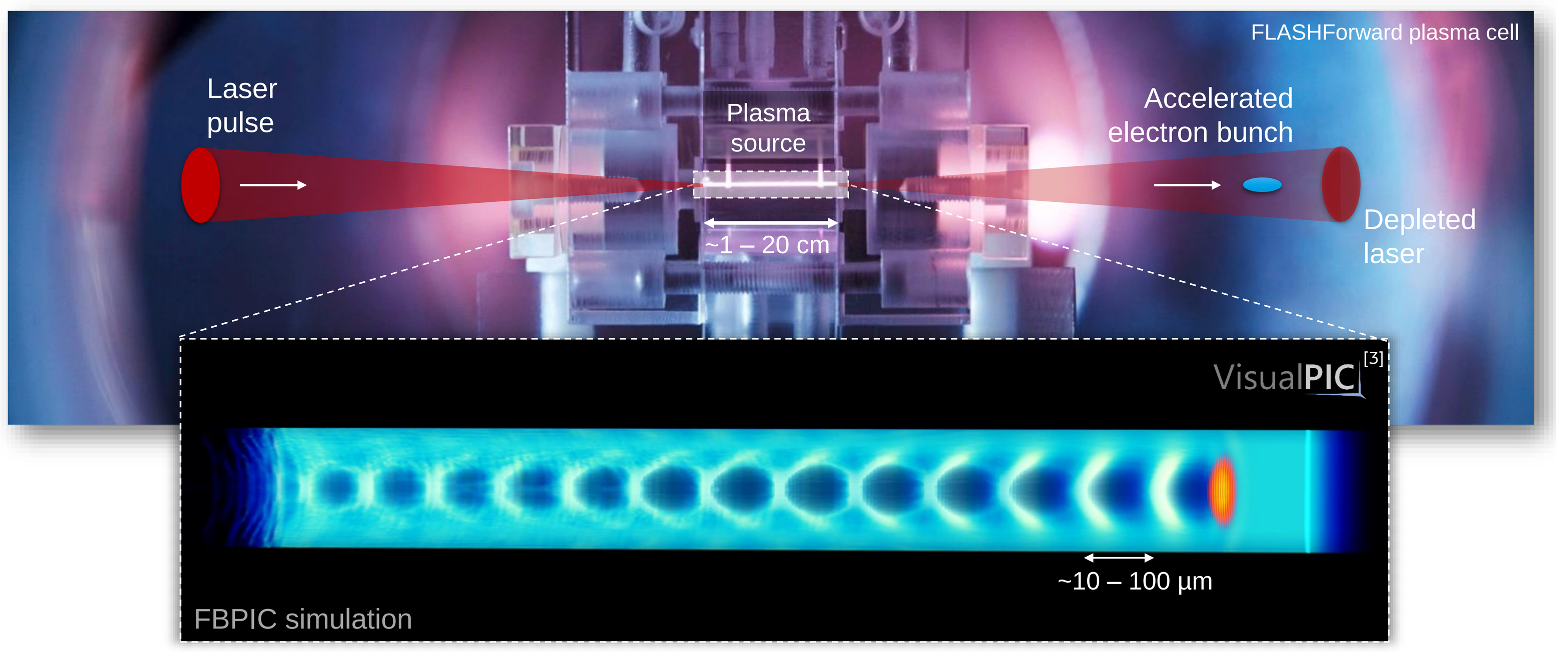
Multitask optimization of laser-plasma accelerators using simulation codes with different fidelities

A. Ferran Pousa [1], S. Jalas [2], M. Kirchen [1], A. Martinez de la Ossa [1], M. Thévenet [1], S. Hudson [3], J. Larson [3], A. Huebl [4], J.-L. Vay [4], R. Lehe [4]

