Monte Carlo Program GF-CAIN for Simulations of Photon Emission in Collisions of Partially Stripped Ion Bunches with Laser-Photon Pulses

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Outline

CAIN

- Stand-alone Monte Carlo program for simulations of **beam–beam interactions** involving **high-energy electrons, positrons and photons**.
- Written by K. Yokoya *et al.*, KEK, Japan, 1984–2011.
- Code is a mixture of FORTRAN 77 and FORTRAN 90/95, $\sim$ 45 000 lines in $\sim$ 400 files
  $\rightarrow$ not well-documented, comments in code scarce.
- Dedicated, elaborate *meta-language* for defining Input/Output (65 pages of description in *User Manual*).
- Output in form of text files with all particle information and TopDrower histograms (no well-defined event record).

ABEL→CAIN history

- It started with program called **ABEL** for **beam–beam interactions** (deformation due to Coulomb field and beamstrahlung) in e^+e^- **linear colliders**.
- Then, after adding interactions with **laser** beams it was renamed to **CAIN**.
- **CAIN 2.0** was written **from scratch** and allowed for **any mixtures** of e^+, e^-, γ and lasers, and **multiple-stage** interactions (input data format completely refreshed).
- Last version: **CAIN 2.42**, 27 June 2011, available at: https://ilc.kek.jp/∼yokoya/CAIN/Cain242/

Physical processes in CAIN 2.42

1. Classical interactions (orbit deform.) due to Coulomb field.
2. Luminosity between beams (e^+, e^-, γ).
3. Synchrotron radiation by electrons/positrons (beamstrahlung) and (coherent) pair creation by high-energy photons due to beam field.
4. **Interactions of high-energy** photon or **electron**/positron **beams** with **laser field**, including non-linear effects of field strength.
5. Classical and Quantum interactions with const. external field.
6. Incoherent e^+e^--pair creation by photons, electrons and positrons.
7. Transport of charged particles through magnetic beamline.
8. **Polarisation effects** can be included in most interactions (through polarisation vector for electron/prositron beams, Stokes parameters for photons).

Output of CAIN

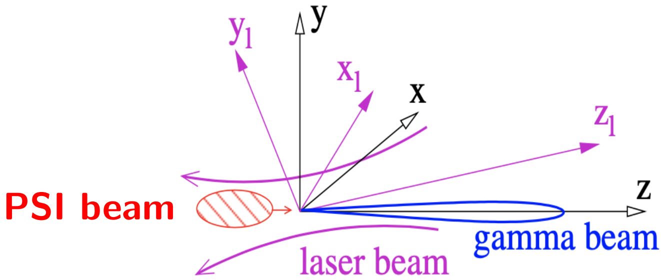
- Output data (particle properties, luminosities, statistics, etc.) can be written in specified files at any moment of job
  $\rightarrow$ **Can be huge!** (for GF up to several GBs)
- Graphical output is written only in **TopDrawer** format
  $\rightarrow$ **Obsolete!**

▷ How to use CERN **ROOT** system for data analysis?

1. For **low** statistics:
   Write particle properties in **CAIN output file** and read them by CERN's **ROOT** data analysis program (in C++).
2. For **high** statistics:
   Transfer **CAIN output** to **input** of **ROOT** data analysis program (run concurrently) through UNIX **named (FIFO) pipes**.

CAIN $\longrightarrow$ **FIFO** $\longrightarrow$ **ROOT data analysis program**

Scattering probability



- **Scattering probability** for a single particle (PSI) in time step Δt:

$$P(\vec{r},\vec{p},\vec{k},t) = \sigma_{\rm abs}(\vec{p},\vec{k})\,(1-\vec{\beta}\cdot\vec{k}/|\vec{k}|)\,n_p(x,y,z,k,t)c\Delta t,$$

where: $\vec{k}$ – photon wave vector, c – velocity of light,
$\vec{p}$, $\vec{\beta}$ – PSI momentum and relativistic velocity,
$n_p(x,y,z,k,t)$ – local density of laser-photon beam,
$\sigma_{\rm abs}(\vec{p},\vec{k})$ – cross section for laser-photon absorption by PSI.

