EPOCH Bremsstrahlung Routine

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Abstract

Two new Bremsstrahlung routines have been developed for *EPOCH*. One has been developed by Jiřı́ Vyskočil, Ondřej Klimo and Stefan Weber at the *ELI*-Beamlines project, and the other by Stuart Morris, a PhD student at the University of York. In this paper, we will outline the methodology of both versions of the Bremsstrahlung routine, specifying how each differ from one another, before presenting the results from running each implemented routine against a test simulation experiment.

1 Introduction

The motivation behind this investigation is the advancements being made in laser technology, and the accessibility of short ultra-intense laser pulses. These have opened new possibilities in generating gamma rays by various processes involving fast electrons which are accelerated during the interaction of an intense laser pulse with a target. These gamma ray sources could have useful applications in various fields including: radiography, photo-nuclear spectroscopy, radiation therapy in medicine, photo-fission for nuclear waste management, and laboratory astrophysics.

One of the most common phenomenon that leads to high energy photon emission, alongside iverse Compton scattering, is Bremßtrahlung. This is the process in which an electron is deflected from its trajectory by the Coulomb attraction of an ion. During this acceleration, the electron emits a photon with energy:

$$\varepsilon_\gamma = \varepsilon_0 - \varepsilon_1 \tag{1}$$

where ε_0 is the initial energy of the electron and ε_1 is the energy of the electron after being scattered. Contemporary and upcoming high-power laser systems will be capable of generating pulses which, when focussed to a spot on the order of a few microns, would attain high intensities of $I \approx 10^{22} - 10^{23}$ W cm^{-2}.

Efficient generation of Bremsstrahlung photons requires a population of fast electrons. These "fast electrons" are produced in two common laser-plasma interactions: a laser interacting with the surface of a solid target, and in Laser Wakefield Acceleration (LWFA).

1.1 Plasma Screening

Plasma screening is the damping of electric fields caused by the presence of mobile charge carriers. In a fluid, with a given permittivity ϵ, composed of electrically charged constituent particles, q_1 and q_2, each pair of particles interacts through the Coulomb force:

$$F = \frac{q_1 q_2}{4\pi\epsilon|r|^3}\vec{r} \tag{2}$$

If the interactions are screened (outside of Debye sphere), then the charge density and electric potential are related by Poisson's equation:

$$-\nabla^2[\Delta\phi(r)] = \frac{1}{\varepsilon_0}[Q\delta(r) - e\Delta\rho(r)] \tag{3}$$

To proceed, need to find a second equation independently relating $\Delta\rho$ and $\Delta\phi$. For this, we can apply the Debye-Huckel model (high Temperatures) or the Thomas-Fermi model (valid at low Temperatures).

2 Method

Bremsstrahlung radiation can be studied by means of Monte Carlo (MC) particle transport simulations which treat electron propagation as a random walk process with the emission of gamma photons due to bremsstrahlung included as 'hard events'. The drawback of this approach is that it requires some description of the fast electron source, it does not generally provide temporal resolution, the trajectories of individual electrons are assumed to be mutually independent.

2.1 ELI's Module

Here's an overview of how the routine works:

- Based on MC code in $PENELOPE$, with Bremsstrahlung differential cross section:

$$\frac{d\sigma}{d\varepsilon_\gamma} = \frac{Z^2}{\beta^2}\frac{1}{\varepsilon_\gamma}\chi(Z,\varepsilon_0,\kappa) \tag{4}$$

- The scaled DCS, χ, is read from a pre-calculated table (Seltzer and Berger)
  - Spans energies from 1 keV to 10 GeV, and for elements with $Z = 1 - 92$
- This value is integrated over ε_γ to obtain σ for each ion species
- Uses computationally less intensive algorithm which always emits photons in the parallel direction
- A more thorough algorithm was implemented, but results were very similar to completely parallel algorithm
- Inside PIC loop:
  - Calculates ion density, n_i
  - It compares a random number $\xi \in [0, 1]$, drawn from a uniform distribution, to the emission probability:

$$g = n_i v_e \sigma \Delta t \tag{5}$$

  - If $\xi < g$ then it produces a photon with momentum parallel to v_e
  - Produced photon has reduced energy κ that is determined by the Probability Distribution Function:

$$p(\varepsilon_0,\kappa) = \frac{1}{\kappa}\chi(Z,\varepsilon_0,\kappa)\Theta(\kappa-\kappa_{cut})\Theta(1-\kappa) \tag{6}$$

