Session 3: Beyond PIC

Smilei) Workshop

Physics Modules

9 November 2023

Francesco Massimo (z10f )
francesco.massimo@universite-paris-saclay.fr

Motivation: missing physics in PIC codes

Vlasov → no interaction between individual particles

Maxwell equations → no quantum effects

Finite grid size → no high-frequency photons

Fixed charge → no atomic physics

Fixed mass → no nuclear physics

Added Physics in Smilei

Ionization

Collisions (interaction at close range)

Nuclear reactions

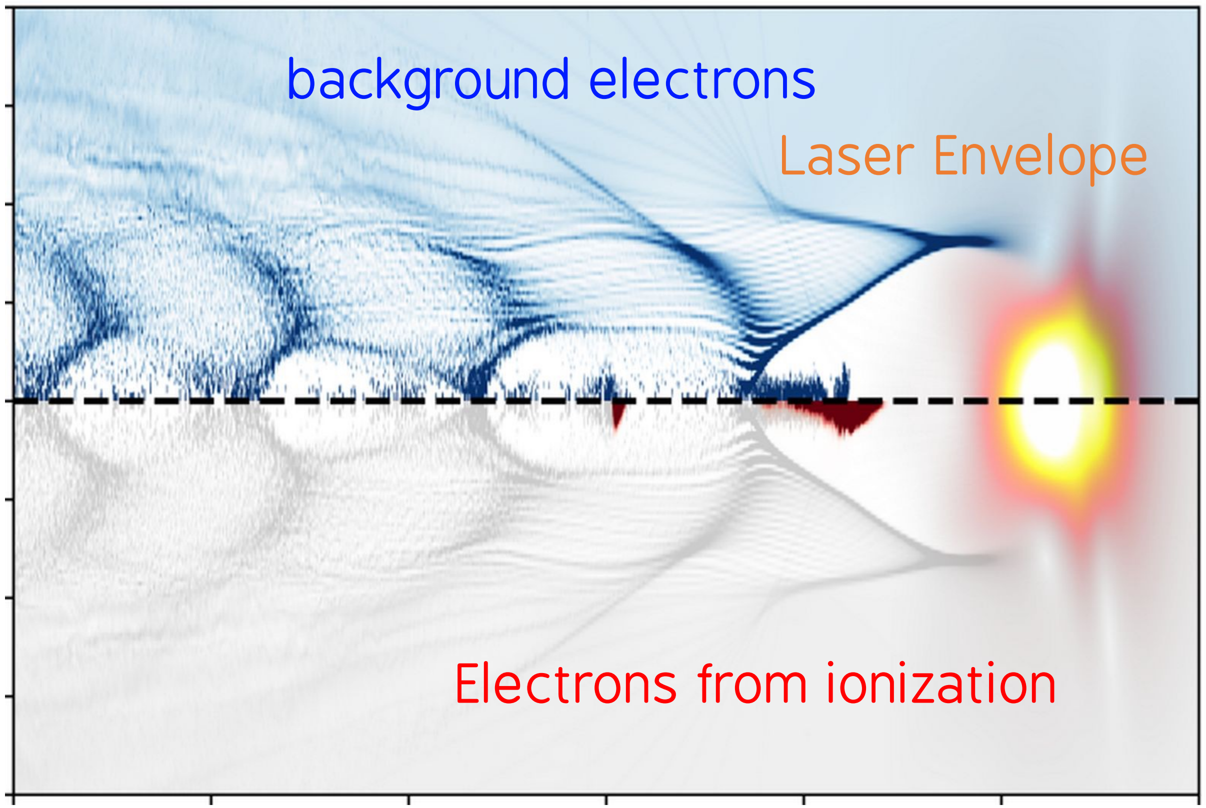
Radiation by accelerated charges at small scales

