Unravelling ultrashort dynamics of plasma-based accelerators

PIConGPU

Leveraging synthetic diagnostics to match PIC simulations with experimental data

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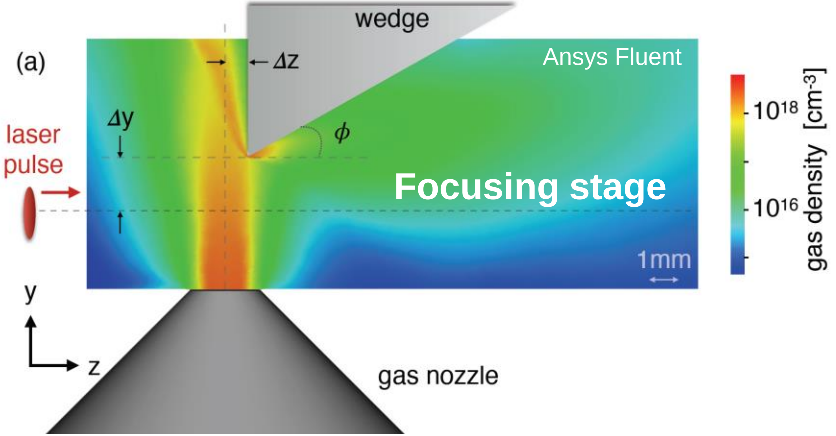
University of Delaware | Georgia Tech | Berkeley Lab | Oak Ridge National Laboratory | Leadership Computing Facility | EuroHPC Joint Undertaking | CASUS Center for Advanced Systems Understanding

Plasma-PEPSC Centre of Excellence

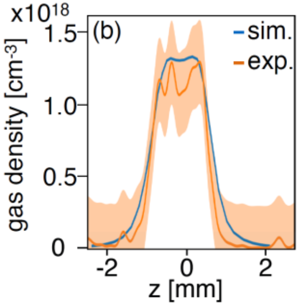
Electron beam focusing by a passive plasma lens

Y. Chang, et al. *under review* **(2023)**

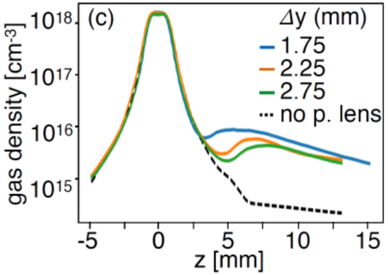


- Metal wedge modifies the gas density to create **a shallow density bump** behind the LWFA stage.
- Gas density peaks ~ 10^{16} cm^{-3} and extends over 20 mm long

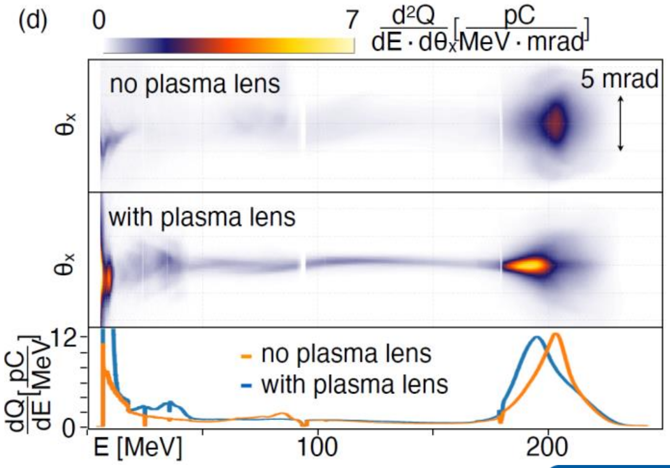
gas density profile
no wedge



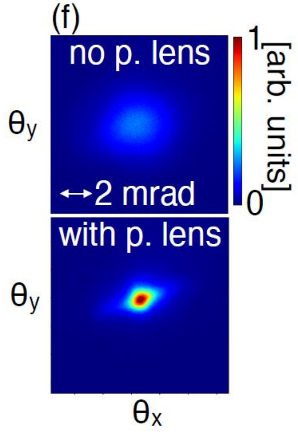
gas density profile
with wedge



Electron spectra

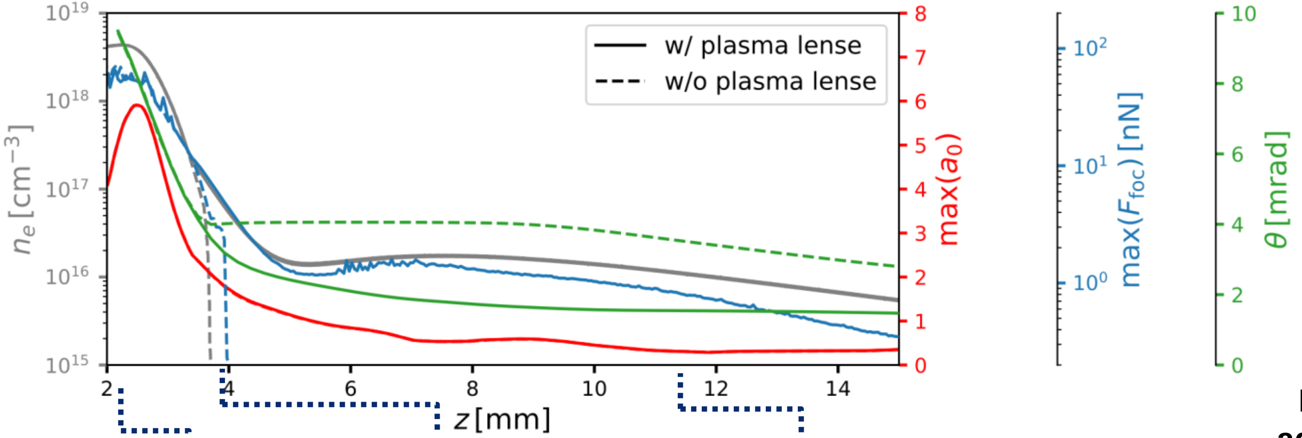


Beam profiler



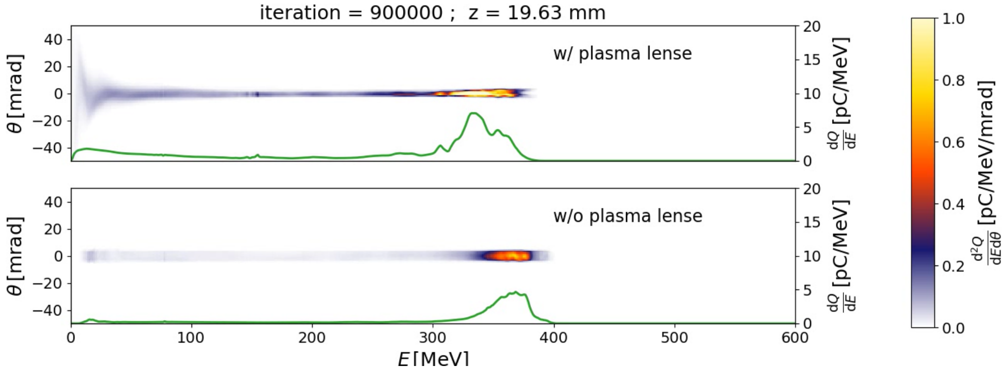
Experiment simulations can be large and extend over multiple scales

