PIConGPU + X

Building blocks for successful Exascale accelerator simulations

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Plasma-PEPSC Centre of Excellence

PIConGPU

github.com/ComputationalRadiationPhysics/picongpu

picongpu.readthedocs.io

PIConGPU is ready for Exascale

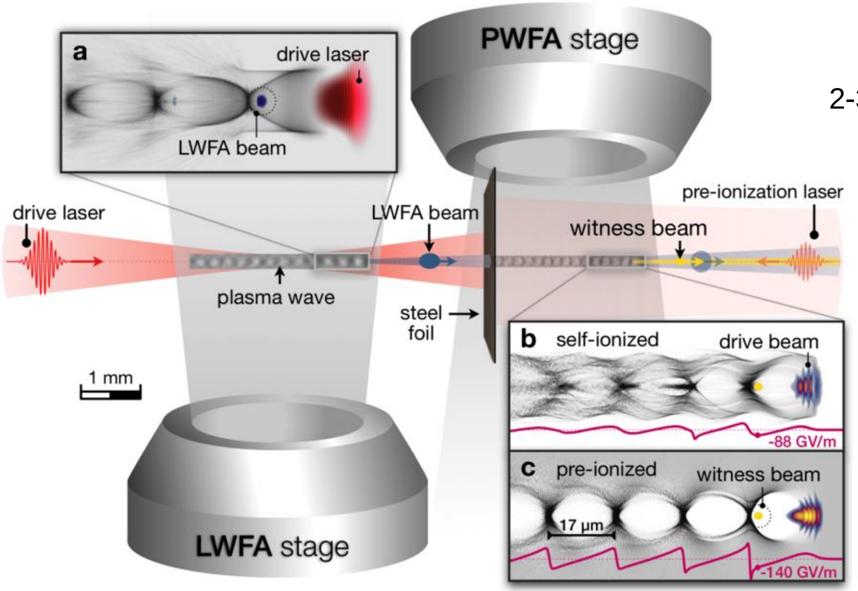
- **Scales up to the largest HPC systems**
- **Performance-portable** via (NVIDIA, AMD, Intel, ARM,...)
- Implements **exascale workflows** for scalable I/O capabilities, such as streaming, data reduction and visualization workflows.

Experiments usually do not have an exascale system nearby…
How do we leverage the power of exascale computing?

HZDR
HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

From laser-plasma accelerator experiments to digital twins

tightening the links by synthetic diagnostics and experimental data reconstruction



~50-100 simulations
2-3 sims per week on 200 GPUs

PIConGPU

Experimental data reconstruction

Synthetic diagnostics & surrogate models

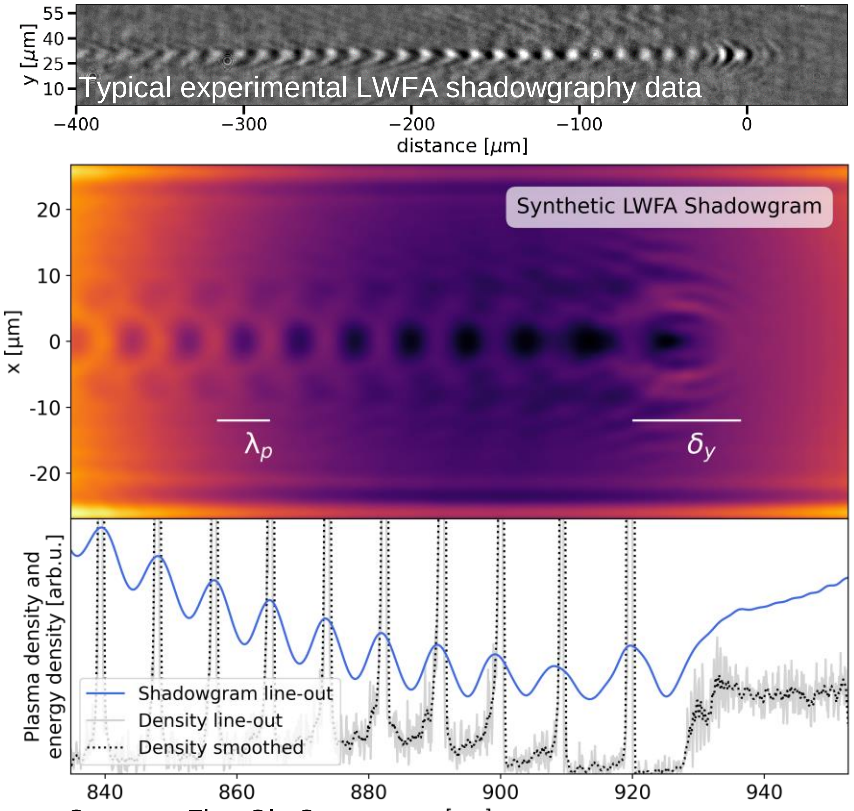
Hybrid LWFA+PWFA accelerator experiment

Large-scale start-to-end simulations

"Matching" the large parameter space of complex experimental designs to simulations needs to be understood and further constrained.

