Changes to EGS4 Since Version 1.0
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This document outlines the changes to the EGS4 code between the SNOMAN 2_07 implementation (EGS4, version 1) and SNOMAN 2_08 (EGS4, version 2) implementation. A brief description of the changes is given, together with my assessment of the relevance to SNO. This document draws heavily on the references contained herein and a set of lecture notes entitled "History and overview of EGS4" [1].

1 Changes to EGS4

All of these changes are optional - they are not included in the default version of EGS4, but must be enabled either at MORTRAN[1] compile time, or via the use of variables at run time. Some are manifestly not relevant to SNOMAN, but are included for completeness.

1.1 PRESTA

PRESTA (Parameter Reduced Electron Step Transport Algorithm) [2] introduces a number of changes to the electron transport:

- A refined calculation of the curvature of each electron substep. This path length correction is based on Molière scattering theory, rather than the Fermi-Eyges theory used in version 1. A more accurate calculation of the electron transport step size (TMXS).
- The addition of a lateral correction algorithm (standard EGS4 code ignores this and thus underestimates the lateral diffusion).
- The introduction of a boundary crossing algorithm, which causes sub steps to become shorter in the vicinity of a boundary, removing transport artifacts associated with the boundary.

Installation of these routines requires the use of a number of macros, provided with the source code. In addition the changes are controlled at run time by software switches shown in Table 1.

In principle all the above are of interest to SNOMAN - the first two definitely improve the simulation, the third might improve the simulation of certain classes of events, and in any case may improve the speed of the EGS4 calculations. In practice, the boundary crossing algorithm cannot currently be implemented as it requires the geometry to be able to calculate the shortest distance to any boundary, an operation not completely supported by the SNOMAN geometry (notably the phototube geometry). This also means that the lateral correction algorithm cannot be used. The path length correction is of particular interest as it alters the path length of charged particles, and thus the amount of Čerenkov light. However, detailed examination suggests that, even at low energies, the path length is corrected by $\leq 0.5\%$.

[1] MORTRAN is a FORTRAN preprocessor, which allows a number of facilities, such as macro for template replacement, and "shorthand". MORTRAN code is first compiled into FORTRAN using the MORTRAN3 compiler supplied with the EGS4 code, and then compiled normally using a standard FORTRAN77 compiler.

Variable	Value	Comment
IPLC	-1	No path-length correction used
	0	New presta path-length correction used
	1	Old EGS4 path-length correction used
IBCA	0	Boundary crossing algorithm invoked
	1	Boundary crossing algorithm not invoked
ILCA	0	Lateral correction algorithm invoked
	1	Lateral correction algorithm not invoked
IOLDTM	0	New TMXS calculation used
	1	Old TMXS calculation used
BLCMIN	0.0	PRESTA selects minimum step-sizes
	1.0	Absolute minimum value

Table 1: PRESTA switches.

1.2 Bremsstrahlung angular distribution

The standard EGS4 approximation is that the photon is emitted at an angle given by $\theta = 1/E$ where E is the energy in units of the electron rest mass. The expectation was that the approximation was valid because at high energies, the distribution would be strongly forward peaked, whilst at low energies, multiple scattering would wash this artifact out. This expectation has been shown to be sadly lacking, even for thick targets at low energies ($\sim$ 10 MeV), where definite calculational artifacts have been demonstrated. An alternative to the standard EGS4 approach is to employ the Schiff formula which, the author notes, does remove the artifacts for thick target studies at medical diagnostic energies (ie the sorts of energies SNO is working at).

The macros to achieve this are already incorporated in the code [3], and are switched on via the (FORTRAN) user flag IBRDST (set to 1 to enable the more complicated formula). A serendipitous side effect of this is that the elemental composition data required for the muon and neutron codes is automatically read in.

1.3 K and L shell fluorescence

Standard EGS4 code does not create or transport fluorescent photons. Although macros and sampling schemes now exist for doing this, the energies make it irrelevant to SNOMAN [4].