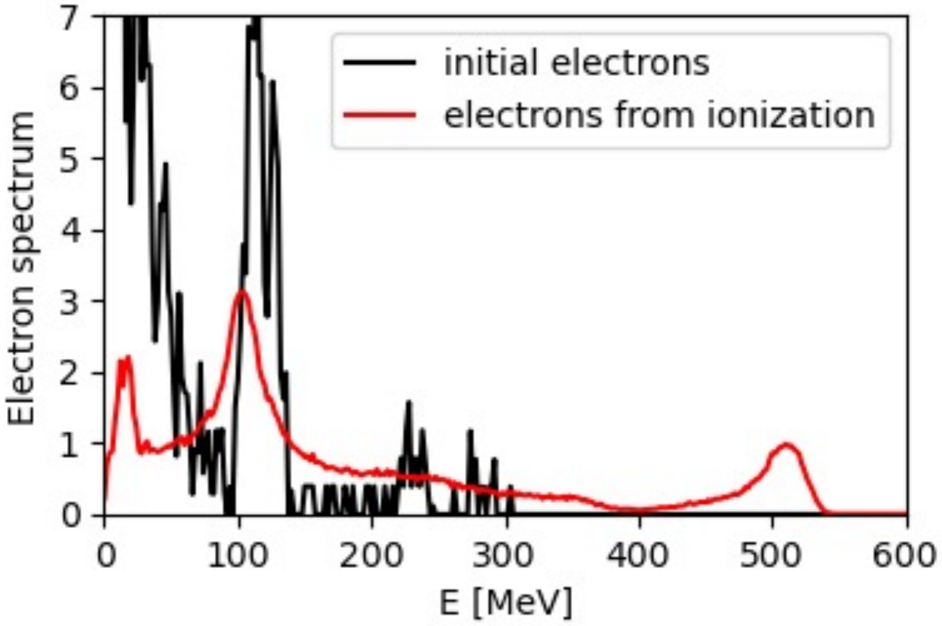
Electron-positron **pair creation**

Field Ionization

Ionization: concept

Example with laser wakefield ionization



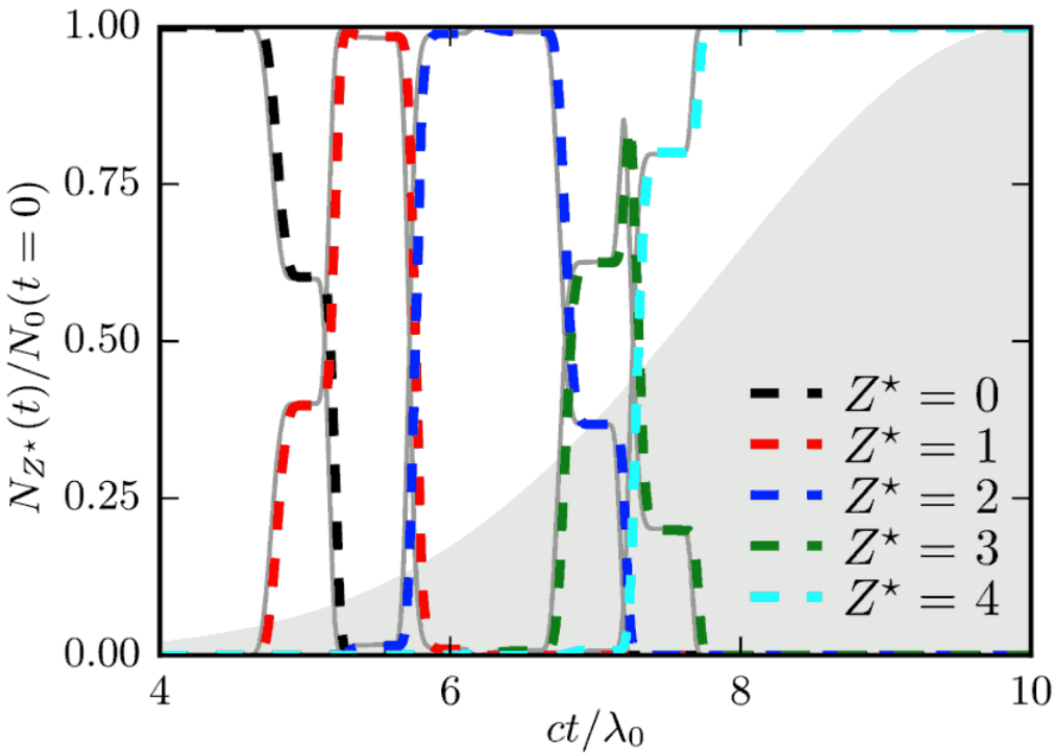


Ionization in Smilei: tunnel ionization

- Multi-level ADK model from [R. Nuter et al., PoP 19, 033107 (2011)]
- Ionization rate Γ from theoretical formula
- Outermost electron is stripped if random number $U > \exp(-\Gamma \Delta t)$
- Multiple ionization in 1 timestep is accounted for
- Envelope ionization discussed in Advanced Modules

