Improved angular sampling for pair production in the EGS4 code system

Alex F. Bielajew

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Ionizing Radiation Standards
Institute for National Measurement Standards
National Research Council of Canada
Ottawa, Canada
K1A 0R6
Tel: 613-993-2715
Fax: 613-952-9865
e-mail: alex@irs.phy.nrc.ca

Abstract

Two new angular distributions for pair production have been implemented in the EGS4 code. This report summarises the method by which the distribution is sampled and documents the revisions to the EGS4 system. A discussion of sampling efficiency and accuracy is given. A minor bug that allowed electrons or positrons with negative kinetic energy to be created (at very low probability) has been corrected. As well, a limitation that prevented very small angle scattering ($< 10^{-5}$ radians) has been relaxed. A realistic example at 50 GeV is given.

1 Introduction

The angular sampling of the newly created e^-e^+ pair in the EGS4 system (Nelson *et al.* 1985) may be oversimplified for some applications. The algorithm currently employed is to set all newly created electrons in motion at a fixed angle with respect to the initiating photon direction. This fixed angle has the form $\Theta_\pm = 1/k$, where $\Theta_\pm$ is the scattering angle of the e^+ or e^- (in radians) and k is the energy of the initiating photon in units of $m_o c^2$, the rest mass of the electron (0.5110034 MeV). This angle represents an estimate of the expected *average* scattering angle.[1] The motivation for employing such a crude approximation was based on the following argument: At high energies the distribution is so strongly peaked in the forward direction that more accurate angular modeling will not significantly improve the shower development. At low energies, particularly in thick targets, multiple scattering of the resultant pair will "wash out" any initial distribution. Therefore, the extra effort and computing time necessary to implement pair angular distributions was not considered worthwhile. It was recognised, however, that the above argument would break down for applications where the e^+e^- pair may be measured before having a chance to multiple scatter sufficiently and obliterate the initial distribution.

In anticipation of the requirement of an improved sampling procedure, two new options for sampling the pair angle are introduced in the two following subsections. Procedures for sampling these formulae are given in the next section along with a discussion of sampling efficiency and timing. A sample problem for measuring the angular distribution of pairs coming from 50 GeV incident photons is given. This report concludes with a listing of the code changes to the EGS system including the patch for the minor bug related to the creation of negative energy electrons or positrons after a pair event and the patch that prevents very small scattering angles ($< 10^{-5}$ radians) from deflecting particles.

The formulae employed in this report were taken from the compilation by Motz, Olsen and Koch (1969).

1.1 Leading order approximate distribution

As a first approximation, the leading order multiplicative term of the Sauter-Gluckstern-Hull formula was used (equation 3D-2000 of Motz *et al.*(1969)):

$$\frac{\mathrm{d}P}{\mathrm{d}\Theta_\pm} = \frac{\sin\Theta_\pm}{2p_\pm(E_\pm - p_\pm\cos\Theta_\pm)^2}, \tag{1}$$

where $\Theta_\pm$ is the $e^\pm$ scattering angle (in radians), $E_\pm$ and $p_\pm$ are the $e^\pm$ total energy and momentum in units of the electron rest-mass energy, $m_o c^2$.

[1] The extremely high-energy form of the leading order approximation discussed later implies that the distribution should peak at $\Theta_\pm = 1/(\sqrt{3}E_\pm)$. However, the Bethe-Heitler cross section used in EGS4 peaks at $E_\pm = k/2$ and the approximation $\Theta_\pm = 1/k$ is a reasonable one on average, given the highly approximate nature of the angular modeling.

This distribution is used by the ETRAN-based codes (Seltzer 1987) and is included for comparison purposes. The Sauter-Gluckstern-Hull formula was derived under the following approximations:

	Approximation	Condition of validity
i)	No screening	Low-Z elements
ii)	First order Born approximation	$(2\pi Z/137\beta_{\pm}) \ll 1$
iii)	Negligible nuclear recoil	$k \gg (1/m_{\rm n}), k \ll m_{\rm n}$ (large angles)

where $m_{\rm n}$ is the rest mass energy of the nucleus in units of $m_{\rm o}c^2$ and $\beta_{\pm}$ is the magnitude of the velocity of the $e^{\pm}$ in units of the speed of light, c.

The full Sauter-Gluckstern-Hull formula differs from the above by a modulating factor that varies between 0 and approximately 2 and thus it is to be regarded as a crude approximation even in its region of validity.

1.2 The Schiff distribution

This formula employed for the angular sampling routine is equation 3D-2003 of Motz *et al.*(1969), which is the cross section, differential in photon energy and angle,

$$\frac{{\rm d}\sigma^2}{{\rm d}E_{\pm}{\rm d}\Omega_{\pm}} = \frac{2\alpha Z^2 r_0^2}{\pi}\frac{E_{\pm}^2}{k^3}\left\{-\frac{(E_+ - E_-)^2}{(u^2+1)^2} - \frac{16u^2E_+E_-}{(u^2+1)^4} + \left[\frac{E_+^2+E_-^2}{(u^2+1)^2} + \frac{4u^2E_+E_-}{(u^2+1)^4}\right]\ln M(y)\right\}, \tag{2}$$

where,

$$u = E_{\pm}\Theta_{\pm}\ ;\ \frac{1}{M(y)} = \left(\frac{k}{2E_+E_-}\right)^2 + \left(\frac{Z^{1/3}}{111(u^2+1)}\right)^2,$$

and, the following definitions for the variables apply:

k	energy of the photon in units of $m_{\rm o}c^2$
E_+, E_-	final $e^{\pm}$ total energy in units of $m_{\rm o}c^2$ ($k = E_+ + E_-$)
$\Theta_{\pm}$	angle between the outgoing $e^{\pm}$ and the incoming photon direction (in radians)
${\rm d}\Omega_{\pm}$	Differential solid angle of the outgoing $e^{\pm}$
Z	atomic number of the target material
r_0	$\equiv e^2/m_{\rm o}c^2$ (classical electron radius)
α	$\equiv e^2/(\hbar c) = 1/137...$ (fine structure constant)

The following table, derived from the Motz *et al.* article, outlines the essential approximations employed in the development of equation 2.

	Approximation	Condition of validity
i)	Approximate screening potential	$(Ze/r)e^{-r/a}$
ii)	First order Born approximation	$(2\pi Z/137\beta_{\pm}) \ll 1$
iii)	Extreme relativistic	$E_{\pm}, k \gg 1$
iv)	Small angles	$\Theta_{\pm} = O(E_{\pm})$
v)	Negligible nuclear recoil	$k \gg (1/m_{\rm n}), k \ll m_{\rm n}$ (large angles)

It should be noted that only the angular distribution part of equation 2 is employed. The cross section differential in electron energy employed by the EGS4 code is far less restrictive (Approximation (iii) plus Thomas-Fermi screening factors).

2 Sampling procedure

The distribution expressed by equation 1 is normalised,

$$\int_0^{\pi} {\rm d}\Theta_{\pm} \left(\frac{{\rm d}P}{{\rm d}\Theta_{\pm}} \right) = 1,$$

and may be sampled from the formulae:

$$\sin\Theta_{\pm} = \frac{2\sqrt{X(1-X)}}{p_{\pm}(2X-1)+E_{\pm}} \; ; \; \cos\Theta_{\pm} = \frac{E_{\pm}(2X-1)+p_{\pm}}{p_{\pm}(2X-1)+E_{\pm}}, \tag{3}$$

where X is a random number uniform on the range $[0,1]$. The $\sin\Theta_{\pm}$ and $\cos\Theta_{\pm}$ forms are related by trigonometric identities but both forms expressed by equation 3 are useful. EGS4 requires both $\sin\Theta_{\pm}$ and $\cos\Theta_{\pm}$ to be calculated. For very small angles $\sin\Theta_{\pm}$ can not be obtained from $\cos\Theta_{\pm}$ using $\sin\Theta_{\pm} = \sqrt{(1-\cos\Theta_{\pm})(1+\cos\Theta_{\pm})}$ without numerical breakdown in single-precision arithmetic. This is because for small angles $\cos\Theta_{\pm} \approx 1 - \Theta_{\pm}^2/2$, and the $\Theta_{\pm}^2/2$ term may be insignificant in comparison to unity.