Smooth **transition** from **laser driven to beam driven regime**

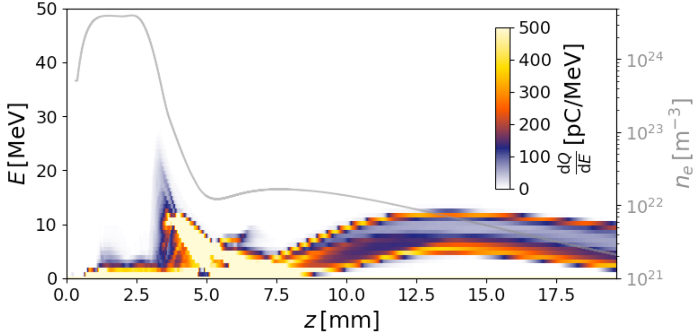


Normal plasma lens simulation
768x V100 GPUs
900k time steps
~24h time to solution

Extended setup to capture low energy injection
6144x V100 GPUs
900k time steps
~18h time to solution



Plasma lensing gives rise to an **additional down-ramp injection**.



PIConGPU

github.com/ComputationalRadiationPhysics/picongpu

picongpu.readthedocs.io

PIConGPU is used at Exascale

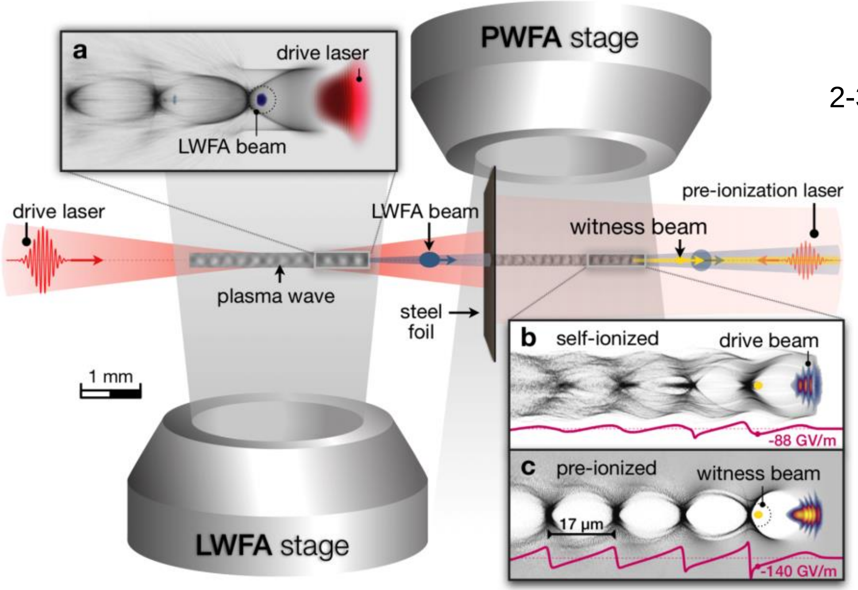
- **Scales up to the largest HPC systems**
- **Performance-portable** via (NVIDIA, AMD, Intel, ARM,...)
- Implements **exascale workflows** for scalable I/O capabilities, such as streaming, data reduction and visualization workflows.

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

HZDR HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

Unravelling ultrashort dynamics of plasma-based accelerators

tightening the links by synthetic diagnostics and experimental data reconstruction