Ionization in Smilei: tutorial Field Ionization

Laser interacting with carbon plasma




```
Species(
    name = 'carbon',
    ionization_model = 'tunnel',
    ionization_electrons = 'electron',
    atomic_number = 6,
    charge = 0.,
    ...
)
```

Collisions

Collisions alter the electron behaviour

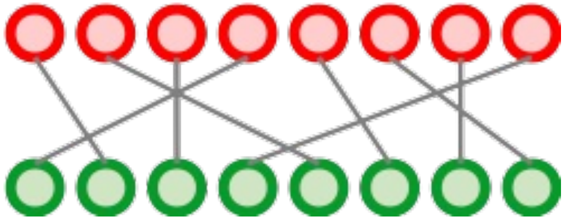
- Electron beam divergence and energy deposition
- Resistive heating by a strong current
- Heat transport (fusion research)

Adding collisions to your namelist:

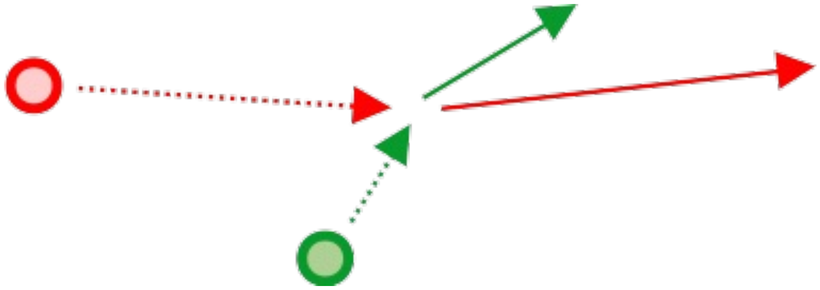
```
Collisions(
    species1 = ['ions1', 'ions2'],
    species2 = ['electrons'],
    #coulomb_log = 3,
)
```

Collisions numerical implementation: a binary process

- Macro-particles are associated 2-by-2 randomly

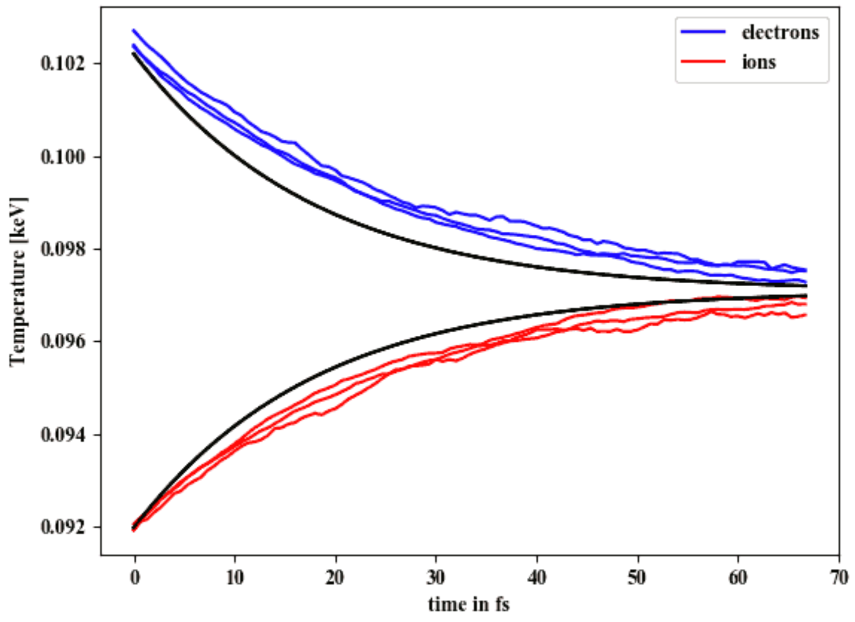


- The collision rate is computed for each pair. It corresponds to a small-angle Rutherford cross-section. [F. Prez et al., PoP 19, 083104 (2012)]
- A random deflection is computed accordingly