Monte Carlo generation

→ **Two stages of Monte Carlo simulation:**

1. According to probability $P(\vec{r}, \vec{p}, \vec{k}, t)$ **scattering event** is sampled using **von Neumann rejection method**.
2. When scattering event occurs **emitted photon** is generated, i.e. its **energy** and **angles** are generated in **PSI rest-frame** according to differential cross section, and then event is **Lorentz-transformed** to **LAB** frame.

▷ The above is repeated for each **macroparticle**, and then generation moves to the **next** time moment, i.e. $t + \Delta t$, ...

- One **macroparticle** represents some **number** of **real** particles (PSI) in a **bunch** (simulations for each real particle may be not feasible if their number is very large!).
- To each **macroparticle** a Monte Carlo **weight** is assigned which is a ratio of the number of real particles to the number of macroparticles (the smaller weight the better).

Cross section

- **Cross section** of photon-absorption by PSI:
  [E.G. Bessonov and K.J. Kim, IEEE PAC 1995:2895–2897]

$$\sigma_{\rm abs}(\vec{p},\vec{k}) = \frac{2\pi r_e c\, f\, \Gamma}{[\gamma\omega(1-\beta\cos\psi)-\omega_0]^2+\Gamma^2}$$

r_e – classical electron radius,
f – oscilator strength,
γ, β – relativistic factor and velocity of PSI,
ω – incoming photon frequency,
ψ – angle between incoming photon and PSI,
ω_0 – PSI transition frequency between states 1 and 2,
$\Gamma = \omega_0^2 r_e f g_1/(c g_2)$ – spontaneous emission half-linewidth,
where $g_{1,2}$ – degeneracy factors of states 1 and 2, respectively.

Emitted photon kinematics

- MC generation of **emitted photon** in **PSI rest-frame**
  $\Rightarrow$ **Unpolarised case so far!**

  1. azimuthal angle ϕ:
  $$\phi \in \mathcal{U}(0,1),$$
  where $\mathcal{U}$ denotes **Uniform** distribution,
  2. polar angle θ:
  $$\cos\theta \in \mathcal{U}(-1,1),$$
  3. angular frequency ω' ($\rightarrow$ energy $E' = \hbar\omega'$):
  $$\omega' \in \mathcal{L}(\omega'_{min}, \omega'_{max}),$$
  where $\mathcal{L}$ – **Lorentzian** distribution with prob. density funct.:
  $$\rho_{\omega_0,\Gamma}(\omega'; \omega'_{min}, \omega'_{max}) = \mathcal{N}\,\frac{\Gamma}{(\omega'-\omega_0)^2+\Gamma^2},$$
  with $\mathcal{N}^{-1} = \arctan([\omega'_{max}-\omega_0]/\Gamma) - \arctan([\omega'_{min}-\omega_0]/\Gamma)$.

Energy spread of laser beam

- **CAIN** assumes monochromatic laser beam (photon energy spread not important for inverse-Compton scattering).
- For **resonant** atomic photon absorption **laser-beam energy spread** can be **comparable** or even **larger** than the **resonance linewidth**, so **it has to be taken into account**!
- In **GF-CAIN** it is done in two ways (inside corresponding routines):
  1. If $\sigma_{\bar{\omega}}/\bar{\omega} < \Gamma/\omega_0$, the **laser-photon energy** $E = \hbar\omega$ is generated from the corresponding **Gaussian distribution**, then the **scattering cross section** is calculated using the **weight** corresponding to $\sigma_{\rm abs}(\vec{p}, \vec{k})$.
  2. Otherwise, the **photon energy** in the PSI-rest frame is generated from the **Lorentzian distribution** of $\sigma_{\rm abs}(\vec{p}, \vec{k})$, then the **scattering cross section** is calculated using the **weight** corresponding to the **Gaussian** function of the **laser-energy spread**.

▷ In this way, Monte Carlo event generation in **GF-CAIN** is **efficient** for an **arbitrary resonance linewidth**!