Hybrid LWFA+PWFA accelerator experiment

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

PIConGPU

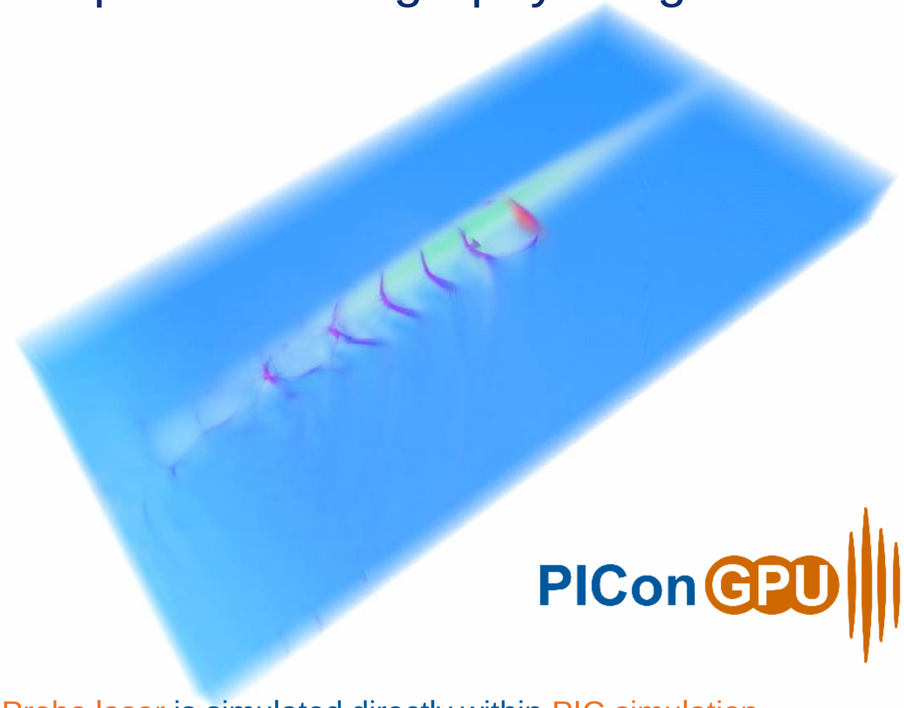
Experimental data reconstruction

Synthetic diagnostics

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



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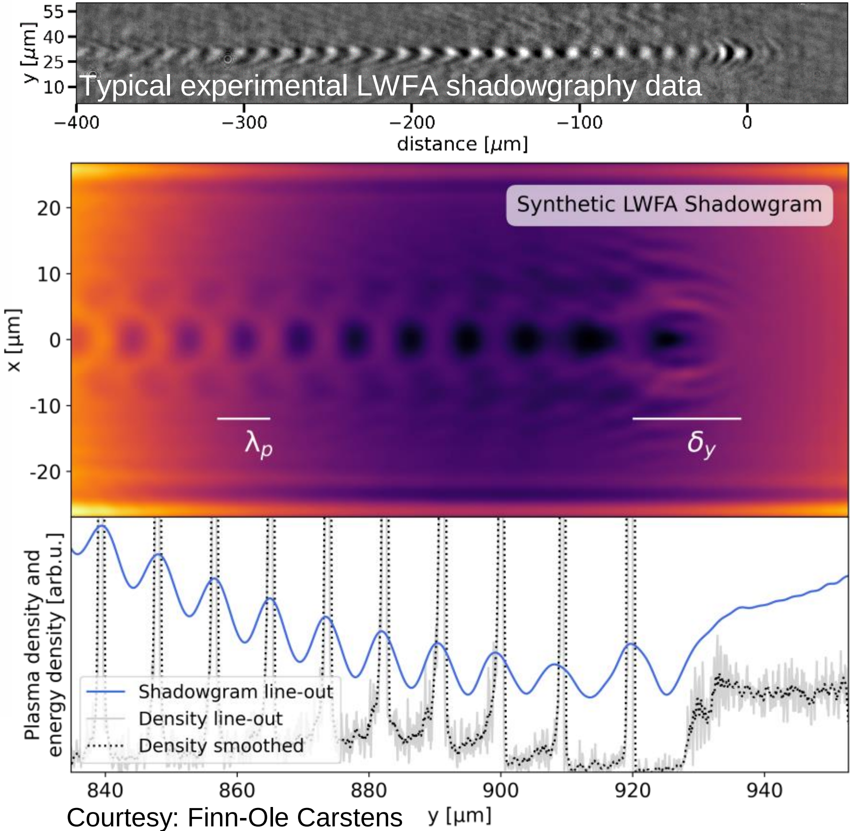
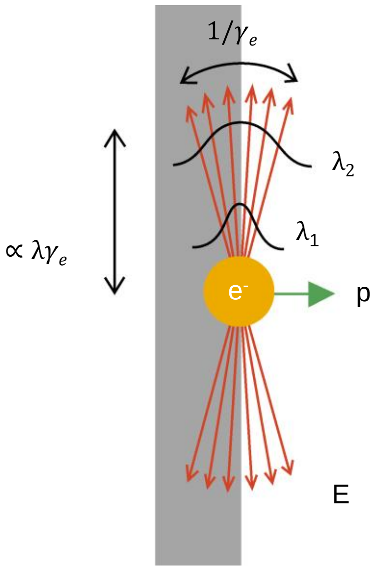


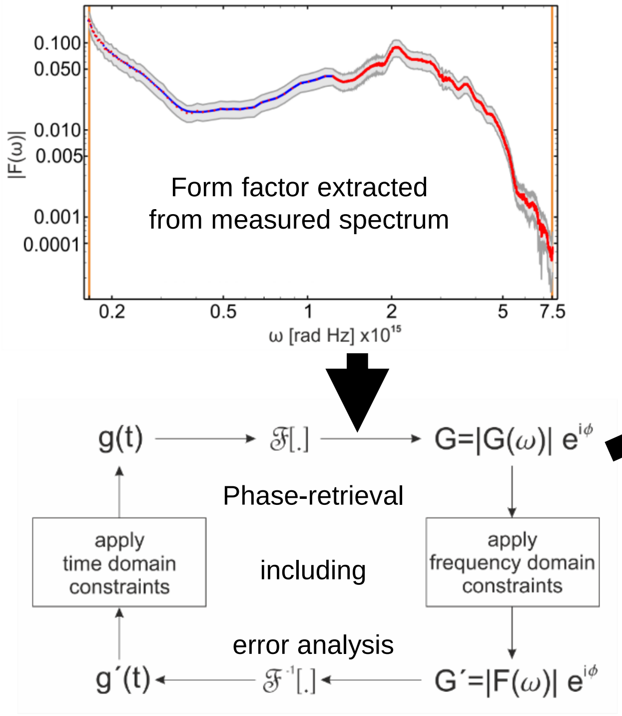
Courtesy: Finn-Ole Carstens

- 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)

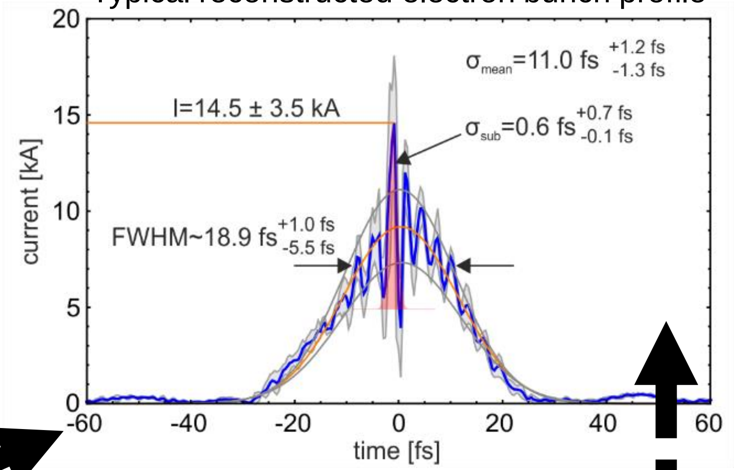
Experimental data reconstruction to infer the longitudinal electron bunch profile from measured CTR spectra