  - PDF is interpolated from the pre-calculated χ table (mentioned above) and by evaluating κ using a combination of numerical inverse transform and rejection method
    - Reduced photon energy: $\kappa = E_\gamma/E_{Kinetic}$
    - This calculation is as described in PENELOPE paper
  - The electron momentum is modified in line with this reduced energy value
  - If $g > 1$ (as a result of a long time-step) then a photon is emitted, but the g is lowered by 1 until its value drops $g < 1$.
- User options:
  - Can specify Minimum energy, ε_{cut}
  - Turn off electron recoil
  - Can apply a multiplication factor to emit photons of lower computational weight with higher probability
- Generated photons are tagged but exist within the Photon species
- Routine is coupled with QED routine need both compiler options switched on, but can turn off additional QED effects in input deck
- This routine does not account for Plasma screening

2.2 York's Module

Stuart Morris' Bremsstrahlung routine is a hybrid model that uses the Seltzer-Berger cross sections, as was done by ELI (see above), and Wu *et al*'s plasma screening.

In Wu *et al*'s plasma screening model, the cross sections are interpolated between the approximate complete screening result and a cross section based on Debye shielding. This is equivalent to including a cross section multiplication factor, valid for Plasmas, F_σ of:

$$F_\sigma = 1 + \frac{Q^2}{Z^2} \frac{\ln\left|c_1 Z^{1/3}\sqrt{\frac{T_e}{n_e}}\right|}{\ln|c_2 Z^{-1/3}|} \tag{7}$$

where $c_1 = \sqrt{\epsilon_0 k_B} m_e c\alpha/1.4\hbar e \approx 7.6 \times 10^{11} K^{-1/2} m^{-3/2}$, and $c_2 = 1.4/\alpha \approx 192$.

Instead of applying F_σ to the approximation which is only valid at high electron energies (as Wu *et al* have done):

$$\sigma = \frac{16}{3}\alpha r_e^2 \ln(10^9) Q^2 \left(\frac{Z^2}{Q^2}\ln\left|\frac{a m_e c}{\hbar}\right| + \ln\left|\frac{\lambda_D}{a}\right|\right), \tag{8}$$

Stuart's routine applies F_σ to Seltzer-Berger cross sections. This method allows the treatment of the increased emission for for ionised media while maintaining the accuracy of the Seltzer-Berger photon spectra.

Similar to the *ELI* routine, Stuart uses a Monte Carlo algorithm, however his definitions are slightly different:

- Probability of reaching L without emission:

$$P(L) = \lim_{N\mapsto\infty}\left(1 - n_i\sigma\frac{L}{N}\right)^N = e^{-n\sigma L} \tag{9}$$

- Therefore, the Culmitaive probability of emission is given by:

$$F(L) = 1 - e^{-n_i\sigma L} = 1 - e^{-\tau} \tag{10}$$

  where $\tau = n_i\sigma L$ is the optical depth. Computationally, this function is replaced with a uniformly distributed number between 0 and 1, i.e $\xi \in [0, 1]$

