FLYonPIC: Atomic Physics for PIC

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MATTER AND TECHNOLOGIES ACCELERATOR RESEARCH AND DEVELOPMENT

HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

PIConGPU **Physics Extension** modelling **Atomic Physics** including **excited states** in **transient** plasmas

PIConGPU :FLYonPIC

Need self consistent Prediction of Excited States in Particle-in-Cell Simulations

Charge State Prediction

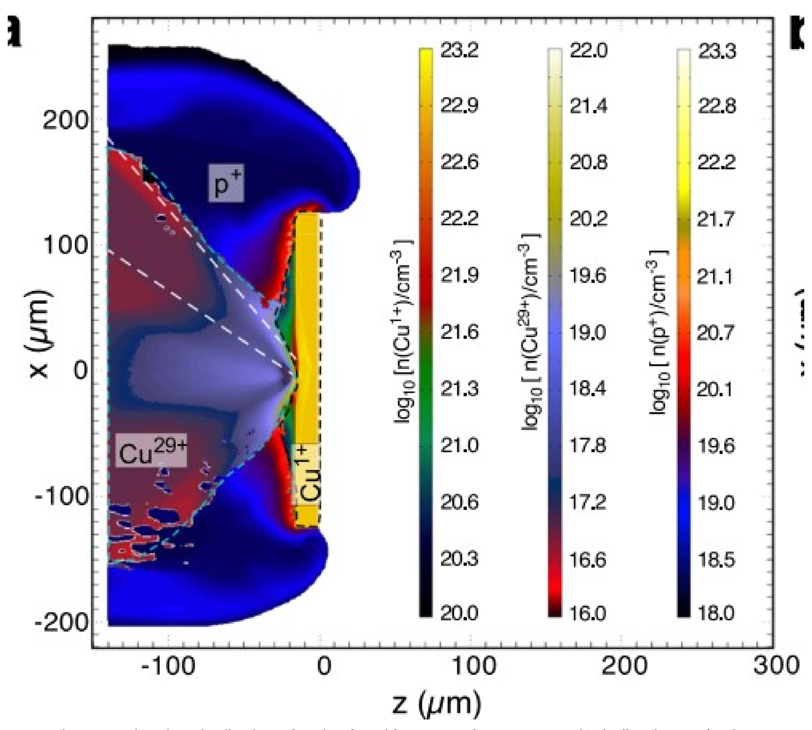


Fig.1: Ion density Distribution of a simulated laser accelerator target (Schollmeier et al. Phys. Plasmas 22, 043116 (2015))

ionization from/to **excited** atomic states

X-ray Probing

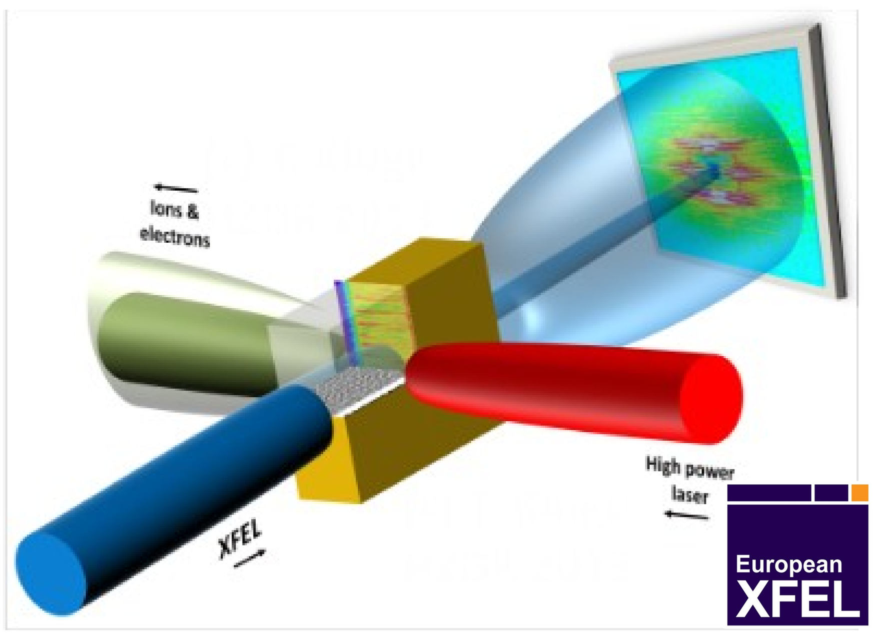


Fig.2: X-ray probing of laser driven for ion acceleration (sketch of HiBEF experimental setup at XFEL)

HiBEF

Modell x-ray absorption/emission/scattering

State of the Art (accept at least one):

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

[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)

Laser plasma accelerators conditions:

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

State of the Art is not sufficient!

