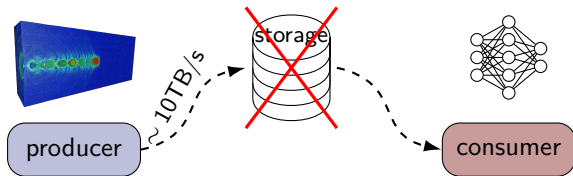
Model Performance:



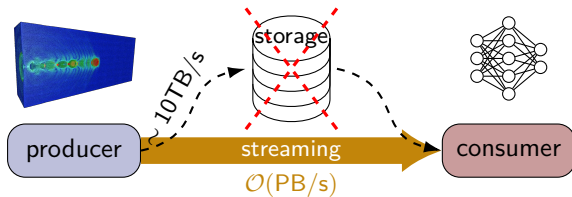
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Recycling Large-Scale Simulation Data for Training

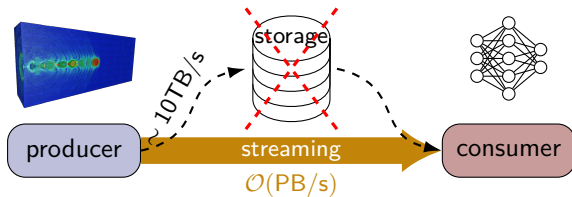


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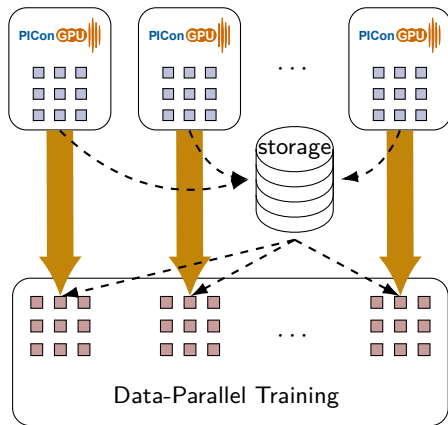


- Extend in experience-replay buffer to storage, for more diverse batches,
- + stream from simulations dynamically.

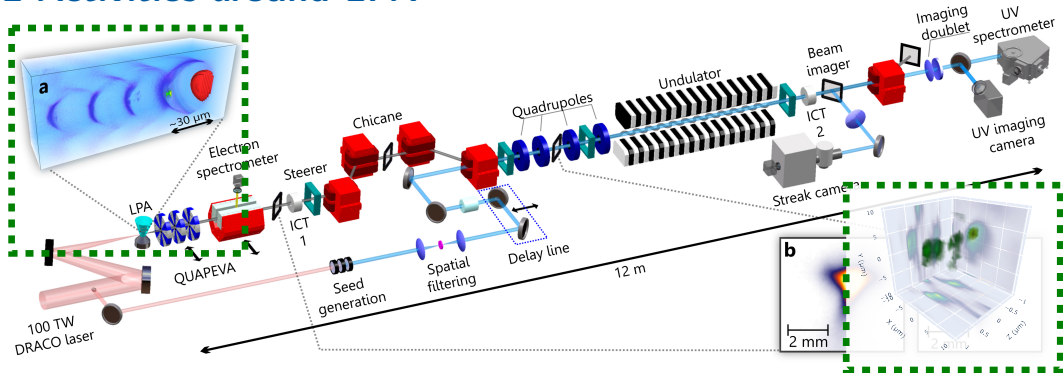
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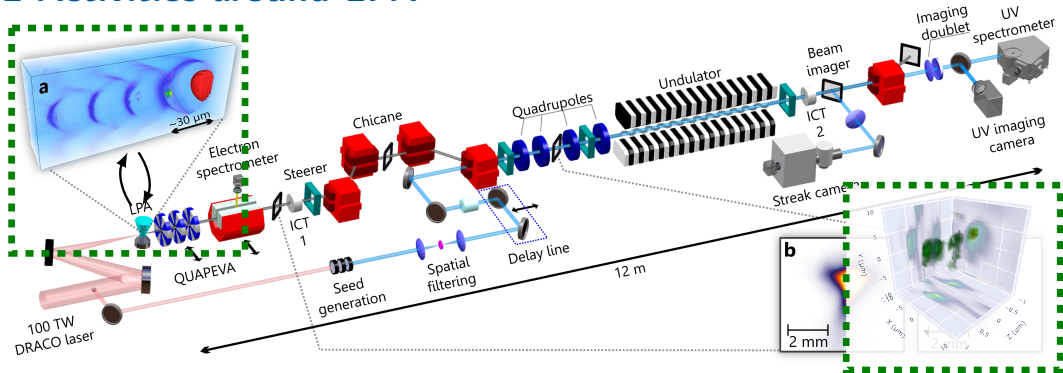
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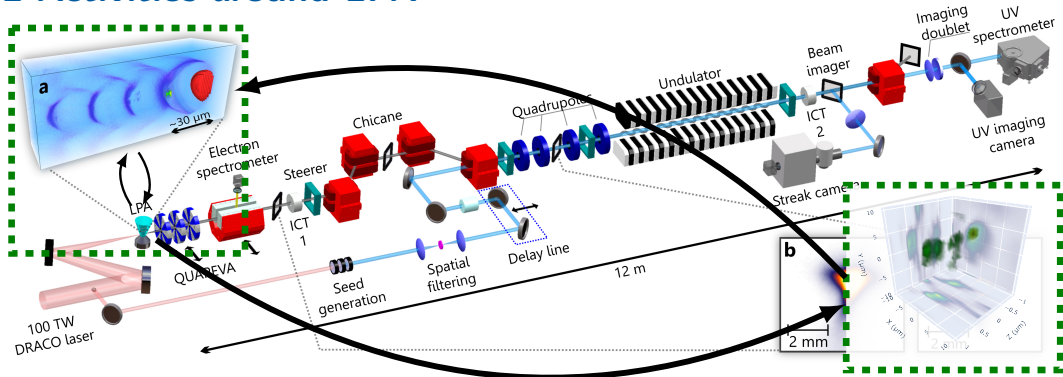
ML Activities around LPA