metal foil

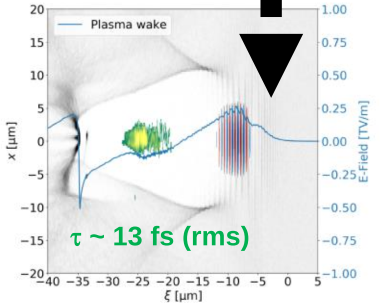


Typical reconstructed electron bunch profile



Electron bunch length agrees with 3D-PIC simulations

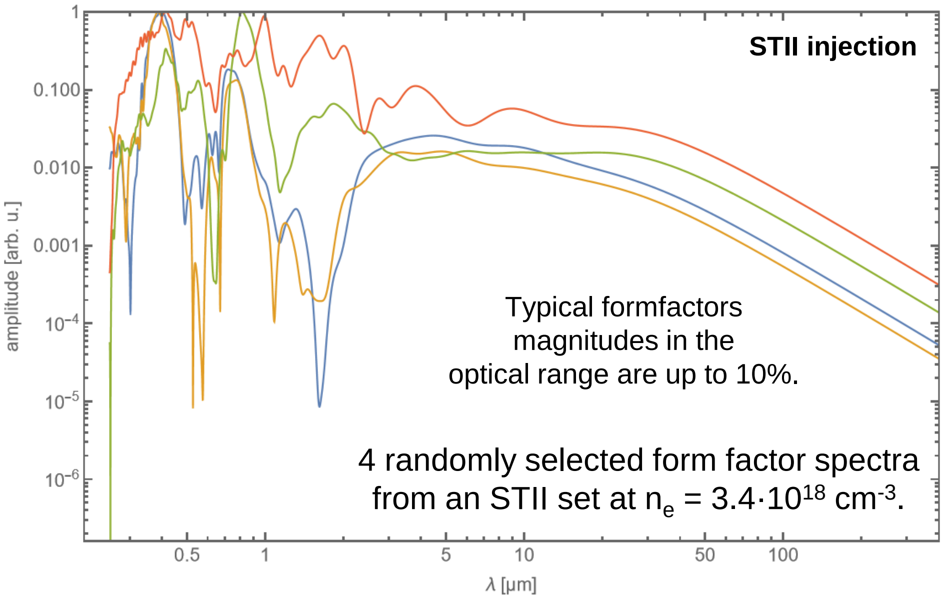
PIConGPU

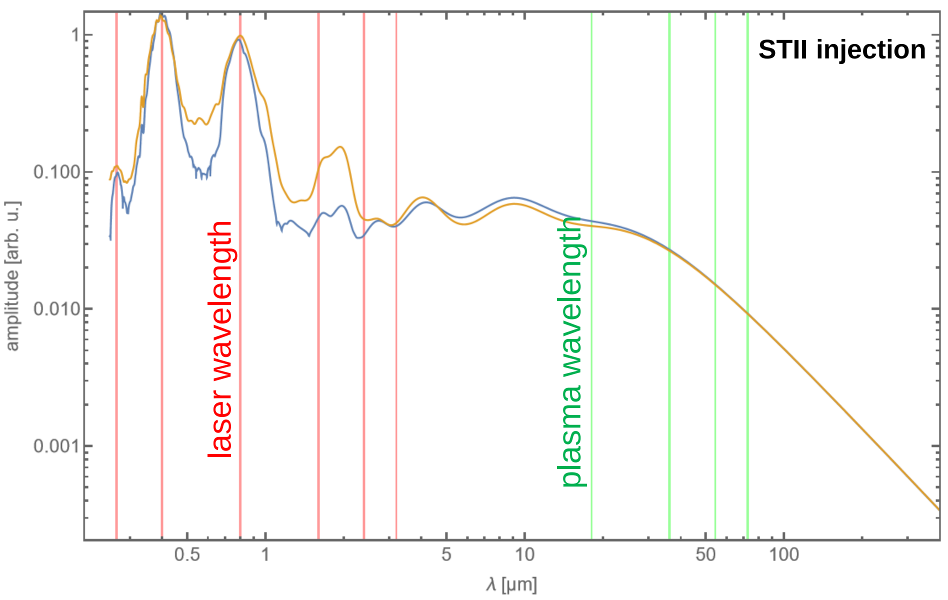


alpaka

Zarini *et al.* (2022), Phys. Rev. Accel. Beams 25, 012801

Typical micro-structures are dominated by the laser wavelength scale

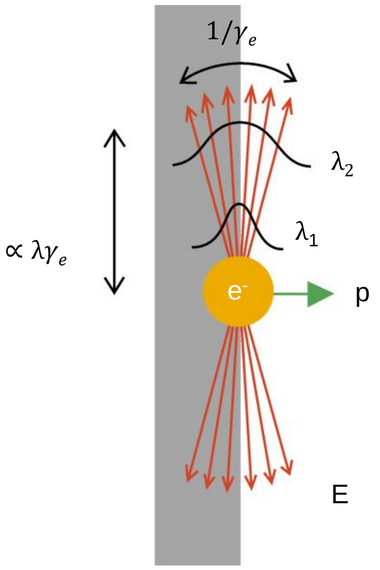


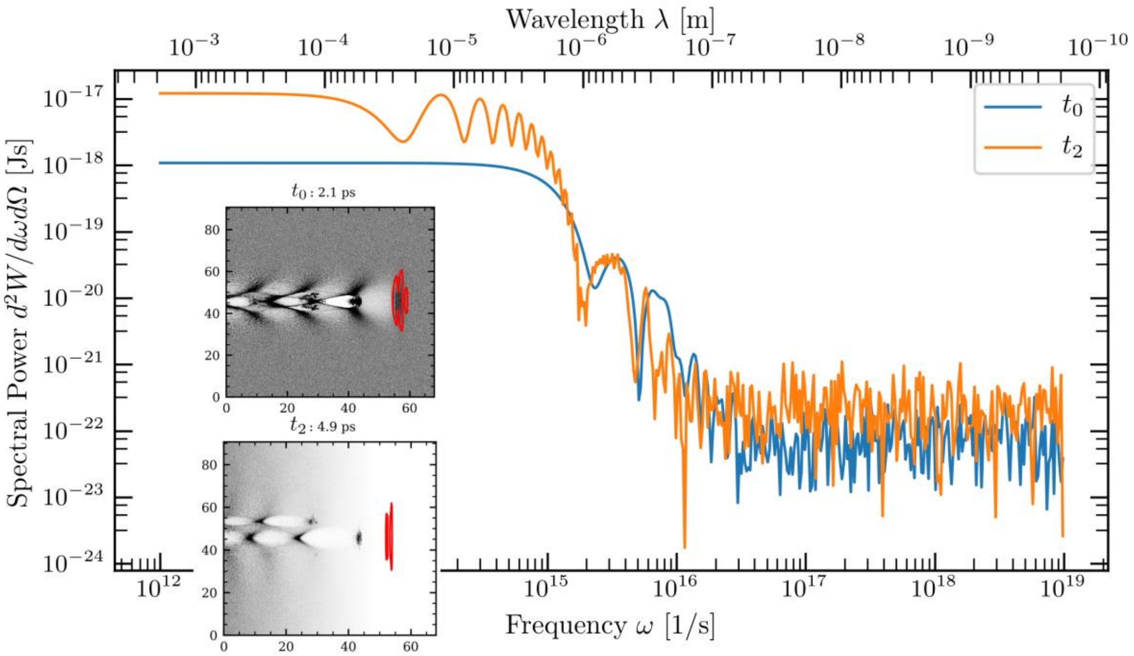


Apply arithmetic (orange) and geometrical (blue) averages on all 58 shots of an STII set at $3.4 \cdot 10^{18}$ cm^{-3}.