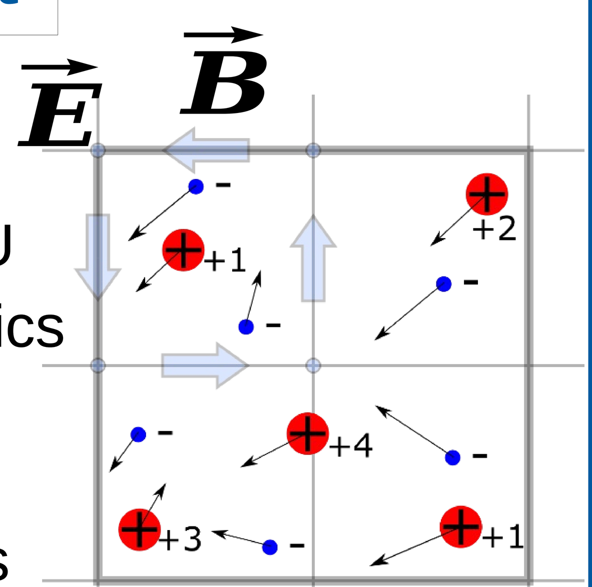
FLYonPIC: High Level Concept

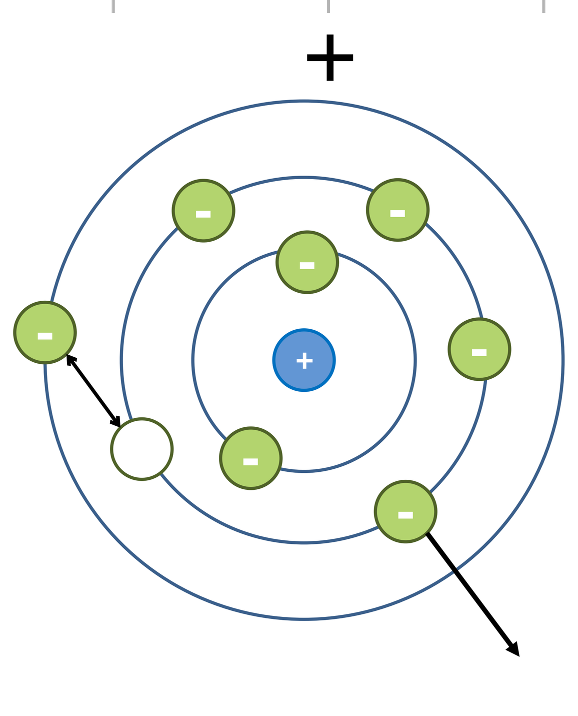
use **PIConGPU** as **Base**:

- fully kinetic modelling of plasma

+ track **excited** atomic **states** in PIConGPU
+ **runtime rate equation solver** for dynamics

- get local paticle-spectrum from PIC (no assumption of temp.)
- time dependent solver for state dynamics (with adaptive sub-stepping)
- feedback to PIC for self consistency (-spectrum and ionization)





Implementation:
direct **inclusion** in PIConGPU

- **simplified atomic state** model
- **one atomic state** per macro particle
- on **super cell level**
- **approximate rate** calculation (reused from flyCHK/SCFLY)
- **Monte Carlo** time dependent rate solver