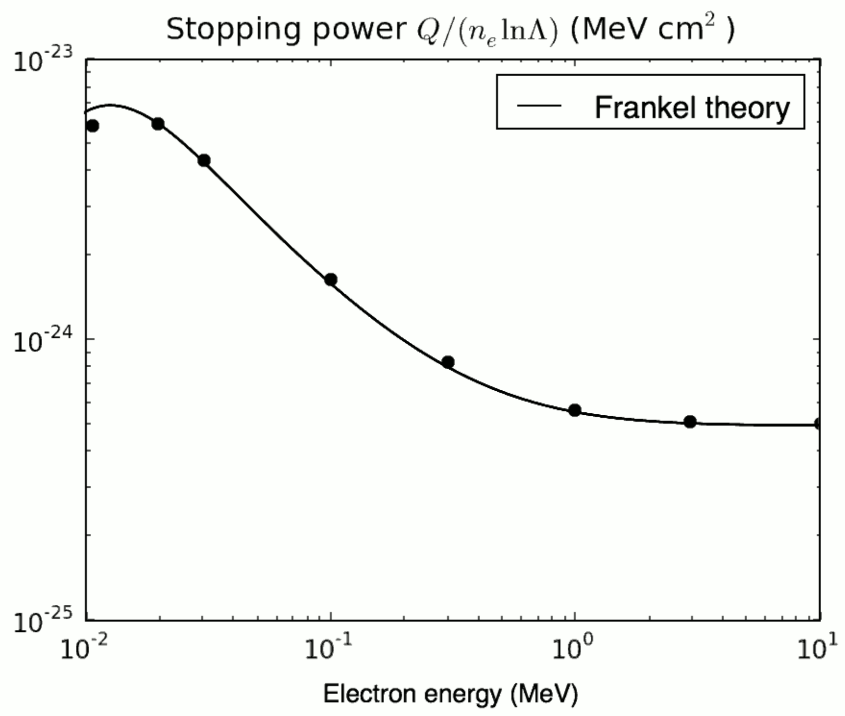


Collisions: comparing the numerical implementation with theory

Thermalization between electrons and ions



e-e stopping power



Collisions: be careful with high collision rates

In Smilei the parameter analogous to a collision rate is

$$s = \tfrac{1}{2} \langle \theta^2 \rangle N$$

Deflection variance

Number of deflections in 1 timestep

Collisions are not correctly computed if $s > 2$

The value of s can be monitored in a debug file

Nuclear Reactions

Occurrence of nuclear reactions in laser-plasma interaction

- Inertial fusion studies
- Neutron sources
- Isotope production

Nuclear reactions occur during collisions

- Adapted from [D. P. Higginson et al., JCP 388, 439 (2019)]
- Cross-section is tabulated. Currently available: $D + D \rightarrow He3 + n$
- New macro-particles creation is sampled randomly
- A rate multiplier *R* is introduced to produce more reactions but with less statistical weight.
- *R* may be automatically calculated to produce ~ as many macro-particles as in the reactants.

Add nuclear reactions in your namelist

```
Species(
    name = "Deuterium",
    atomic_number = 1,
    mass = 3870.5,
    ...
)
Species(
    name = "Helium",
    atomic_number = 2,
    mass = 5497.9,
    ...
)
Species(
    name = "neutron",
    atomic_number = 0,
    mass =  1838.7,
    ...
)
```

```
Collisions(
    species1 = ['Deuterium'],
    species2 = ['Deuterium'],
    nuclear_reaction = ['Helium','neutron'],
)
```

