Portable solutions for Digital Twins
A worst case scenario

Michael Bussmann @ LEAPS Integrated Platform Workshop

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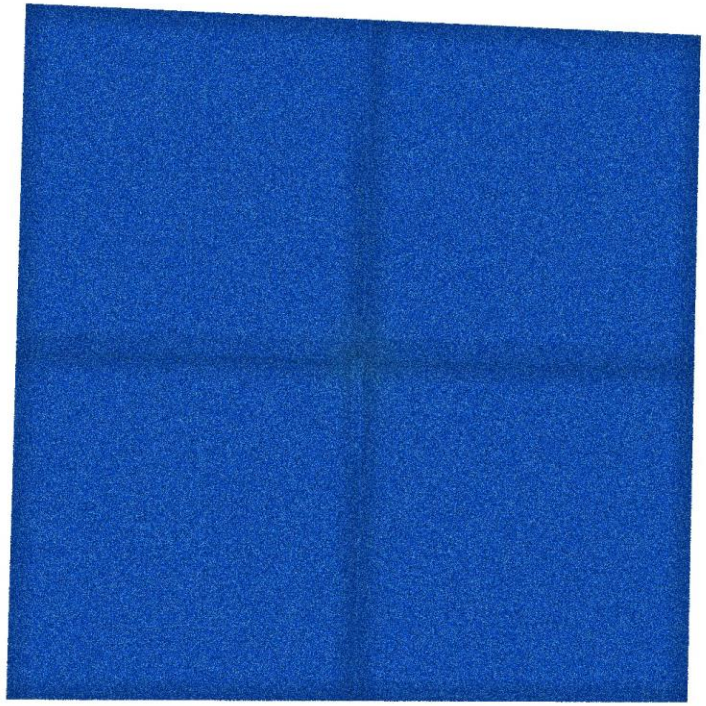
Worst case scenario: Plasma Accelerators for Electron Beams

When your machine is your experiment

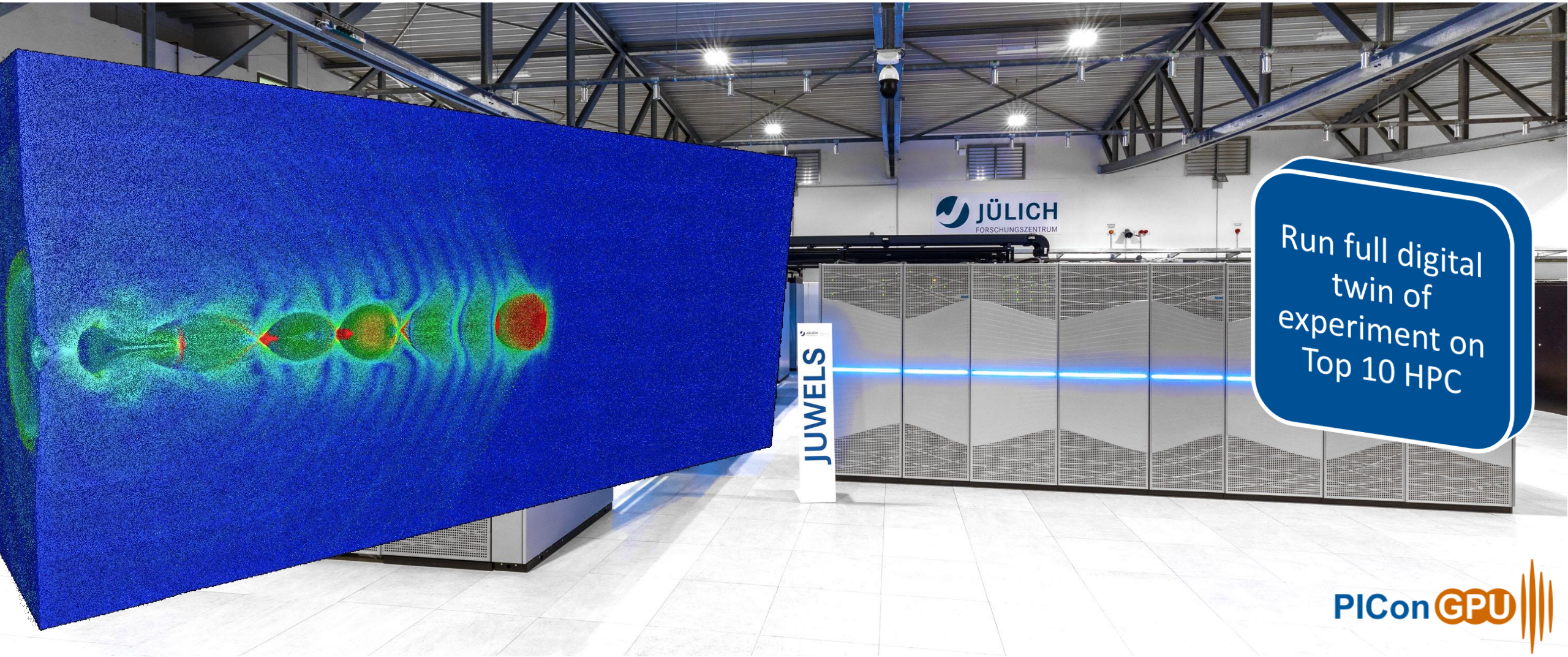
- **Compact** setup (cm long plasma)
- **Driver** is either a laser or a particle beam
- **Special:** Low transverse emittance, fs, nC, GeV
- **Challenge 1:** Highly nonlinear
- **Challenge 2:** fs diagnostics & control needed
- **Challenge 3:** Scalability