- The optical depth travelled by an electron moving with energy E in a timestep Δt is given by:

$$\Delta\tau = n_i(x)\sigma(E)v\Delta t \tag{11}$$

- Photon emission occurs when $\Delta\tau > \xi$
- Photons emitted in direction of electron motion
- Radiating electron's momentum reduced to account for the emission of the photon
- Upon emission, a new optical depth is sampled for the next emission event of the electron
- The energies of the photons are calculated from a cumulative distribution function $F(k)$

$$F(k) = \frac{1}{\sigma}\int_{k_{cut}}^{k} \frac{d\sigma}{dk'} dk' \tag{12}$$

  - Several methods for doing this (Wu *et al* method)
  - In hybrid model, then routine uses look-up tables from GEANT4
  - These tables contain k/T, $\ln(T)$, and $(\frac{\beta}{Z})^2 k\frac{d\sigma}{dk}$
  - Table has been pre-processed using *tableGenerator.m* program
  - This Monte Carlo treatment is analogous to the process used in the QED module
- Effects of nuclear recoil have been assumed to be neglible, therefore not included

2.3 Benchmarking

Both routines have been benchmarked to test that they are obtaining the correct results. They have chosen different ways of doing this but both have used external software, and both have promising results.

2.3.1 ELI

"The algorithm has been succesfully validated against PENELOPE by running a simulation of a bunch of 511 MeV electrons propagating through bulk Au target with immobile ions for 2 ps. The comparison of the resulting spectra is shown in Figure 1."

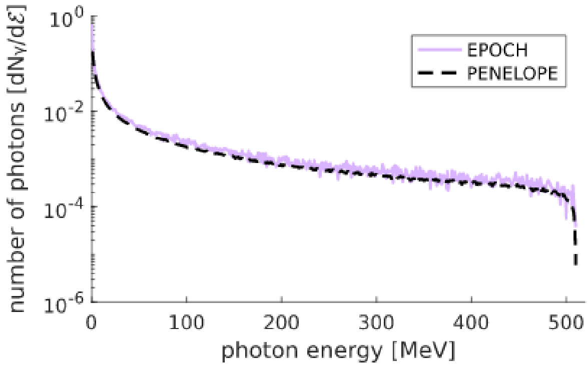


Figure 1: Comparison of photon spectra of bremsstrahlung radiation generated by a 511 MeV electron bunch propagating through an Au target for 2 ps from a PIC simulation (*EPOCH*) and a MC simulation (PENELOPE).

2.3.2 York

"The code has been benchmarked in two ways. The first consideres the spectra of high energy electrons passing through atomic targets, and compares the results against the spectra of an equivalent set-up run in GEANT4. The second tests the implementation of the plasma enhancement factor F_σ, by comparing the photon spectra of electrons passing through an atomic target against electrons traversing half the distance in a target heated to make $F_\sigma = 2$."

GEANT4 benchmarking

- Recreation of test performed by Wan *et al*
- 100,000 electrons positioned in the first cell in the x direction, and the central cells in the y and z directions for higher dimensional codes.
- Assigned a drift momentum along x, with initial energies of either 100 MeV or 1 GeV.
- Background of solid density, neutral atoms (Al or Au) used as a Bremsstrahlung target
- Look at the specta of the electron bunch and Bremsstrahlung photons after they had travelled 5 mm
- This was repeated for a range of particles per cell and in 1, 2, and 3-dimensions

Here is the result of the 3D simulation:

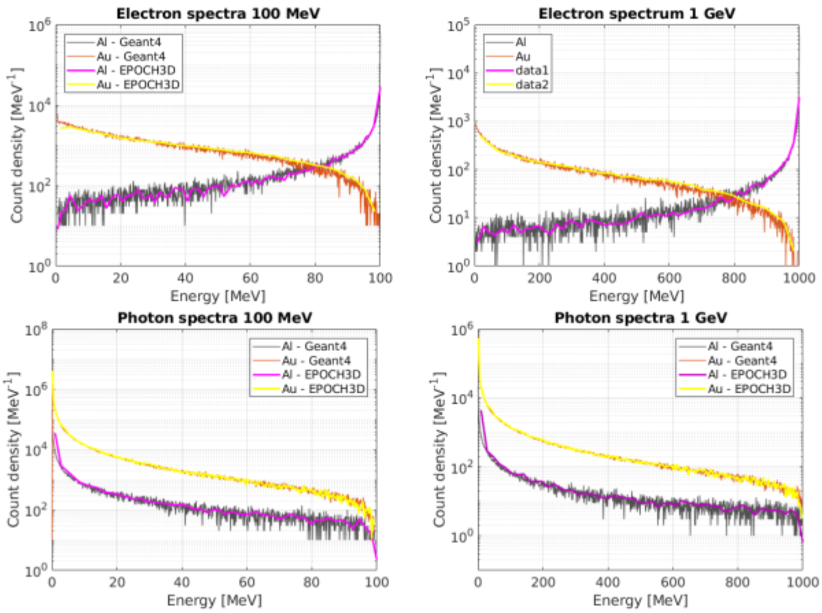
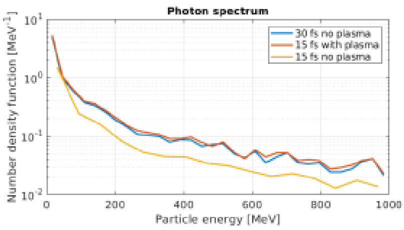