In-situ synthetic diagnostics give insights into the plasma dynamics
Acquire shadowgraphy images for comparison to experiment

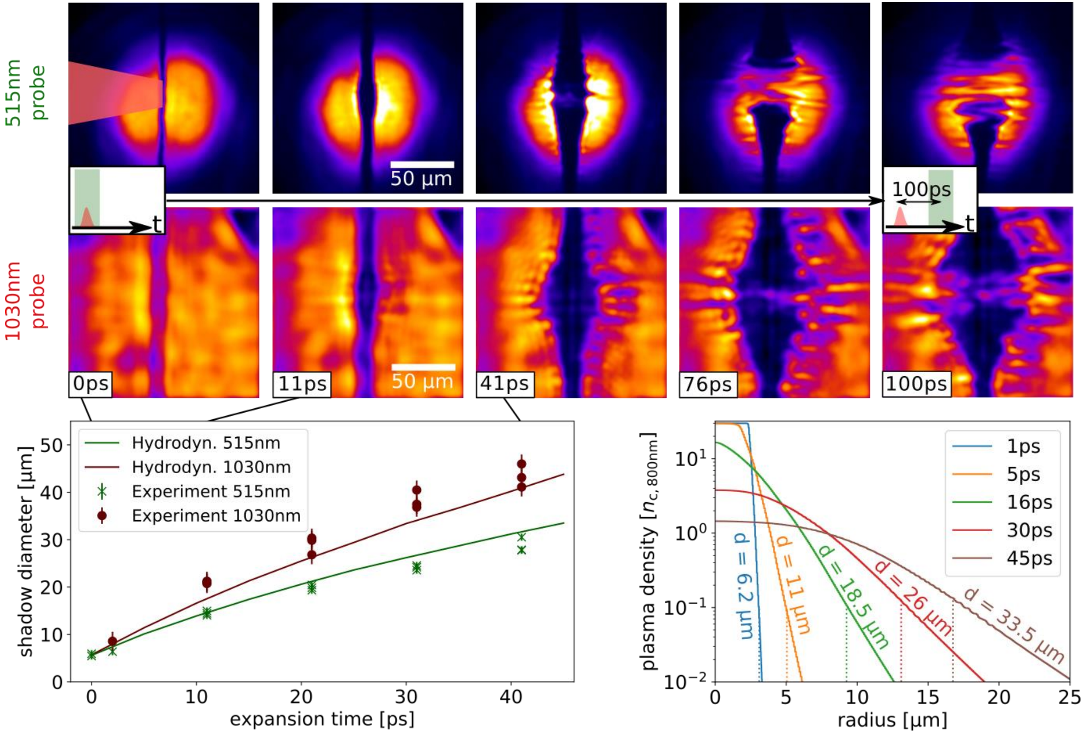
PIConGPU



Courtesy: Finn-Ole Carstens

- Probe laser is simulated directly within PIC simulation
- Propagation to camara modeled in-situ
  by a plugin, i.e. no post-processing needed.
- First results already show characteristics not observed
  in static simulations (e.g. from strong fields or relativistic particles)

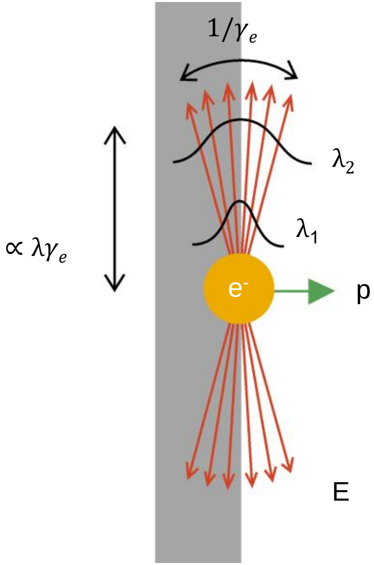
In-situ synthetic diagnostics give insights into the plasma dynamics
Acquire shadowgraphy images for comparison to experiment