1.4 Electromagnetic field transport

The EGS4 subroutine ELECTR now contains macro replacement templates to allow for transport of particles through a user specified configuration of electric and magnetic fields. Not relevant to SNOMAN.

1.5 ICRU37 collision and radiative stopping powers

PEGS4 (the pre-processor for EGS) has been altered to make the radiative stopping powers compliant with ICRU Report 37 [5]. This will make changes in the bremsstrahlung cross section for particles below $\sim$ 50 MeV, and will make a significant difference below a few MeV where the bremsstrahlung production is small [6]. This is included in the PEGS code via a run time flag, and will be implemented in SNOMAN version 2_08.

1.6 Improved photon cross sections

The standard EGS4 code uses the photon cross sections of Storm and Israel [7]. An alternative is the more modern PHOTX library, for which the major change is to the low energy photo-electric cross section. This suggests that it will make very little difference to SNOMAN [8].

1.7 Photoelectron angular distribution

In the standard EGS4 code, the electron produced when a photon is absorbed by an atom is assumed to have the same directional cosines as the incoming photon. This is obviously only an approximation, and the theory of Sauter has been coded as an optional extra. SNOMAN currently ignores photoelectrons, so their angular distribution is irrelevant [9].

1.8 Pair production angular distributions

The standard EGS code uses the assumption that the electron and positron produced in pair production are emitted at an angle $\theta = 1/E$ with respect to the photon's direction. E is the photon's energy in units of the electron rest mass. This is analogous to the Bremsstrahlung angular distribution discussed earlier and is justified in a similar manner. The assertion is made that at high energies, the distribution will be strongly peaked, and at low energies, the effects of the assumption will be washed out by multiple scattering. However, as has been discussed in a previous section, this may not be the case, and macros have been installed in the code to allow for two improved approximations to the angular distribution [11]:

- The leading order approximation, which is considered by the authors to be "a crude approximation, even in its region of validity". However, the region of validity does cover all the SNO materials, and solar neutrino energies.
- The Schiff distribution, an extremely high energy approximation which fails completely at 4.14 MeV.

Which of these options is used is controlled by a run time switch IPRDST (0 gives the old distribution, 1 gives the leading order approximation, 2 gives the Schiff distribution, but using the leading order approximation below 4.14 MeV) [10]. Given that pair production is dominant at high energies, it seems reasonable to use the full Schiff distribution.

1.9 Low energy electron cross section modelling

The standard EGS4 code exploits the fact that at high energies the cross sections for discrete interactions drop with decreasing energy. Although this is a good approximation in the relativistic regime, it fails in the non relativistic regime when the cross sections starts to rise with decreasing energy. Although not of particular interest to the modelling of high energy and solar energy neutrinos, this may have a pronounced effect on the light produced from low energy events, such as PMT $\beta - \gamma$s [12]. The effect of this is that all path lengths (for solar neutrino energy electrons) are reduced by $\sim 0.5\%$, with the consequent effect on the number of Čerenkov photons produced.

1.10 More accurate trigonometric functions

Because of the time used in evaluating sines and cosines, the standard EGS4 code makes use of a precalculated look up table for these functions. This can lead to problems for small angle modelling, and macros are available to recover the native FORTRAN trigonometric functions, or install other systems.

1.11 Single elastic scattering

There is no code yet available for this, but I suspect it does have a bearing on recent discussions as it concerns work to modify EGS4 to use single electron scattering rather than Molière formalism. Interested readers are directed to [13, 14].

1.12 Binding effect in the Compton interaction

The standard EGS4 code treats any candidate Compton scattered electron as being free, and ignores any atomic binding energy. This is generally a good approximation for photon energies down to a few

tens of keV, but can have an effect on low energy studies ($\sim 40 - 200$ keV, depending on the materials under study) [15]. Irrelevant for SNOMAN.

