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FLUKA and PENELOPE simulations of 10 keV to 10 MeV photons in LYSO and soft tissue

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HIGHLIGHTS

- Monte Carlo simulations of electromagnetic particle interactions and transport by FLUKA and PENELOPE were compared.
- 10 keV to 10 MeV incident photon beams impinged a LYSO crystal and a soft-tissue phantom.
- The pulse height spectra, depth doses central-axis as well as off-axis were found to agree within statistical uncertainty; no systematic difference was observed.

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ABSTRACT

Monte Carlo simulations of electromagnetic particle interactions and transport by FLUKA and PENELOPE were compared. 10 keV to 10 MeV incident photon beams impinged a LYSO crystal and a soft-tissue phantom. Central-axis as well as off-axis depth doses agreed within 1 s.d.; no systematic under- or over-estimate of the pulse height spectra was observed from 100 keV to 10 MeV for both materials, agreement was within 5%. Simulation of photon and electron transport and interactions at this level of precision and reliability is of significant impact, for instance, on treatment monitoring of hadrontherapy where a code like FLUKA is needed to simulate the full suite of particles and interactions (not just electromagnetic). At the interaction-by-interaction level, apart from known differences in condensed history techniques, two-quanta positron annihilation at rest was found to differ between the two codes. PENELOPE produced a 511 keV sharp line, whereas FLUKA produced visible acolinearity, a feature recently implemented to account for the momentum of shell electrons.

1. Introduction

FLUKA (Ferrari et al., 2005; Battistoni et al., 2007) and PENELOPE (Salvat et al., 2001; Sempau et al., 1997, 2003) are Monte Carlo codes for simulating radiation transport and calculating radiometric quantities. Independently developed, the former is reputed for seamless handling of a broad variety of particle types and heavy ions from eV to TeV range, whereas the latter specializes on electromagnetic showers (i.e. electron, positron and photon only). Within the electromagnetic domain the codes differ notably in the treatment of charged particle scattering and energy loss.

This work focuses on the domain where FLUKA and PENELOPE overlap, and draws on the opportunity to validate simulation output on measurable quantities (e.g. pulse height spectra from a scintillator crystal, 3D dose distributions) as well as quantities which are inaccessible physically (e.g. double-differential energy–angle correlation at the point of interaction). Whereas the *ultimate* benchmark would be to compare simulation against measurement, inter-code comparison allows clean and controlled access to quantities of interest untainted by inherent cross-calibration factors and confounding factors arising from the experimental environment.

2. Simulations

Simulations were ran in pairs using FLUKA version 2012 and PENELOPE version 2011. A 1 cm $\times$ 1 cm square field impinged the 3 cm $\times$ 3 cm face of a 12 cm-deep LYSO crystal ($Lu_{1.8}Y_{0.2}SiO_5$; density 7.40 g/cm^3; mean excitation energy 411.0 eV), divided into 4 segments by a 0.2 mm-thick septa ($C_{12}H_{22}O_5$; density 1.13 g/cm^3; mean excitation energy 69.3 eV) which form a cross in the beam's eye view. Pairs of simulations were ran

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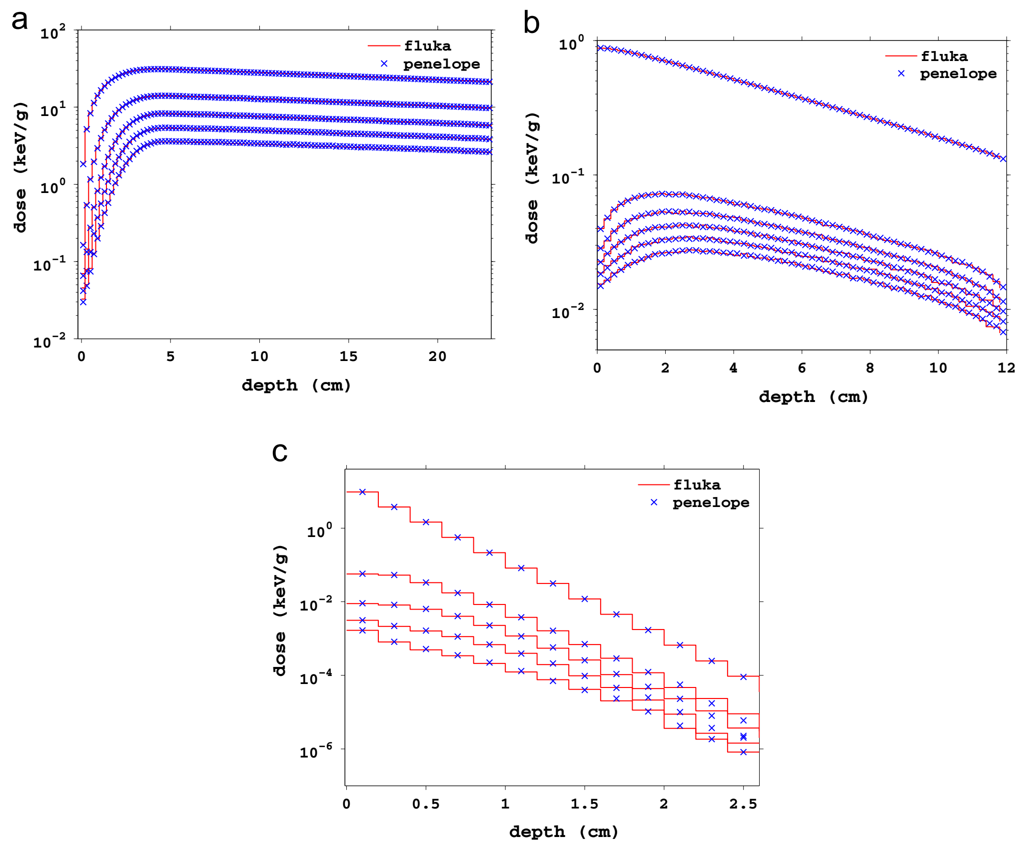