To sample the angular distribution expressed by equation 2, a rejection technique is applied following a change of variables. Consider the change of variables:

$$\xi = \frac{1}{u^2+1} \; ; \; \frac{1}{1+E_{\pm}^2\pi^2} \leq \xi \leq 1.$$

Then, applying the small angle approximation, ${\rm d}\Omega_{\pm} \longrightarrow 2\pi\Theta_{\pm}{\rm d}\Theta_{\pm}$, the angular distribution rejection function, g, has the form:

$$\frac{{\rm d}g}{{\rm d}\xi} = N_g\{2 + 3(r+r^{-1}) - 4[(r+r^{-1}+4\xi-4\xi^2][1+\ln m(\xi)/4]\}, \tag{4}$$

where

$$m(\xi) = \left(\frac{(1+r)(1+r^{-1})}{2k} \right)^2 + \left(\frac{Z^{1/3}\xi}{111} \right)^2 \; ; \; r = E_-/E_+,$$

and N_g is a normalisation factor that should be chosen so that

$$g(\xi) \leq 1 \; \forall \; \xi \in \left[\frac{1}{1+E_{\pm}^2\pi^2}, 1 \right].$$

The position of the maximum of the function g proved difficult to characterise accurately and two-step iterative scheme was developed based upon the slow variation of the logarithmic term, $[1+\ln m(\xi)/4]$, in equation 4 and the observation that the position of the maximum was relatively independent of the value of r. For the purposes of estimating the maximum value of g, r was set equal to 1.

A satisfactory algorithm for N_g was found to be

$$N_g = 1.02 \max \left[g\left(\frac{1}{1+E_{\pm}^2\pi^2} \right), g(\xi_{\max}^{(1)}) \right], \tag{5}$$

where $\xi_{\max}^{(1)}$ is an estimate of the position of the maximum of g after a one-step iteration. The zeroth-order estimate is:

$$\xi_{\max}^{(0)} = \max \left\{ 0.01, \max \left[\frac{1}{1+E_{\pm}^2\pi^2}, \min \left(0.5, \frac{222}{k^2 Z^{1/3}} \right) \right] \right\},$$

and the second iteration yields:

$$\xi_{\max}^{(1)} = \max \left\{ 0.01, \max \left[\frac{1}{1+E_{\pm}^2\pi^2}, \min \left(0.5, \frac{1}{2} - \frac{\alpha'}{3\beta'} + \mathrm{sgn}(\alpha') \sqrt{\left(\frac{\alpha'}{3\beta'} \right)^2 + \frac{1}{4}} \right) \right] \right\}$$

where

$$\alpha' = 1 + \ln m(\xi_{\max}^{(0)})/4 - \beta'(\xi_{\max}^{(0)} - 1/2),$$

$$\beta' = \frac{\xi_{\max}^{(0)} (Z^{1/3}/111)^2}{2m(\xi_{\max}^{(0)})}.$$

and

$$\mathrm{sgn}(\alpha') = \begin{cases} +1 & \text{if } \alpha' \geq 0 \\ -1 & \text{if } \alpha' < 0 \end{cases}$$

The extra 1.02 in equation 5 is a "safety factor" which will be motivated later.

To justify this prescription, consider the plots of g depicted in figures 1 and 2 for two elements, $Z = 1$ and $Z = 100$. These plots span the dynamic range of EGS4. Each figure contains five curves for g corresponding to $r = \frac{1+f(k-2)}{k-1}$ for $f = 0$ (*i.e.* $E_{\pm} = 1$, short-dashed line), $\frac{1}{5}, \frac{2}{5}, \frac{3}{5}, 1$ (*i.e.* $E_{\pm} = k/2$, long-dashed line). (Equation 4 has symmetry under interchange of r and r^{-1} and thus plotting values in the range $[r_{\min}, 1]$ is complete.[2])

[2] This is an accidental symmetry. In the Born approximation there is the basic symmetry that $\frac{\mathrm{d}\sigma^2}{\mathrm{d}E_- \mathrm{d}\Omega_-}$ may be obtained from $\frac{\mathrm{d}\sigma^2}{\mathrm{d}E_+ \mathrm{d}\Omega_+}$ through the interchange $(E_+, p_+, \Omega_+) \rightleftharpoons (E_-, p_-, \Omega_-)$. Equation 4 just happens to be itself symmetric under $E_+ \rightleftharpoons E_-$.