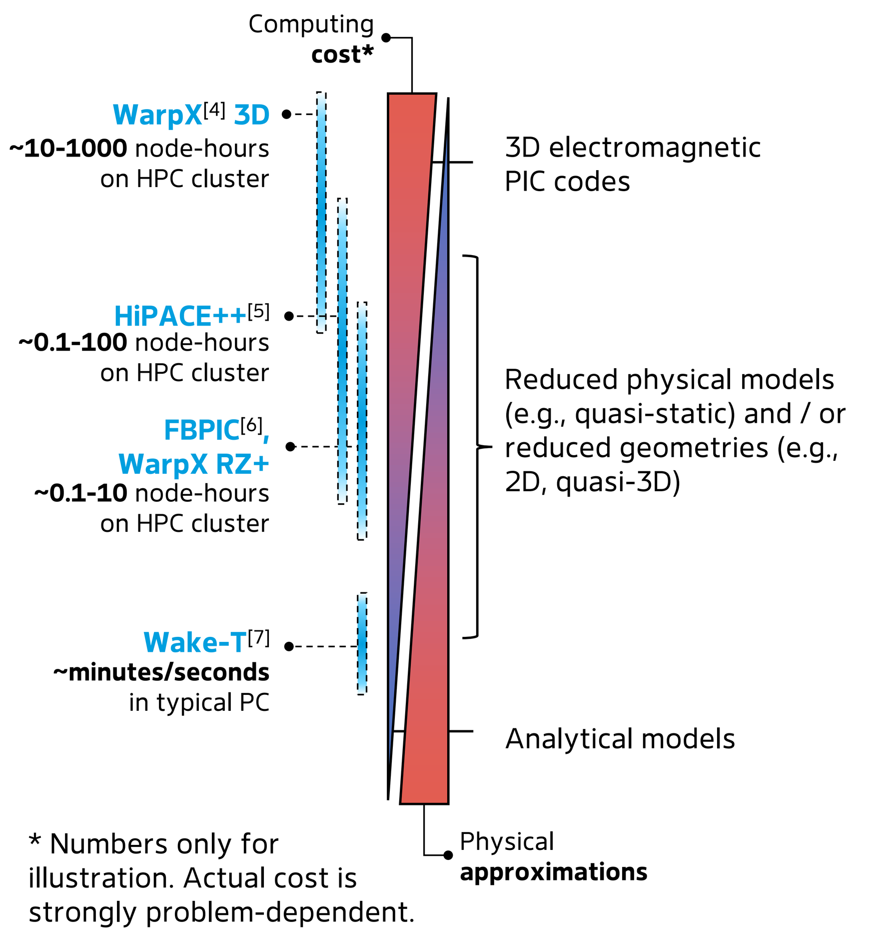
[1] Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany
[2] Department of Physics Universität Hamburg, Hamburg, Germany
[3] Argonne National Laboratory, Lemont, USA
[4] Lawrence Berkeley National Laboratory, Berkeley, USA