Li-like Pb, H-like Pb and He-like Ca

- PSI's cannot be defined by **CAIN** input – they are implemented in **CAIN** routine `LNCPGN`:
  - Lithium-like ${}^{208}_{82}\mathrm{Pb}^{79+}$ in file `src/GF/Pb/lncpgn-Pb_Li-like.f`
  - Hydrogen-like ${}^{208}_{82}\mathrm{Pb}^{81+}$ in file `src/GF/Pb/lncpgn-Pb_H-like.f`
  - Helium-like ${}^{40}_{20}\mathrm{Ca}^{18+}$ in file `/src/GF/Ca/lncpgn-Ca_He-like.f`
- They are copied into **CAIN**'s file `/src/lncpgn.f` in `Makefile` when the corresponding PSI-run is chosen by a `make` command, e.g.
  - `make run-PbLi`
  - `make run-PbH`
  - `make run-CaHe`

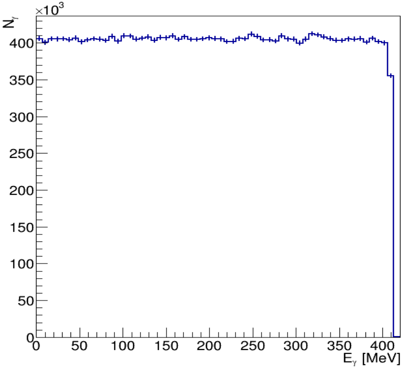
  and then an appropriate input file is read.
- **Spontaneous** emission **delay** and **stimulated** emission have been added – important for PoP experiment Pb^{79+} as well as for Ca^{18+}
  → appropriate modifications of **CAIN** **event record** as well as 'drift' routines were necessary.
- Other PSI's can be implemented in a similar way – not elegant, but easier than modifying complicated **CAIN** input!

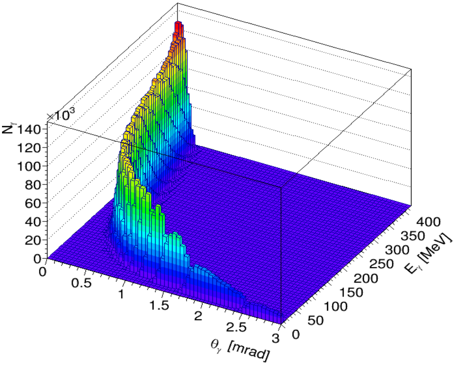
H-like Pb – input parameters (based on Bessonov et al.)

- **PSI beam:** ${}^{208}_{82}\mathrm{Pb}^{81+}$ with transition: $1s^1\ {}^2S_{1/2} \rightarrow 2p^1\ {}^2P_{1/2}$
  - transition energy: $\hbar\omega_0 = 68.7\,\mathrm{keV}$; $f = 0.416$, $g_1 = 1$, $g_2 = 3$
  - ion mass: $M_i = 193.687\,\mathrm{GeV/c^2}$
  - ion energy and relative spread: $E_i = 579\,\mathrm{TeV}$, $\sigma_E = 2 \cdot 10^{-4}$
  - relativistic factor: $\gamma_i = 2989$
  - number of ions per bunch $N_i = 9.4 \cdot 10^7$
  - beta function in IR: $\beta_x = \beta_y = 0.5\,\mathrm{m}$
  - geometric emittance: $\epsilon_x = \epsilon_y = 3 \cdot 10^{-9}\,\mathrm{m\,rad}$
  - r.m.s transverse beam size: $\sigma_x = \sigma_y = 38.73\,\mu\mathrm{m}$
  - r.m.s. bunch length $\sigma_z = 15\,\mathrm{cm}$
- **Laser:** Gaussian spatial and time profiles
  - photon energy and rel. spread: $E_\gamma = 11.45\,\mathrm{eV}$, $\sigma_\omega = 2 \cdot 10^{-4}$
  - photon wavelength: $\lambda_\gamma = 108.28\,\mathrm{nm}$
  - pulse energy: $W_l = 56\,\mu\mathrm{J}$
  - peak power density: $P_{00} = 1.1 \cdot 10^{13}\,\mathrm{W/m^2}$
  - r.m.s. transverse beam size at focus: $\sigma_x = \sigma_y = 25.42\,\mu\mathrm{m}$
  - Rayleigh length: $R_{L,x} = R_{L,y} = 7.5\,\mathrm{cm}$
  - r.m.s. pulse length: $\sigma_z = 15\,\mathrm{cm}$