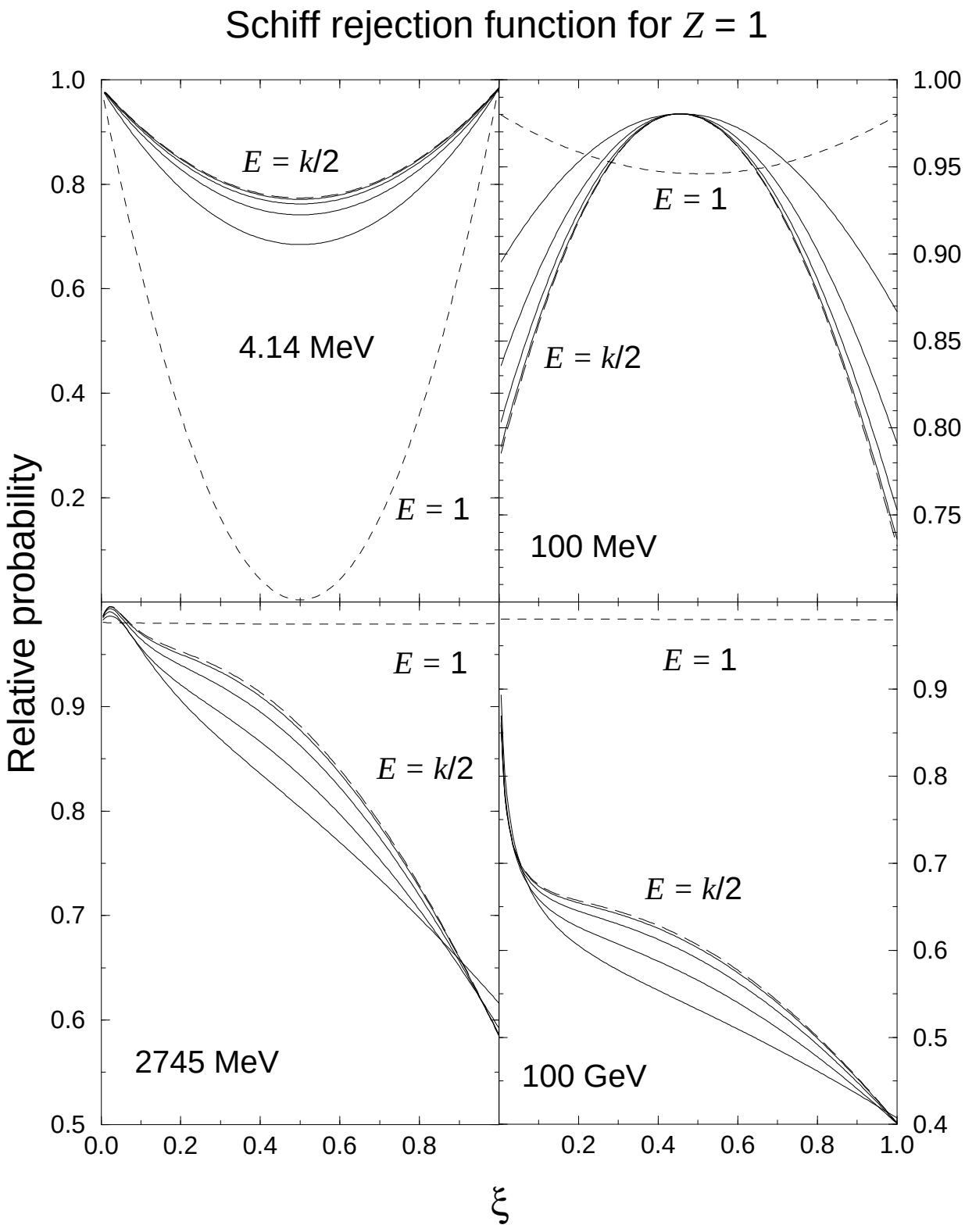

Figure 1: The function g with various values of r for 4.14, 100, 2745, and 100,000 MeV in H ($Z = 1$). $E_{\pm} = 1$ (short-dashed line), $E_{\pm} = k/2$ (long-dashed line). The solid lines are in between these extremes. There exact values of r are described in the text.

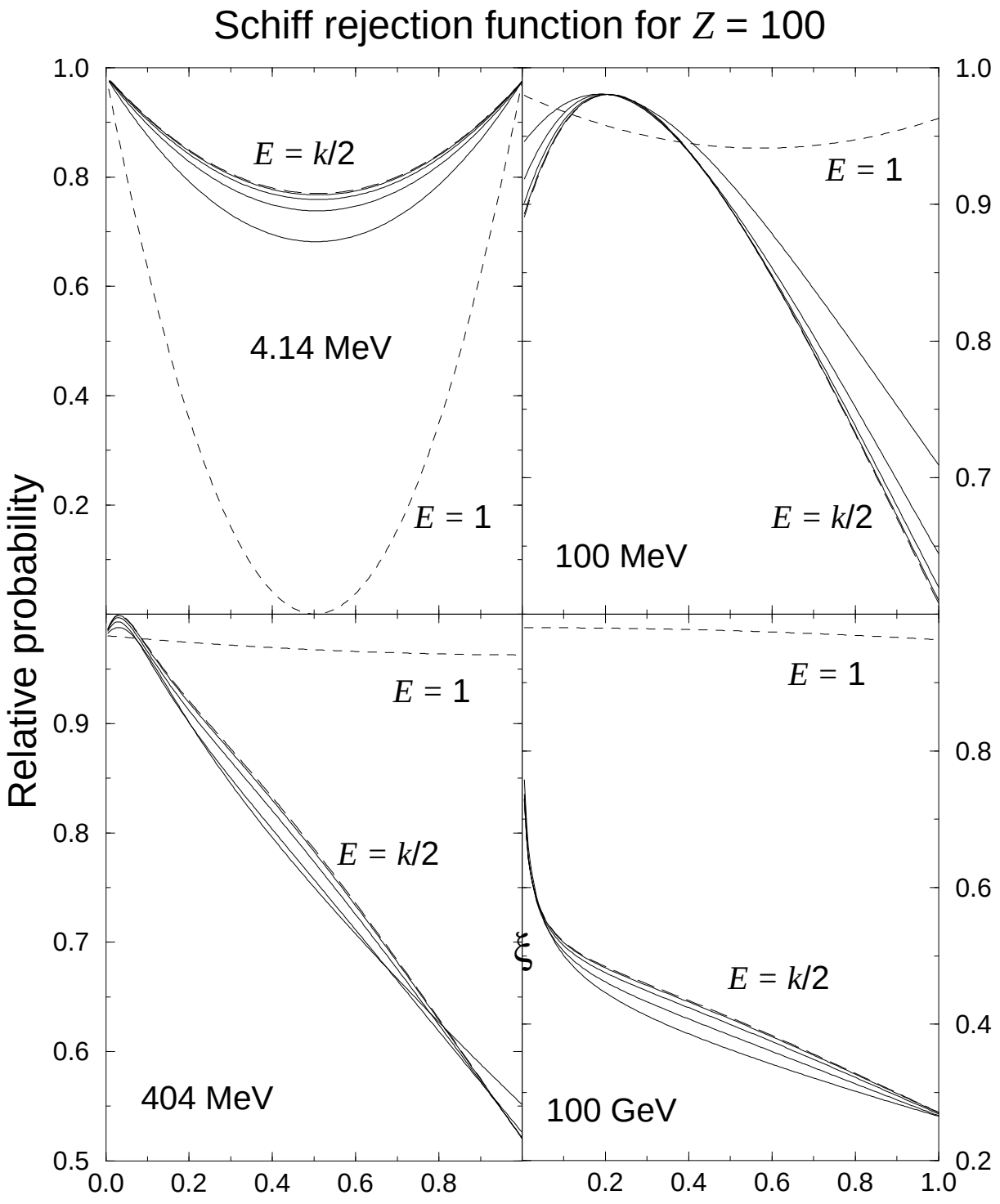

Figure 2: The function g with values of r as described in the text for 4.14, 100, 404, and 100,000 MeV in Fm ($Z = 100$). $E_{\pm} = 1$ (short-dashed line), $E_{\pm} = k/2$ (long-dashed line). The solid lines are in between these extremes. There exact values of r are described in the text.

The lowest energy depicted is for $E_\gamma = 4.14$ MeV which is a threshold below which the distributions can be negative and hence, non-physical. In this region the validity criteria are being violated severely and it is not surprising to observe non-physical characteristics from the distributions. This behaviour is the result of the extremely high-energy approximation of the Schiff formula. The Sauter-Gluckstern-Hull formula does not exhibit this anomalous behaviour despite violating the validity criteria arising from the first Born approximation. The two plots for $E_\gamma = 2745$ in H and $E_\gamma = 404$ in Fm motivate the inclusion of the 1.02 "safety factor". In the vicinity of these energies g approaches unity abruptly owing to a mathematical quirk of the normalisation procedure.

2.1 Sampling efficiency

Given the initial values of E and k, the theoretical efficiency of the above sampling technique can be expressed as:

$$\epsilon(E,k,Z) = \frac{N_g \int_{(1+E_\pm^2\pi^2)^{-1}}^{1} \mathrm{d}\xi \; g(\xi)}{\int_{(1+E_\pm^2\pi^2)^{-1}}^{1} \mathrm{d}\xi}. \tag{6}$$

which should be proportional, on average, to the fraction that the rejection technique is successful on a given pass. This sampling efficiency is plotted in figure 3 for energies from 4.14—10^7 MeV for $Z = 1$ and 100 and for the extrema of r. Taking into account that the cross section differential in energy peaks at $E_\pm = k/2$, one notes that the sampling efficiency worsens as energy increases and with increased Z. The small "kinks" in the $E = k/2$ curves occur near $E = 2745$ MeV for $Z = 1$ and $Z = 404$ for $Z = 100$ are quirks in the method of normalisation discussed previously which necessitated the safety factor of 1.02. A better maximum-finding algorithm would probably eliminate this but may not be worth the extra computing time.