Radiation and energy losses by accelerated charges

Accelerated charges emit radiation

- Charge **loses energy** and **emits photons**

Probability increases with particle energy

and field strength

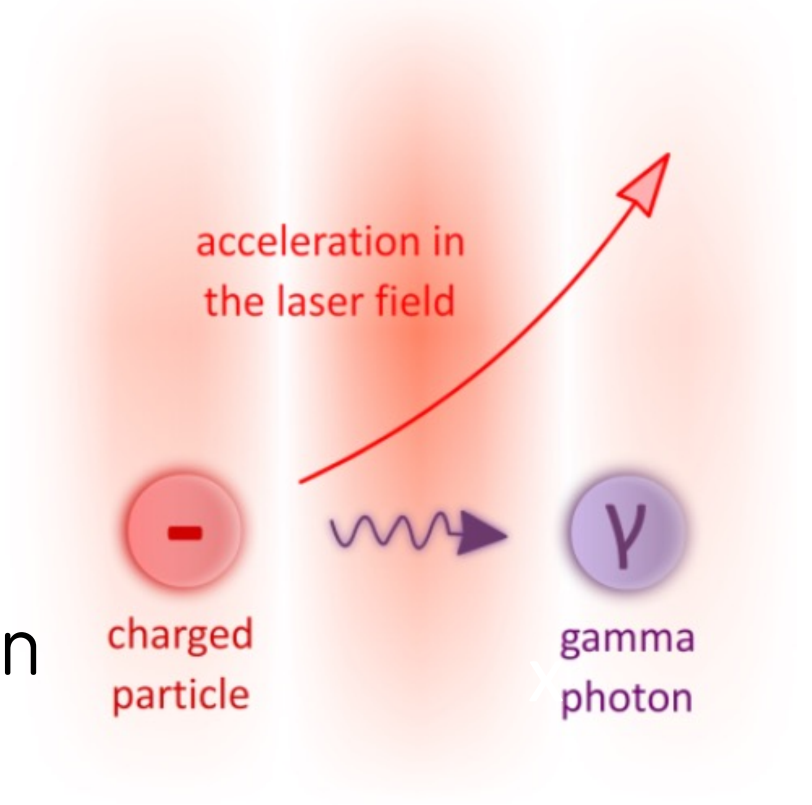
In Smilei:

- Inverse Compton Scattering

fast electron + strong field → high-energy photon

- Bremsstrahlung (not yet)

fast electron + nucleus → high-energy photon



Inverse Compton Scattering assumptions

- Relativistic particle $\gamma \gg 1$
- Relativistic field $a_0 \gg 1$
- Fields below the Schwinger limit ~ 10^{18} V/m , $4*10^{29}$ W/cm2
- Incoherent radiation between neighbors

Quantum parameter χ decides the regime

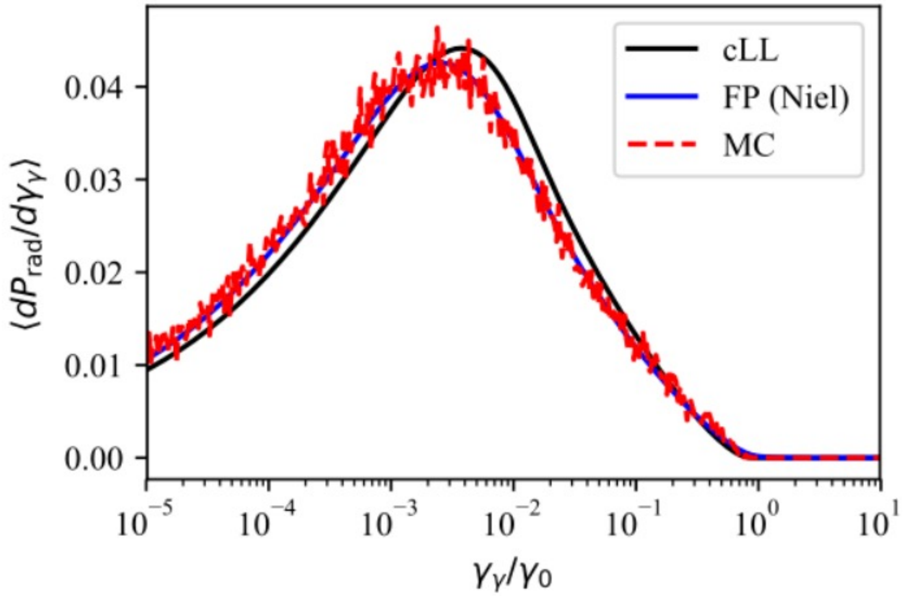
$$\chi = \frac{\gamma}{E_s}\sqrt{(\vec{E}+\vec{v}\times\vec{B})^2-(\vec{v}\cdot\vec{E})^2/c^2} \sim \gamma\frac{E}{E_s}$$