However, beam micro-structures are complex, feature significant shot-to-shot variations and raise the question of their physics origins.

Synthetic in-situ diagnostics in PIConGPU
to simulate the measured CTR spectrum



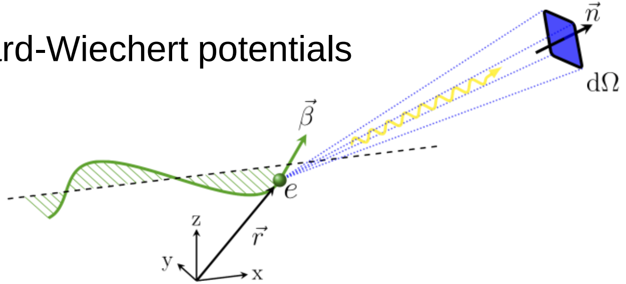


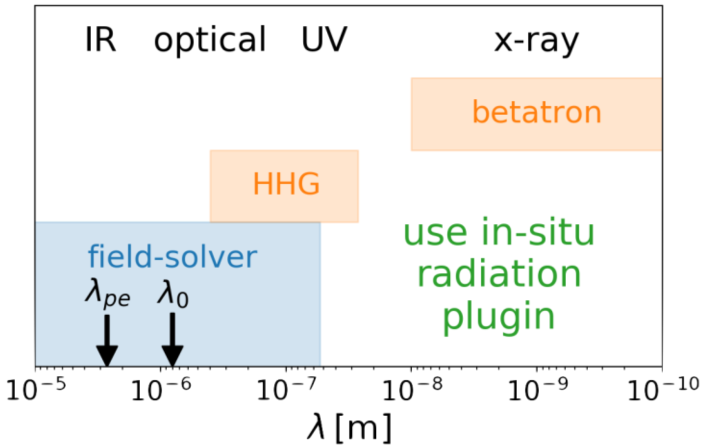
Allows for direct comparison with non-reconstructed measured CTR data.
Provides high-quality data for testing & refining reconstruction routines.

In-situ radiation diagnostic: Study HHG reflections in solid-density targets

$$\frac{\mathrm{d}^2 I}{\mathrm{d}\Omega \mathrm{d}\omega} = \frac{q^2}{16\pi^3 \varepsilon_0 c} \cdot \left| \sum_{i=1}^{N} \int \frac{\vec{n} \times \left[\left(\vec{n} - \vec{\beta}_i \right) \times \dot{\vec{\beta}}_i \right]}{\left(1 - \vec{\beta}_i \cdot \vec{n} \right)^2} \cdot e^{\mathrm{i}\omega \left(t - \frac{\vec{n}\vec{r}_i}{c} \right)} \mathrm{d}t \right|^2$$

Based on Liénard-Wiechert potentials

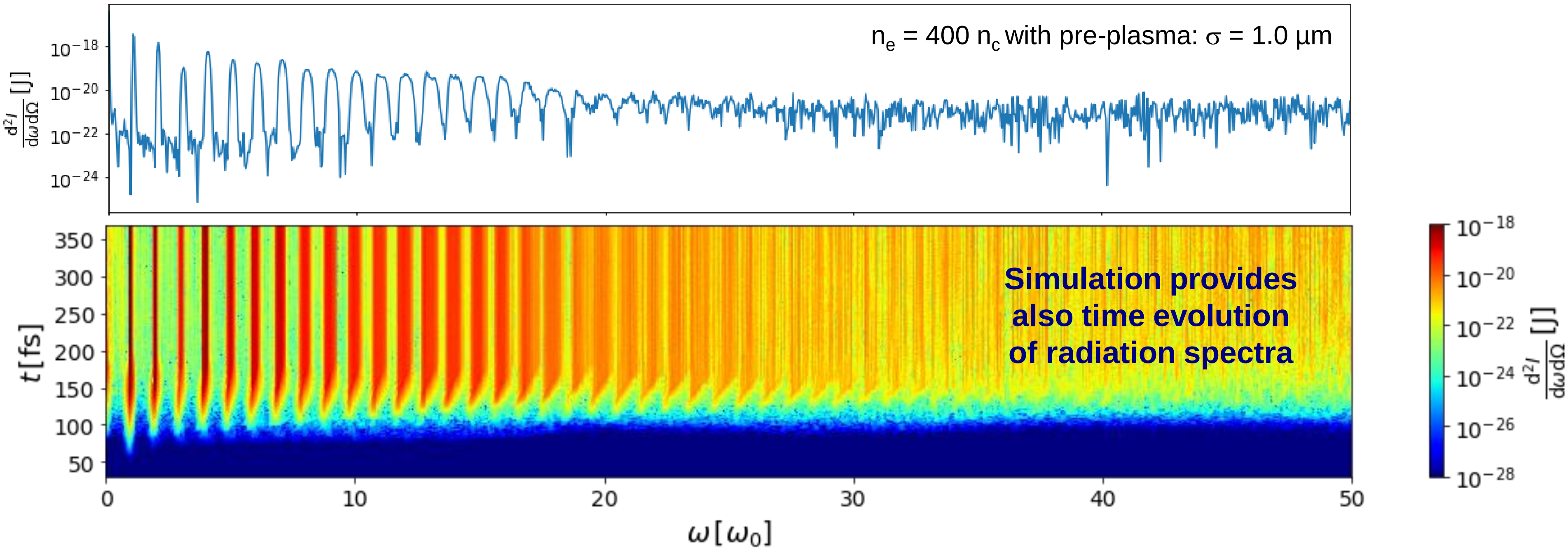




- Spectral range from **IR to x-ray**
- Resolves **coherent** and **incoherent** radiation **simultaneously**
- Includes **polarization** properties
- Resolves **temporal evolution** of spectra
- Computes radiation of all **billions of particles** in the simulation