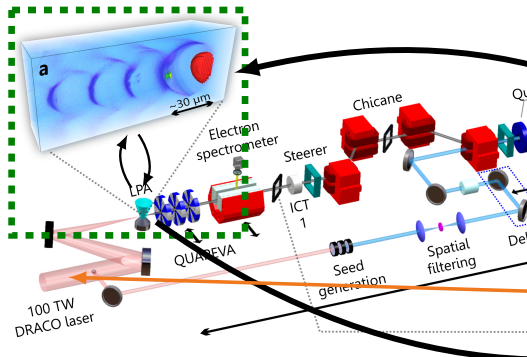
ML Activities around LPA



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ML Activities around LPA



Patch-MLP-Based Predictive Control: Simulation of Upstream Pointing Stabilization for PHELIX Laser System

HZDR
HELMHOLTZ ZENTRUM
DRESDEN ROSENDOF

J. Wang¹, J.B. Ohland², Y. Chang³, V. Pandi⁴, S. Bock⁵, A.H. Okunura^{6,7}, U. Eisenhardt⁸, A. Imran⁹, M. Busemann¹⁰, U. Schramm¹¹, J. Küling¹²

¹ Helmholtz-Zentrum Dresden-Rossendorf, Germany; ² Technische Universität Dresden, Germany; ³ GSI Helmholtzbeschleuniger für Schwerionenforschung, Germany; ⁴ Amplitude laser group - Dresden operations, Germany; ⁵ Chemnitz University of Technology, Chemnitz, Germany; ⁶ Extreme Light Infrastructure - Nuclear Physics, National Institute for Physics and Nuclear Engineering, University of Bucharest, Ilfov, Romania; ⁷ Engineering and Applications of Lasers and Accelerators Doctoral School (EALAS), Romania; ⁸ Extreme Light Infrastructure - Nuclear Physics, National Institute for Physics and Nuclear Engineering, Ilfov, Romania

Introduction

- Jitter: Slow drift → 100 Hz passively low-bandwidth loops leave residue
- Upstream stabilization: avoids lever-arm amplification, clipping, downstream load
- Proportional-Integral-Derivative Controller (PID) limit: inertia of large optics → misses fast jitter
- Solution: → PHELIX MAG data → MLP at Pre-Amplifier design
- Result: Patch-Based MLP extends PID bandwidth, stabilizes high-energy beams



Methodology



- Traditional PID:
 - Limited by inertia & computation delay → leaves residual jitter
 - MLP-driven PID:
 - Adds short-horizon forecasting with an MLP predictor
- Patch-Based MLP design:
 - Splits sequence into short patches → captures local temporal patterns
 - Lightweight, low-latency → real-time capable
 - Robust to noise → stable performance in practice



Simulation Results



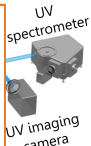
- System modeling:
 - Data from PHELIX Laser
 - Mirror as damped 2nd-order system
- Traditional PID baseline:
 - Tuned parameters → optimal response (Orange curve)
- Predictive approach:
 - Prediction 5 points (~1.2 ms) → Applied to system → improved response (Green curve)

