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## Automated optimization workflow to translate laser plasma acceleration experiments into PIC simulations

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Modern laser-plasma accelerators require large-scale particle-in-cell (PIC) simulations to realistically model the three-dimensional relativistic laser-plasma interactions. The large number of possibly unknown laser and target parameters and their uncertainties in experimental setups prevent a simple translation of experimental setups into simulations and thus make meaningful statements about the prevailing dynamics difficult. In order to efficiently reproduce experiments PIC simulations were performed and their deviation from experimental results evaluated. To minimize this deviation, a feedback loop using Bayesian optimization was used to determine the next set of input parameters. We employed this method to self-truncated ionization injection experiments for electron acceleration at HZDR. It resulted in good agreement between simulation and experimental results after only a few simulations. Thus, saving computational resources compared to random parameter sampling. The simulations were performed using the open-source software PConGPU, a multi-GPGPU PIC code that generates openPMD output at high throughput. It allows the simulation of dispersive lasers and their propagation over hundreds of thousands of time steps through complex targets. The iterative optimization scheme was implemented using Snakemake, a Python-based workflow engine that allows any number of computational jobs to be organized in a directed acyclic graph (DAG) and submitted to different compute clusters. The combination of PConGPU and Snakemake allowed simulations to be compiled, run, and evaluated in an automated and parallel fashion, and the results used directly in the Bayesian optimization algorithm to obtain new input parameters. The developed workflow interface can be easily applied to any other multi-parameter PConGPU simulation campaign and is now part of the publicly available PConGPU codebase.

### Speed talk:

Normal speed talk selection

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