Fig. 1. Depth dose in soft tissue by (a) 10 MeV; (b) 100 keV; (c) 10 keV photon beam. From top to bottom, where present: 0 cm, 0.5 cm, 0.7 cm, 0.9 cm, 1.1 cm and 1.3 cm off beam central axis.

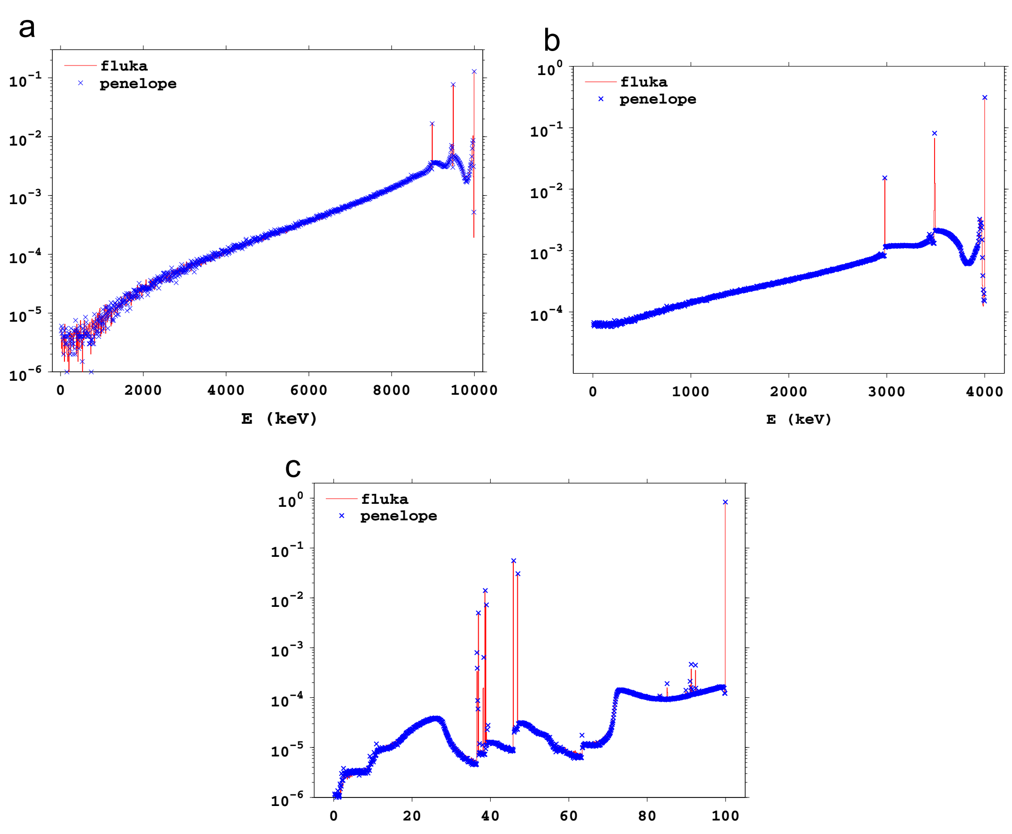

Fig. 2. Pulse height spectra in LYSO by a (a) 10 MeV; (b) 4 MeV; (c) 100 keV photon beam.

