Joint surrogate modelling and reconstruction of Laser-Wakefield Acceleration by invertible neural networks

F. Bethke, R. Pausch, P. Stiller, A. Debus, M. Bussmann, N. Hoffmann

HZDR HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

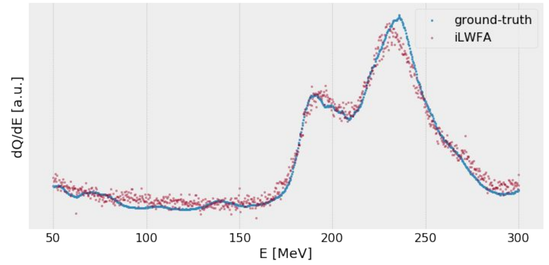
CASUS CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

HELMHOLTZ AI | ARTIFICIAL INTELLIGENCE COOPERATION UNIT

Motivation

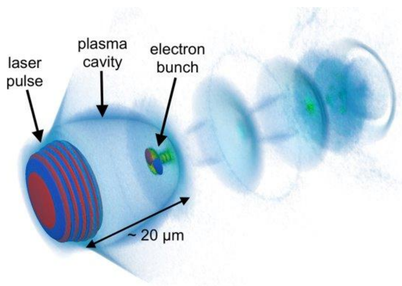
Surrogate model for computationally demanding Laser-Wakefield Acceleration

→ Reconstruction of experimental diagnostics requires fast approximation of non-linear mapping



Energy spectrum: generated

Simulation



Method

Invertible Neural Network

→ simulation and reconstruction done by same network

→ trained bi-directionally

→ resolves ambiguous inverse problems

→ uncertainty quantification for inverse pass

Results

Comprehensive study on 2.7 TB of training data generated by PIConGPU.

- inference time: 5 ms
- surrogate model: MSE < 0.007
- reconstruction: relative error < 8.2%

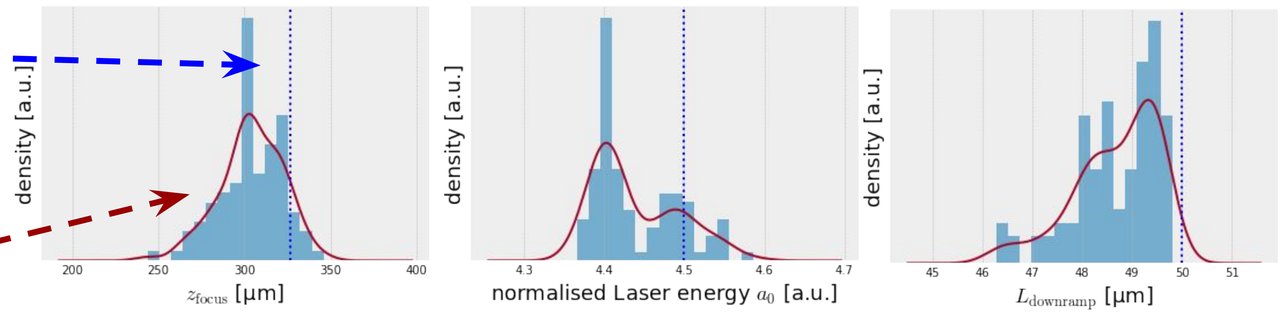
Network

Invertible Neural Network

Parameters: reconstructed

ground-truth

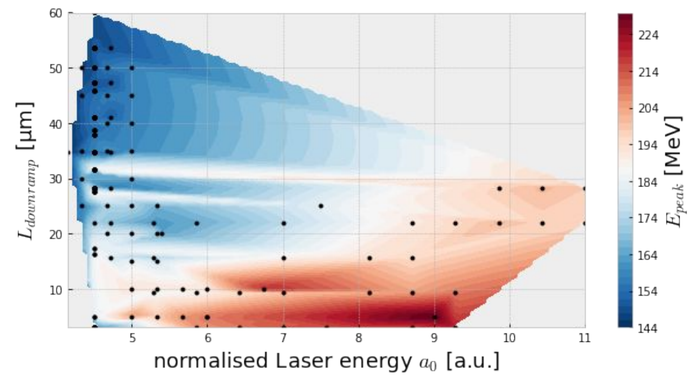
Posterior of INN
each mode = possible parameter configuration