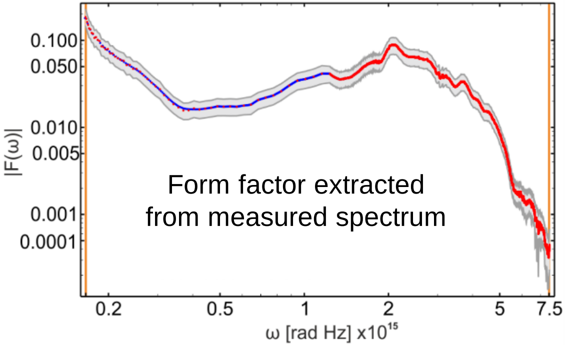
Courtesy: Constantin Bernert

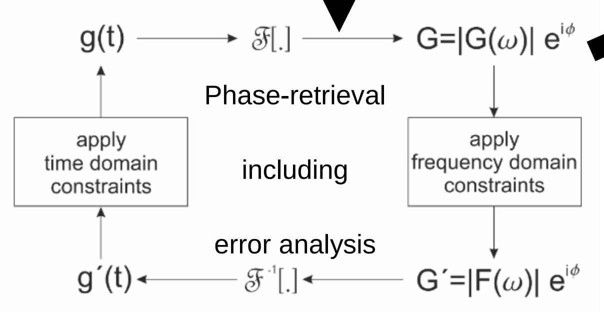
- Synthetic, in-situ shadowgraphy diagnostics enable analyzing expansion measurements of time-resolved shadowgraphy at near-critical hydrogen jet targets.
- PIC simulations need to ensure correct initial conditions for ion acceleration. In-situ synthetic shadowgram diagnostics now can check for consistency with experiment.

Experimental data reconstruction to infer the longitudinal electron bunch profile from measured CTR spectra