PIConGPU ► OCELOT ► GENESIS

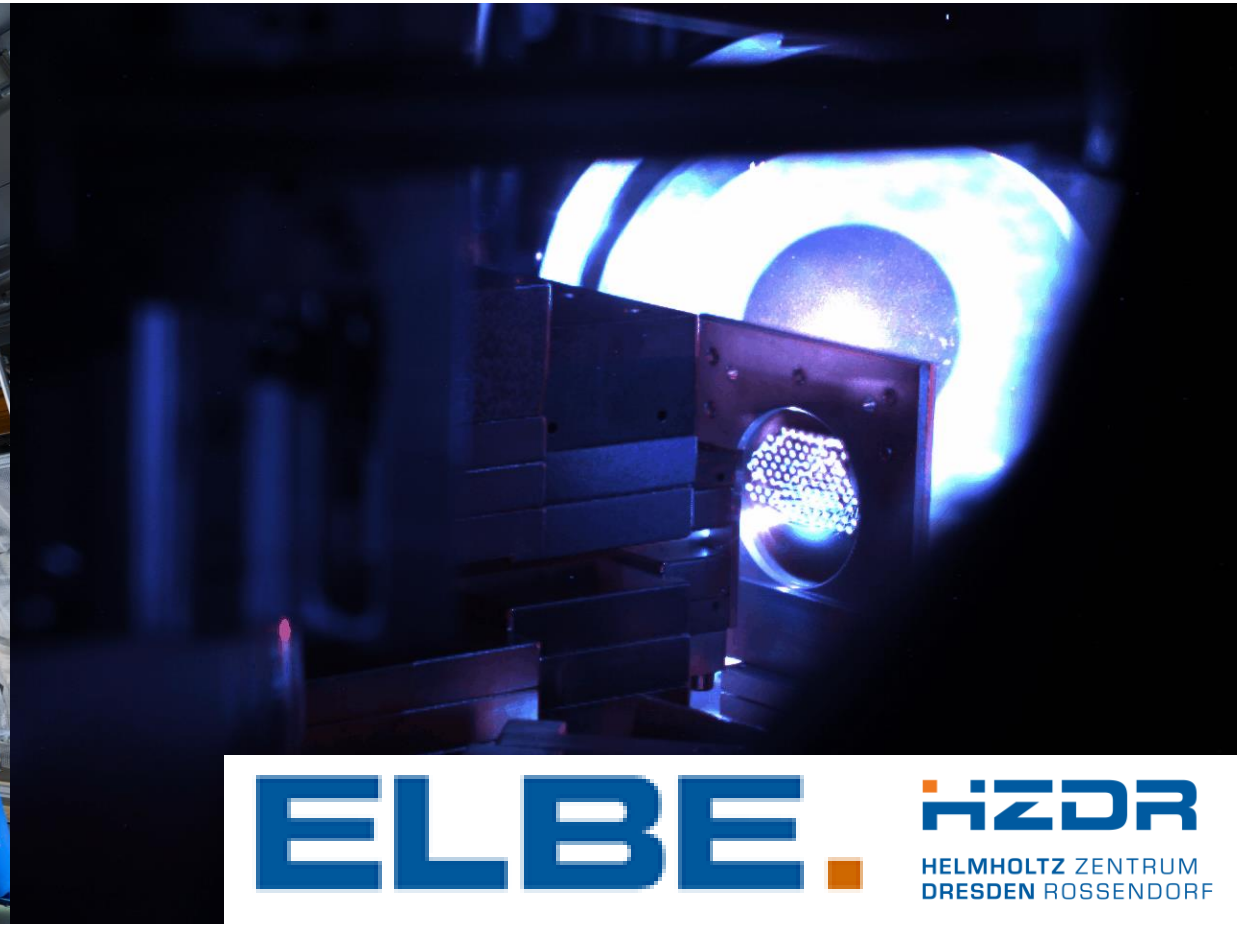
Digital Twins of Plasma Accelerators for Electron Beams

Use Europe's largest Supercomputers

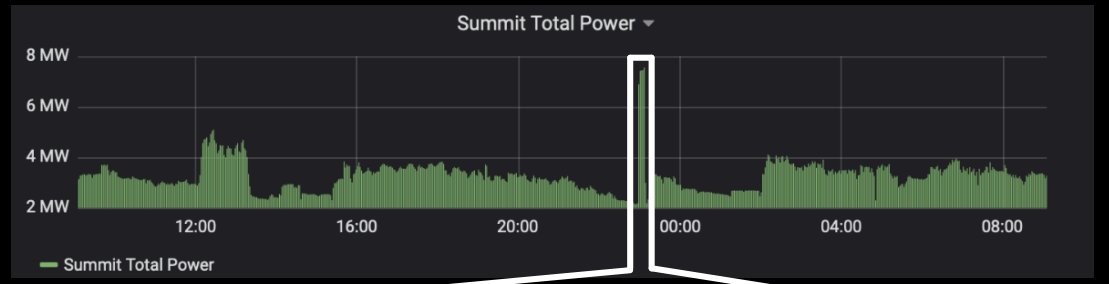


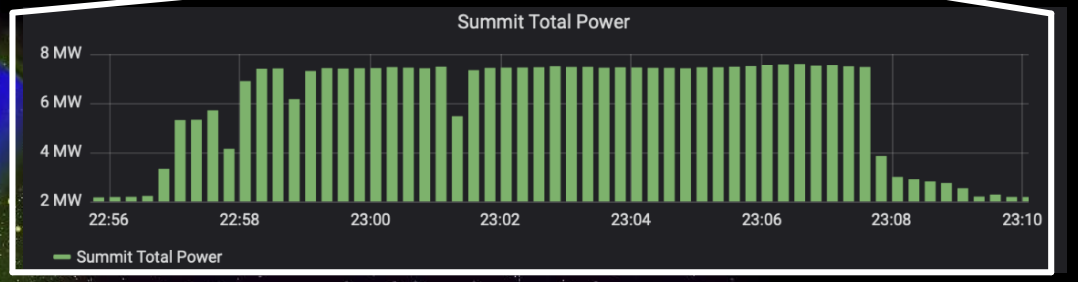
Beyond worst case scenario: Plasma Accelerators for Ion Beams

Helmholtz International Beamline for Extreme Fields @ HED/EUXFEL



Simulations on Summit
10 Trillion (10^{13}) Particles
400 Billion (4×10^{11}) Cells
27600 GPUs