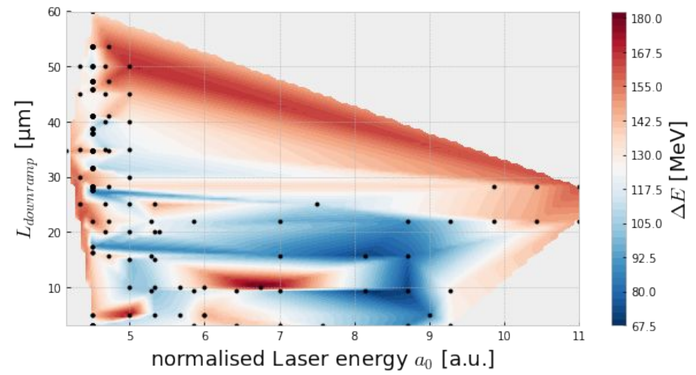
Application in Radiation Physics

Very fast **interpolation in derived moments** of energy spectrum.

1) Peak Energy



2) Full Width at Half Maximum



DRESDEN concept

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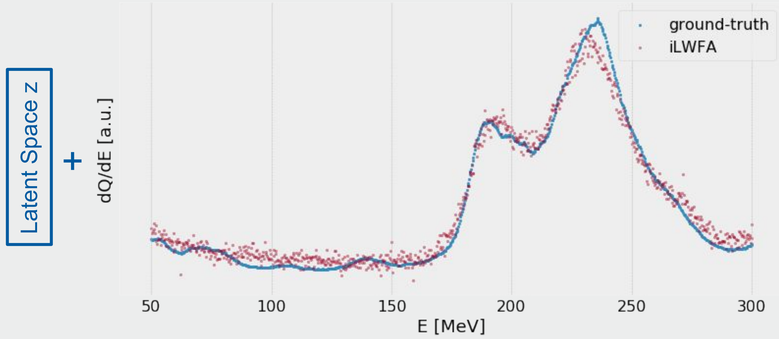
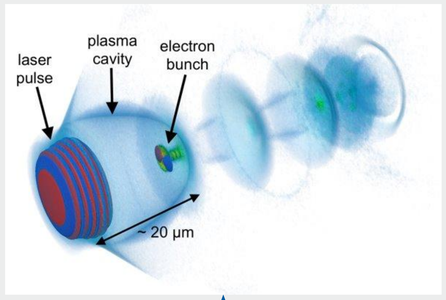
- **Surrogate model for Laser-Wakefield Acceleration simulation Data** is highly desirable since the simulations are highly computationally demanding even for highly-optimized particle-in-cell codes

➔ Fast approximation of highly non-linear process to increase the applicability of LWFA techniques



Energy spectrum

Simulation



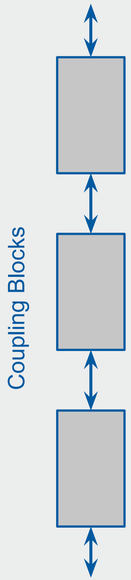
Method

- **Invertible Neural Network** with multiple coupling blocks, each having multi-layer subnetworks

➔ Can run in Forward and Reverse mode

➔ Subnetworks do not have to be inverted

➔ Otherwise lost information is projected to the latent space z



Goals

- **Predict the final energy spectrum** of a laser-wakefield acceleration simulation from simulation parameters and vise versa using an invertible neural network (INN)
- 2.7 Terabytes of training data, generated by large scale PIConGPU simulations