Emitted photon energy in LAB

- Number of **macroparticles** generated in **GF-CAIN**: $9.4 \cdot 10^7$
- Spontaneous emission **delay** included (small in this case)



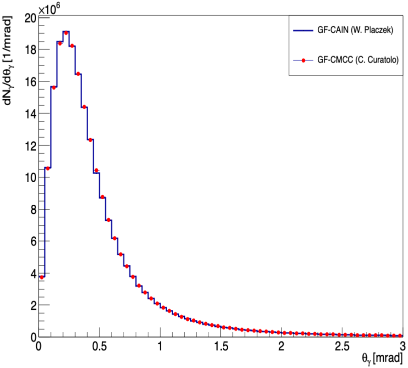


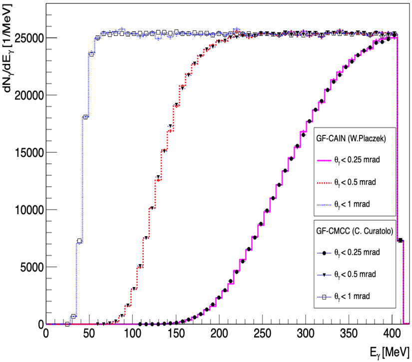
→ Half of most energetic photons within $\theta < 1/\gamma_{\rm i}$

→ Number of emitted **photons** per **ion**: $N_\gamma / N_{\rm i} = 0.11$

Comparisons: GF-CAIN vs. GF-CMCC

▷ Comparisons with the independent Monte Carlo program **GF-CMCC** of Camilla Curatolo (INFN-Padova)





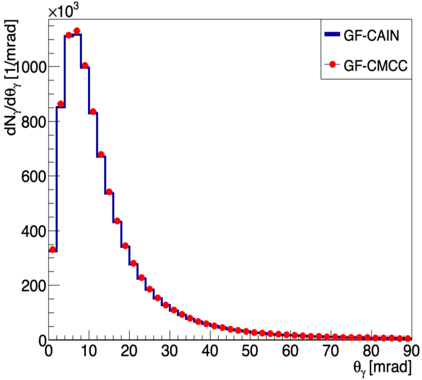
→ **Very good agreement of the two MC programs!**

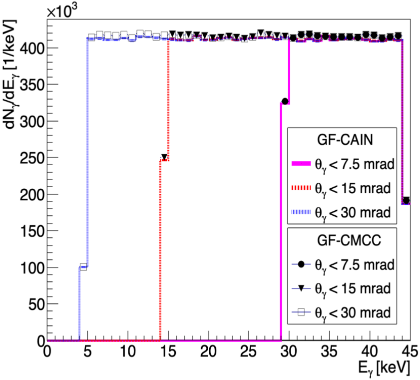
Lithium-like Pb ion for PoP – input parameters (LoI)