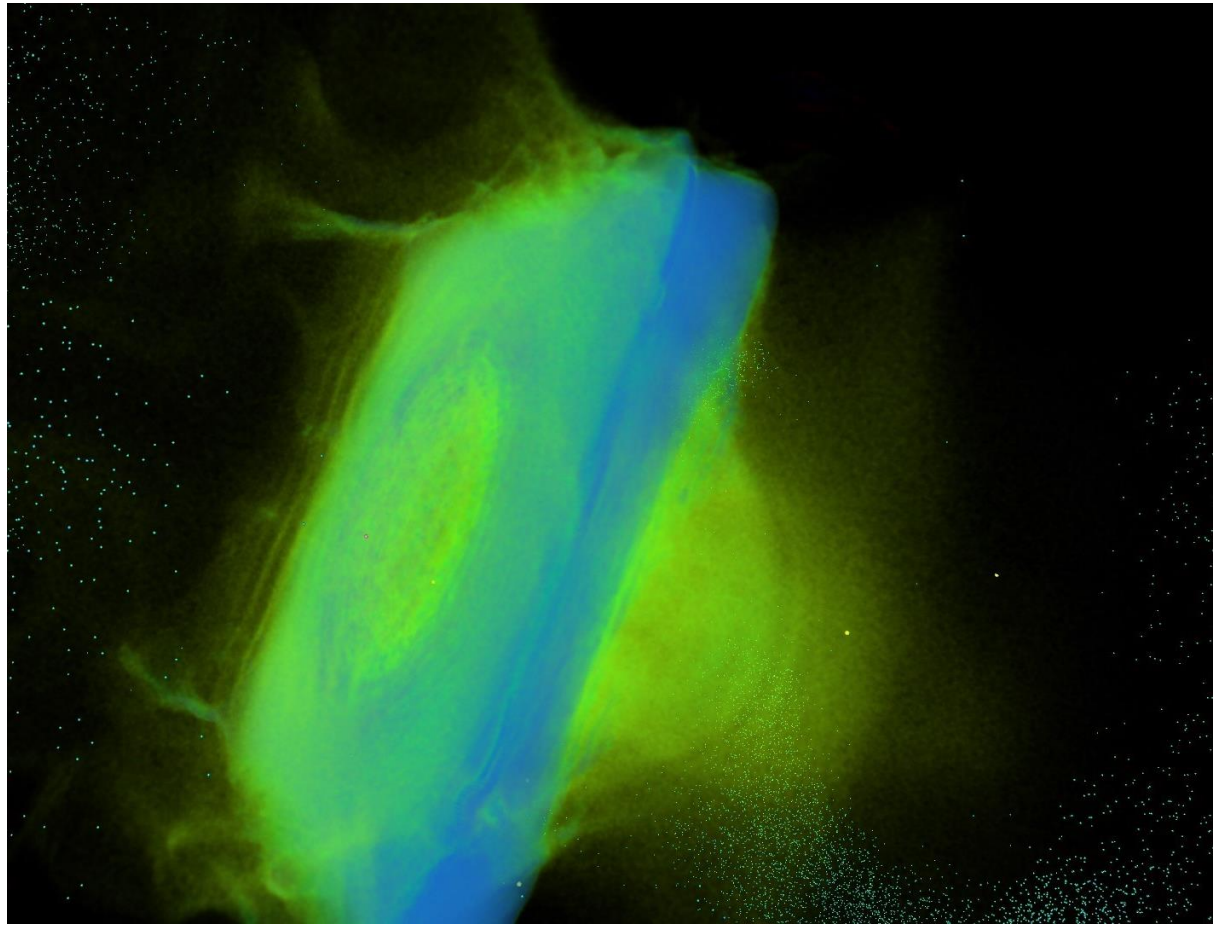


PIConGPU ISAAC

Beyond worst case scenario: Plasma Accelerators for Ion Beams

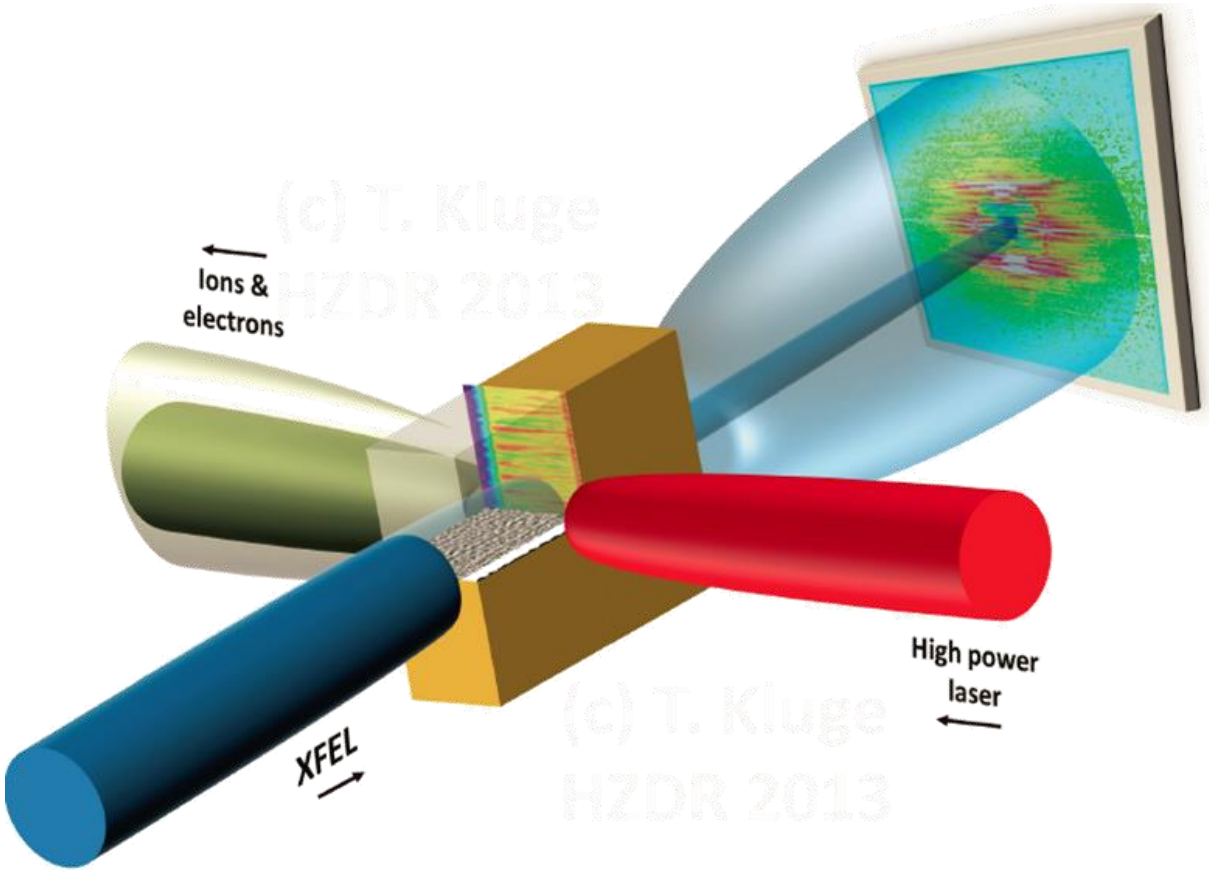
A highly nonlinear, dynamical system with o(Avogadro) particles

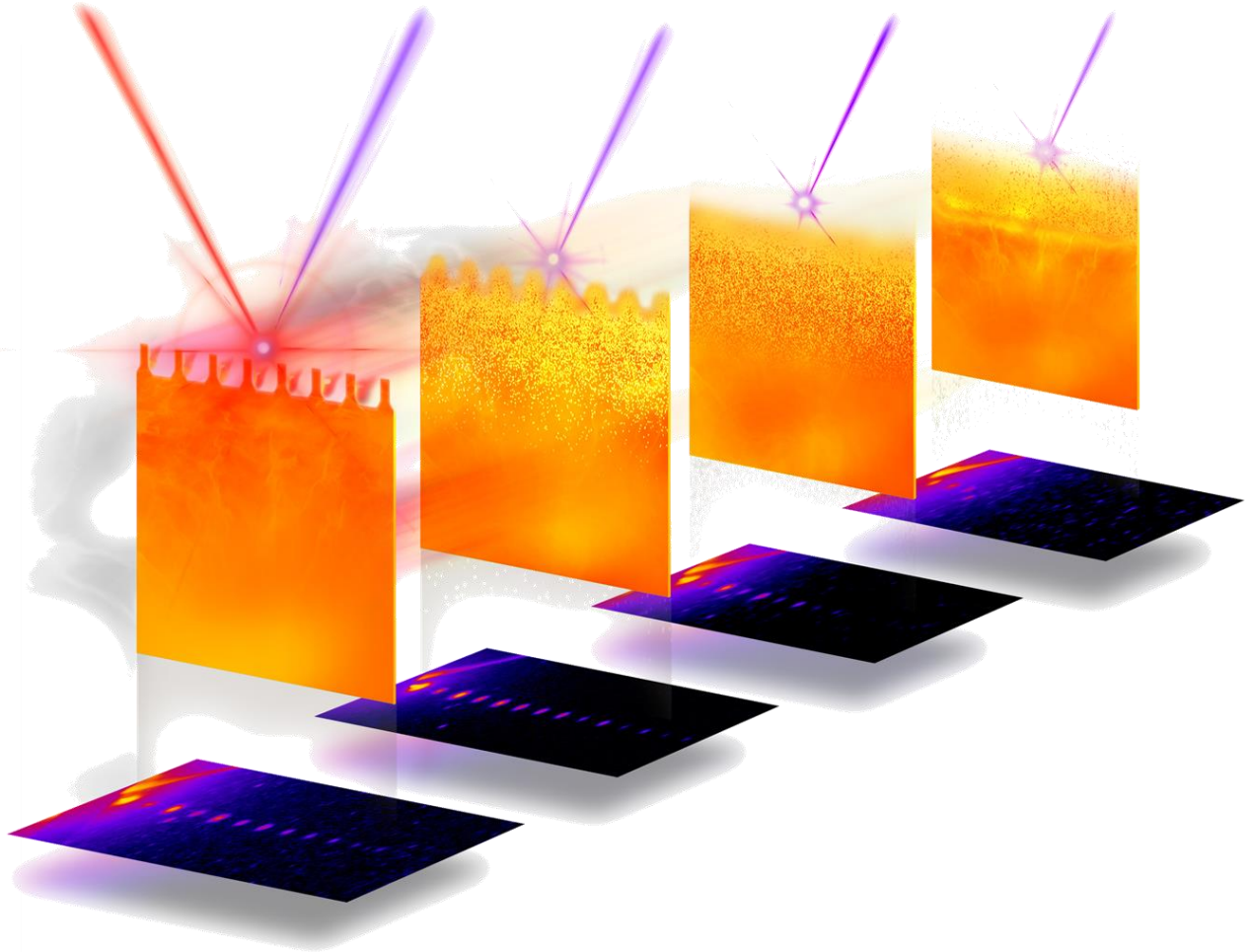
- **Solid density**
- **Atomic** time & length scales
- **Dynamic, transient** plasma
- **Radiation transport** + Background
- **Experimental Reproducibility** low
- **Initial parameters** not well known
- **Multi-modality** diagnostics needed