Studying changes in HHG reflection via synthetic radiation

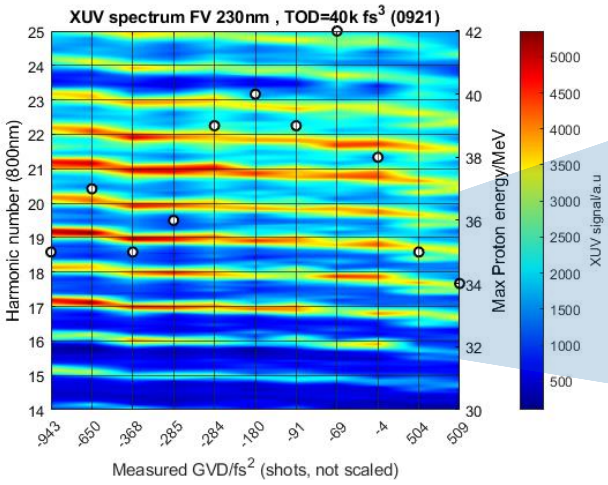
To understand **experimental correlation** between **proton energy and harmonics**



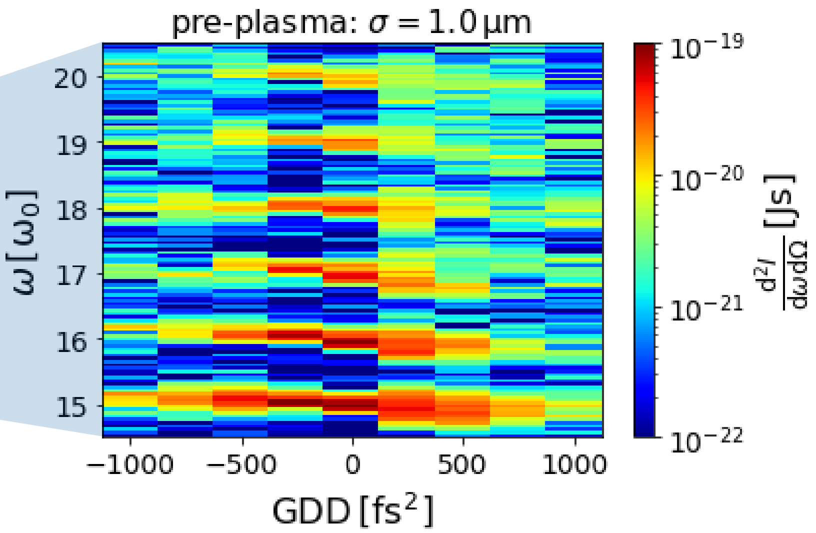
Changes in harmonics

Experiment – Simulation – Theory – agreement on frequency shifts

Experiment



Simulation

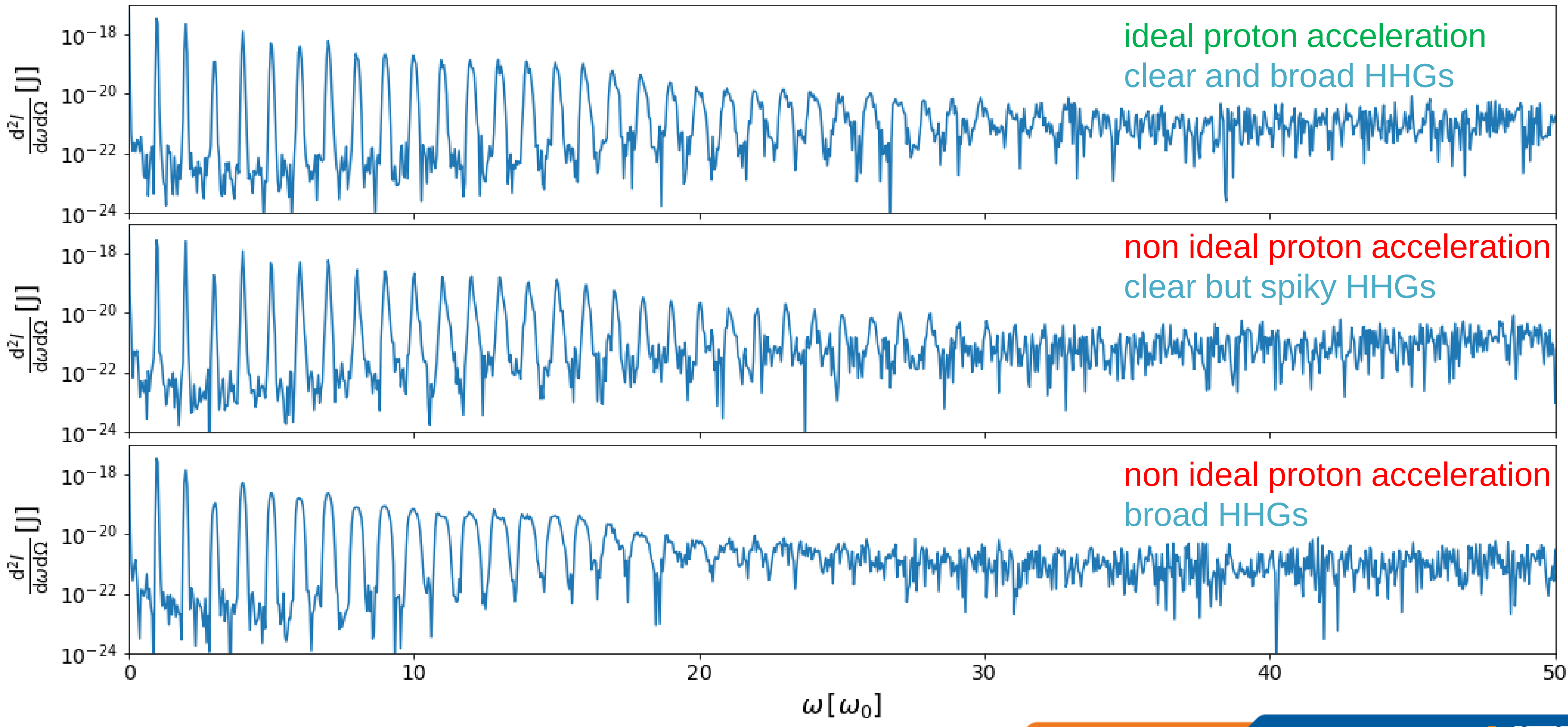


Frequency shifts in **experiments and simulations** over GDD **agree with theoretical predictions**:
E. Porat et al. PRR 4 L022036 (2022)