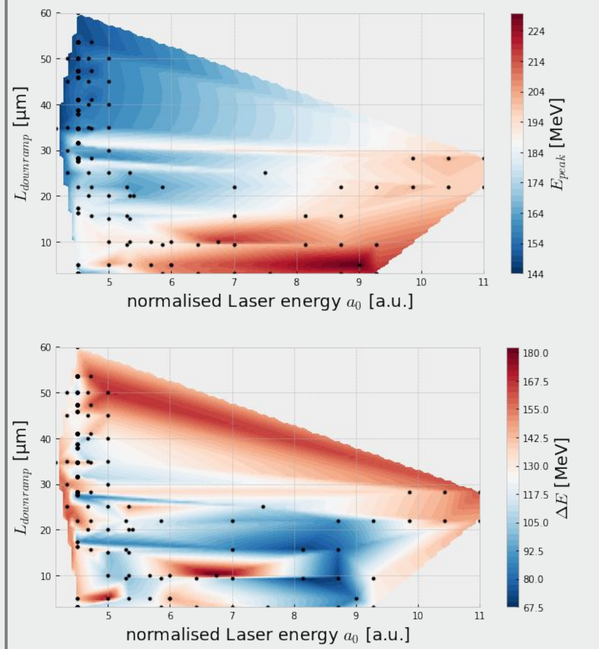
- **Recover simulation parameters** from simulation output through sampling the posterior predictive distribution using the latent space of the INN

➔ Resolve ambiguous mapping

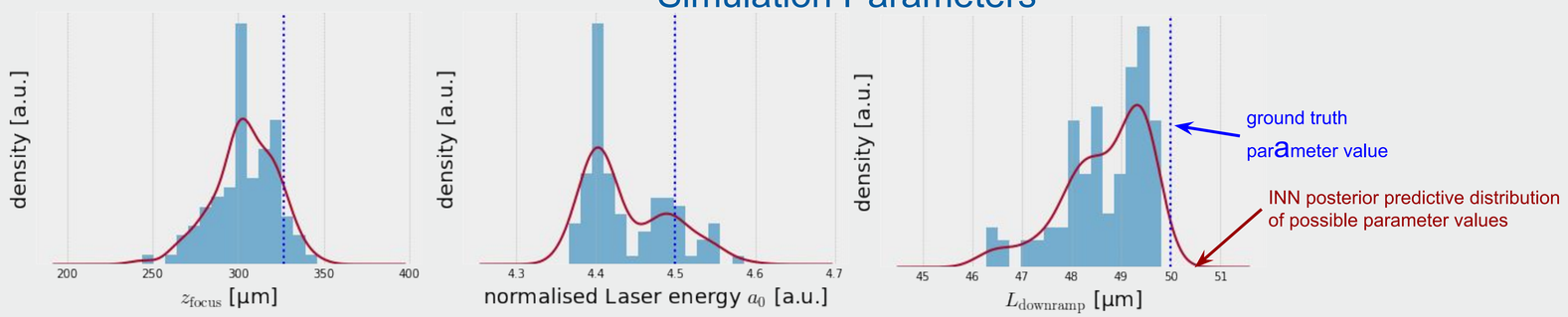
➔ Uncertainty quantification

Physical Application

- **Fast approximation of the simulation output** with the surrogate model to maximise certain diagnostics on the predicted energy distribution



Simulation Parameters



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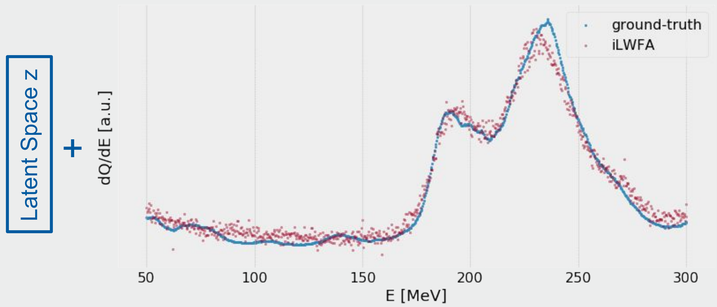