The ultimate test of sampling efficiency is determined by the degradation of overall timing. This is discussed in a later section.

2.2 Sampling accuracy

This section concerns the incorporation of the new sampling routine into the EGS4 code and the verification that the sampling procedure works as expected. This is accomplished by comparing Monte Carlo sampled angular distributions with the theoretical expressions, equations 1 and 2. Three examples are presented. In figure 4, angular distributions $\mathrm{d}P/\mathrm{d}(E_\pm\Theta_\pm)$ are plotted for 4 MeV photons in C ($Z = 6$), 150 MeV photons in W ($Z = 74$) and 2000 MeV photons in Cu ($Z = 29$), for both extremes of r and for one intermediate energy. The 4 MeV case employed the lowest order approximate distribution (because of the 4.14 MeV threshold described earlier) while the two other cases employ the Schiff distribution. The dashed lines are the theoretical predictions from either equation 1 or 2. The normalisations are absolute. Evidently, the sampling routines are working as expected. A specialised user code, `PAIRTEST`, was written for

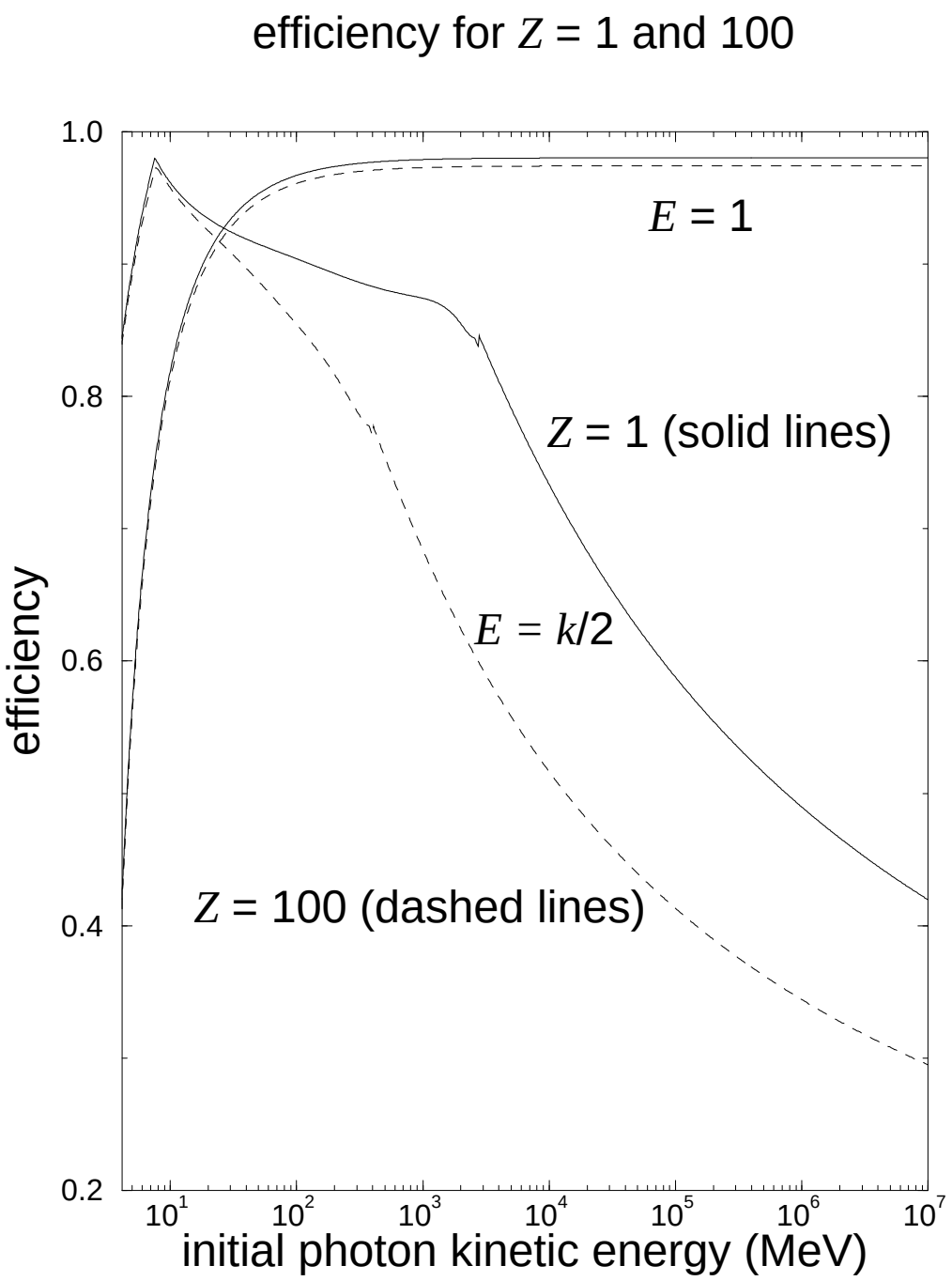

Figure 3: Sampling efficiency for energies from 4.14—10^7 MeV for $Z = 1$ and 100 and for $E_\pm = 1$ and $k/2$.

