AN INVERSE-COMPTON SCATTERING SIMULATION MODULE FOR RF-TRACK

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Abstract

A simulation module implementing Inverse-Compton scattering (ICS) was added to the tracking code RF-Track. The module consists of a special beamline element that simulates the interaction between the tracked beam and a laser, making RF-Track capable of simulating a complete ICS source in one go, from the electron source to the photons. The description of the laser allows the user to thoroughly quality the laser in terms of wavelength, pulse energy, pulse length, incoming direction, M² parameter, aspect ratio, polarisation and whether the laser profile should be Gaussian or uniform. Furthermore, as the code implements fully generic expressions, the scattering between photons and different particles than electrons can be simulated. A benchmark against CAIN showed excellent agreement and that RF-Track outperforms CAIN in terms of computational speed by orders of magnitude.

INTRODUCTION

Light sources based on Inverse Compton Scattering are attracting growing attention due to their compactness, high brilliance, and the capability to reach a wide range of photon energies, from X-rays (few keV) to gamma rays (few MeV), the latter inaccessible to most light sources including synchrotrons.

Inverse Compton scattering takes place when a charged particle transfers a fraction of its momentum to a photon, increasing its energy. The maximum final photon energy achievable in an ICS interaction occurs in case of a *head-on* collision. If the initial energy of the photon is E_i , the final energy E_f is given by

$$E_{\rm f} = 4\gamma^2 E_{\rm i},$$

where γ is the relativistic factor of the scattering particle [1]. In the case of ultra-relativistic electrons, the photon's energy can increase by several orders of magnitude.

While designing an ICS source, the simulation of ICS is crucial to assess the scattered photons' spectral properties, bandwidth, and angular distribution. The most accredited code for simulating Inverse Compton Scattering is probably CAIN, written by Yokoya et al. [2]. CAIN is a stand-alone Monte Carlo program that simulates beam-beam interactions involving high-energy electrons, positrons, and photons. The code covers the classical and quantum domains in linear and weakly nonlinear regimes. The interaction is described as the scattering between particles and has been extensively tested and compared to experimental results. Despite its excellent reputation, the practical application of CAIN towards optimising an ICS-based facility is hindered by two primary limitations: (1) it operates rather slowly, and (2) as a standalone code, it requires an interface with conventional particle tracking codes that can transport electrons through the accelerator to the interaction point (IP), making integrated performance optimisation challenging.

To circumvent these limitations, the author of this paper developed a simulation module as a part of the tracking code RF-Track [3]. Since RF-Track can track particles with any charge through an accelerator while accounting for the effects of space charge, beam loading, wakefields, etc., this module enables the simulation of an ICS source from cathode to X-rays in one go. This unlocks a thorough optimisation of the source being designed.

The module was written in parallel C++ and showed simulation speed orders of magnitude faster than CAIN. This paper provides a detailed description of the implementation and two benchmarking cases.

IMPLEMENTATION

To the user, the collision point consists of a specialised lattice element called "LaserBeam" that simulates the scattering between the tracked beam and a laser. This element allows the user to define the key laser parameters: wavelength, pulse energy, pulse length, incoming direction (which can be arbitrarily chosen over the entire solid angle), the M² parameter, the aspect ratio, the degree of linear polarisation (optional), and whether the laser beam has a Gaussian or a uniform profile.

LaserBeam is a time-dependent element that the user can synchronise to the beam or an absolute clock. Like any other RF-Track's lattice element, it can be arbitrarily displaced by any offset and angle, allowing for misalignment imperfection studies. The element can have a length or be thin; in either case, the entire three-dimensional structure of the bunch is reconstructed during the computation.

The scattering is computed in the rest frame of the charged particle as a Monte Carlo process. When the photon's energy is much lower than the particle's rest energy, its absolute momentum and wavelength remain unchanged during the collision. In this case, the scattering is elastic and is called *Thomson scattering*. Proper *Compton scattering* occurs at higher photon energies when there is a momentum transfer between the particle and the photon, and the scattering is inelastic. After the computation of the scattering, the phasespace variables of particle and photon are updated and moved back to the laboratory frame, where tracking continues for both species.