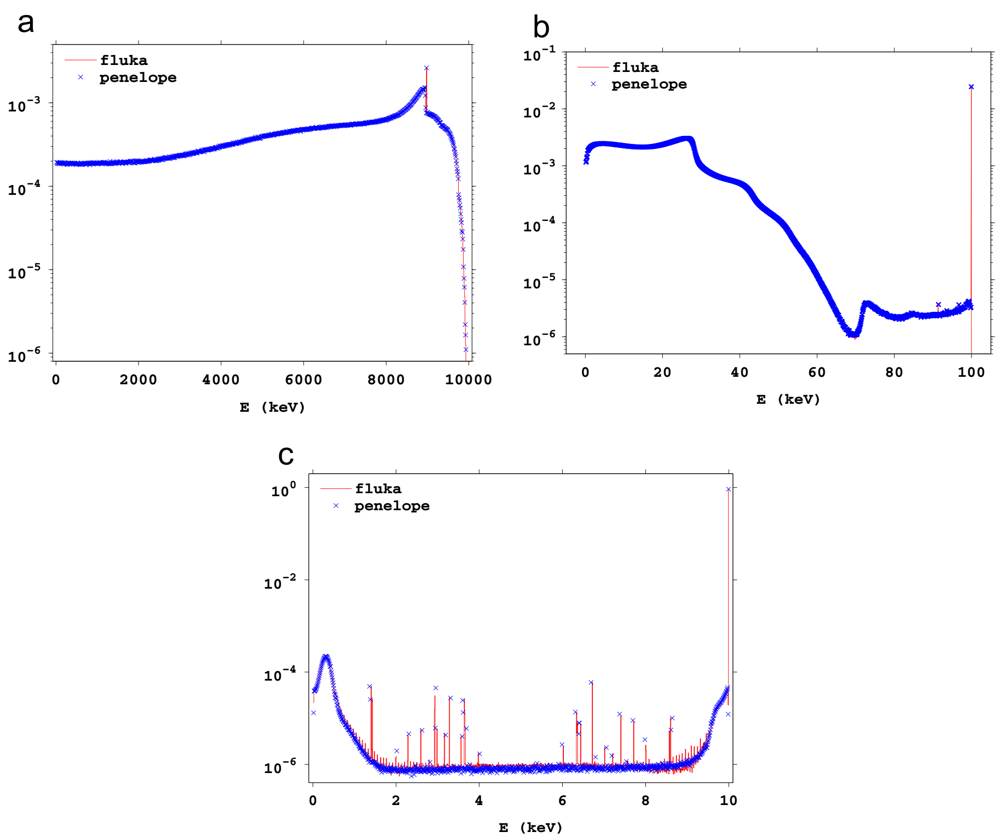

Fig. 3. Pulse height spectra in soft tissue by a (a) 10 MeV; (b) 100 keV; (c) 10 keV photon beam.

independently with 100 keV, 4 MeV and 10 MeV photons incident on the LYSO crystal. Next, with a target of identical dimensions but instead filled with ICRP Soft Tissue, simulation pairs were repeated for 10 keV, 100 keV and 10 MeV photons. In the case of 10 MeV beams the depth of the target was doubled. For all runs transport and production thresholds were set to 1 keV.

The following quantities were scored: 3D dose distribution at 2 mm intervals, 1024-channel pulse height spectrum, as well as the phase-space attributes at each interaction. This scoring combination is to minimize the chances of observing *apparent agreements*, where underlying differences could be masked by canceling effects or loss of details due to averaging. Whereas the dose distribution is averaged over all histories, the pulse height spectrum tests correlation at a history-by-history level. It follows that attributes scored at each interaction test conservation laws at the collision-by-collision level.

3. Results

From the mean free path of the primary photon, as expected photon cross-sections were found to be the same for FLUKA and PENELOPE for all beam–target combination studied. Depth dose distribution along the central beam axis, and that along different off-axis positions, agreed within statistical uncertainty (Fig. 1), addressing the absorption as well as lateral scatter of both codes. No systematic difference between FLUKA and PENELOPE was observable. Pulse height spectra in LYSO as well as soft tissue showed tight agreement between FLUKA and PENELOPE over five orders of magnitude (Figs. 2 and 3), agreeing in photo-peaks, escape peaks and Compton edges.

Photon pairs emitted from positron annihilation at rest were found to be 511.0 keV, sharp, in PENELOPE. FLUKA, however,

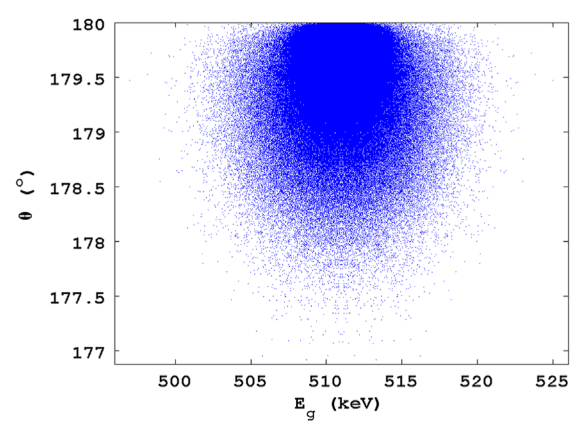

Fig. 4. Energy spectrum of photons emitted from positrons annihilating at rest as produced by FLUKA; the spread is absent in PENELOPE. Data shown is for the 4 MeV-LYSO setup.