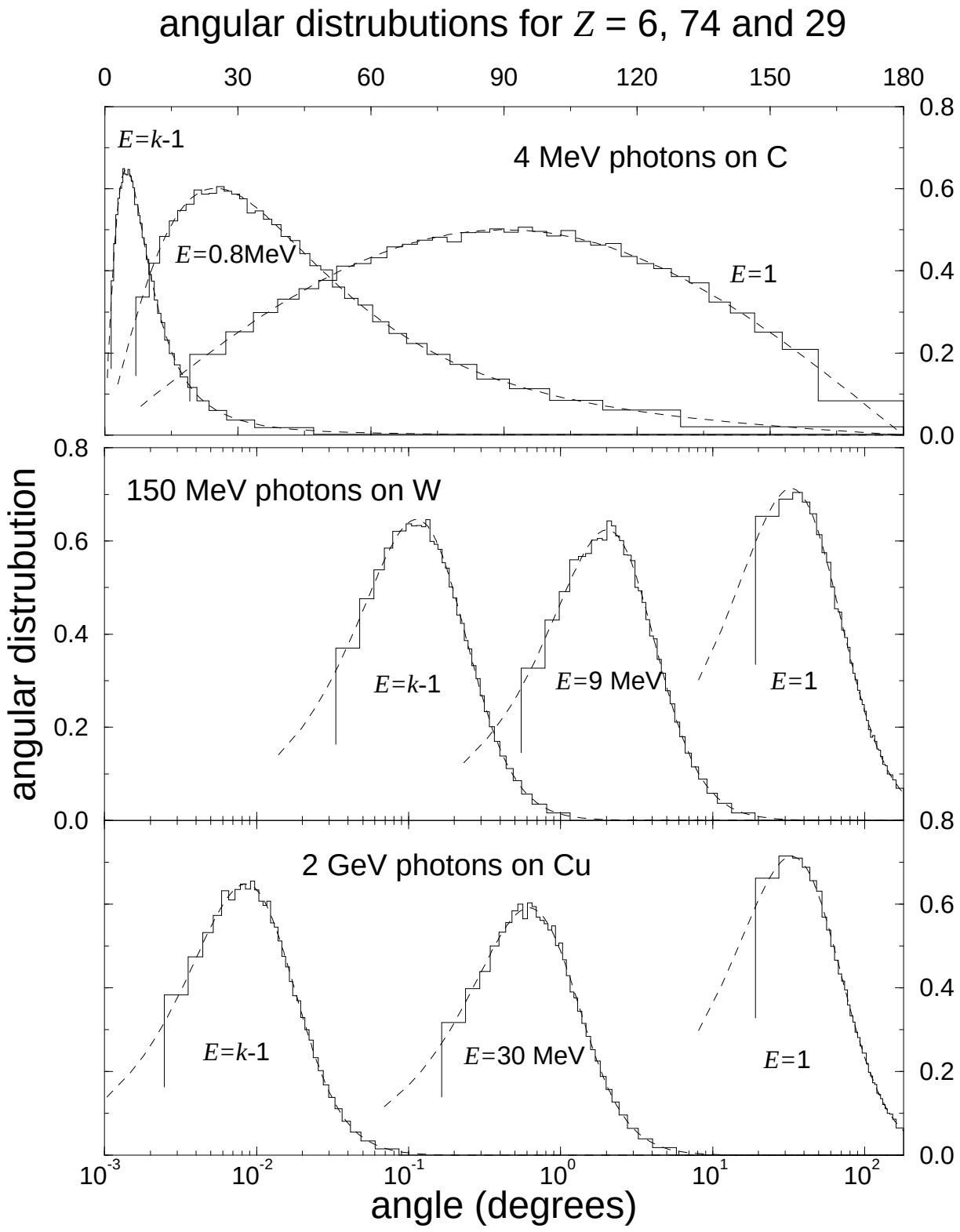

Figure 4: Angular distributions $\mathrm{d}P/\mathrm{d}(E_{\pm}\Theta_{\pm})$ for 4 MeV photons in C ($Z = 6$), 150 MeV photons in W ($Z = 74$) and 2000 MeV photons in Cu ($Z = 29$). The 4 MeV curves employ the lowest order approximate distribution because the energy is below the 4.14 MeV threshold. The two other energies employ the Schiff distribution.

this purpose. It calls the sampling subroutine `PAIR` directly, avoiding particle transport and allows the user to pick the fraction of incident energy going into the initial e^+ or e^-.

2.3 Timing comparisons

With respect to performance, an upper limit on the timing degradation can be gleaned from the test programme, `PAIRTEST`, turning off all scoring and just cycling the subroutine `PAIR`. The results for this extreme case are given in Table 1. These data were obtained

E_γ (MeV)	Z	Default EGS4	Lowest Order	Schiff
2000	29	$\equiv 1$	1.13	1.91
150	74	$\equiv 1$	1.07	1.78
4.14	6	$\equiv 1$	1.03	1.39

Table 1: Timing comparisons for three methods of sampling angular distributions

on a Sun SparcStation2 cycling the subroutine `PAIR` 10^6 times. Any scoring or particle transport makes these ratios better.

The above data represent a worst case. In a total absorption simulation of 500 MeV photons in Tungsten, no degradation of timing performance was noticed within the timing resolution of the computer.

3 Implementation in the EGS4 code

3.1 Effective Z

To account for pair production in the field of an atomic electron and to consider materials other than pure elements, the Z in equation 2 has to be estimated. The dependence of the angular distributions on Z is weak and the following estimate has been effected:

$$Z_{\rm eff} = \sqrt{\sum_{i=1}^{N_{\rm e}} p_i Z_i (Z_i + 1)}, \tag{7}$$

where $N_{\rm e}$ is the number of elements in the material, p_i is the proportion by number of the $i^{\rm th}$ element of the material properly normalised so that $\sum_{i=1}^{N_{\rm e}} p_i = 1$, and Z_i is the atomic number of the $i^{\rm th}$ element. The factor $Z_i(Z_i + 1)$ is intended to account for pair production in the field of an atomic electron in an approximate fashion. Equation 7 is used for all materials, elemental (*i.e.* $N_{\rm e} = 1$) or not. The $Z_{\rm eff}$ factor is identical to that employed in the new angular distributions for bremsstrahlung photons (Bielajew, Mohan and Chui 1989). In fact, the Schiff formula employed in this report is an inverse process of a similar relation for the bremsstrahlung cross section (Koch and Motz 1959) and the

pair and bremsstrahlung cross sections can be obtained from one another by symmetry relations.

The change to subroutine `HATCH` and the additions to the standard macro set, `EGS4MAC.MORTRAN` are documented in the Appendix.

3.2 Schiff threshold

As seen previously, the Schiff distribution breaks down mathematically for $E_\gamma < 4.14$MeV. To prevent non-physical modeling, if a user has requested the Schiff distribution but the photon energy is less than the 4.14 MeV threshold, the lowest order approximate distribution, equation 1, is used for subthreshold energies. The user may change this threshold by resetting the macro `$BHPAIR` documented in the Appendix.

3.3 Sampling algorithm

The following algorithm is employed to sample the lowest order approximate angular distribution:

1. Pick a random number X on the interval $[0, 1]$.
2. Evaluate $\sin\Theta_\pm$ and $\cos\Theta_\pm$ using equation 3.
3. Repeat for the charge of the other sign, reversing the sign of $\sin\Theta_\pm$.

The following algorithm is employed to sample the Schiff angular distribution:

1. Calculate N_g from equation 5.
2. Pick a candidate ξ_{test} uniform on the range $[0, 1]$.
3. Evaluate $g_{\text{test}} = N_g g(\xi_{\text{test}})$.
4. Express ξ_{test} in terms of an angle, $\Theta_{\text{test}} = (\sqrt{1/\xi_{\text{test}} - 1})/E_\pm$
5. Pick a random number X on the interval $[0, 1]$.
6. If $X \leq g_{\text{test}}$ and $\Theta_{\text{test}} \leq \pi$, accept ξ_{test}, else, go back to step 2.
7. Repeat for the charge of the other sign, reversing the sign of $\sin\Theta_\pm$.

This is essentially the process executed by the selection macros described in the Appendix. A final subtlety concerns the sign reversal of $\sin\Theta_\pm$ for the second charged particle. This is done to cause the emergent pair to be set in motion in opposite directions from each other in the plane perpendicular to the line of motion of the initiating photon. This azimuthal angle should actually be a distributed, stochastic quantity. It could be sampled

from, for example, equation 3D-3000 of Motz *et al.* (1969) but the distribution, expressible in terms of elliptic functions, would be difficult to sample from. This effort is probably not warranted unless it were required to simulate an e^+e^- correlation experiment.

Angular distributions (with the energies of the resultant pair products selected stochastically) are plotted in figure 5. The old EGS4 results are given as single-valued vertical lines, the lowest order angular distribution by solid lines and the Schiff distribution by the dashed lines. Note that the 4.15 MeV case just exceeds the sampling threshold discussed earlier.

3.4 User control

One implements the new sampling routines by using the new versions of `EGS4.MORTRAN` and `EGS4MAC.MORTRAN`, recompiling one's user code, and including the common block `BREMPR` in a code segment where one sets the switch `IPRDST=1` for the lowest order angular distribution or `IPRDST=2` for the Schiff angular distribution. The redefinition of the common `BREMPR` is documented in the Appendix as well as the changes to `EGS4.MORTRAN` and `EGS4MAC.MORTRAN`. If one does not set the switch `IPRDST` or sets it to any value other than 1 or 2, the old EGS4 sampling algorithm is employed.

3.5 Other minor modifications to the EGS system

In EGS4, subroutine `PAIR` can allow negative kinetic energy electrons and positrons to be created since the branching ratio that splits the photon energy between the outgoing electron and positron total energy is allowed to approach zero. A patch for this is given in the Appendix. If the total energy of an outgoing particle is less than the rest mass, the energy sampling procedure is recycled.