Model stability

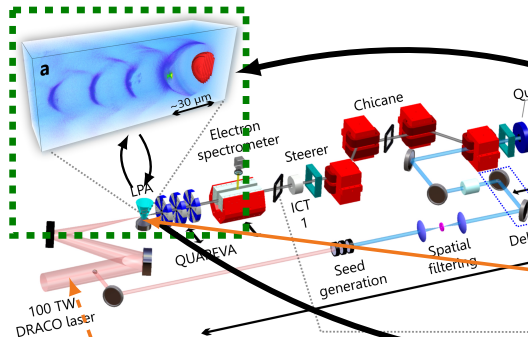
- Long-term test: 10 hours of data
- Sampling: 1 min every 5 min
- Result: no major failures observed
- Note: brief deterioration caused by new vibration sources

Outlook

- Implementation: Patch-MLP PID at PHELIX Pre-Amplifier Bridge
- Testing: under varied rep. rates, thermal loads & vibrations
- Evaluation: compare with traditional PID → validate, reveal challenges, guide optimization



ML Activities around LPA



A Roadmap Towards Direct Imaging of Plasma Targets During Laser Acceleration using Computational X-Ray Holography

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Motivation

Laser-plasma acceleration (LPA) needs non-invasive, single-shot diagnostics. Gas jets evolve on μs -scales with strong shot-to-shot variability; invasive probes disturb the target. X-rays enable direct imaging of dense, thick targets with phase sensitivity to weak refractive index changes, penetrating where optical diagnostics fail.

In-line holography or Phase Contrast Imaging (PCI) are fast but ill-posed. Robust phase retrieval requires physics-aware regularization and careful experiment design (energy, distance, detector).

A unified, differentiable toolbox is missing. Separate simulators and reconstructions slow iteration and make it hard to optimize geometry, priors, and noise budgets end-to-end.

Differentiable Materials

- Complex refractive index: $n = 1 - \delta + i\beta$ (1)
- δ : phase shift decrement; β : absorption index
- Use lookup table of materials^[1]
- An X-ray source traversing a field has the field: $\Psi(x, y) = \exp[-i\mu(x, y)z] \exp[i\phi(x, y)]$ (2)
- $\mu = 4\pi\beta/\lambda$; $\phi(x, y) = -2\pi\delta(x, y) = -k \int \rho(x, y) dz$
- λ : wavelength; k : wave number; ρ : density projection

Differentiable Propagator/Forward Model

Forward model for near-field imaging: Fresnel-free space propagator or near-field propagator^[2]

$$D(W) = \mathcal{F}^{-1}[\exp(-im)(\mathcal{F}H)^2 + \sigma^2) \mathcal{F}[W]] \quad (3)$$

$\mathcal{F}$: 2D Fourier transform; m : Fresnel number ($m = k d^2 / 2z$); d : detector pixel size; z : propagation distance

Differentiable[†] optical propagators expose gradients, enabling end-to-end calibration, design, tuning, and learning-based reconstruction.

[†]With the use of machine learning framework (PyTorch)



General Workflow

Data Generation
(Clean source, photon energy E , object materials, and wave field ρ)

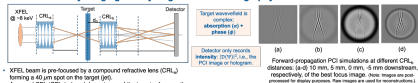
Wave Optics Propagation
(Classical Fresnel propagating system, choose appropriate forward model)

Phase Reconstruction
(Choosing an iterative procedure, choose appropriate reconstruction algorithm)

Phase Reconstruction Suite
(Choosing an iterative (Transport-of-Intensity Equation (TIE), iterative algorithms (Error Reduction/Gerchberg-Saxton, Hybrid Input Output))

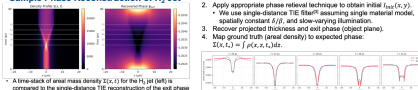
Physics-informed machine learning (unrolled/regularized) methods for robust, single-shot phase recovery

Use Case: X-Ray Imaging of a Hydrogen Jet with Holography/PCI



X-ray beam is pre-focused by a compound refractive lens (CRL₁) forming a 40 μm spot on the target (jet). A second CRL (CRL₂) placed downstream of the target refocuses the beam, after which it propagates to a detector. This provides the resolution of a near-field detector while retaining a far-field geometry.