produced photon pairs with a visible acolinearity effect which translates into a spread in both energy and angle (Fig. 4). Note that the FWHM of energy spread is no more than 2 keV, finer than the bin size of energy spectra shown in preceding plots. This is due to non-negligible momentum of shell electrons, recently implemented and benchmarked in FLUKA (Böhlen et al., 2012). The spread differs from that by positron annihilation in-flight, where both codes produced comparable double-differential characteristics (Fig. 5).

4. Discussion

The pulse height spectra produced by FLUKA and PENELOPE agreed very well despite the independent condensed history

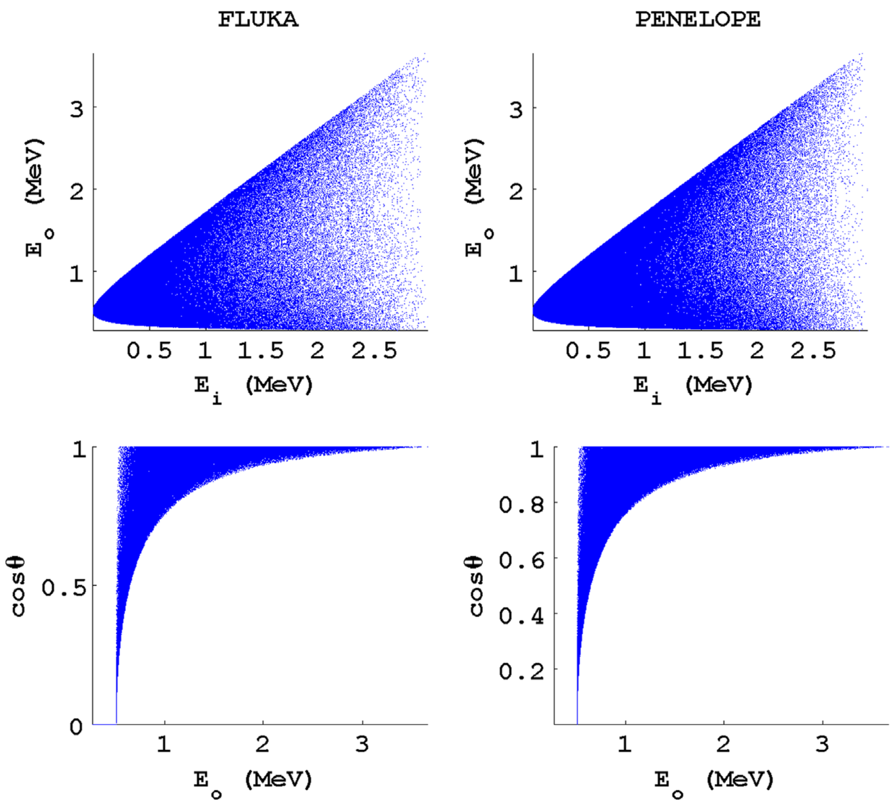

Fig. 5. Two-quanta positron annihilation in-flight: photon energy (E_i), positron energy (E_o) and angle between photon pair (θ). Data shown is for the 4 MeV-LYSO setup.

models. This homes in on the point of the condensed history technique—itself unphysical yet provides good representation of physical processes. While PENELOPE does go up to GeV energies, the incident energies chosen for this work were kept ≤10 MeV so as to avoid the onset of photonuclear reactions, which goes beyond the overlap between the two codes.

The beam–target combinations tested are of significant interest in various detector, dosimetry and medical applications. The 4 MeV-LYSO setup simulated here is in fact an excerpt from a larger experiment (Agodi et al., 2012), for hadrontherapy, where a 80 MeV/u carbon beam hit a PMMA target, emitting polyenergetic photons (among them, 4 MeV) to be measured by a LYSO detector. The application was on the prospects of deducing the position of the Bragg peak from measured photon profiles.

A notable difference between the two codes was observed at the interaction level: PENELOPE does not model acolinearity effects following positrons annihilating at rest, which is negligible for most applications, except, for instance, positron emission tomography (PET), where minor effects become observable.

5. Conclusion

Excellent agreement between FLUKA and PENELOPE was found in the pulse height spectra and dose distribution produced by 10 keV to 10 MeV photon beams impinging LYSO and soft tissue. Seamless simulation of radiometric quantities under such intermediate-energy and heterogeneous configurations addresses exactly the concerns where the radiation physics community needs confidence in, e.g. treatment monitoring of hadrontherapy.

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