Laser-plasma acceleration

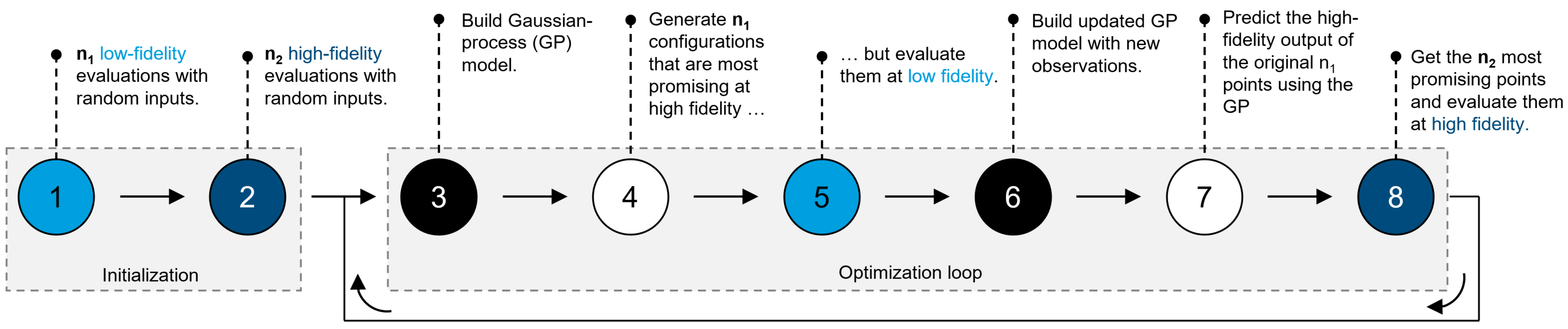


- Laser-plasma accelerators are **ultra-compact** (cm-scale) sources of **GeV** beams[1].
- Performance strongly depends on optimizing a wide range of plasma, laser, and electron beam parameters[2].
- Modeling with high-fidelity 3D particle-in-cell (PIC) simulations is computationally demanding (~1000 of node-hours on HPC clusters).
- Thus, **optimization over large parameter spaces** with 3D PIC codes becomes **prohibitively expensive**.

Enabling efficient high-fidelity optimization by introducing reduced-model simulations

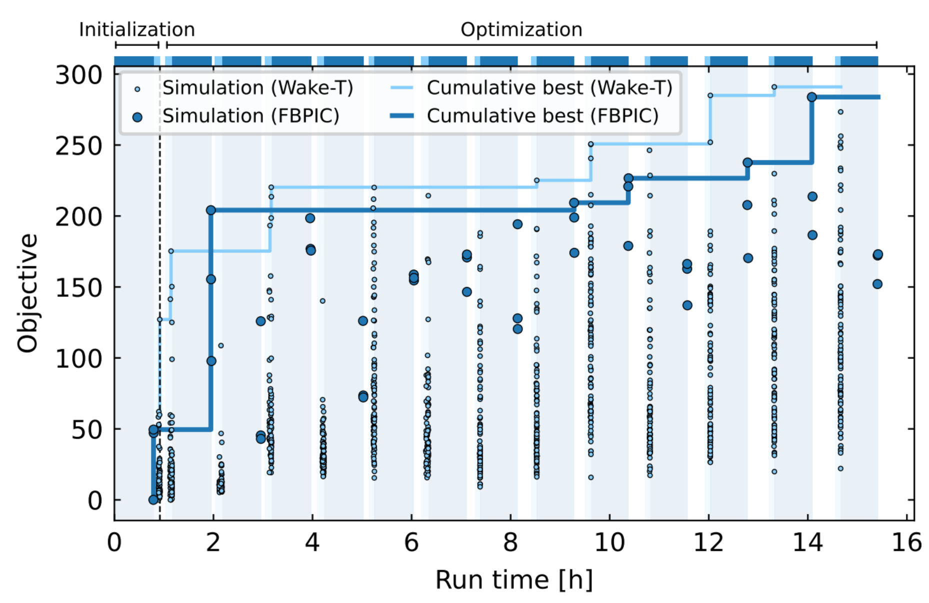


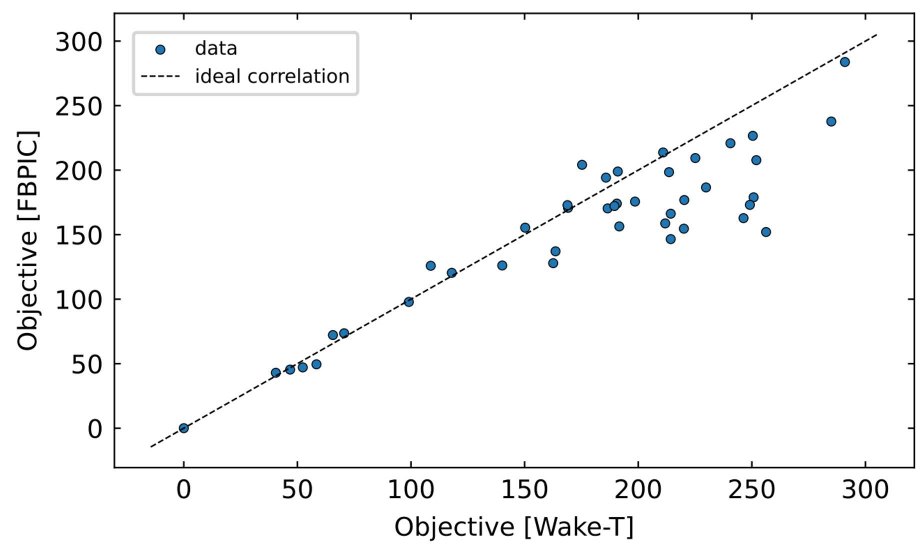
- Several plasma simulation codes have been developed based on **reduced physical models**.
- Although **less accurate/general**, they allow for **speedier** simulations and **broad parameter exploration**.
- Here, we show that incorporating reduced-model simulations into an optimization can strongly decrease the number of required high-fidelity simulations.
- This is enabled by the **multitask Bayesian optimization** algorithm[8,9]:



Proof-of-principle optimization study combining Wake-T and FBPIC

- **Goal:** Optimize beam current profile to achieve highest charge with lowest energy spread.
- 4 parameters: current at the head and tail, beam length, and distance to laser driver.
- Objective to maximize: $f = \frac{k_Q E_{MED}[GeV]}{k_{MAD}}$ with $k_Q = \frac{Q_{tot}}{Q_{ref}}$; $k_{MAD} = \frac{\Delta E_{MAD}}{\Delta E_{MAD,ref}}$
- **High-fidelity** code: **FBPIC** – Quasi-3D electromagnetic PIC (~45 min on single GPU).
- **Low-fidelity** code: **Wake-T** – 2D r-z quasi-static + laser envelope model (~5 min on single CPU core).



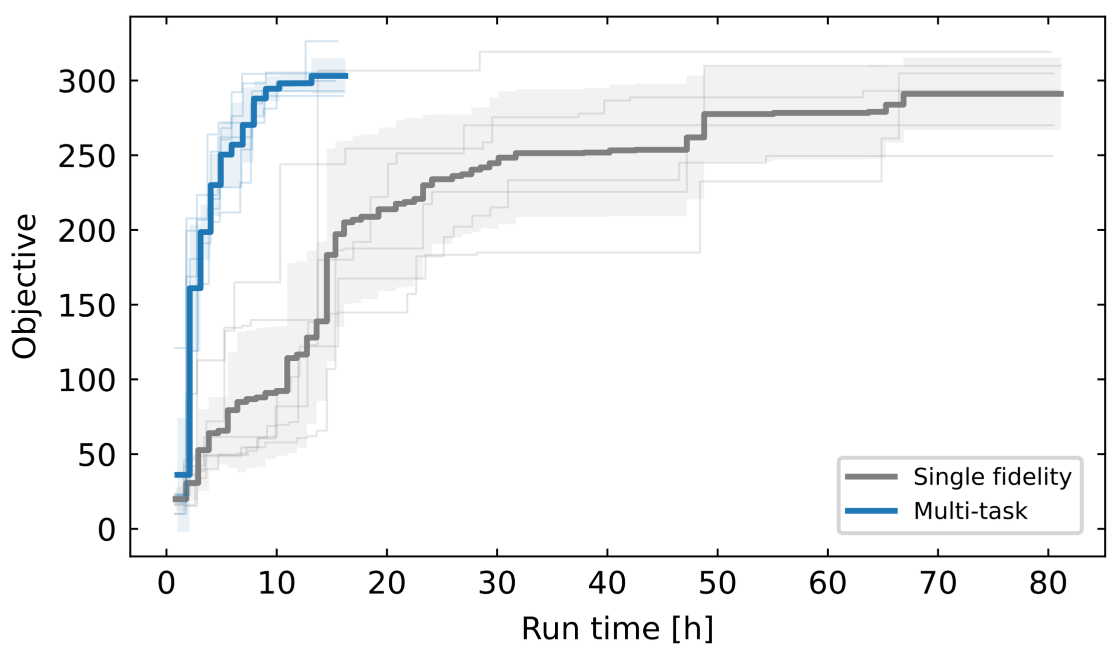


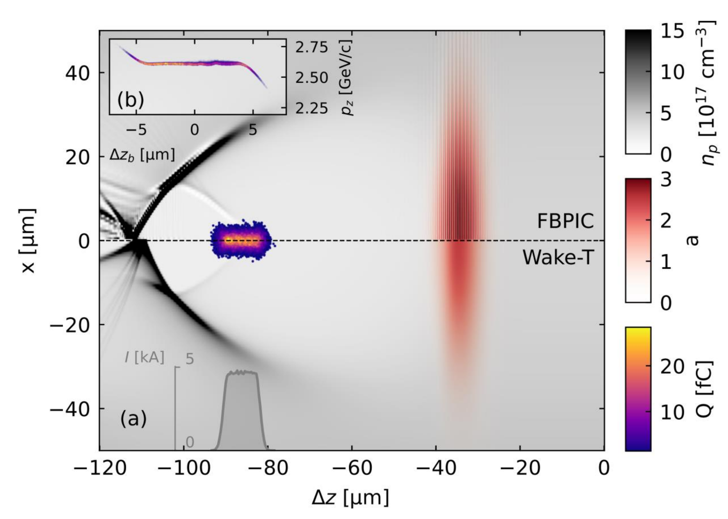
Optimizer effectively learns from low-fidelity simulations