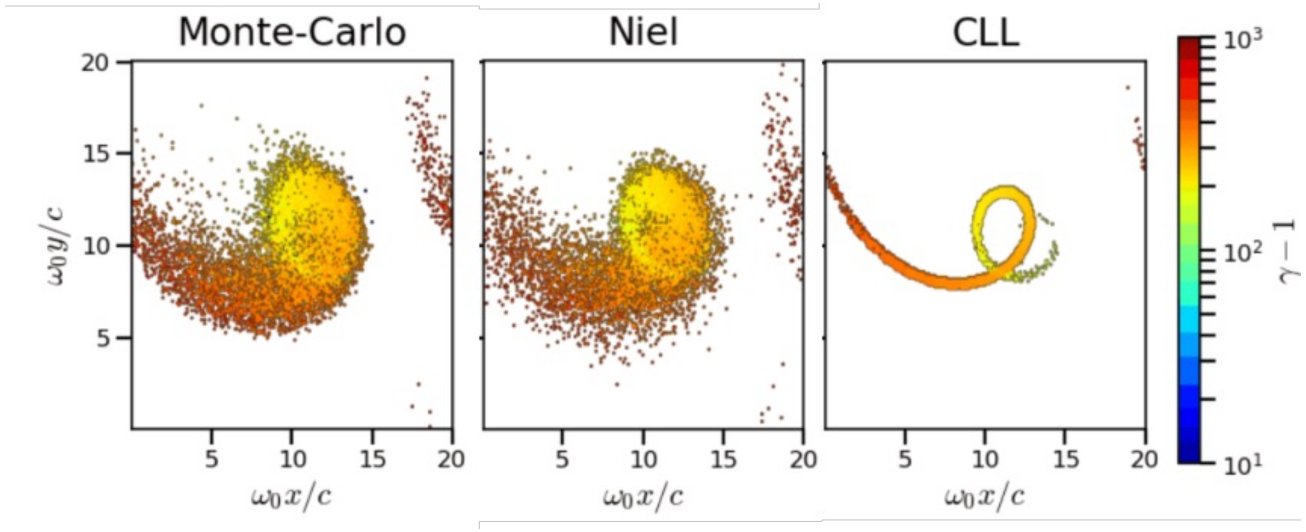
- Classical regime $\chi \sim 10^{-3}$ $\rightarrow$ **Landau-Lifshitz** model, deterministic
- Semi-classical regime $\chi \sim 10^{-2}$ $\rightarrow$ **corrected Landau-Lifshitz**
- Weak quantum regime $\chi \sim 10^{-1}$ $\rightarrow$ **Niel model**, stochastic
- Quantum regime $\chi \sim 1$ $\rightarrow$ **Monte-Carlo model**, stochastic

Produces high-energy macro-photons

Examples of Inverse Compton Scattering

Photon energy distribution emitted by an ultra-relativistic electron bunch in a constant magnetic field. $\chi = 1$





Electron bunch traveling in a constant magnetic field and losing energy over time.