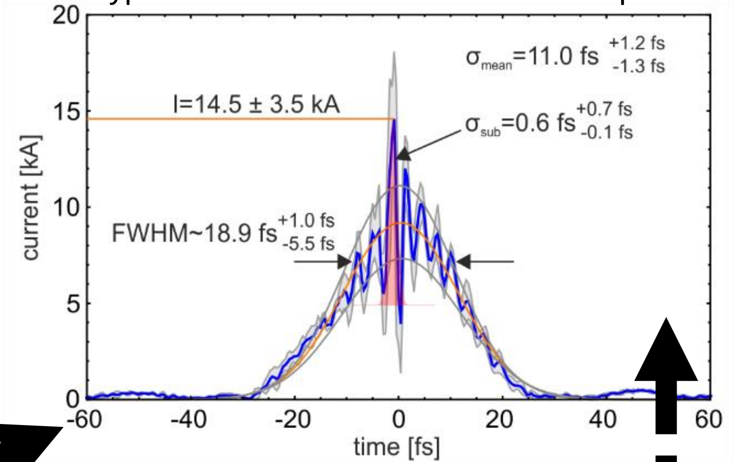


metal foil



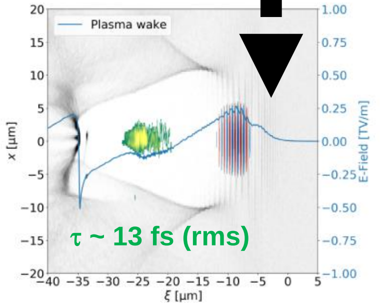


Typical reconstructed electron bunch profile



Electron bunch length agrees with 3D-PIC simulations

PIConGPU

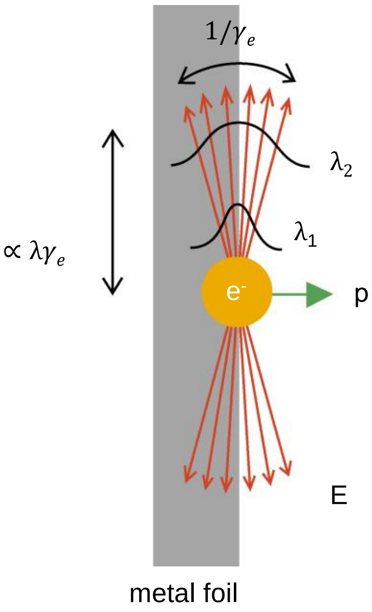


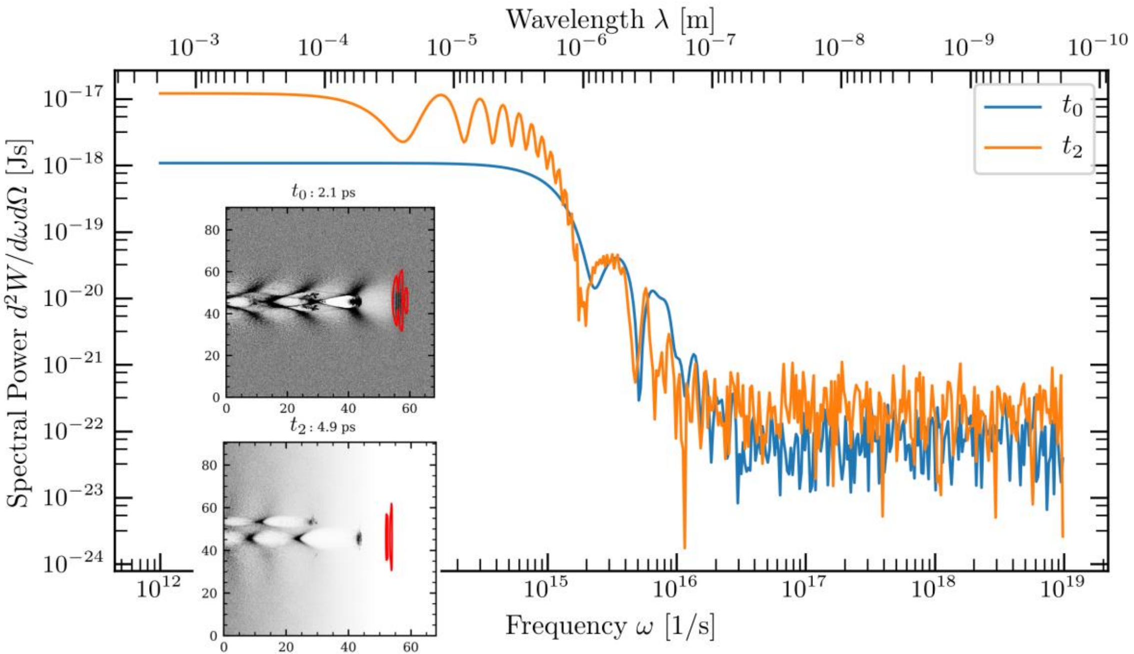
alpaka

Zarini *et al.* (2021), Phys. Rev. Accel. Beams 25, 012801

Synthetic in-situ diagnostics in PIConGPU

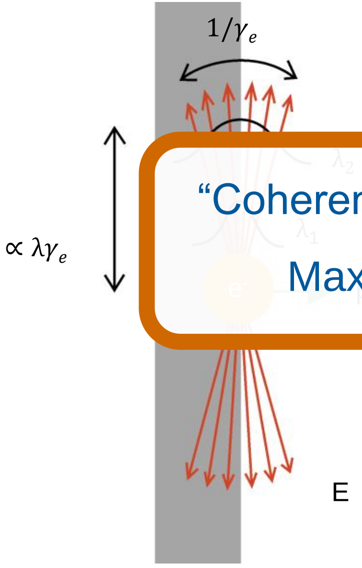
to simulate the measured CTR spectrum

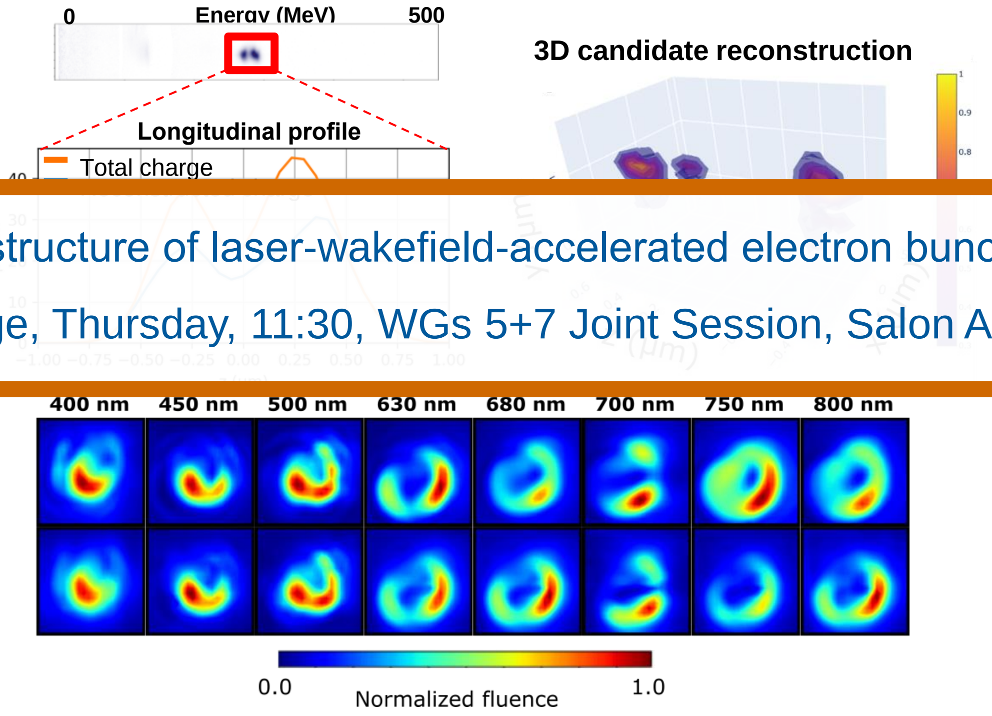




Allows for direct comparison with non-reconstructed measured CTR data.
Provides high-quality data for testing & refining reconstruction routines.