FLYonPIC Current State

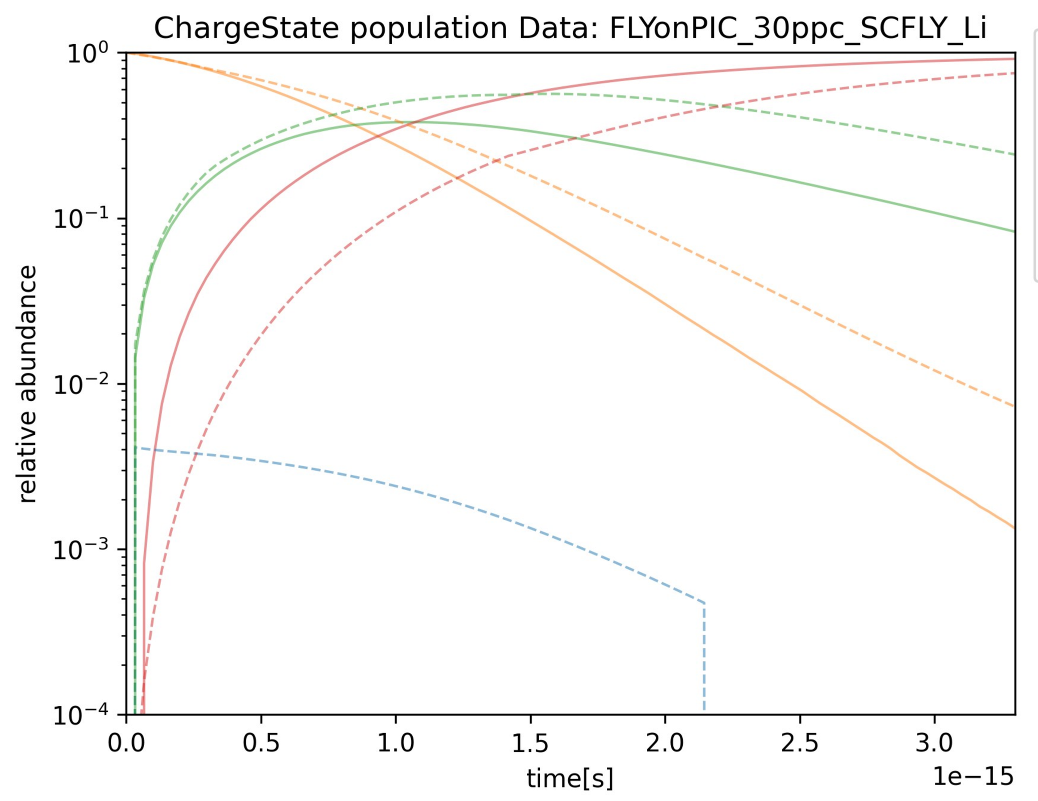
Currently implemented:

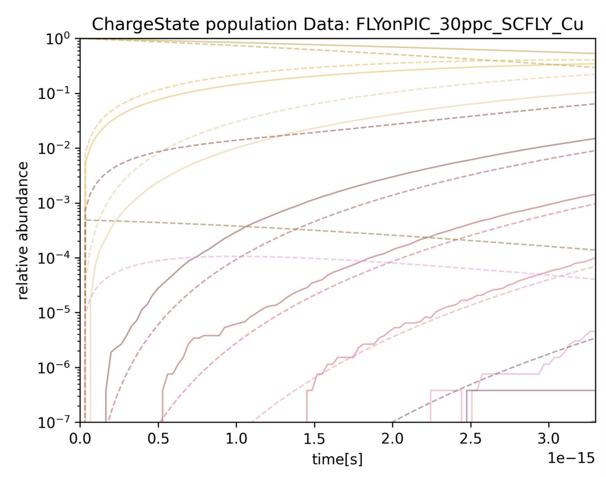
- electronic collisional de-/excitation
- spontaneous deexcitation
- electronic collisonal ionization
- autonomous ionization