The linear correlation between Wake-T and FBPIC data allows the optimizer to gain valuable information from inexpensive Wake-T simulations.

Multitask method enables 10x faster optimization

when compared to a single-fidelity case with exclusively FBPIC simulations. (average over 6 runs)



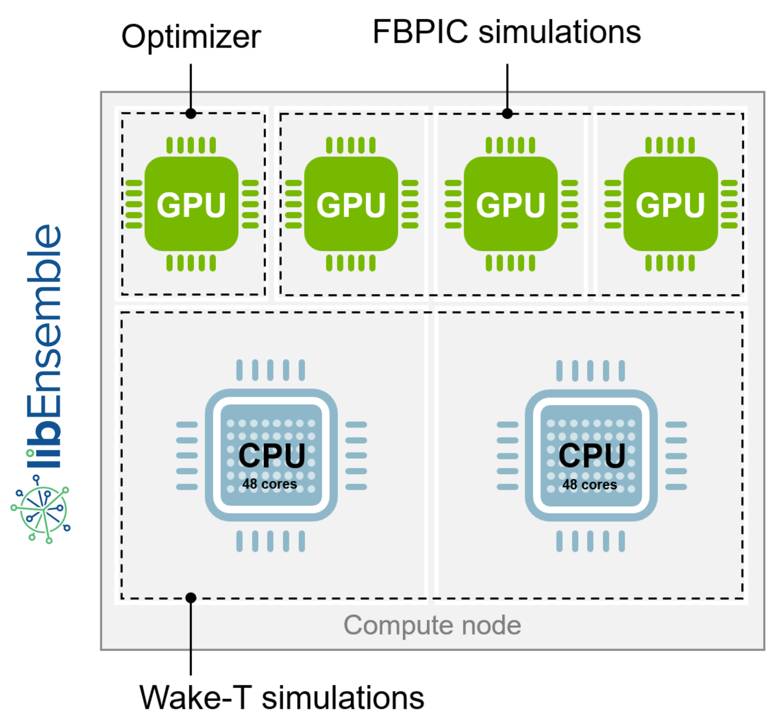


Optimal beamloading achieved

FBPIC/Wake-T comparison for the highest-scoring configuration

Optimization carried out on an HPC node

- 4 NVIDIA A100 GPUs and 2 48-core AMD EPYC CPUs.
- Communication and resource allocation orchestrated by libEnsemble[10].
- Optimizer (Ax[11]) runs on a GPU and can perform batches of 3 FBPIC simulations (GPU) or 90 Wake-T simulations (CPU).



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Deutsches Elektronen-Synchrotron DESY
Ein Forschungszentrum der Helmholtz-Gemeinschaft