Good longitudinal and transverse coherent transition data
is key to revealing 3D electron beam structures on a µm and fs scale





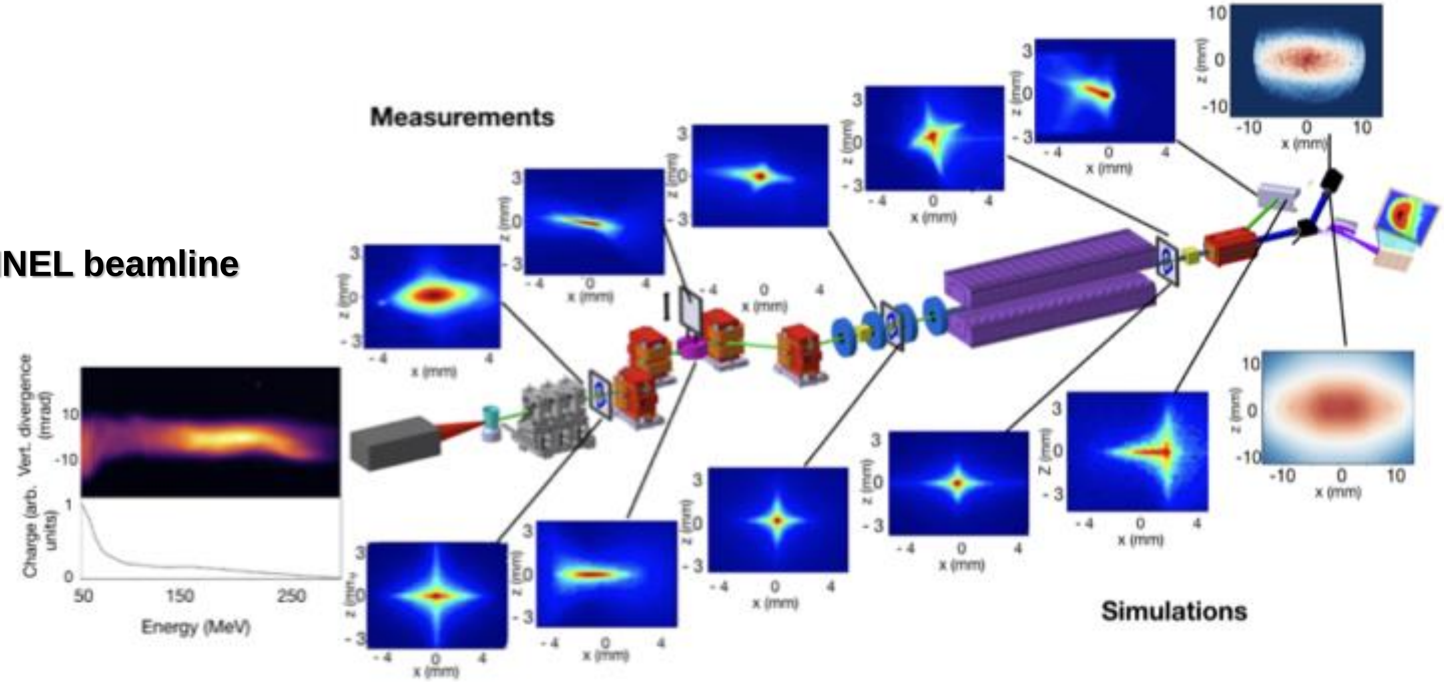
"Coherent 3D microstructure of laser-wakefield-accelerated electron bunches"