- **PSI beam:** $^{208}_{82}\mathrm{Pb}^{79+}$ with transition: $1s^2 2s^1\ {}^2S_{1/2} \to 1s^2 2p^1\ {}^2P_{1/2}$
  - transition energy and lifetime: $\hbar\omega_0 = 230.81\,\mathrm{eV}$, $\tau_0 = 76.6\,\mathrm{ps}$
  - ion mass: $M_i = 193.687\,\mathrm{GeV/c^2}$
  - ion energy and relative spread: $E_i = 18.65259\,\mathrm{TeV}$, $\sigma_E = 2 \cdot 10^{-4}$
  - relativistic factor: $\gamma_i = 96.3$
  - number of ions per bunch $N_i = 0.9 \cdot 10^8$
  - Twiss parameters: $\alpha_x = \alpha_y = 0$, $\beta_x = 70.30\,\mathrm{m}$, $\beta_y = 44.23\,\mathrm{m}$
  - geometric emittance: $\epsilon_x = \epsilon_y = 1.558 \cdot 10^{-8}\,\mathrm{m\,rad}$
  - r.m.s transverse beam size: $\sigma_x = 1.047\,\mathrm{mm}, \sigma_y = 0.83\,\mathrm{mm}$
  - r.m.s. bunch length $\sigma_z = 6.386\,\mathrm{cm}$
- **Laser:** Gaussian spatial-time profiles, beam angle: 2.6°
  - photon energy and rel. spread: $E_\gamma = 1.2\,\mathrm{eV}$, $\sigma_\omega = 2 \cdot 10^{-4}$
  - photon wavelength: $\lambda_\gamma = 1034\,\mathrm{nm}$
  - pulse energy: $W_l = 5\,\mathrm{mJ}$
  - peak power density: $P_{00} = 2.684 \cdot 10^{14}\,\mathrm{W/m^2}$
  - r.m.s. transverse beam size at focus: $\sigma_x = \sigma_y = 0.65\,\mathrm{mm}$
  - Rayleigh length: $R_{L,x} = R_{L,y} = 5.135\,\mathrm{m}$
  - r.m.s. pulse length: $\sigma_z = 0.8394\,\mathrm{mm}$

Comparisons: GF-CAIN vs. GF-CMCC

▷ Comparisons with the independent Monte Carlo program **GF-CMCC** of Camilla Curatolo (INFN-Padova)

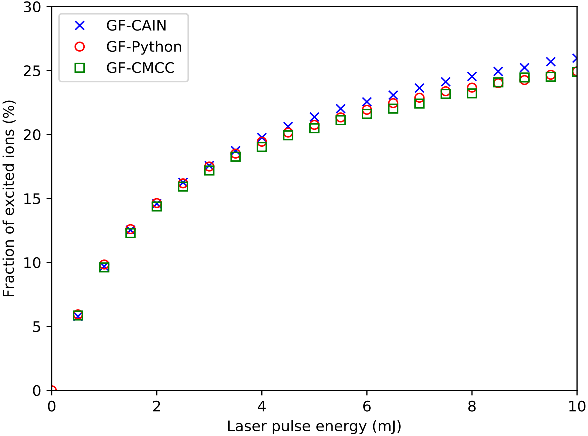




→ **Very good agreement of the two MC programs!**

Fraction of excited ions

- ▷ Predictions of independent Monte Carlo programs **GF-CMCC** (Camilla Curatolo) **GF-Python** (Alexey Petrenko) and **GF-CAIN**



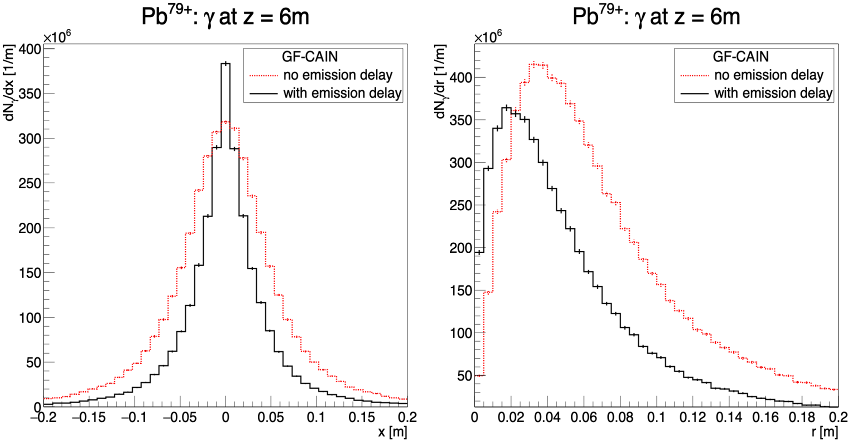
→ **Good agreement between the three programs!**