Sample Phase Reconstruction of H₂ Jet

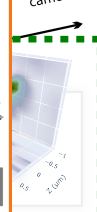
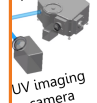


A time-stack of small mass density $\Sigma(x, t)$ for the H₂ jet (left) is compared to the single-distance TIE reconstruction of the exit phase ϕ_{exit} (right). The line plots (red line: $\Sigma(x, t)$; blue dashed: ϕ_{exit} after affine scaling) show close shape agreement consistent with $\phi \propto -\Sigma$. Small knowledge discrepancies expected from the TIE low-pass regularization and single-material assumptions.

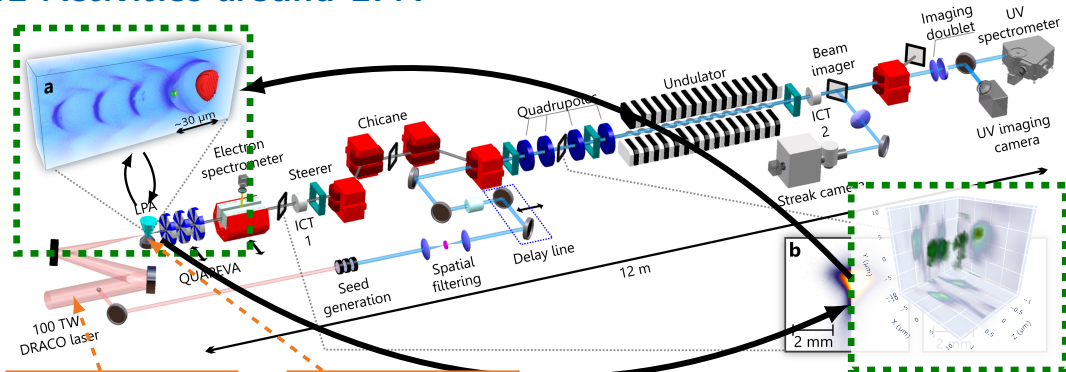
References

- X-Ray Database: https://henlo.de/gov/visual_content/
- J. Gerchberg, Introduction to Fourier Optics (1988).
- D. Paganini et al., J. Microscopy (2002).

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ML Activities around LPA



Patch-MLP-Based Predictive Control: Simulation of Upstream Pointing Stabilization for PHELIK Laser System

HZDR
HELMHOLTZ-ZENTRUM
FÜR ENERGIEFORSCHUNG

Introduction

- The laser system is a high-power laser system used for the production of ultra-short laser pulses.
- The system is composed of several stages, including a seed generation stage, a delay line, and a chicane.
- The system is used for the production of ultra-short laser pulses, which are used for the study of ultra-fast processes.

Methodology

- The methodology involves the use of a Patch-MLP-based predictive control system.
- The system is trained on a dataset of laser pulses, which are used to predict the system's behavior.
- The system is then used to stabilize the laser system, ensuring that the laser pulses are produced with the desired characteristics.

A Roadmap Towards Direct Imaging of Plasma Targets During Laser Acceleration using Computational X-Ray Holography

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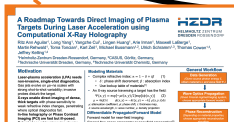
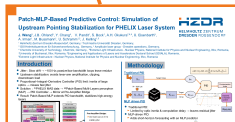
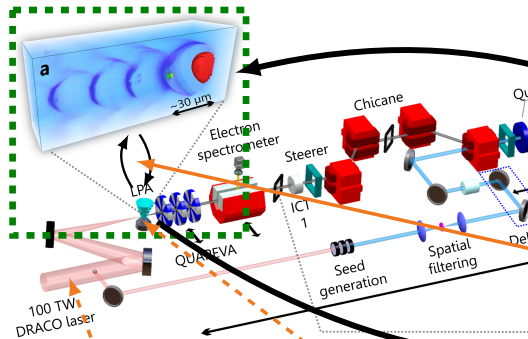
Introduction

- The roadmap involves the development of a computational X-ray holography system.
- The system is used for the direct imaging of plasma targets during laser acceleration.
- The system is trained on a dataset of plasma targets, which are used to predict the system's behavior.

Methodology

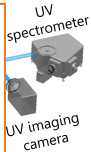
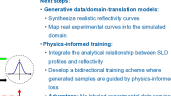
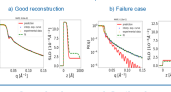
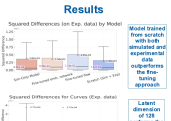
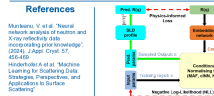
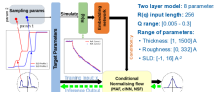
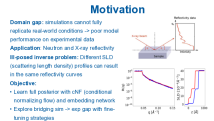
- The methodology involves the use of a computational X-ray holography system.
- The system is trained on a dataset of plasma targets, which are used to predict the system's behavior.
- The system is then used to directly image plasma targets during laser acceleration.