Maxwell LaBerge, Thursday, 11:30, WGs 5+7 Joint Session, Salon A

Data-driven Digital Twin of Free Electron Laser

Surrogate models can provide close to real-time feedback during experiment

COXINEL beamline

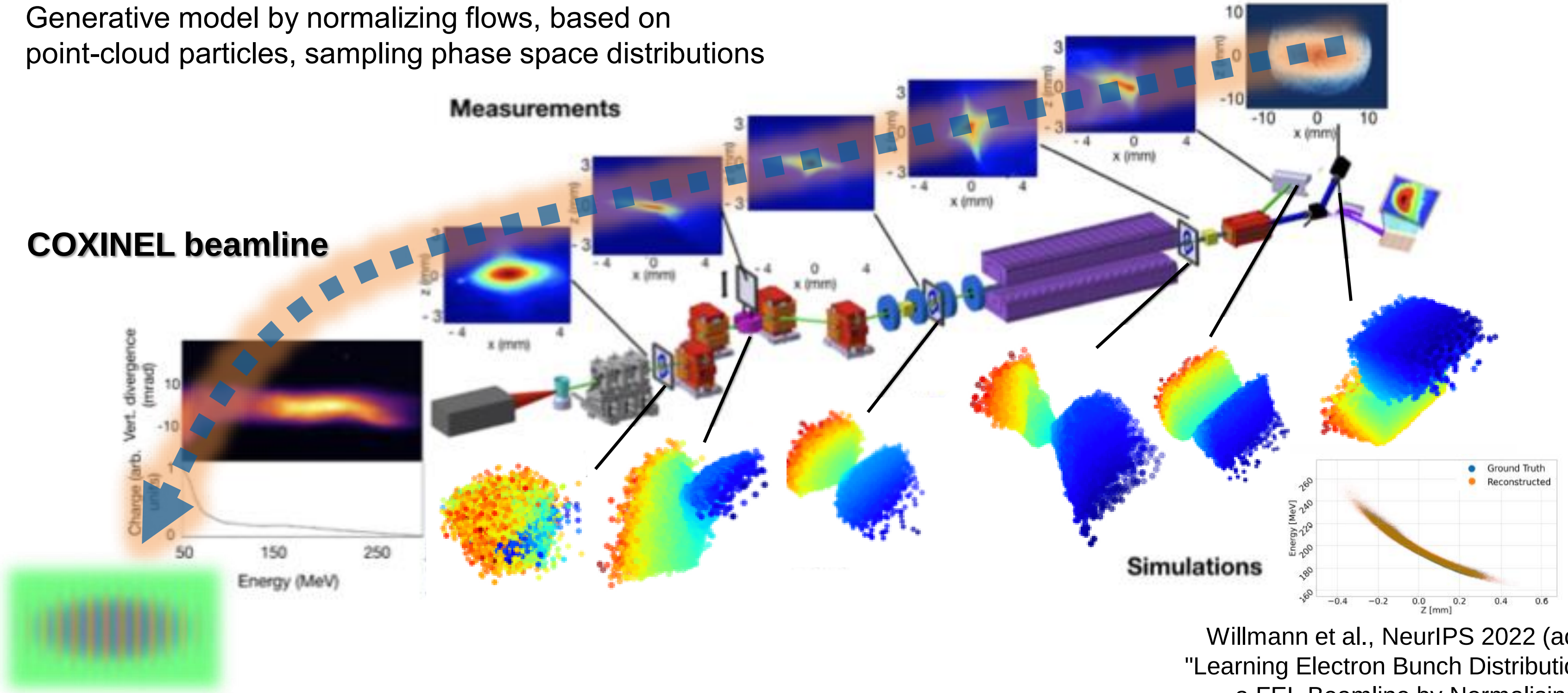


SOLEIL @ HZDR, COXINEL collaboration

Fig: Couprie *et al* 2020 *J. Phys.: Conf. Ser.* **1596** 012040)

Data-driven Digital Twin of Free Electron Laser
Surrogate models can provide close to real-time feedback during experiment

- Surrogate model of COXINEL FEL beamline at HZDR
- Generative model by normalizing flows, based on point-cloud particles, sampling phase space distributions