Spontaneous emission delay and stimulated emission

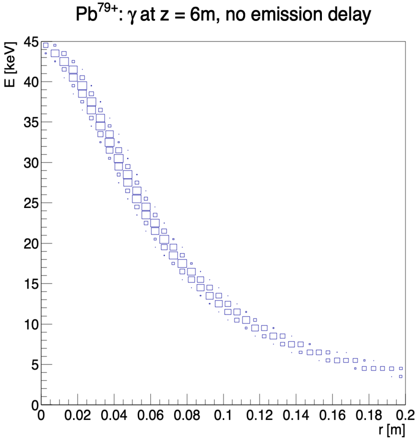
- Mean path of PSI in excited state in LAB $\approx 2.2\,\mathrm{m}$
  $\rightarrow$ Two important effects included in **GF-CAIN**:
  1. **time delay of spontaneous emission** – generated from the **exponential distribution** with the mean-time τ_0, and the **excited** ion is **propagated** until it **de-exites**: (1) after the generated **time** τ by **spontaneous emission** or (2) immediately by **stimulated emission**, or **reaches** a given z or t coordinate (e.g. detector) in the **exited** state.
  2. **stimulated emission** – generated according to the **probability** $P'(\vec{r},\vec{p},\vec{k},t) = (g_1/g_2)P(\vec{r},\vec{p},\vec{k},t)$, where $P(\vec{r},\vec{p},\vec{k},t)$ is the photon-absorption probability and $g_{1,2}$ are the state-degeneracy factors, and when the event is **accepted**, the ion returns to the **ground** state while the two **photons** are **discarded**.

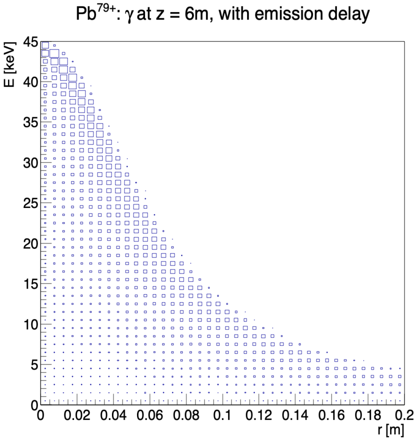
GF-CAIN simulation results at $z = 6\,\mathrm{m}$:	$\mathrm{N}_\gamma/\mathrm{N}_\mathrm{i}$
No spontaneous emission **delay**:	20.1%
With spontaneous emission **delay**:	15.7%
With spont. emission **delay** and **stimulated** emission	13.3%

Photon x-coordinate and radius distributions at $z = 6\text{m}$



Photon radius vs. energy distributions at $z = 6\text{m}$

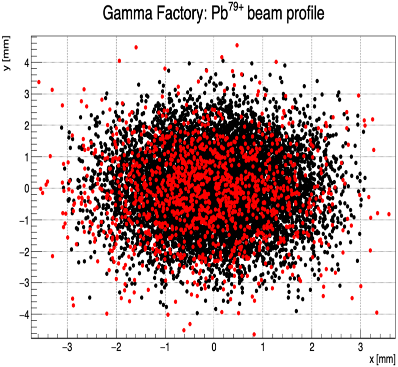


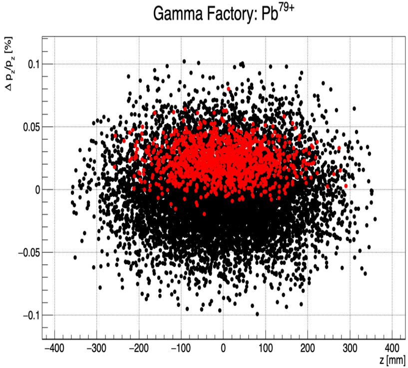


Example for Doppler cooling of PSI beam

- Laser energy lowered by $2\sigma_\omega$ w.r.t. resonance energy

● excited ions ● ground-state ions





▷ Fraction of excited ions: $\mathrm{N_{exited}}/\mathrm{N_{all}} = 9.7\%$
(with spontaneous emission delay and stimulated emission)

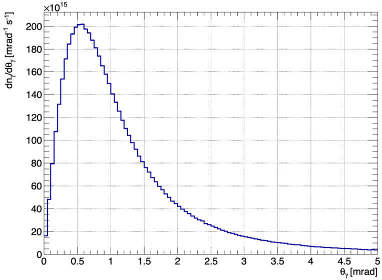
Helium-like Ca ion – input parameters (transmutations)