In EGS4, subroutine `UPHI`, the multi-purpose deflection subroutine, does not apply rotations for $\sin\Theta < 10^{-5}$. This causes artefacts for angular distributions from pair and bremsstrahlung interactions at energies greater than a few tens of GeV. This limit was lowered to 10^{-10} via a macro described in the Appendix.

4 Sample problem at 50 GeV

The recent development of silicon strip detectors permits high-resolution detection of very tight angular distributions[3]. Indeed, it is possible to measure the angular distribution of pairs resulting from 50 GeV photons despite characteristic angles of the order of 10^{-5}

[3]The possibility of performing experiments of this nature was communicated to me by Dr Jim Spencer of SLAC.

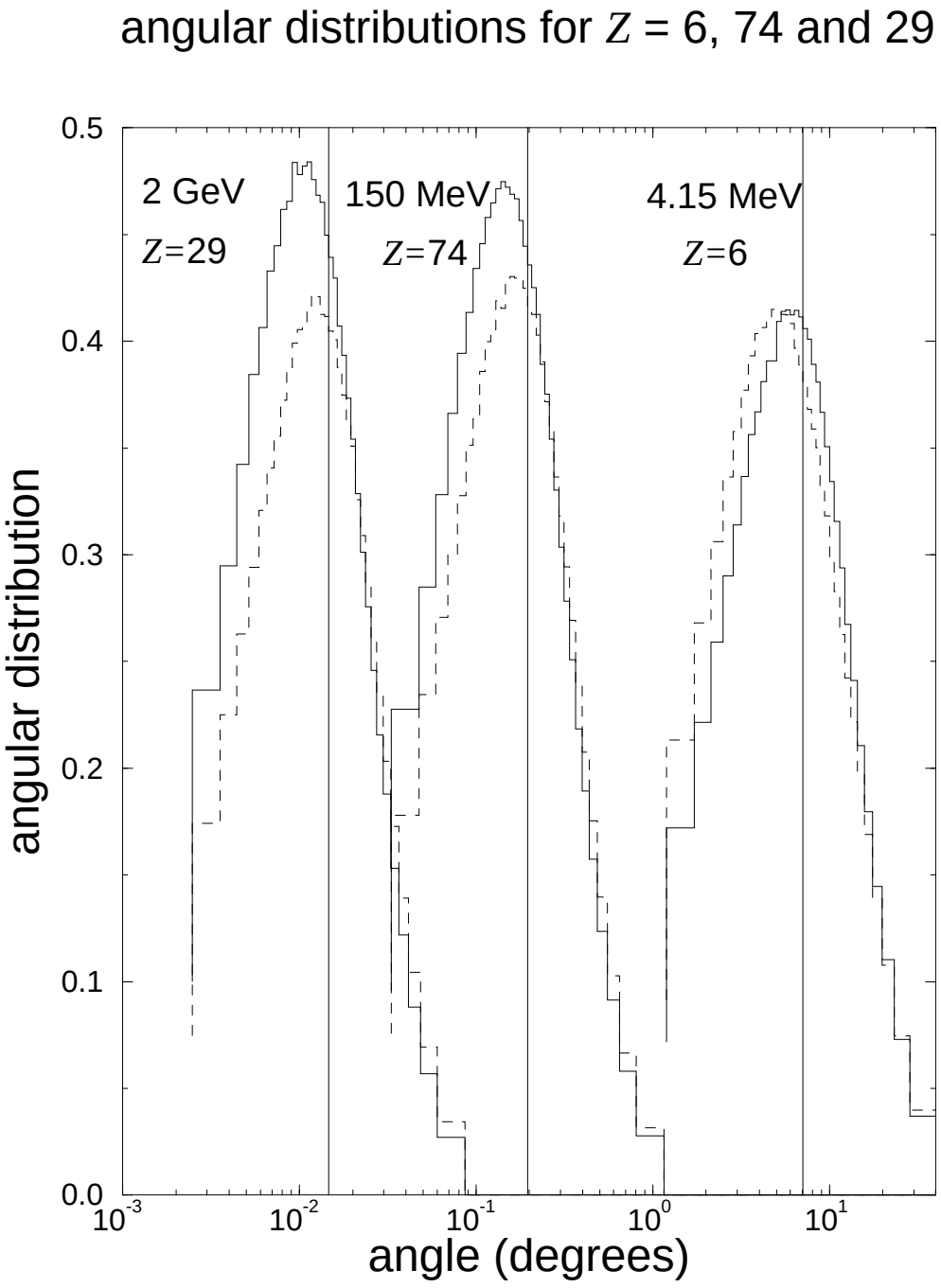

Figure 5: Angular distributions $\mathrm{d}P/\mathrm{d}(E_{\pm}\Theta_{\pm})$ for 4.15 MeV photons in C ($Z = 6$), 150 MeV photons in W ($Z = 74$) and 2000 MeV photons in Cu ($Z = 29$). In this case, the energies of the resultant pair products were selected stochastically.

radians. Silicon strip detectors can be made as thin as 100μ with $x-y$ resolution of the order of 25μ.

A simulation was performed of a 50 GeV photon pencil beam incident on 100μ of Si followed by 10 m of vacuum and a second 100μ of Si. Energy deposit per unit mass in the second Si slab in 25μ radial bins was scored. The solid histogram in figure 6 shows the results employing default EGS4. The artefact results in an anomalous peak in the 125–150μ radial bin. The default fixed-angle algorithm projects all electrons produced by the pair interaction in the first Si slab towards a radial displacement of 140μ in the second slab, represented by the vertical line in figure 6. The structure about this line arises from multiple scattering, primarily in the first Si slab. The dotted histogram shows the results employing the Schiff distribution. The anomalous structure in the 125–150μ radial bin is no longer evident. The result of turning off multiple scattering but still employing the Schiff angular distribution is depicted by the dot-dashed line. Clearly, the initial angular distribution from the pair interaction dominates the structure of the angular distribution curve.