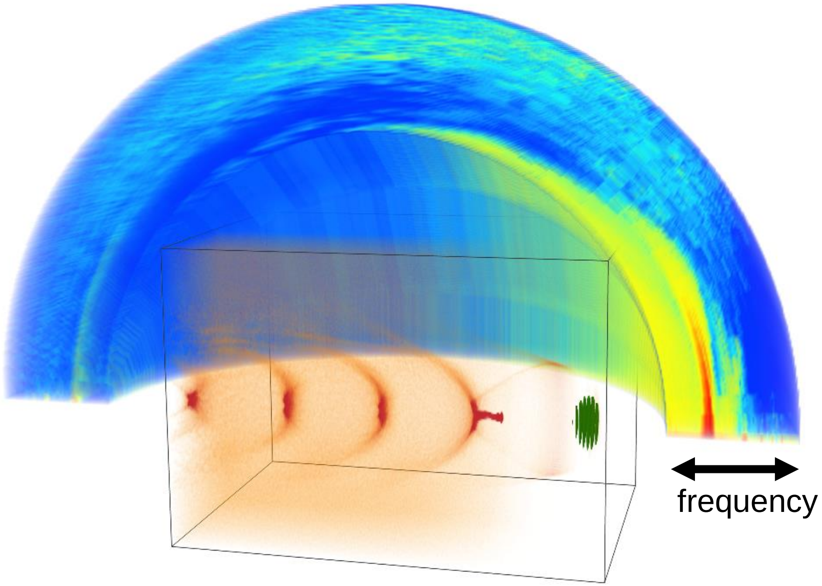


Willmann et al., NeurIPS 2022 (accepted) "Learning Electron Bunch Distribution along a FEL Beamline by Normalising Flows"

Fig: Couprie *et al* 2020 *J. Phys.: Conf. Ser.* **1596** 012040)

An exascale knowledge extraction challenge:

What is the physics origin of emitted plasma radiation by LWFA?



Radiation simulations are computationally very expensive!

- 512 frequencies IR-VIS-UV
- 250 virtual observers on half-dome
- Computed for ~10^9 particles at each time step
- **Over 20x more compute intensive than simulation without radiation**

Courtesy: Richard Pausch

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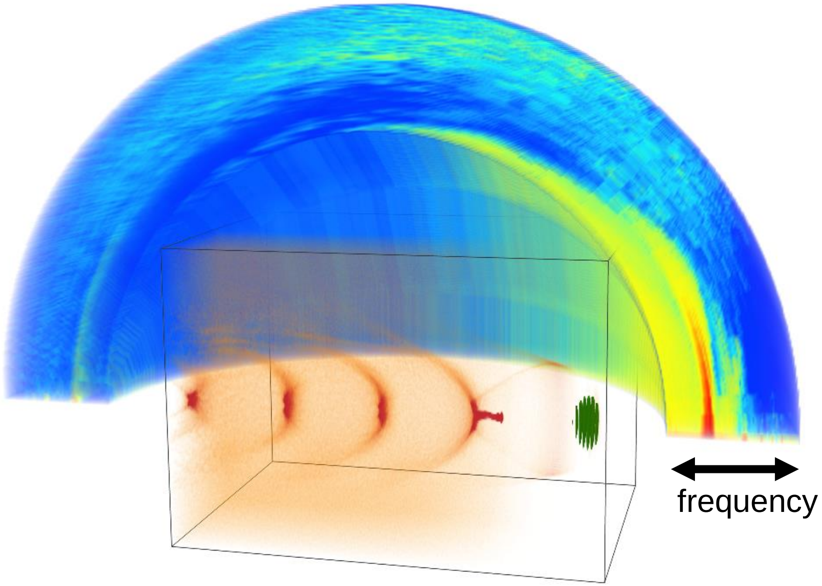
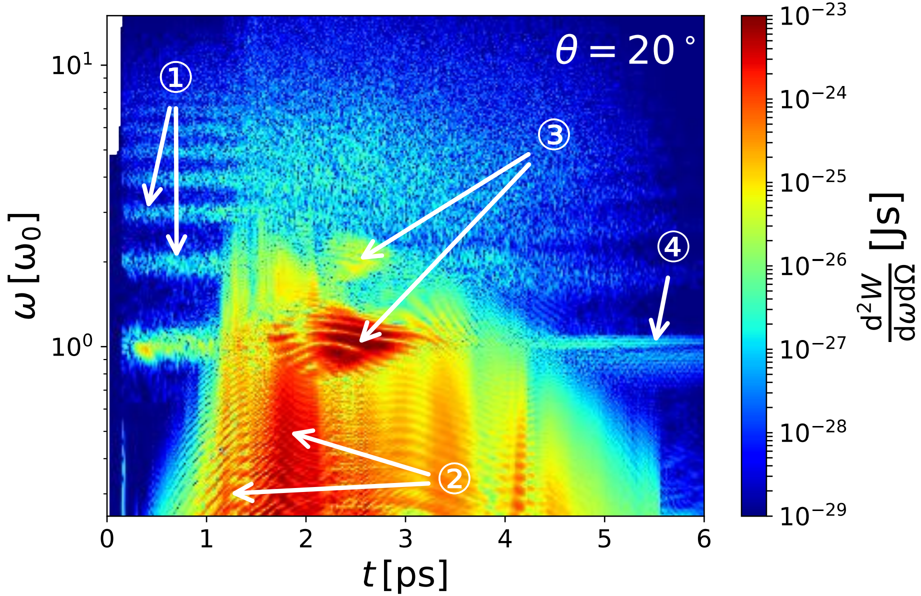