Using the European XFEL & HIBEF as a Microscope

Studying Plasma Accelerators for Ion Beams at the atomic Level





Recreating Experiments virtually via Digital Twins

X-ray Laser, complex System, Scattering and Detectors simulated

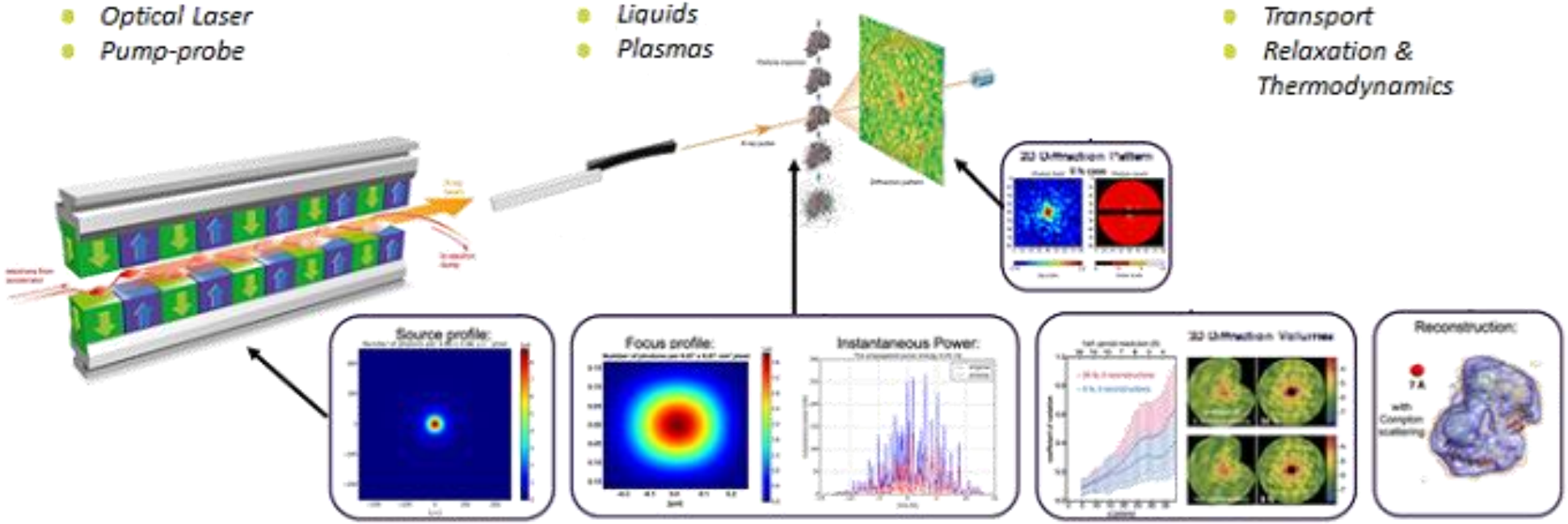
Photon Source
- XFEL
- Synchrotron
- Optical Laser
- Pump-probe

Photon Waveguide
- Lenses
- Mirrors

Target/Sample
- Single particles
- Solids, surfaces
- Liquids
- Plasmas

Detection
- Spectroscopy
- Imaging

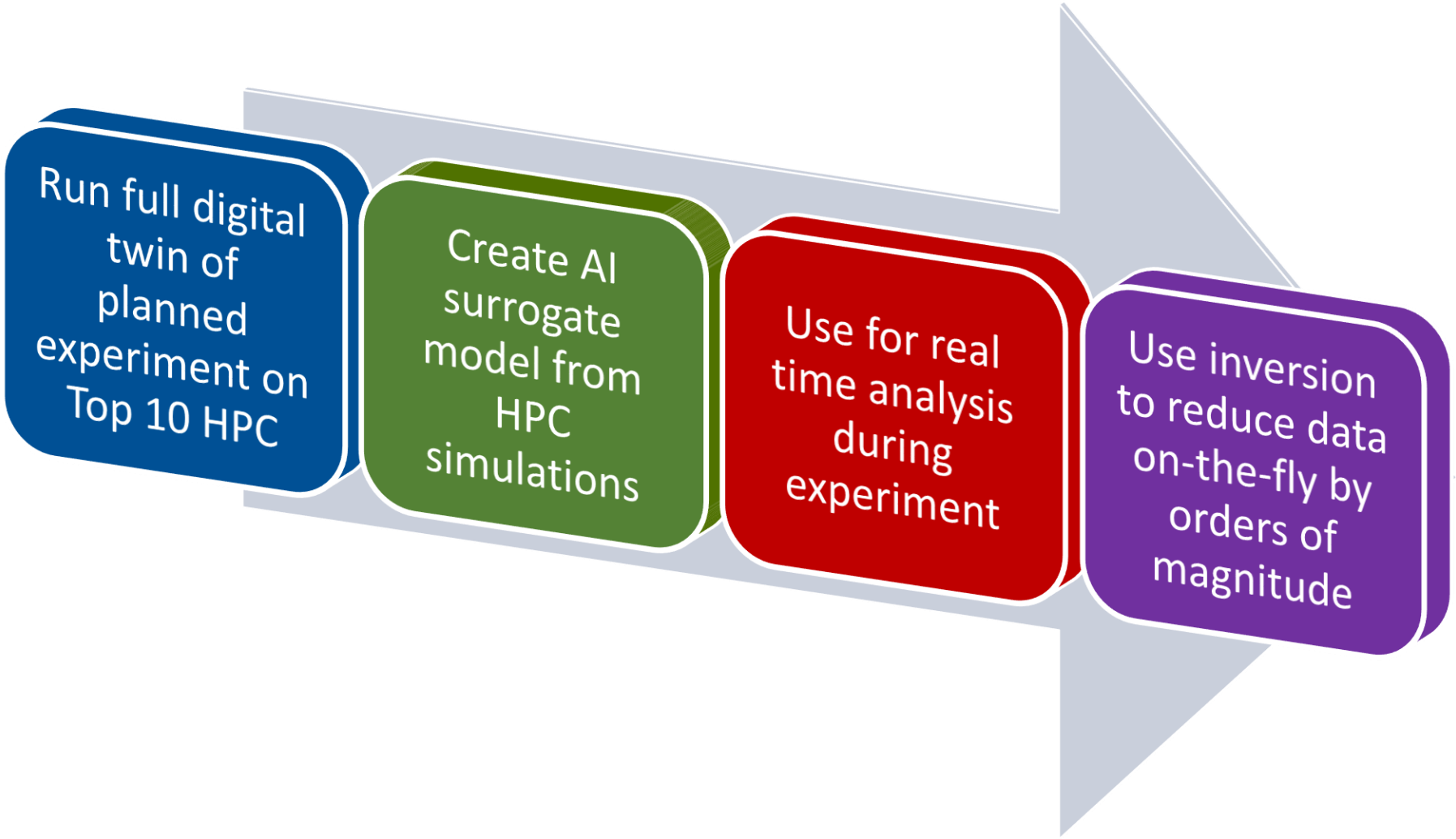
Photon Data Analysis
- Structure determination
- Electronic structure
- Transport
- Relaxation & Thermodynamics