6144 x 6144 cells (2D), cell width = 4nm, 60k time steps
radiation in 16 directions and 256 frequencies
run time: 3h 39min on 32x V100 GPUs

Changes in harmonics similar to experiments

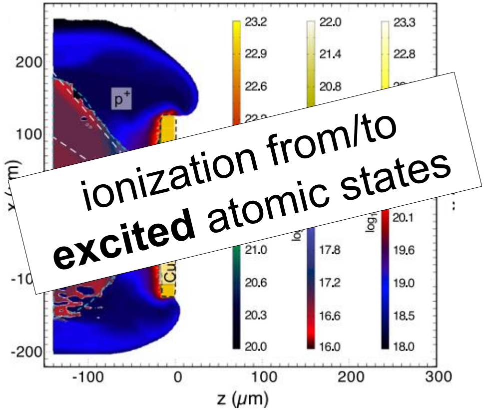
Initial conditions define acceleration – HHG allow direct look at foil at peak laser intensity



For predictive simulations of Laser Plasma Accelerators we also need to care about atomic physics!

State-of-the Art (pick at least one!)

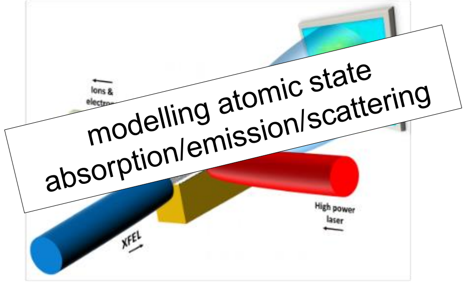
- ground states only, e.g. PIC
- post processing only, e.g. flyCHK[1,2]
- thermal distributions, e.g. PICLS, Calder



Ion density distribution of a simulated laser accelerator target (Schollmeier et al. Phys. Plasmas 22, 043116 (2015))

Laser plasma accelerators can feature

- **transient, high laser intensity** dynamics
- **coupled** atomic state distributions and plasma dynamics (via ionization)
- **non-equilibrium** particle distributions



X-ray probing of laser driven for ion acceleration (sketch of HiBEF experimental setup at XFEL)

State-of-the-Art not sufficient!

[1] T.Kluge et. al. Phy. Plasmas 23, 033103 (2016) and T.Kluge et. al. Phy. Plasmas 24, 102709 (2017)
[2] L.Gaus et. al. Phy. Rev Research 3, 043194 (2021)

PIConGPU :FLYonPIC

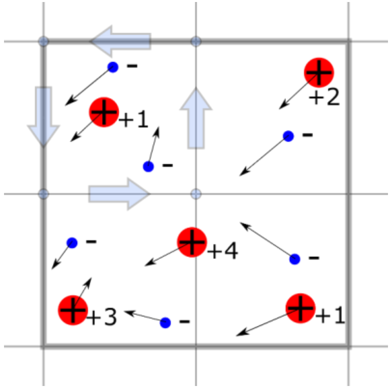
Excited Atomic States in PIC

Use **PIC (PIConGPU)** as basis
for full kinetic modelling

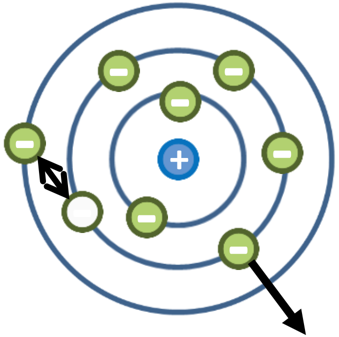
+ track **excited** atomic **states**

+ **runtime rate equation solver** for dynamics

- Obtain local spectrum from PIC
  (no assumption of temp.)
- time dependent solver for dynamics
- feedback to PIC
  (update-spectrum and ionization of ions)

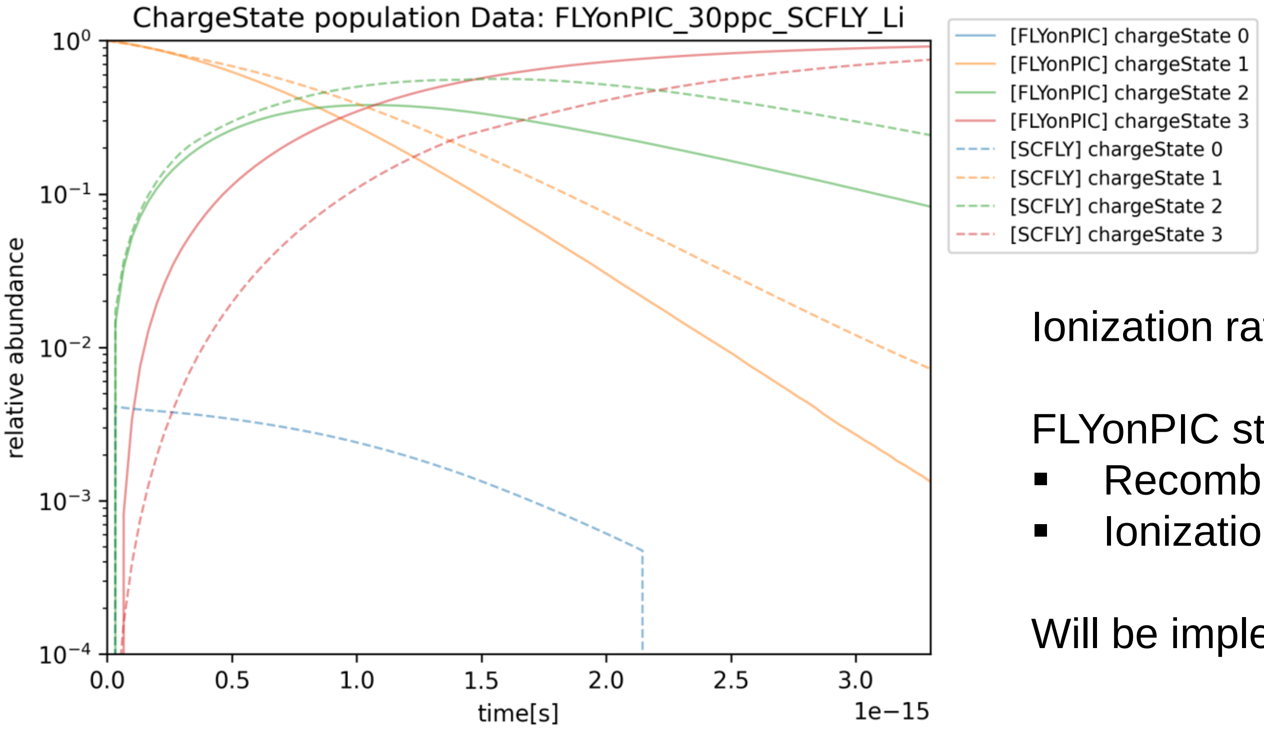


+



Does FlyonPIC work? Yes!