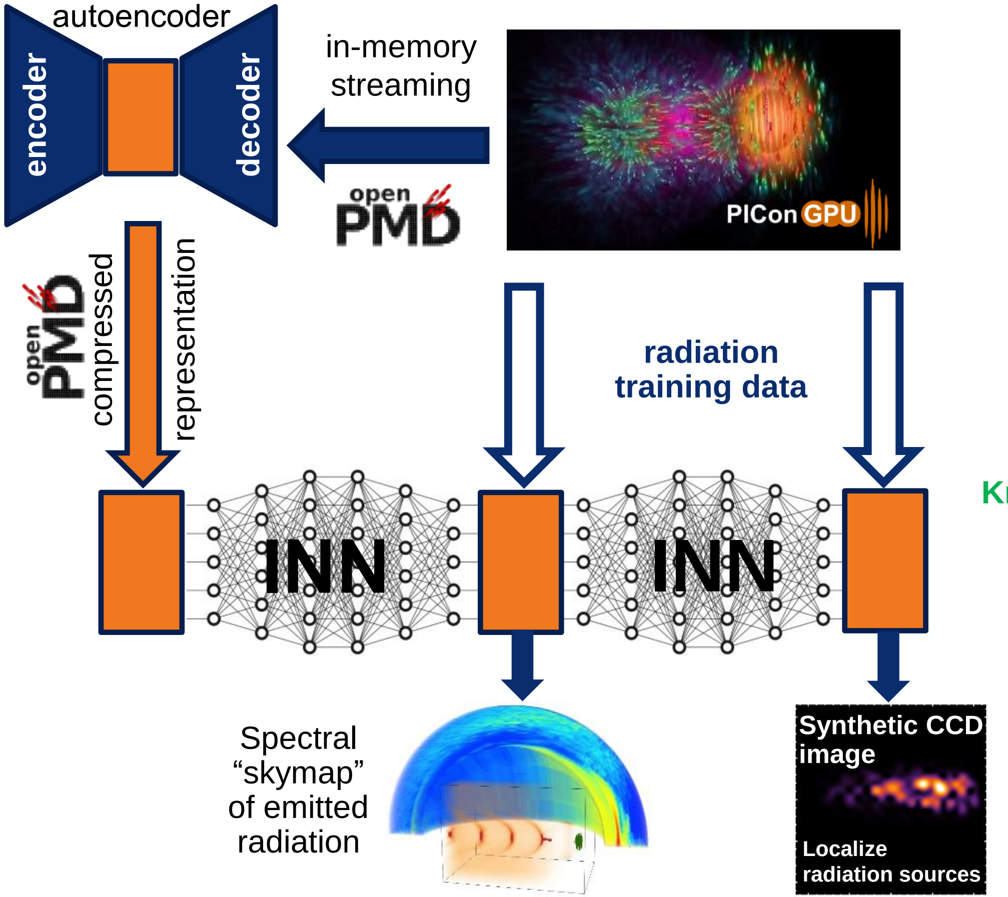


Current state-of-the art of knowledge extraction:
PhD student brain power and running lots of reduced-model simulations.

Courtesy: Richard Pausch

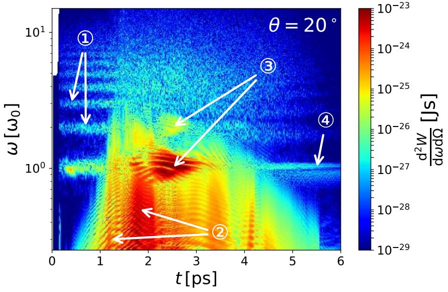
Outlook & vision – Generate surrogate models on exascale machines to infer the physics origin of plasma radiation emissions

Data source from PIConGPU
9D unstructured point-cloud data
For each macroparticle every time step:
Position, Momentum, Acceleration



Knowledge extraction

by exploiting INN inverse mapping



Conclusions

- **PIConGPU is performance portable and scales up to exascale machines (Summit and Frontier).**
  “Matching” the large parameter space of complex experimental designs to simulations needs to be understood and further constrained.

- **In-situ synthetic diagnostics** in particle-in-cell simulations (PIConGPU), such as shadowgraphy, facilitate direct and quantitative comparison to experimental data.

- **Fast inverse-problem solving** including uncertainty quantification requires access to suitable compute resources. Such experiments often start with a lack of high-quality ground truth-data, PIC simulations can provide large quantities of training & test data.

- **Surrogate models** trained by extensive simulations can provide close to real-time feedback during experiment.

LWFA in-situ live visualization using ISAAC on PIConGPU (Felix Meyer)
Helmholtz Best Scientific Image Award 2022 (2nd place)