SimEx (see Talk by Juncheng E)

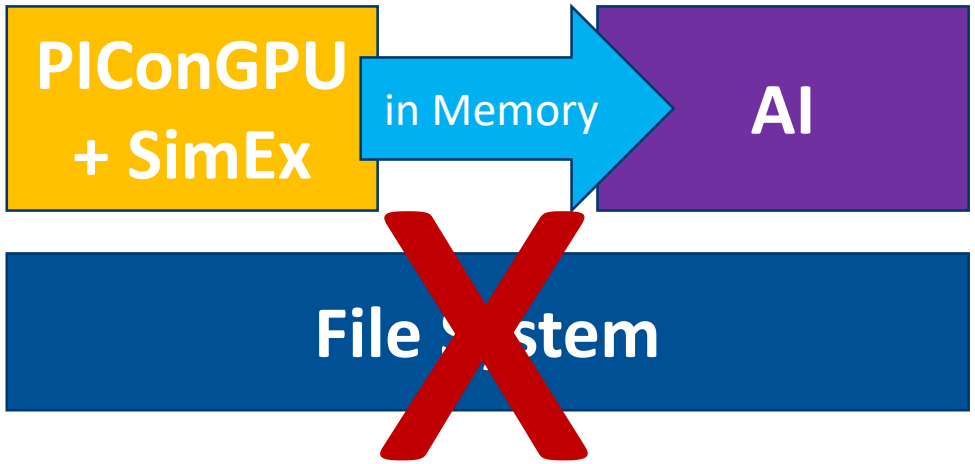
This is the way

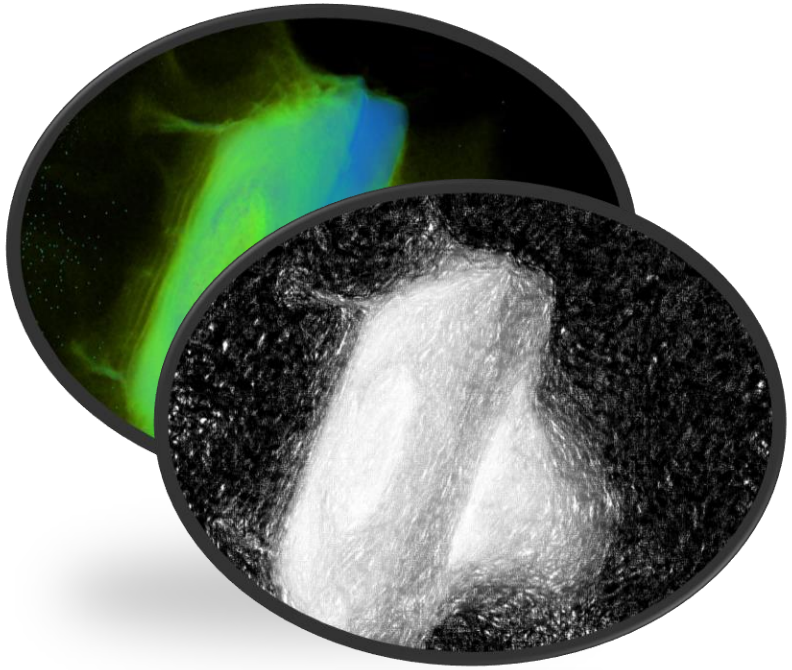
Towards full Digital Twins of Laser Plasma Accelerators



Digital Twins and AI on Top 10 HPC Systems

Coupling a full Digital Twin to large-scale AI for in-Memory Learning





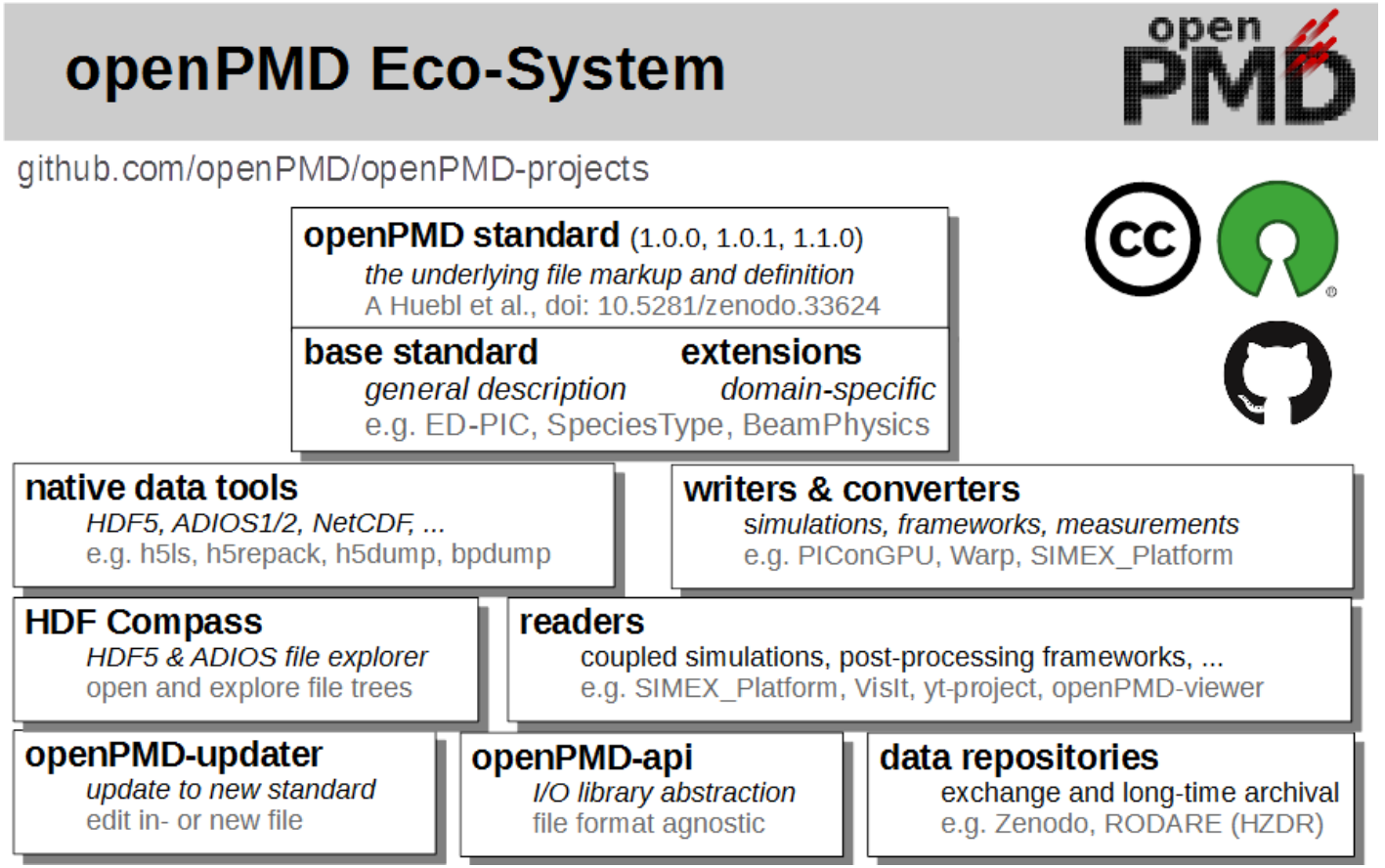
Create AI surrogate model from HPC simulations