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Calculating the final state of the interacting particles requires knowledge of the total and differential cross-sections. The total cross-section is needed to determine λ , the particle's mean free path, that is, the distance a particle travels before it collides with a photon. The angular differential cross-section is needed to calculate the energy and deflection angle of the scattered photon and the recoil of the incident particle.

Since these cross-sections assume different expressions depending on whether the incoming photons are polarised, RF-Track effectively implements four scattering processes: Thomson or Compton, polarised or unpolarised. The following subsections provide the detailed expressions used in the code.

Case of Thomson Scattering

The Thomson differential cross-section of an arbitrary particle at rest with mass m and charge q elastically colliding with a photon is [4],

$$\frac{d\sigma}{d\Omega} = r^2 f\left(\theta, \varphi, P\right),$$

where $r = \frac{q^2}{4\pi\epsilon_0 mc^2}$ is the classical radius of the particle, θ and φ correspond to the photon's incidence direction, and $d\Omega = \sin \theta \, d\theta \, d\varphi$ is the standard differential element of solid angle. The function $f(\theta, \varphi, P)$ accounts for the cross-section's dependence on the direction and polarisation of the incoming photon.

In the assumption of unpolarised photons, the function f must be averaged over all incoming polarisation angles and it reduces to [4]

$$f_{\text{unpolarized}}\left(\theta\right) = \frac{1+\cos^{2}\theta}{2},$$

showing that the scattered photon is isotropic with respect to the azimuthal angle φ .

In the case of a beam of linearly polarized photons, with polarization $P = \sin \phi$ where ϕ is the polarisation angle, the angular dependence of the differential cross-section reads:

$$f_{\text{polarized}} (\theta, \varphi, P) = \left(\left(2P^2 - 1 \right) \sin^2 \varphi - P^2 \right) \sin^2 \theta + \dots$$
$$\dots + 2P\sqrt{1 - P^2} \cos \varphi \, \sin \varphi \, \sin^2 \theta + 1,$$

and the outcoming photon is no longer isotropic in φ .

The total cross-section, needed to compute the mean free path λ , is the integration of the differential cross-section over the whole solid angle,

$$\sigma = \iint_{\Omega} \left(\frac{d\sigma_t}{d\Omega} \right) d\Omega = \frac{8\pi}{3} r^2 = \frac{8\pi}{3} \left(\frac{q^2}{4\pi\epsilon_0 mc^2} \right)^2$$

For electrons and positrons, this is the well-known constant $\sigma_{\text{Thomson}} = 66.5 \text{ fm}^2$. In RF-Track, however, this quantity is computed event by event, allowing for the scattering simulation of any charged particle.

Case of Compton Scattering

For an incident unpolarized photon of energy E_{γ} , the differential cross section is given by the Klein-Nishina formula [4]:

$$\frac{d\sigma_{\text{unpolarized}}}{d\Omega} = \frac{1}{2}r^2 \left(\frac{\lambda}{\lambda'}\right)^2 \left[\frac{\lambda}{\lambda'} + \frac{\lambda'}{\lambda} - \sin^2\theta\right],$$

where λ/λ' is the ratio of the wavelengths of the incident and scattered photons. The angular-dependent ratio of the photon wavelengths is

$$\frac{\lambda}{\lambda'} = \frac{1}{1 + \epsilon (1 - \cos \theta)}.$$

The quantity $\epsilon = E_{\gamma}/(mc^2)$ is the energy of the incident photon normalised to the particle's rest energy.

For a linearly polarized photon, the differential cross section is instead given by [5]

$$\frac{d\sigma_{\text{polarized}}}{d\Omega} = \frac{1}{2}r^2 \left(\frac{\lambda}{\lambda'}\right)^2 \left[\frac{\lambda}{\lambda'} + \frac{\lambda'}{\lambda} - 2\sin^2\theta\cos^2\varphi\right].$$

In this case, the scattered photon is no longer isotropic in the azimuthal angle φ .

ALGORITHM

The interaction is computed over the overlap region in a user-defined number of steps, each with length ΔL . Slicing the computation enables the simulation of multiple scatterings during the collision.