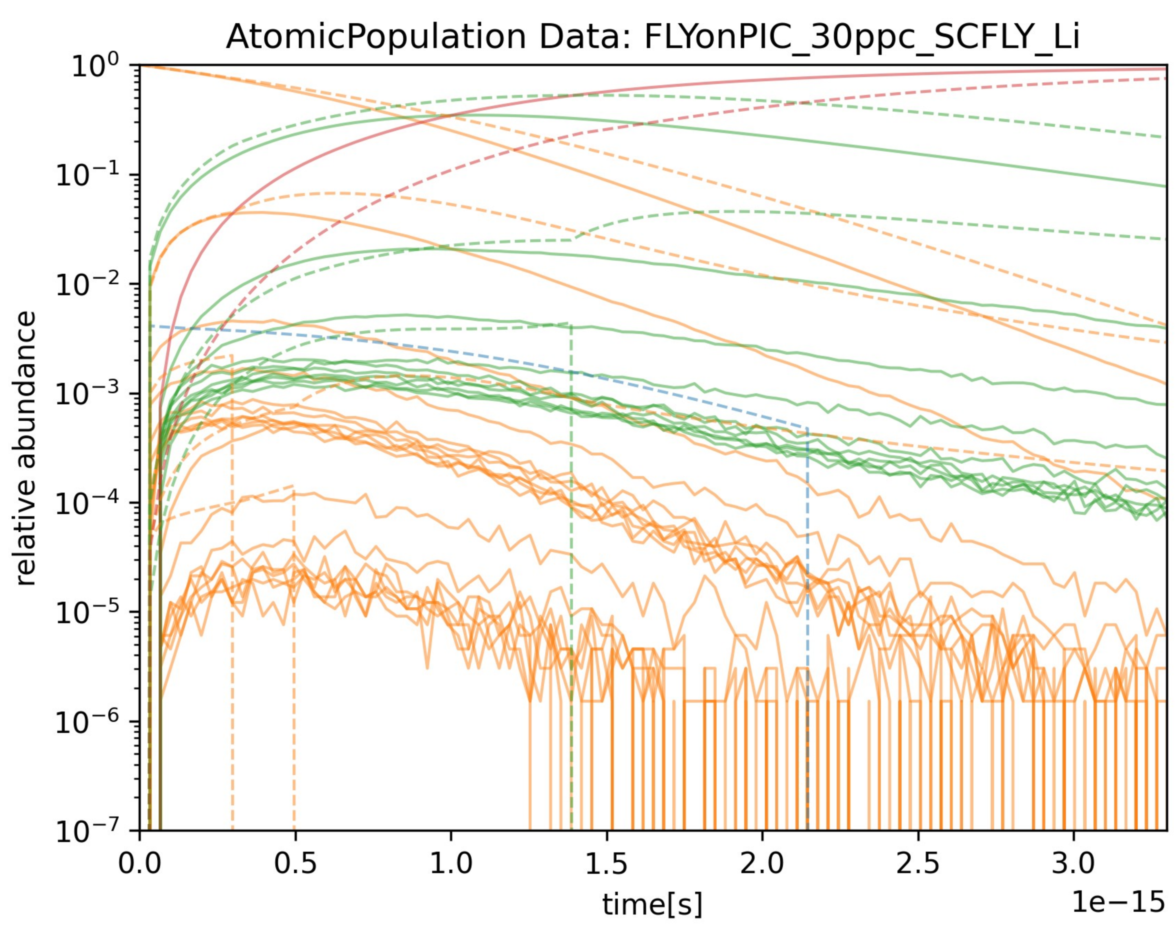
To come:

- radiative-/dielectronic recombination
- Field Ionization (ADK and BSI)
- Pressure Ionization (IPD)

Does it work? Yes!







Lithium test simulation

- homogenous ion density 10^{23} 1/cm^{-3}
- fixed electron temperature at 1keV
- 28^3 cells (4^3 super-cells), 30ppc
- Initial state: 2+ ground state