Exascale F.A.I.R. Workflows

Open & F.A.I.R high performance I/O coupling with openPMD

The openPMD Standard:

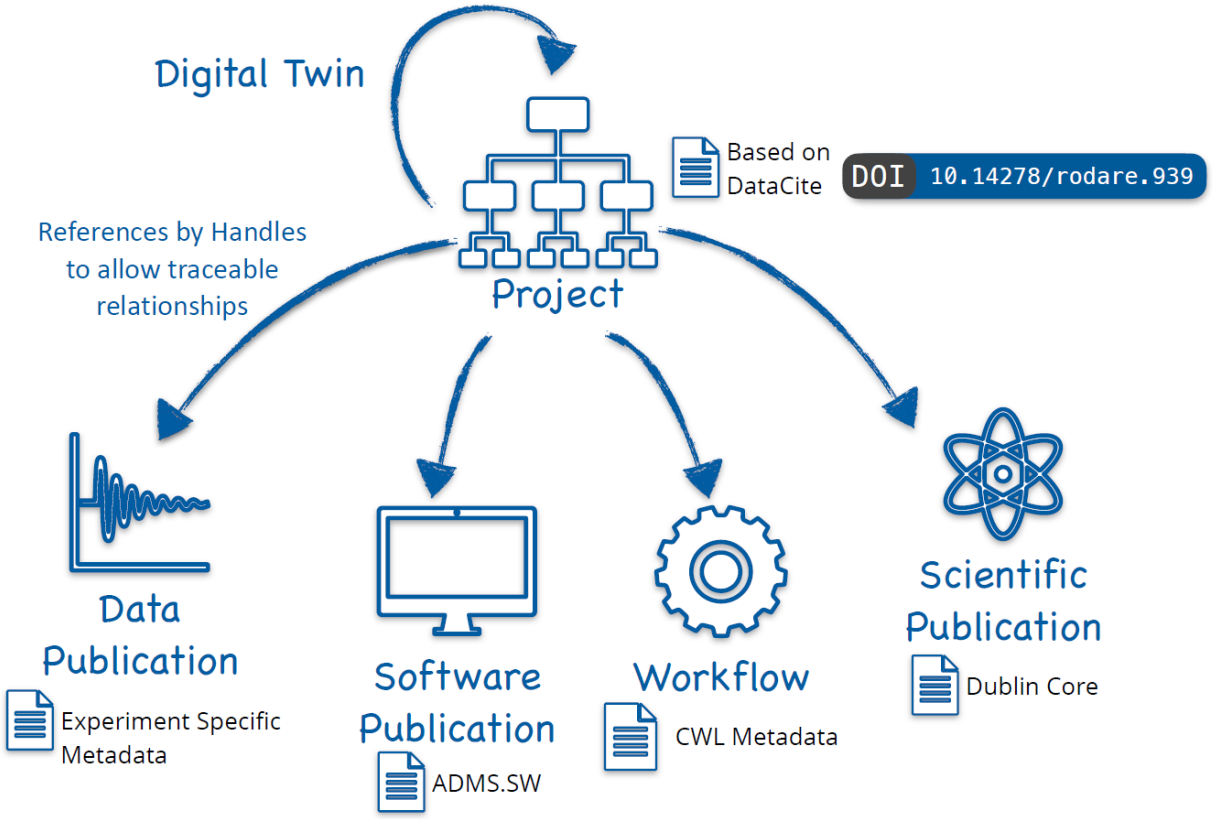
- **Open** standard
- **Self-describing**
- Particle + Mesh data
- **Exascale I/O**
- **In-memory** coupling
- **Ecosystem**: API, viewers, analysis, reduction (e.g. phase space), interpolation (e.g. fields)



PIConGPU, WarpX, FBPIC, SMILEI, SimEx, Ocelot, Paraview, ...