Figure 2: Results comparing $EPOCH$ and GEANT4 spectra from EPOCH3D. Ran with $nx = 64$,, $ny = nz = 6$, $npart = 16 * nx * ny * nz$

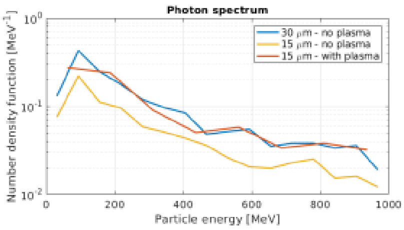
The figure shows that the Bremsstrahlung routine is in good agreement with GEANT4. Stuart does mention that there is some difference on the accuracy of the simulations determined by the resolution of the simulation domain. "Poorer grid resolution will make timesteps longer, and as only one emission from an electron is possible per timestep, there is a certain *dead period* between an emission event and the resetting of the optical depth of an electron. The particle may travel in this time, but the optical depth it will have moved during this time, is not recorded. The result is that poorer resolution will lead to fewer photon emissions, which would explain why the final electron spectra in $EPOCH$ are a little more skewed towards the initial energy values, than the GEANT4 results. This is more noticeable on the gold target, as gold has a greater bremsstrahlung cross section than aluminium.

Plasma screening tests

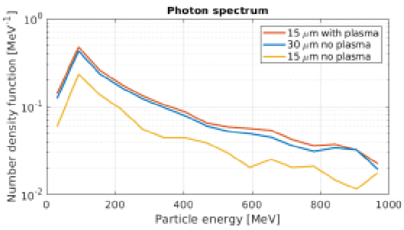
- "There is currently no experimental data on the nature of bremsstrahlung in a heated, ionised target or simulation tool which we can benchmark this feature against"
- Benchmark routine against itself
- Simulate passage of 100,000 electrons of energy 1 GeV through an aluminium target, but this time we simulate fully ionised ($Q = Z$) and heated aluminium
- Use solid density Al
- Temperature for $F_\sigma = 2$ is $T \approx 6.01 \times 10^9 K$
- Passage of electrons through 30 μm without screening should give same result as electrons passing through 15 μm with screening (optical depth should increase twice as fast)
- Results are shown in the Figure below



(a) `EPOCH1D`: nx=256, $npart = 1024 * nx$.



(b) `EPOCH2D`: $nx = 128$, $ny = 8$, $npart = 64 * nx * ny$



(c) `EPOCH3D`: $nx = 64$, $ny = 6$, $nz = 6$, $npart = 256 * nx * ny * nz$

Figure 3: Results comparing the bremsstrahlung photon spectra of 10^5 electrons of energy 1 GeV when passing through distances of fully ionised aluminium with an electron termperature of 6.01×10^9 K, using different bremsstrahlung models. If the code works correctly, the 15 μm results with plasma screening should match the 30 μm results without. The 15 μm results without plasma are shown for context.