Add radiation in your namelist

```
Species(
    name = "electron",
    ...
    radiation_model = "Monte-Carlo",
    radiation_photon_species = "photon",
)

Species(
    name = "photon",
    mass = 0,
    ...
)

RadiationReaction(
    ...
)
```

Electron-positron pair creation

Add pair creation in your namelist

```
Species(
    name = "electron",
    ...
    radiation_model = "Monte-Carlo",
    radiation_photon_species = "photon",
)
Species(
    name = "positron",
    ...
    radiation_model = "Monte-Carlo",
    radiation_photon_species = "photon",
)

Species(
    name = "photon",
    mass = 0,
    ...
    multiphoton_Breit_Wheeler = ["electron","positron"],
)
```

```
RadiationReaction(
    ...
)
MultiphotonBreitWheeler(
    ...
)
```

Various quantum effects could be included

- Breit-Wheeler pair creation

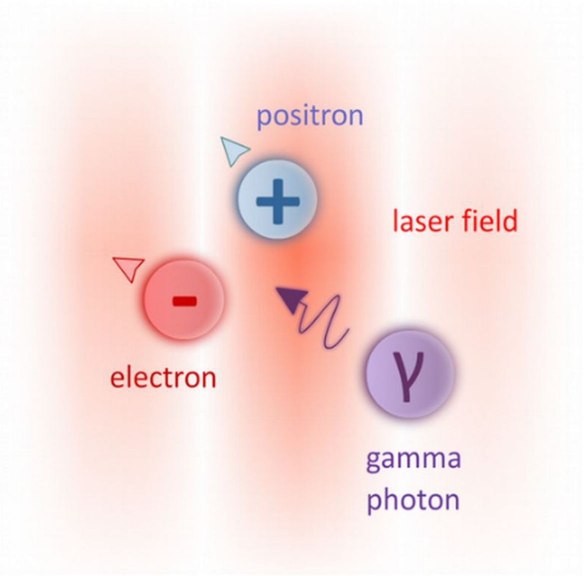
  high-energy photon + strong field → e- / e+ pair

- Bethe-Heitler pair creation (not yet)

  high-energy photon + nucleus → e- / e+ pair

- Photon-photon interaction …

Breit-Wheeler effect creates e+/e- pairs



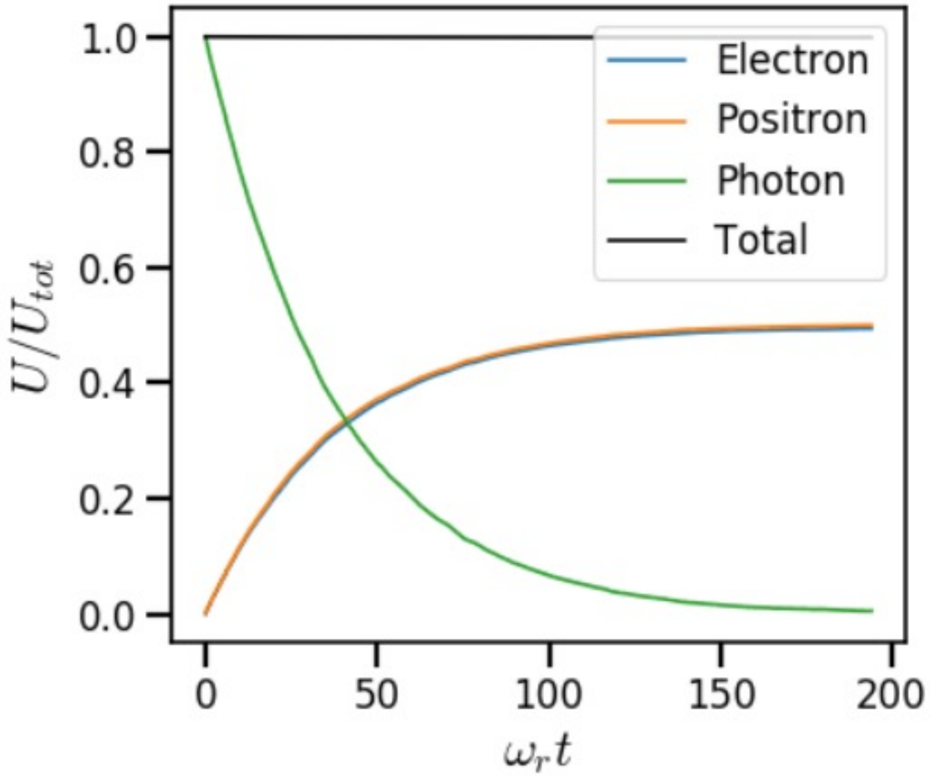
- High-energy photons exist as macro-particles (from inverse Compton scattering)
- **Photon** + **strong field** → e- / e+ pair
- Probability increases with photon energy and field strength
- Assumptions: $\chi_\gamma > 10^{-2}$, $\gamma_\gamma > 2$, $a_0 \gg 1$