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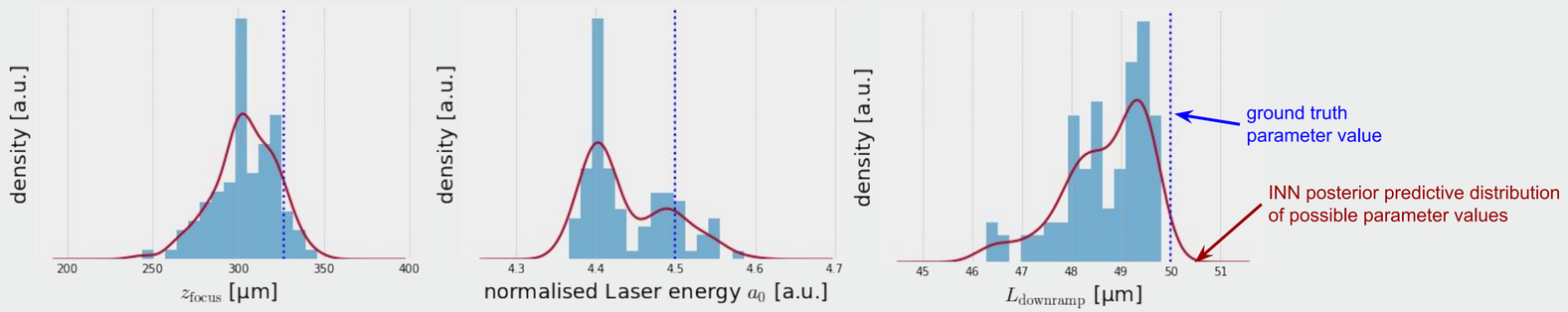

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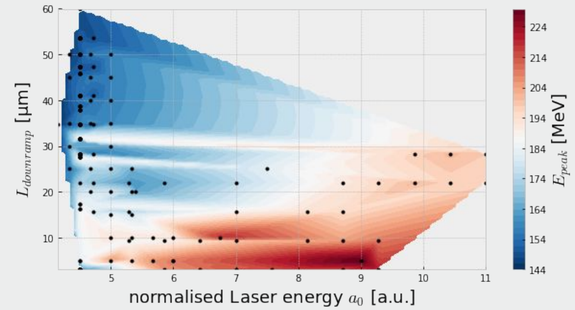

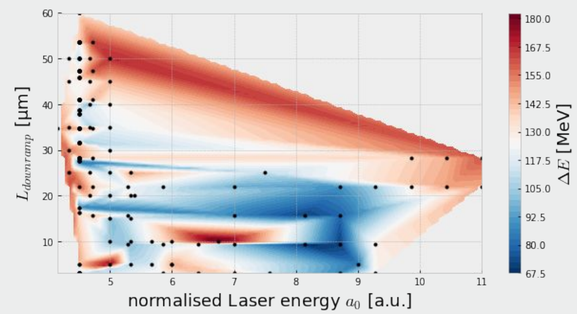

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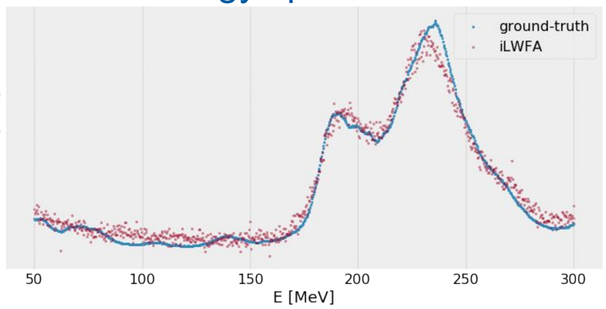
Energy spectrum

Latent Space z + dQ/dE [a.u.]



Coupling Blocks

- ➔ **Invertible Neural Network** with multiple coupling blocks, each having multi-layer subnetworks
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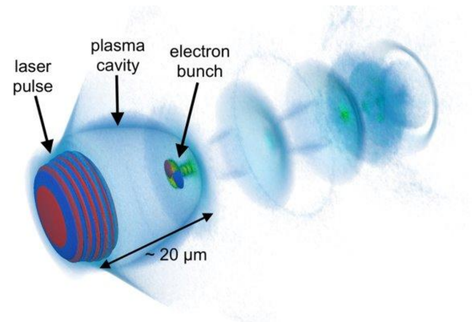
Simulation