"While EPOCH1D and EPOCH2D show consistent photon spectra, EPOCH3D seems to be over-estimating with the plasma screening correction. I believe this is due to the poor resolution at which the particular result was run for, causing the background target atoms to be less uniformly distributed cell to cell. Running with the plasma correction tends to slow the code, typically by a afactor of 1.9 in EPOCH2D. Results from profiling suggest this is due to the expensive calculation of finding the temperature across the grid at each timestep, to obtain a T_e value. If this model were ever to be ignored or tested, it is important to know which parameters would produce the greatest deviation from the Seltzer-Berger cross sections."

3 Results

3.1 Hot Electron Temperature Measurement

3.1.1 Experimental Setup

Here are the conditions for Jiri's simulation of a laser interacting with a thin ($\sim \mu m$), fully ionised metal/plasma target:

- 2D domain with $x \in (-5, 25)\mu m$ and $y \in (-60, 60)\mu m$
- Cell size = 10×10 nm
- Laser properties:
  - Investigated a range of Intensities: $3 \times 10^{21} - 1 \times 10^{23}$ W cm^{-2}
  - $\lambda = 1\mu m$
  - Gaussian spatial and temporal profile
  - FWHM duration of $\tau = 30$fs
  - Focused to a $w = 3\mu m$ spot
  - Pulse emitted from $x = -5\mu m$
  - Propagating along the x axis
  - Peak intensity at $t = 60$fs
- Target properties:
  - Investigated three different materials: Mylar (CH), Al, and Au
  - Fully ionised Al plasma with $n_e = 770n_c$
  - Fully ionised Au^{+51} with $n_e = 2680n_c$
  - Fully ionised CH with $n_e = 289n_c$
  - Critical density:
$$n_c = \frac{\epsilon_0 m_e \omega^2}{e^2} \tag{13}$$
  - Investigated a range of target thicknesses: $d = 1, 2, 5, 10, 15, 20\mu m$
- Assume very good laser pulse contrast
- Simulations included a current smoothing algorithm and third order particle weighting to limit noise and numerical heating
- In their paper then Vyskocil *et al* use a target with regions of different particle per cell densities. We will not be implementing this structure in these test experiments.

3.2 Electron Temperature Results

Here are the results for extracting the hot electron temperature from the simulations. We extracted the temperature by looking at both; the electron spectra, and the Bremsstrahlung spectra.

<u>Method</u>
We extract the electron/Bremsstrahlung spectra at all times of the population:

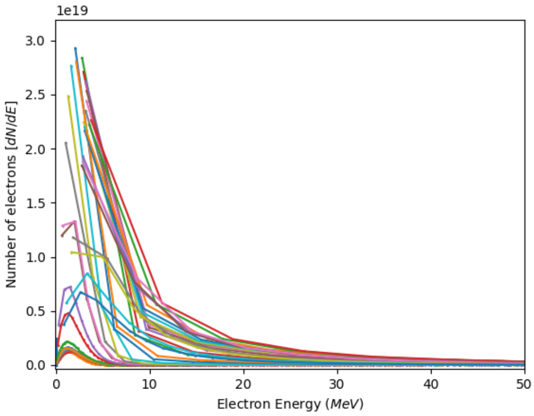


Figure 4: Electron spectra from all outputted timesteps of the simulation. Note that the number of electrons increases as the simulation progresses, since the laser is interacting with the plasma and increasing the energy of the electrons.

Then we look at the time-integrated spectrum from the entire simulation:

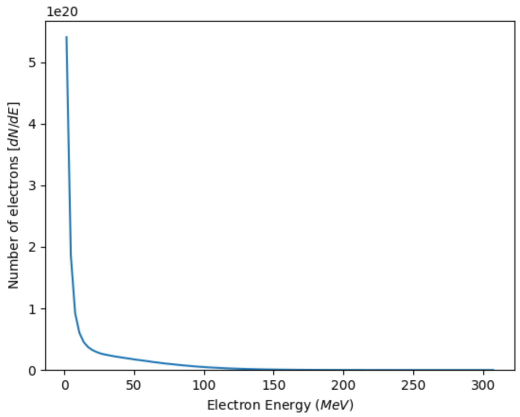


Figure 5: Time-integrated electron spectrum from all timesteps of the simulation.