ML Activities around LPA

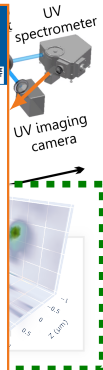
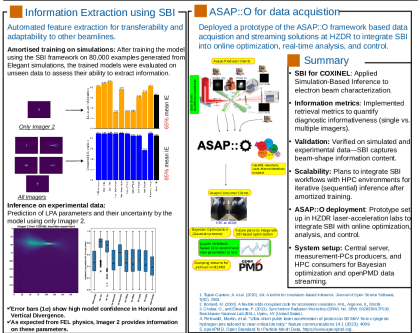
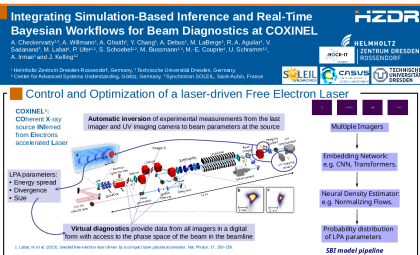
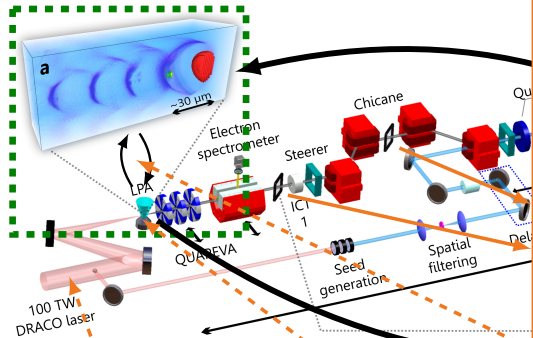


Domain Transfer from Simulation to Experimental Neutron and X-ray Reflectivity Data Using Probabilistic Generative Models

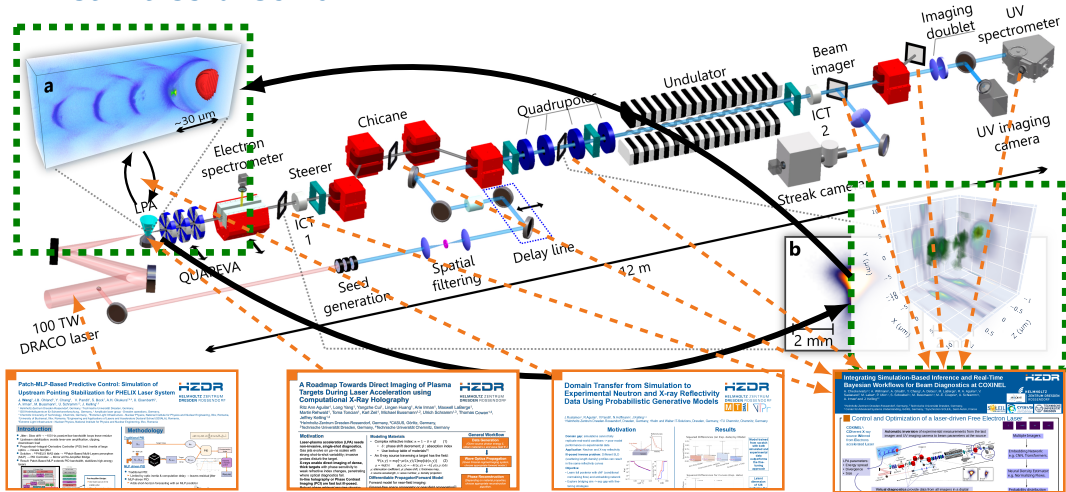
J. Rustenau, R. Aguilera, V. Pandit, N. Hoffmann, J. Kelling, H. Helmoltz-Zentrum Dresden-Rossendorf, Dresden, Germany, Helm and Walter IT-Solutions, Dresden, Germany, ITU Chemnitz, Chemnitz, Germany



ML Activities around LPA



ML Activities around LPA



End.



End.



- Arie Irman, Armin Gaith, Franziska Herrmann, Susanne Schöbel, ...
- Richard Pausch, Klaus Steiniger, Franz Pöschel, ...
- Alexander Debus, Maywell LaBerge, ...
- Thomas Kluge, Vidisha Rana, ...
- Hans-Peter Schlenvoigt, Martin Rehwald, Karl Zeil, ...
- Partners from GSI, ORNL, UDeI

Thank You.