For each slice and each charged particle in the beam, the simulation algorithm repeats the following seven steps until the colliding bunches no longer overlap:

- 1. Determine the average density and direction of the incoming photon beam at the particle's location.
- 2. Perform a Lorentz boost of the average photon into the rest frame of the scattered particle.
- 3. Check whether it is a Thomson or a Compton scattering; then, compute the total cross-section σ to evaluate the particle's mean-free path $\lambda = 1/(\rho \sigma)$, with ρ the volume number density of the photons.
- 4. Given λ and ΔL , compute the probability of scattering. If $\lambda \gg \Delta L$, force a scattering event and produce a weighted photon based on the weight of the charged particle.
- Using a Monte Carlo method, utilise the appropriate differential cross-section to evaluate the energy and the 3D direction (θ, φ) of the scattered photon.
- 6. Given the scattered photon's direction and energy, resolve the kinematics of the scattering, update the particle's phase-space variables, and perform a Lorentz boost into the lab frame.

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7. Add the scattered photon to the beam's data structure and advance both particle and photon through the next slice.

These computations are performed in parallel over the beam's particles.

BENCHMARK AND PERFORMANCE

The RF-Track's implementation was compared with CAIN in the ThomX and ELI-NP cases. Figure 1 compares X-ray beam-defining plots at the IP, obtained in RF-Track and CAIN for the ThomX source [6]. The expected Compton edge of 45 keV is determined from both codes. Other X-ray beam parameters obtainable in RF-Track, e.g., beam size, $\sigma_x = 58 \,\mu\text{m}, \sigma_y = 52 \,\mu\text{m}$, and beam divergence, 9 mrad, correspond to the simulations from CAIN. These results show that RF-Track and CAIN are in excellent agreement. Output photon parameters were also compared for ELI-NP-GBS [7] in Table 2. The value for the scattered photon flux is the only notable difference between the two codes.

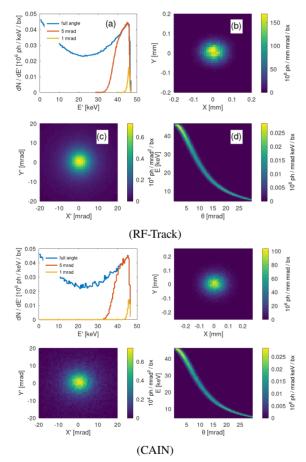


Figure 1: ICS beam-defining plots of ThomX, simulated using RF-Track (top) and CAIN (bottom). (a) The energy spectrum of photons travelling in all directions and through a 1 mrad and 5 mrad collection angle. (b) The transverse source size. (c) The angular emission distribution. (d) The number of ph/mrad²/s as a function of energy and collection angle.

A summary of the performance of RF-Track and CAIN is shown in Table 1. RF-Track can compute the results from Figure 1 several orders of magnitude faster than CAIN. The longer computation runtime of CAIN can be attributed to its requirement for a larger number of electron macroparticles to generate sufficient statistics, given the smallness of the scattering cross-section. RF-Track can enforce a minimum number of scattered photon macroparticles per slice, which relaxes the requirement on the number of electron macroparticles.

Table 1: Comparison Between RF-Track and CAIN in the ThomX Case

Parameter	CAIN	RF-Track
Input electron ⁽¹⁾	5×10^{7}	104
Output X-rays ⁽¹⁾	12,700	1,350,311
Runtime (s)	2,545	0.67
Total flux (10^{13} ph/s)	2.65 ± 0.02	2.50 ± 0.01

⁽¹⁾ Number of simulated macro particles

Table 2: Comparison Between RF-Track and CAIN in the ELI-NP Case (Courtesy of Gianfranco Paternò)

Parameter	CAIN	RF-Track
Mean energy (keV)	9118.63	9117.61
Peak energy (keV)	10025.00	10025.00
Max energy (keV)	10130.17	10129.02
Relative energy bandwidth ⁽²⁾	6.74%	6.77%
Nb. of photons ⁽²⁾	2.82×10^{5}	2.57×10^{5}
Fraction of photons ⁽²⁾	0.2558	0.2546

 $^{(2)}$ Within a cone $\theta < 0.5 \, \rm{mrad}$

CONCLUSIONS

The capability to simulate linear Thomson and Compton scattering has been implemented in the RF-Track particle tracking code. This development enables integrated start-toend simulations of ICS sources from cathode to X-rays. A benchmark against CAIN showed that RF-Track's results are in excellent agreement, while RF-Track outperforms CAIN's computational speed by orders of magnitude.

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