Without Metadata on Workflows we are lost

HELIPORT as a step towards F.A.I.R. Digital Twins

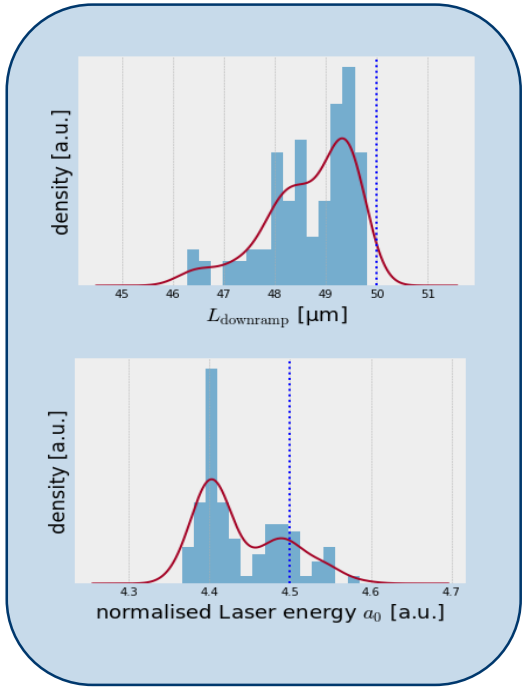


HELIPORT HELmholtz Scientific Project WORkflow PlaTform

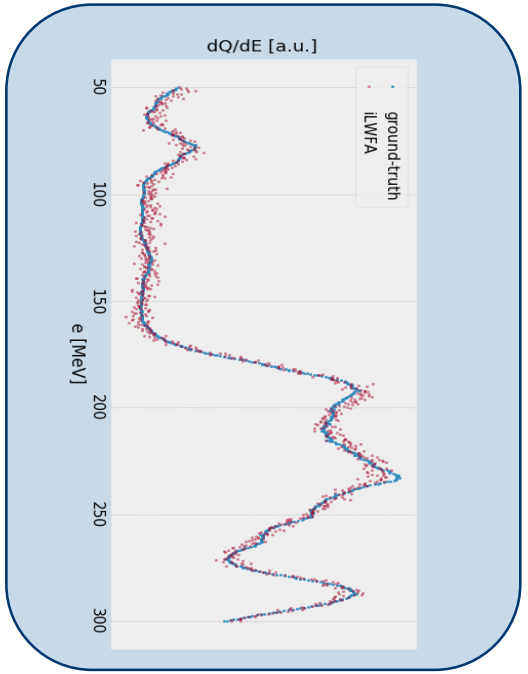
See talk by Oliver Knodel

Digital Twins and AI on Top 10 HPC Systems

Creating Surrogate Models of Plasma Accelerators using AI



Invertible Neural Network



Benefits

- Recover ambiguous mapping
- Uncertainty quantification

Inputs:
Laser Energy
& Plasma Profile

Output:
Particle Energy Spectrum

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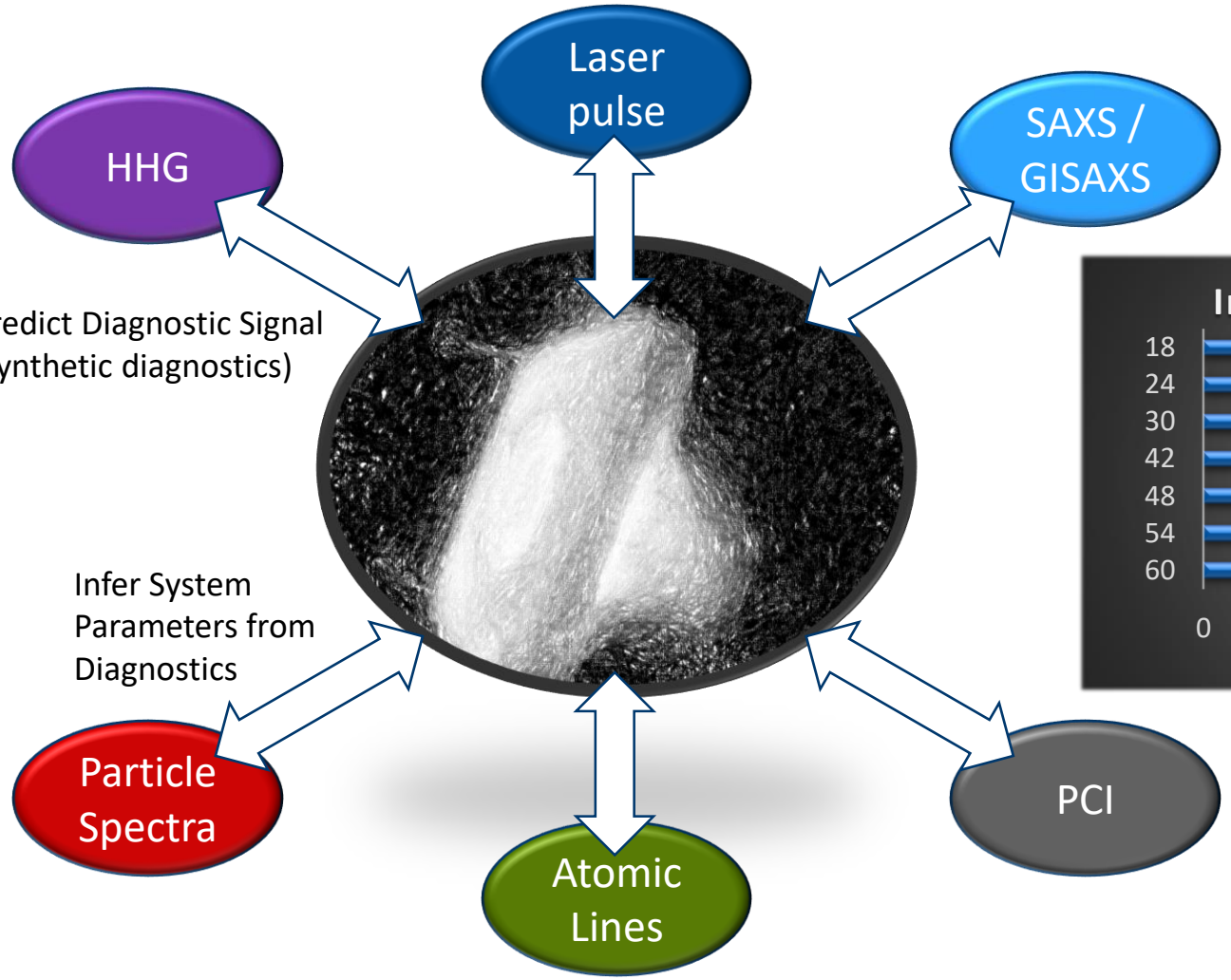
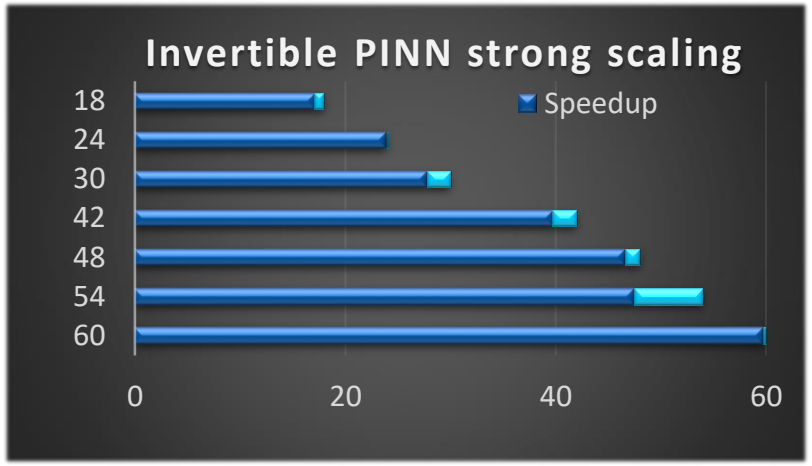
Surrogate Models of Experiments

AI real time Digital Twin Operations with Invertible PINNs





Use for real time analysis during experiment

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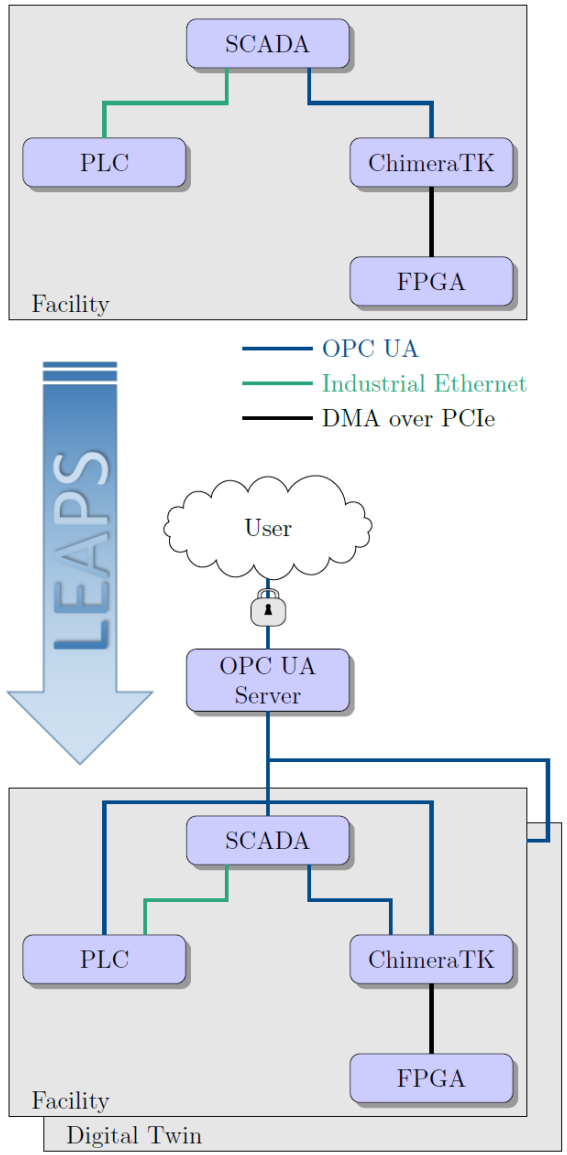
A Digital Twin should be a twin of the machine