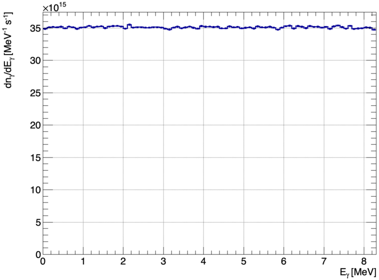
- **PSI beam:** ${}^{40}_{20}\mathrm{Ca}^{18+}$ with transition: $1s^2\ {}^1S_0 \to 1s^1 2p^1\ {}^1P_1$
  - transition energy and lifetime: $\hbar\omega_0 = 3.9023775\,\mathrm{keV}$, $\tau_0 = 8.8\,\mathrm{fs}$
  - ion mass: $M_i = 37.332\,\mathrm{GeV/c^2}$
  - ion energy and relative spread: $E_i = 39.72\,\mathrm{TeV}$, $\sigma_E = 2\cdot 10^{-4}$
  - relativistic factor: $\gamma_i = 1064$
  - number of ions per bunch $N_i = 3\cdot 10^9$
  - Twiss parameters: $\alpha_x = \alpha_y = 0$, $\quad \beta_x = \beta_y = 50\,\mathrm{m}$
  - geometric emittance: $\epsilon_x = \epsilon_y = 3\cdot 10^{-10}\,\mathrm{m\,rad}$
  - r.m.s transverse beam size: $\sigma_x = \sigma_y = 0.1225\,\mathrm{mm}$
  - r.m.s. bunch length $\sigma_z = 15\,\mathrm{cm}$
- **Laser:** Gaussian spatial-time profiles, beam angle: 0°
  - photon energy and rel. spread: $E_\gamma = 1.833824\,\mathrm{eV}$, $\sigma_\omega = 2\cdot 10^{-4}$
  - photon wavelength: $\lambda_\gamma = 676.1\,\mathrm{nm}$
  - pulse energy: $W_l = 0.5\,\mathrm{mJ}$
  - peak power density: $P_{00} = 2.822\cdot 10^{13}\,\mathrm{W/m^2}$
  - r.m.s. transverse beam size at focus: $\sigma_x = \sigma_y = 0.15\,\mathrm{mm}$
  - Rayleigh length: $R_{L,x} = R_{L,y} = 41.81996, \mathrm{cm}$
  - r.m.s. pulse length: $\sigma_z = 1.49896\,\mathrm{cm}$ $\;(\sigma_t = 50\,\mathrm{ps})$

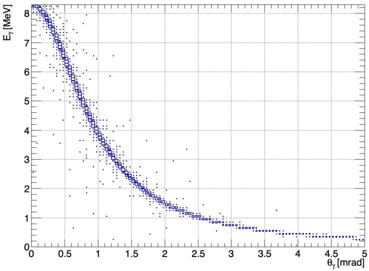
Photon emission angle and energy

- ▷ Repetition rate: 20 MHz
- ▷ Emission rate: $N_\gamma / N_{PSI} \approx 5$

→ For $\sigma_t = 500$ ps: $N_\gamma / N_{PSI} \approx 30$







Summary

- **CAIN** code has been customised to **compile** with **gfortran** (GNU Fortran) and **run** on Linux and macOS systems
  $\rightarrow$ with the use of customised Makefile
- **CAIN** Monte Carlo program has been **debugged** and **adapted** to **laser-photon pulse** collisions with **PSI beams** of ${}^{208}_{82}\mathrm{Pb}^{81+}$, ${}^{208}_{82}\mathrm{Pb}^{79+}$ and ${}^{40}_{20}\mathrm{Ca}^{18+}$ (**Gamma Factory**) $\Rightarrow$ **GF-CAIN**.
- **Spontaneous** emission **delay** and **stimulated** emission have been implemented – important for PoP experiment.
- **GF-CAIN** output has been interfaced with **ROOT** data analysis program via UNIX **named (FIFO) pipes**.
- **Good agreement** with independent Monte Carlo event generators **GF-CMCC** of Camilla Curatolo and **GF-Python** of Alexey Petrenko.
- Statistics of $\sim 10^8$ **macroparticles** can be generated on medium PC.