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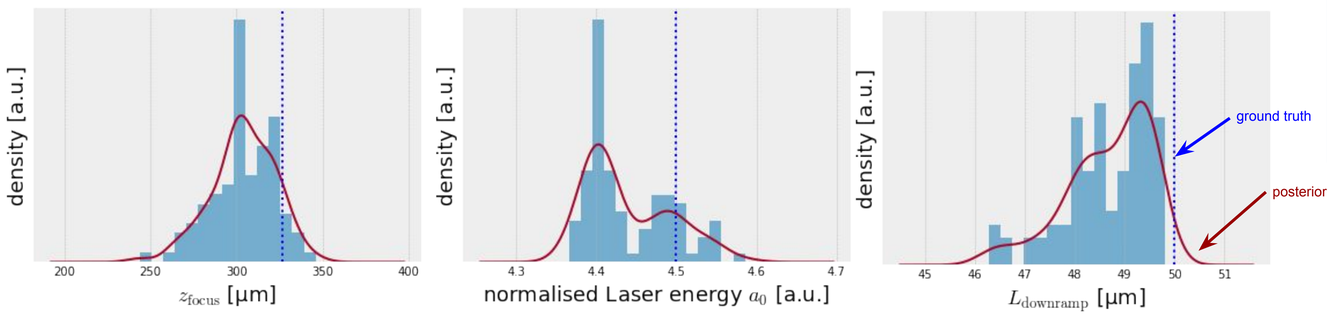
Simulation Parameters



- **Recover simulation parameters** from simulation output through sampling the posterior predictive distribution using the latent space of the INN
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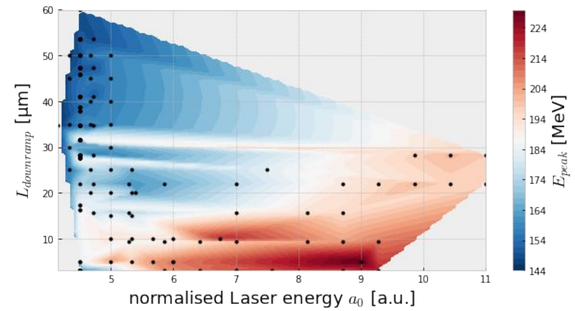

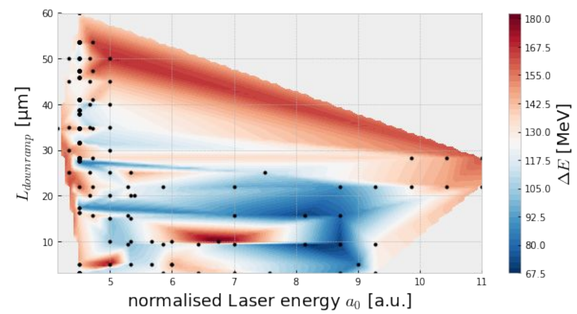

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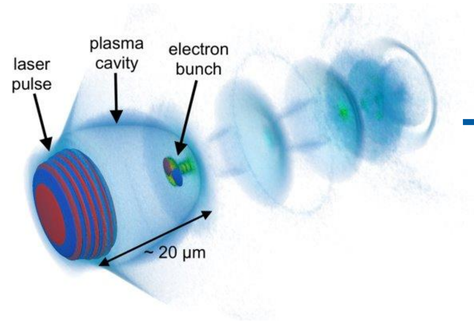
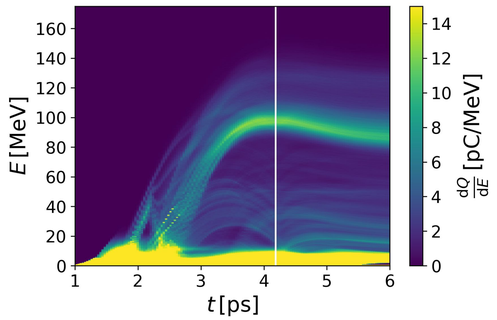
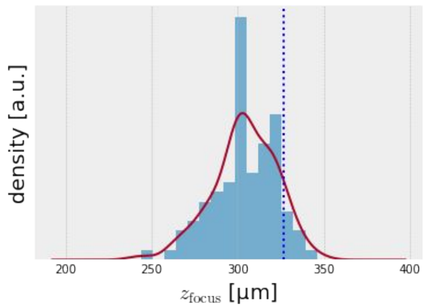
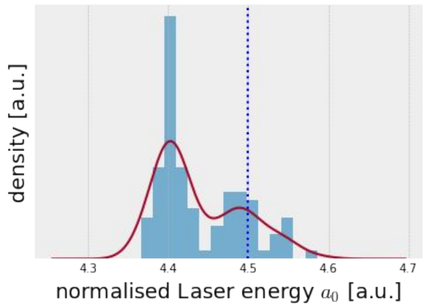
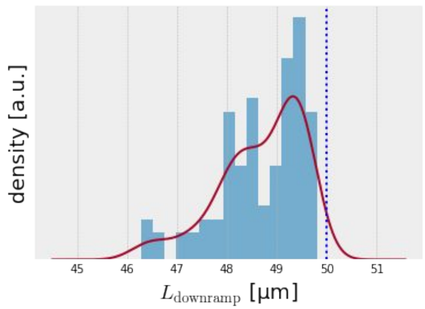