Stochastic scheme (purely quantum effect)

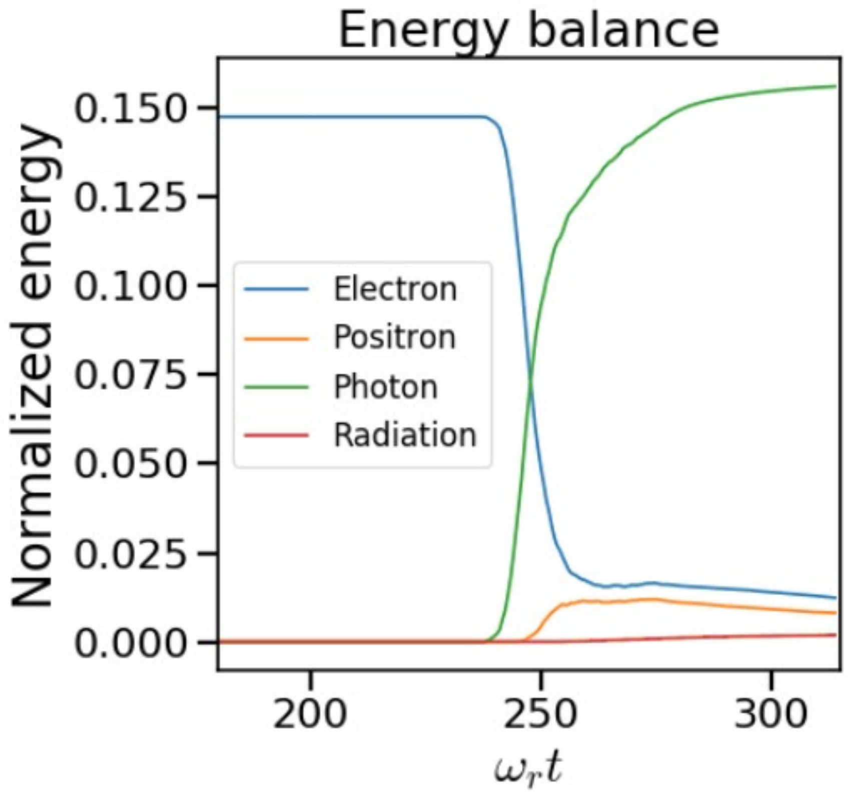
- Maximum optical depth randomly sampled for each photon (given by theoretical formula)
- When optical depth is reached, pair is created
- Electron / positron energy randomly sampled
- Photon deleted

Examples of Breit-Wheeler pair creation

Photon bunch traveling
in a constant magnetic field



Electron bunch
colliding with a laser



Summary: available physics modules

- **Ionization** by fields and by collisions
- **Collisions** between macro-particles(correction for degenerate plasmas)
- **Nuclear reactions**
- **Radiation** of accelerated charges (classical + QED)
- Breit-Wheeler **pair production**
- Projects: Bremsstrahlung, Bethe-Heitler pairs

Thank you for your attention!

Thanks for supporting this event

eli beamlines

PLAS@PAR Plasmas à Paris

GdR APPEL
Groupement de Recherche Accélérateurs Plasma PompÉs par Lasers

Contributing labs, institutions & funding agencies

MAISON DE LA SIMULATION

PLAS@PAR Plasmas à Paris

P2IO Physique des 2 Infinis et des Origines

PALM Laboratoire d'Excellence Physique : Atomes Lumière Matière

LPP

irap astrophysique & planétologie

iris

intel

CELIA

GdR APPEL
Groupement de Recherche Accélérateurs Plasma PompÉs par Lasers

Physique des Infinis
Une Initiative Sorbonne Université

AIDAS
AI Data Analytics and Scalable Simulations

cnrs

cea

SORBONNE UNIVERSITÉ

université PARIS-SACLAY

ÉCOLE POLYTECHNIQUE

INSTITUT POLYTECHNIQUE DE PARIS