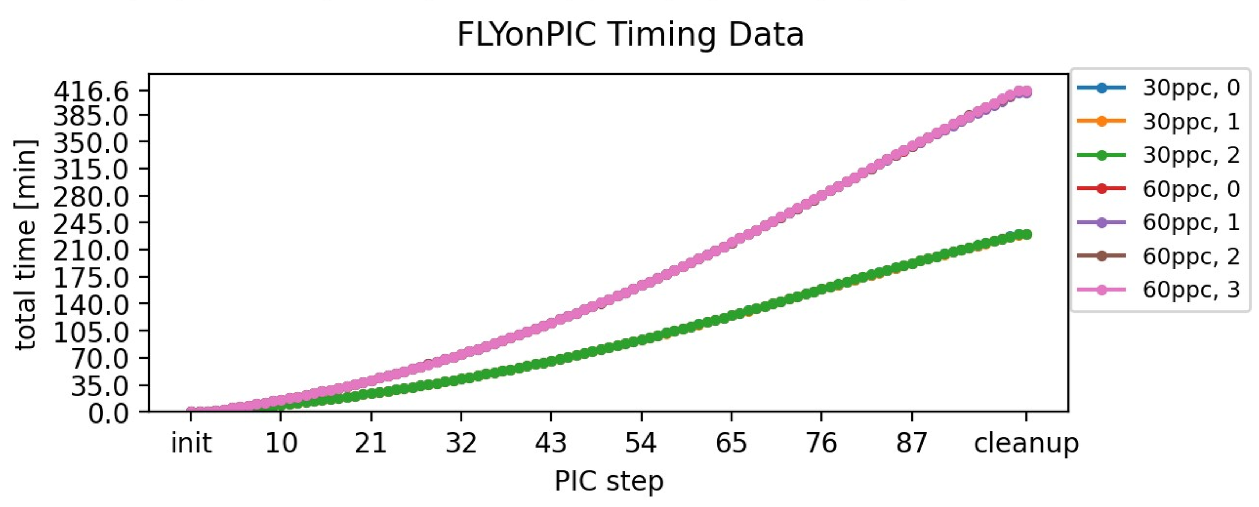
Copper test simulation

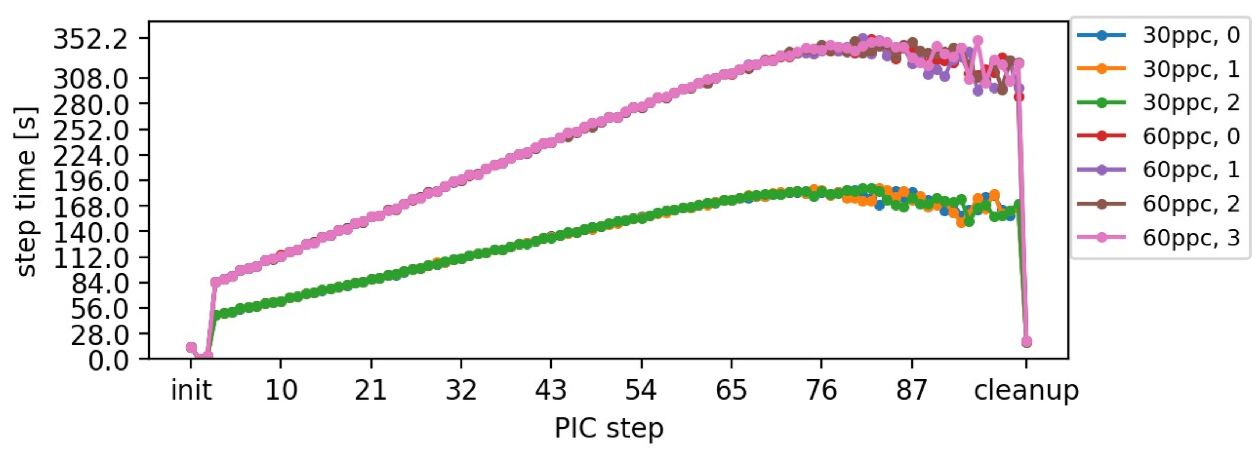
- homogenous ion density 10^{22} 1/cm^{-3}
- fixed electron temperature at 1keV
- 28^3 cells (4^3 super-cells), 30ppc
- Initial state: 9+ ground state

Future: Radiation Transport Modelling

(radiative de-/excitation and ionization)

How to fill an Exascale Cluster: Initial Performance Test





Argon test simulation

- homogenous ion density 10^{22} 1/cm^{-3}
- fixed electron temperature at 1keV
- 28^3 cells (4^3 super-cells), 30/60 ppc
- Initial state: 2+ ground state

on 1x NVidia-V100 GPU

PIC simulation without FLYonPIC: ~ 50ms per PIC-step

Simulation repeated 4x for statistics (□ case numbers)

~300 Atomic Physics subs steps per PIC step

Potential for 1-2 order of magnitude speedup by storing local probability maps.

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