PIConGPU
:FLYonPIC



Courtesy: Brian Marré

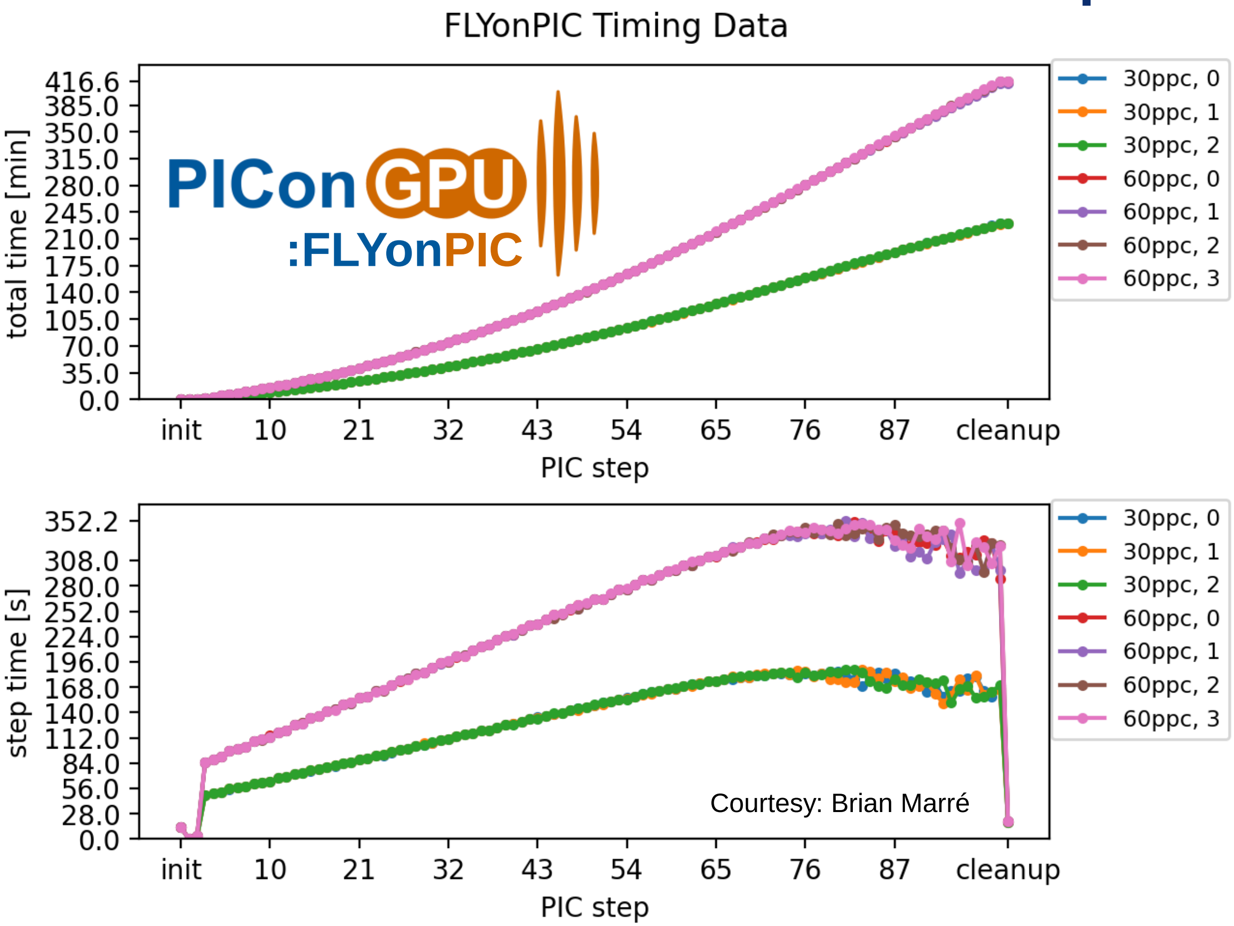
Ionization rate is too high.

FLYonPIC still lacks

- Recombination
- Ionization Potential Depression

Will be implemented soon.

How to kill an Exascale cluster: Initial performance tests



- **Argon test simulation**, homogenous ion density 10^{22} cm^{-3}, fixed electron temperature at 1keV
- PIC simulation without FLYonPIC: 50ms per PIC-step
- 28^3 cells (4^3 super-cells), 30/60 ppc on 1x NVidia-V100 GPU
- Simulation repeated 4x for statistics (→ case numbers)
- ~30 atomic physics subs steps per PIC step
- Potential for 1-2 order of magnitude speedup by storing local probability maps.

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 few-cycle shadowgraphy, coherent transition radiation and Liénard-Wiechert far-field radiation facilitate direct and quantitative comparison to experimental data.
- FLYonPIC is an novel addition to PIConGPU, an in-situ rate equation solver, modeling time-dependent atomic physics including excited states, without temperature assumptions.
  - Quantitative physics tests show encouraging results.
  - Runtime tests show that including atomic physics at scale will require post-exascale systems.

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

An Exascale-ready software stack for simulations & more

Driving the science behind advanced particle accelerators

PIConGPU — Exascale-ready Plasma Simulations

alpaka, LLAMA, cupla — Performance Portability (GPUs, CPUs, FPGAs)

openPMD — F.A.I.R. Exascale I/O + in-memory coupling

ISAAC — In-situ, interactive, live visualization

PICMI Standard — Define simulation runs via common interface

Team behind PIConGPU

github.com/ComputationalRadiationPhysics/picongpu













HZDR

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