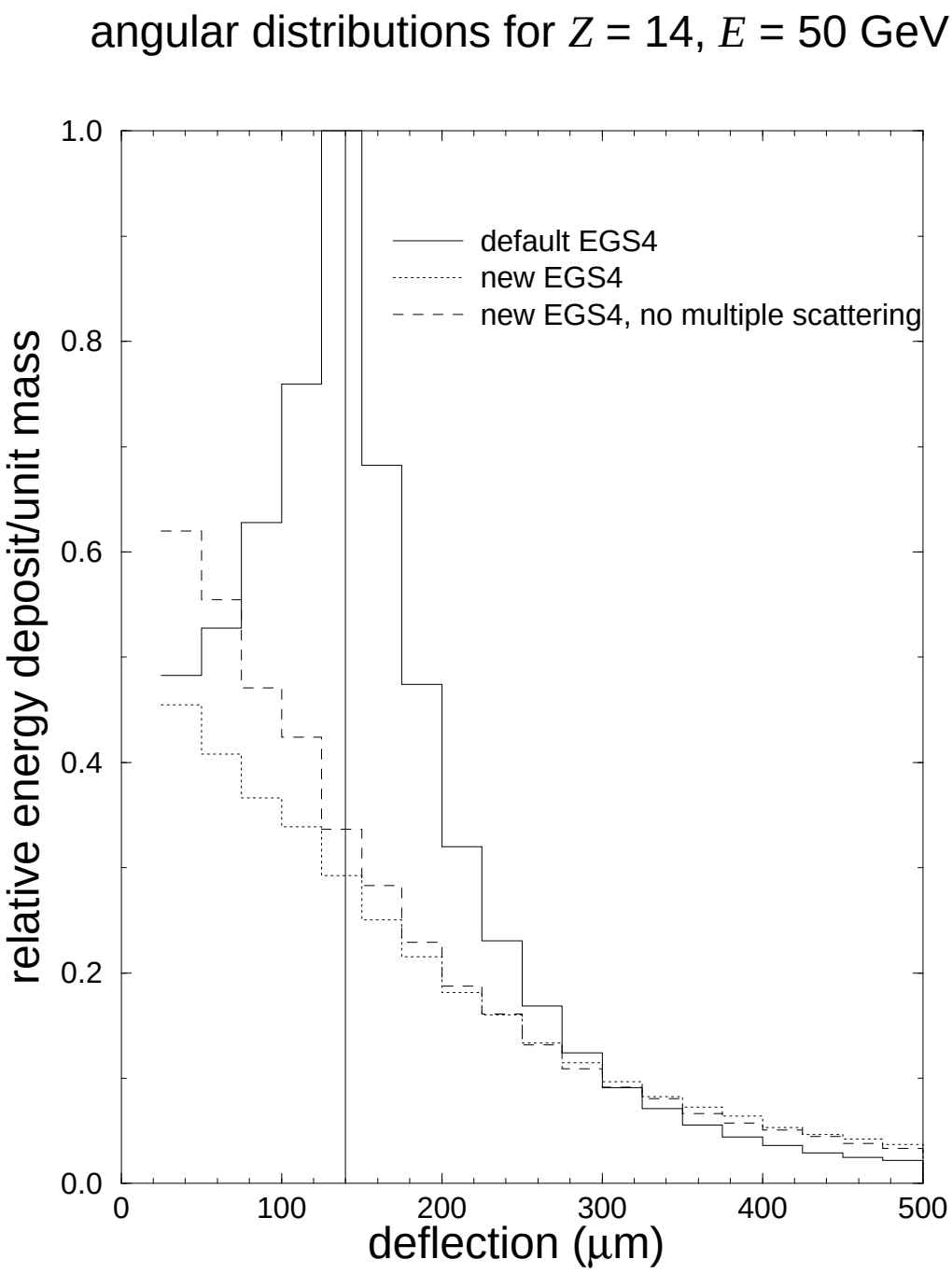

Figure 6: Energy deposit per unit mass in 25μ radial bins for a 100μ Si slab following transport through an initial 100μ Si slab and 10 m of vacuum. A pencil beam of 50 GeV photons was incident on the first Si slab. The solid histogram is for default EGS4, the dotted histogram employs the Schiff pair angular distribution, and the dot-dashed curve switches off multiple scattering while employing the Schiff distribution.

5 Acknowledgement

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References

Bielajew A F, Mohan R and Chui C-S 1989 *Improved bremsstrahlung photon angular sampling in the EGS4 code system* (NRCC report:PIRS-0203)

Koch H W and Motz J W 1959 Bremsstrahlung cross-section formulas and related data *Rev. Mod. Phys.* **31**, 920–55

Motz J W, Olsen H A and Koch H W 1969 Pair Production by Photons *Rev. Mod. Phys.* **41**, 581–639

Nelson W R, Hirayama H, and Rogers D W O 1985 The EGS4 Code System *Stanford Linear Accelerator Report SLAC-265 (Stanford, CA 94305)*

Seltzer S M 1987 *An overview of ETRAN Monte Carlo Methods* in Monte Carlo Transport of Electrons and Photons eds. Jenkins T E, Nelson W R, Rindi A, Nahum A E, and Rogers D W O (Plenum Press:New York)

Appendix A Code changes for the EGS4 system

To get the new sampling macros, please contact the author (AFB) and request them. The following changes were made to the EGS4 system:

In SUBROUTINE PAIR, part of EGS4.MORTRAN, the following patch eliminates the minor bug that allowed negative kinetic energy in one of the pair products:

```
                                .
                                .
                                .
]UNTIL RNSCRN.LE.REJF; "RETRY UNTIL ACCEPTED"
                                .
                                .
                                .
```

was changed to:

```
                                .
                                .
                                .
]UNTIL ((RNSCRN.LE.REJF).AND.(BR.GE.(RM/EIG))); "RETRY UNTIL ACCEPTED"
                                .
                                .
                                .
```

In SUBROUTINE HATCH, part of EGS4.MORTRAN, the insertion of the template $INITIALIZE-PAIR-ANGLE; allows the reading in of material dependent quantities needed by the sampling routine:

```
                                .
                                .
                                .
IF (RHOR(JR).EQ.0.0)[RHOR(JR)=RHO(MD);]
]]

"BREMSSTRAHLUNG ANGULAR DISTRIBUTION INITIALIZATION - DEFAULT IS NULL"
"NEXT LINE ADDED AFB 88/05/31"
$INITIALIZE-BREMS-ANGLE;

"PAIR ANGULAR DISTRIBUTION INITIALIZATION - DEFAULT IS NULL"
"NEXT LINE ADDED AFB 91/05/29"
$INITIALIZE-PAIR-ANGLE;

"   SETUP IS NOW COMPLETE"
IF (NMED.EQ.1)[OUTPUT;
                                .
                                .
                                .
```