Then we fit a curve to the tail of the distribution to extract the temperature:

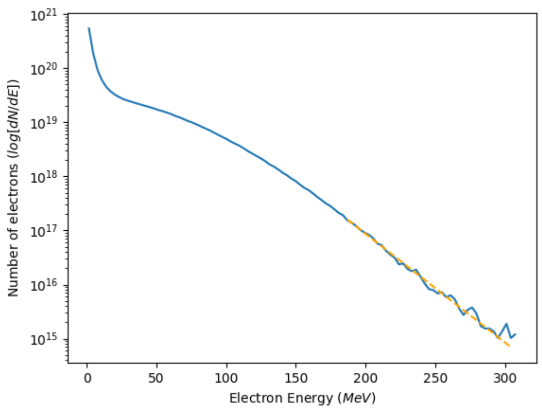


Figure 6: Time-integrated electron spectrum with an exponential curve fitted to the tail. Note that the y axis has a logarithmic scale.

We assume that the tail of the distribution has an exponential temperature fit:

$$N_\gamma \approx \exp(-\varepsilon_\gamma / k_B T_\gamma) \tag{14}$$

Therefore, the gradient of the exponential fit, $m = -1/k_B T_\gamma$, can be used to calculate the temperature of the hot electrons.

Electron Spectra

The figure below shows the results of the hot electron temperature as a function of laser intensity/normalised potential a_0.

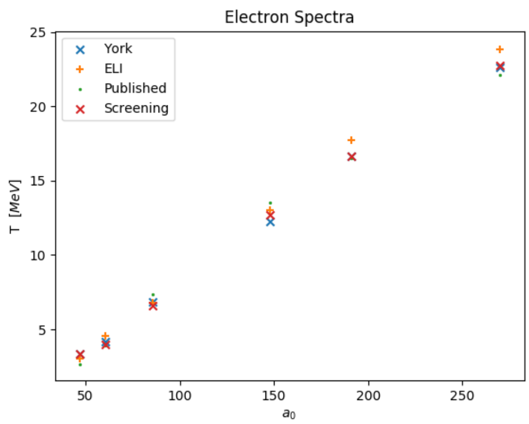


Figure 7: The measured electron temperature as a function of the normalised potential a_0. Note that all three data sets show a linear relation.

All of the data points are in close agreement with each other, this is largely due to the fact that the electron species is well populated (10^{16}) at large energies, whereas the Bremsstrahlung photons have significantly less (10^4).

Bremsstrahlung spectra

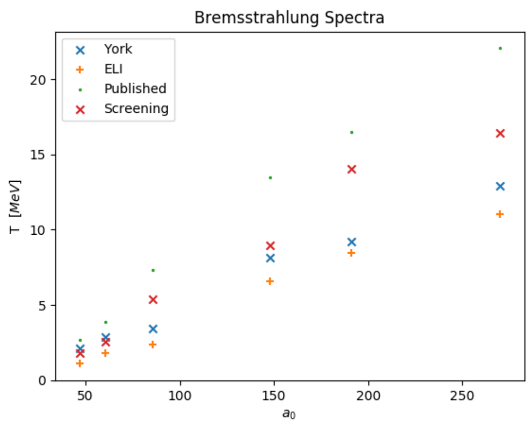


Figure 8: The measured electron temperature as a function of the normalised potential a_0. Note that all three data sets show a linear relation.

There is a larger variance in results from the Bremsstrahlung spectra, but once again, all three sets of results are in relatively close agreement with each other. Note that the data set which most closely resembles the published data set is the York routine with the plasma screening enabled. The average difference between the Photon temperature and Electron Temperature is 1.44. For the York routine without plasma screening then the difference is 1.68. For the ELI routine, the difference is 2.39.

Ponderomotive Scaling

Note that none of these data points comes anywhere near following Ponderomotive scaling. This can be seen in the figure below.