OPC-UA — Unified control, info & feedback

LEAPS WG2 WP1 proposal

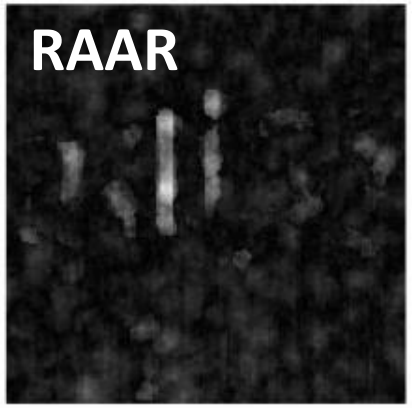
- **Open Standard** for **information modeling** and machine-to-machine **communication**
- Built-in **scalable security & authentication**
- **Industry** standard (e.g. PLC integration)
- **Portable**, platform-independent
- **Testbed** at HZDR ELBE-Facility, evaluated for DALI THz Facility Digital Twin
- **Interface** to ChimeraTK, e.g. for FPGAs

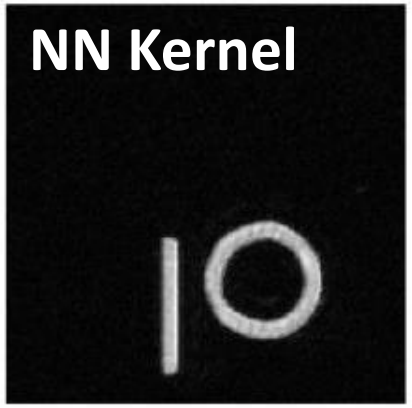


Klaus Zenker
ELBE

Retrieve System Parameters from Experiments in Real Time

AI Phase Retrieval from Small Angle X-Ray Scattering





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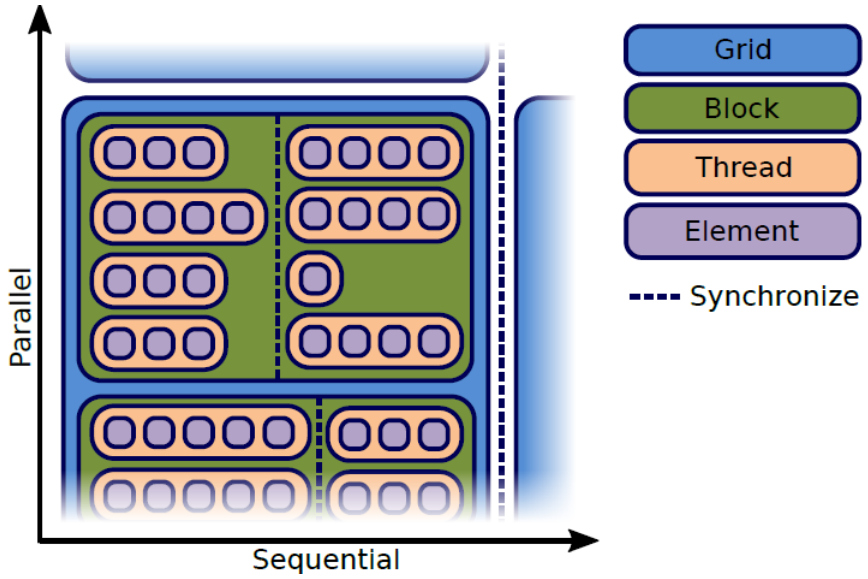
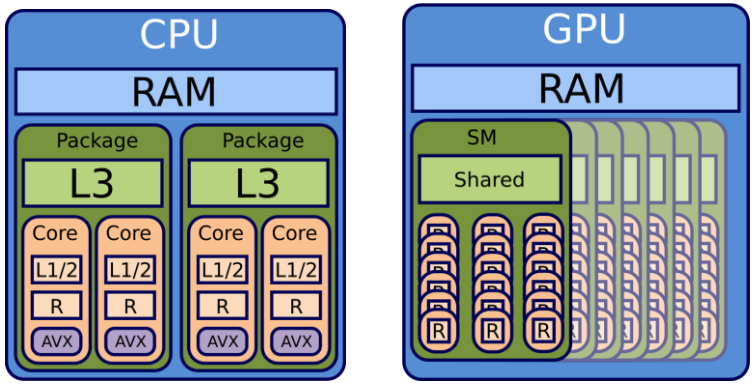
Retrieve System Parameters from Experiments in Real Time

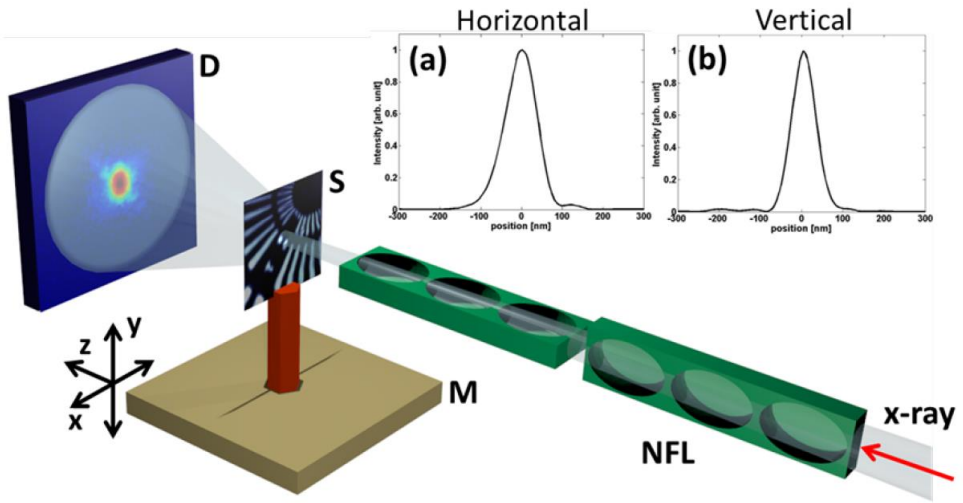
Single-source C++ CPU/GPU/FPGA parallel codes with Alpaka

Alpaka:

- **Single-source** C++
- Parallel
- Multi-Accelerator
- **CPU, GPU, FPGA**
- Portable







DESY ePIE Ptychography Algorithm

This is the way!

Open, portable solutions for Digital Twins

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Exascale Plasma Accelerator Simulations	PIConGPU
In-situ, steerable, live, Tbyte/s visualization	ISAAC
Self-descriptive Exascale I/O and in-memory coupling	openPMD
F.A.I.R. Workflow metadata lifecycle management	HELIPORT HELmholtz Scientific Project WORkflow PlaTform
Photon Science Experiment Digital Twins	SimEx
Invertible, multimodal AI Surrogate Models	HELMHOLTZAI Nico Hoffmann YIG 
Open information modeling & control	OPC UA
Single source parallel code for CPUs, GPUs, FPGAs	alpaka

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