The following macros have been included in EGS4MAC.MORTRAN:

```
                                .
                                .
                                .
"-------------------------------------------------------------------"
"  PAIR ANGLE SELECTION MACROS                                      "
"-------------------------------------------------------------------"

"THESE MACROS ARE EXPLAINED IN NRCC REPORT # PIRS0287 BY BIELAJEW    "

;
"MACRO TO INITIALIZE DATA FOR PAIR PRODUCTION                        "
"THE QUANTITY ZBRANG IS ( (1/111)*Zeff**(1/3) )**2                   "
"WHERE Zeff IS DEFINED IN EQUATION (7) OF PIRS0287                   "
"THIS MACRO GOES IN SUBROUTINE HATCH                                 "
"THIS MACRO IS IDENTICAL TO THE $INITIALIZE-BREMS-ANGLE DEFINED ABOVE "
"                                                                    "
REPLACE {$INITIALIZE-PAIR-ANGLE;} WITH {;
    IF(IPRDST.GT.0)[
        DO IM=1,NMED[
            ZBRANG(IM)=0.0;PZNORM=0.0;
            DO IE=1,NNE(IM)[
                ZBRANG(IM)=
                  ZBRANG(IM)+PZ(IM,IE)*ZELEM(IM,IE)*(ZELEM(IM,IE)+1.0);
                PZNORM=PZNORM+PZ(IM,IE);
                ]
                ZBRANG(IM)=(8.116224E-05)*(ZBRANG(IM)/PZNORM)**(1./3.);
            ]
        ]
}
;
"THRESHOLD BELOW WHICH ONLY LOWEST ORDER ANGULAR DISTRIBUTION OF THE  "
"PAIR ANGLE IS EMPLOYED. SCALE IS ENERGY (MeV).                      "
"USERS MAY OVERRIDE THIS WITH A HIGHER VALUE BUT A LOWER VALUE WILL  "
"CAUSE NON-PHYSICAL SAMPLING                                         "
"                                                                    "
REPLACE {$BHPAIR} WITH {4.14}
;
"THIS MACRO ENABLES VERY SMALL ANGLE SAMPLING TO BE     "
"ACCUMULATED. THE LIMIT OF 1.0E-10 BREAKS DOWN AROUND   "
"50 GEV OR SO (THETA=RM/E, FOR BOTH PAIR AND BREM).     "
"THIS MACRO REPLACES CODE IN UPHI AND IN THE PRESTA     "
"MACROS FOR THE LATERAL CORRELATION PART $PRESTA-LCDV.  "
;
REPLACE{(SINPS2.LT.1.0E-10)} WITH {(SINPS2.LT.1.0E-20)}
;
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"THE FOLLOWING REPLACES THE EGS4 DEFAULT $SET-PAIR-ANGLE MACRO    "
"IT'S USE REQUIRES AN ASSOCIATE MACRO $SET-PAIR-REJECTION-FUNCTION"
"DEFINED BELOW                                                    "
"                                                                 "
"USAGE: IPRDST=0 => EGS4 DEFAULT ANGLE SELECTION                  "
"       IPRDST=1 => LOWEST ORDER ANGULAR DISTRIBUTION             "
"                                                                 "
"              d(Probability)            sin(theta)               "
"              -------------- = --------------------------------  "
"                 d(theta)      2*P*[E_total - P*cos(theta)]**2   "
"                                                                 "
"       IPRDST=2 => MOTZ, OLSEN AND KOCH (1969) EQ. 3D-2003       "
"                   IF IPRDST IS NON-ZERO AND E_PHOTON < $BHPAIR  "
"                   THE IPRDST=1 DISTRIBUTION IS USED             "
"                                                                 "
REPLACE {$SET-PAIR-ANGLE;} WITH {;
    IF((IPRDST.EQ.1).OR.((IPRDST.EQ.2).AND.(EIG.LT.$BHPAIR)))[
        DO ICHRG=1,2[
            IF(ICHRG.EQ.1)[ESE=PESE1;]ELSE[ESE=ESE2;]
            PSE=SQRT((ESE-RM)*(ESE+RM));
            $RANDOMSET COSTHE;COSTHE=1.0-2.0*COSTHE;
            SINTHE=RM*SQRT((1.0-COSTHE)*(1.0+COSTHE))/(PSE*COSTHE+ESE);
            COSTHE=(ESE*COSTHE+PSE)/(PSE*COSTHE+ESE);
            IF(ICHRG.EQ.1)[CALL UPHI(2,1);]
            ELSE[NP=NP+1;SINTHE=-SINTHE;CALL UPHI(3,2);]
            ]
        $RANDOMSET RNNO34;      "jan 15 added this line  DR"
        IF (RNNO34.LE.0.5)[IQ(NP)=1;IQ(NP-1)=-1;]
        ELSE[IQ(NP)=-1;IQ(NP-1)=1;]
        RETURN;
        ]
    ELSEIF((IPRDST.EQ.2).AND.(EIG.GE.$BHPAIR))[
        "ZBRANG=( (1/111)*Zeff**(1/3) )**2"
        ZTARG=ZBRANG(MEDIUM);
        "TTEIG = TOTAL INITIAL PHOTON ENERGY IN ELECTRON REST MASS UNITS"
        TTEIG=EIG/RM;
        DO ICHRG=1,2[
            IF(ICHRG.EQ.1)[ESE=PESE1;]ELSE[ESE=ESE2;]
            "TTESE = TOTAL FINAL ELECTRON ENERGY IN ELECTRON REST MASS UNITS"
            TTESE=ESE/RM;
            "TTPSE = TOTAL FINAL ELECTRON MOMENTUM IN ELECTRON REST MASS UNITS"
            TTPSE=SQRT((TTESE-1.0)*(TTESE+1.0));
            "THIS IS THE RATIO (r IN PIRS0287)"
            ESEDEI=TTESE/(TTEIG-TTESE);
            ESEDER=1.0/ESEDEI;
            "DETERMINE THE NORMALIZATION "
            XIMIN=1.0/(1.0+(3.141593*TTESE)**2);
            $SET-PAIR-REJECTION-FUNCTION(REJMIN,XIMIN);
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            YA=(2.0/TTEIG)**2;
            XITRY=MAX(0.01,MAX(XIMIN,MIN(0.5,SQRT(YA/ZTARG))));
            GALPHA=1.0+0.25*LOG(YA+ZTARG*XITRY**2);
            GBETA=0.5*ZTARG*XITRY/(YA+ZTARG*XITRY**2);
            GALPHA=GALPHA-GBETA*(XITRY-0.5);
            XIMID=GALPHA/(3.0*GBETA);
            IF(GALPHA.GE.0.0)[
                XIMID=0.5-XIMID+SQRT(XIMID**2+0.25);
                ]
            ELSE[
                XIMID=0.5-XIMID-SQRT(XIMID**2+0.25);
                ]
            XIMID=MAX(0.01,MAX(XIMIN,MIN(0.5,XIMID)));
            $SET-PAIR-REJECTION-FUNCTION(REJMID,XIMID);
            "ESTIMATE MAXIMUM OF THE REJECTION FUNCTION"
            "FOR LATER USE BY THE REJECTION TECHNIQUE  "
            REJTOP=1.02*MAX(REJMIN,REJMID);
            LOOP[
                $RANDOMSET XITST;
                $SET-PAIR-REJECTION-FUNCTION(REJTST,XITST);
                $RANDOMSET RTEST;
                "CONVERT THE SUCCESSFUL CANDIDATE XITST TO AN ANGLE"
                THETA=SQRT(1.0/XITST-1.0)/TTESE;
                "LOOP UNTIL REJECTION TECHNIQUE ACCEPTS XITST"
                ]UNTIL((RTEST.LE.(REJTST/REJTOP)).AND.(THETA.LT.PI));
            SINTHE=SIN(THETA);COSTHE=COS(THETA);
            IF(ICHRG.EQ.1)[CALL UPHI(2,1);]
            ELSE[NP=NP+1;SINTHE=-SINTHE;CALL UPHI(3,2);]
            ]
        $RANDOMSET RNNO34;      "jan 15 added this line  DR"
        IF (RNNO34.LE.0.5)[IQ(NP)=1;IQ(NP-1)=-1;]
        ELSE[IQ(NP)=-1;IQ(NP-1)=1;]
        RETURN;
        ]
    ELSE[
        THETA=RM/EIG;
        ]
}
;
```

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"THIS IS THE FUNCTION d[G(XI)]/(d XI) OF PIRS0287    "
"THE RESULT IS RETURNED IN {P1} AS A FUNCTION OF {P2}"
"I.E. {P1}=G({P2}) WHERE {P2}=XI                     "
"                                                    "
REPLACE {$SET-PAIR-REJECTION-FUNCTION(#,#);} WITH {;
    {P1} = 2.0+3.0*(ESEDEI+ESEDER) -
        4.00*(ESEDEI+ESEDER+1.0-4.0*({P2}-0.5)**2)*(
            1.0+0.25*LOG(
                ((1.0+ESEDER)*(1.0+ESEDEI)/(2.*TTEIG))**2+ZTARG*{P2}**2
                )
            )
        ;
}
;
"THIS COMMON HAS BEEN EXTENDED BY THE PAIR ANGLE SELECTION FLAG"
"IPRDST                                                      "
"                                                            "
REPLACE {;COMIN/BREMPR/;} WITH
   {;COMMON/BREMPR/
     $LGN(DL(6,$MXMED)/1,2,3,4,5,6/),
     $LGN(ALPHI,BPAR,DELPOS(2,$MXMED)),
     ASYM($MXMED,$MXEL,2),
     $LGN(WA,PZ,ZELEM,RHOZ($MXMED,$MXEL)),
     PWR2I($MXPWR2I),
     $LGN(DELCM,NNE,ZBRANG($MXMED)),
     IBRDST,IPRDST;
     $TYPE ASYM;
    }
                                .
                                .
                                .
```