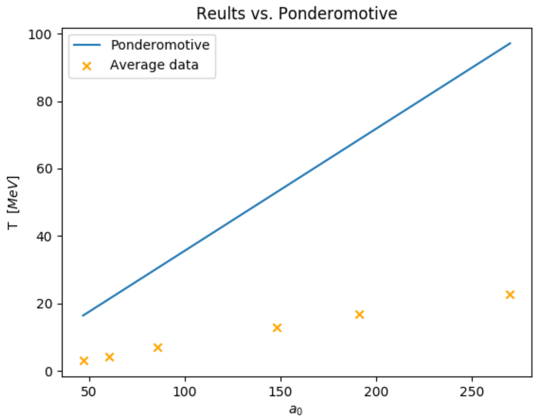
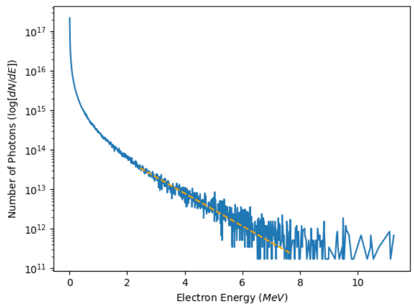


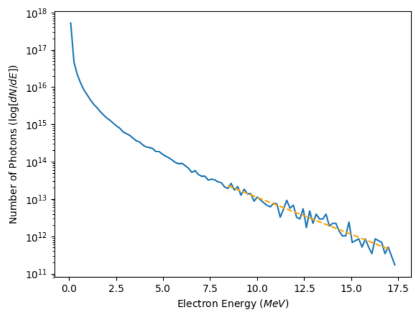
Figure 9: The average electron temperature from all data sets plotted against the theoretical Pondermotive scaling.

Quality of Results

Note that both simulations included a bremsstrahlung photon multiplication factor of 1000 in order to increase the number of photons being created to make the spectra more complete. From the results, then we can see that the York routine is able to recreate Bremsstrahlung spectra which are more accurate. This can be seen in the quality of the raw spectra:



(a) The Time-integrated Spectra from the ELI routine for a laser of Intensity $I = 3 \times 10^{21}$ Wcm^{-2}. Note that the data is very stochastic near the higher energies.

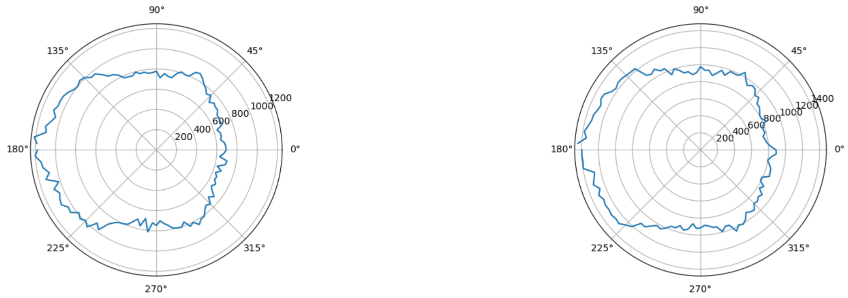


(b) The Time-integrated Spectra from the $York$ routine for a laser of Intensity $I = 3 \times 10^{21}$ Wcm^{-2}. Note that the data is much smoother in comparison.

Figure 10: A figure comparing the output Bremsstrahlung spectra from both routines.

3.3 Angular Distribution

Refluxing electrons play a large role in the emission angle of the Bremsstrahlung photons. In their paper, then Vyskocil *et al.* study the emission angle of the electrons for targets of varying thickness. Form their results, then a clear “Butterfly” pattern should emerge. So far, I have been unable to replicate their results:



(a) ELI Routine: The emission angle for the simulation with a laser intensity of $I = 1 \times 10^{22}$ $\mathrm{Wcm}^{-2}/a_0 = 86$

(b) $York$ Routine: The emission angle for the simulation with a laser intensity of $I = 1 \times 10^{22}$ $\mathrm{Wcm}^{-2}/a_0 = 86$

Figure 11: A figure comparing the output Bremsstrahlung spectra from both routines.