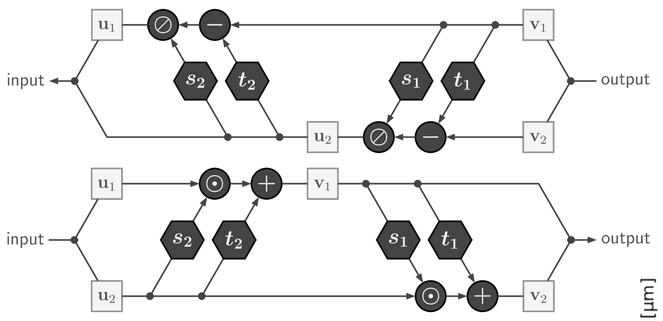


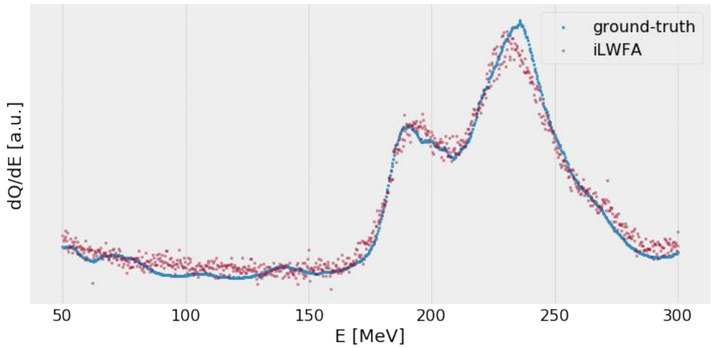


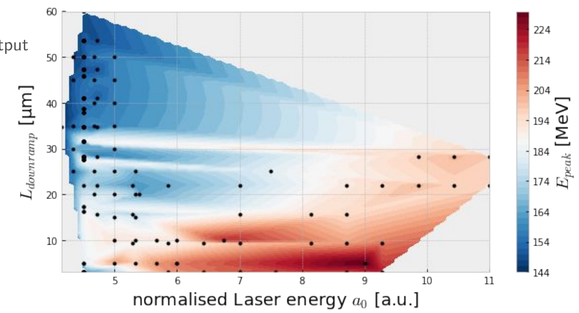


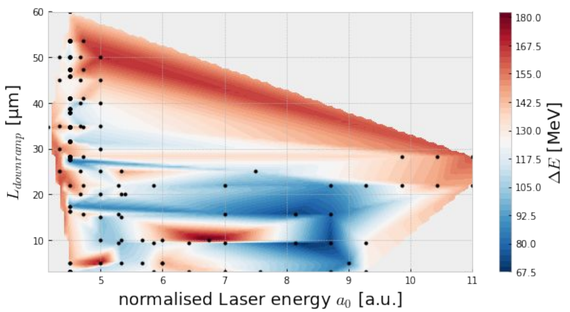
Invertible Neural Network

Coupling Blocks with subnetwoks s/t









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