1.13 Doppler broadening

In addition to the previous point, the motion of the electrons in the atomic cloud is ignored by the default EGS4 code. Code has been developed to model this, but the effect is only notable at low energies (one study was done at 40 keV) and is thus irrelevant to SNOMAN [16].

1.14 Linearly polarised photon scattering

The standard EGS4 cross sections are summed over all possible incoming and outgoing polarisations. This has been shown to produce errors at low energies (40-250 keV), and would produce errors in any simulation involving polarised electrons, but is once again not of importance in SNOMAN (unless some calibration source is likely to produce polarised electrons) [16].

2 Current Implementation

Of the changes mentioned above, five warrant our attention:

1. PRESTA;
2. Bremsstrahlung and pair production angular distributions;
3. ICRU-37 stopping powers;
4. low energy cross section modelling;
5. single electron scattering.

Of those, one (ICRU-37) will be included automatically, two (PRESTA and the angular distribution stuff) are switchable at run time, allowing them to be removed from the simulation at the flick of a software switch, one (low energy cross sections) is hardwired, but could be made switchable if required, and one is pending, with no code currently available.

2.1 Bugs

- The EGS4 code contains a rather nasty potential problem. The routine UPHI uses three local variables (A, B, C) to store information between calls. This is not technically valid under the FORTRAN77 standard, and is certainly not valid on any machines using dynamic memory allocation, where it will result either in an error or outright nonsense, depending on how well designed the FORTRAN77 compiler is. A SAVE A,B,C statement solves this problem. There is a secondary problem in that the PRESTA routines also use a variable B (from Molière theory). The SAVE statement thus introduces a conflict with the declaration of B as a common variable in COMMON/USERPR/ (whilst the common block is used, the specific variable is not). For safety, the local variables A, B, C have been renamed in routine UPHI.

- Routine HATCH contains a compiler dependent bug. The source of the bug is that individual entries in the PEGS file will have one line different depending on whether the line is a gas or not. Consider the following code fragment:

```
      READ(KMPI,1,ERR=1270) (MBUF(I),I=1,5),RHO(IM),NNE(IM),IUNRST(IM)
     * ,EPSTFL(IM),IAPRIM(IM)
1     FORMAT(5A1,5X,F11.0,4X,I2,9X,I1,9X,I1,9X,I1)
      GO TO 1280
1270  BACKSPACE(KMPI)
      READ(KMPI,2)(MBUF(I),I=1,5),RHO(IM),NNE(IM),IUNRST(IM),EPSTFL(IM
```

```
     *  ), IAPRIM(IM)
2        FORMAT(5A1,5X,F11.0,4X,I2,26X,I1,9X,I1,9X,I1)
1280     CONTINUE
```

This reads the file in the more common format, and, if it gets an error, interprets that as a signal that the other format is required. The file is then backspaced and reread in the other format. This doesn't work on the RS6K, which despite realising the problem, helpfully sets the variables to zero and continues as if nothing were wrong. Curiously, the compiler recognises a problem (IOSTAT is returned as 97), but the ERR flag appears to be unset. The reason for this problem is unclear, though may be a manifestation of the fact that END= and ERR= are obsolete in the FORTRAN90 standard. Replacing the code with:

```
        READ (KMPI,1270)ADUMMY1
1270    FORMAT(A80)
        BACKSPACE(KMPI)
        ADUMMY2 = ADUMMY1(29:32)

        IF(ADUMMY2.NE.'GASP')THEN
          READ(KMPI,1) (MBUF(I),I=1,5),RHO(IM),NNE(IM),
     *                 IUNRST(IM),EPSTFL(IM),IAPRIM(IM)
1         FORMAT(5A1,5X,F11.0,4X,I2,9X,I1,9X,I1,9X,I1)
        ELSE
          READ(KMPI,2)(MBUF(I),I=1,5),RHO(IM),NNE(IM),IUNRST(IM),
     *                EPSTFL(IM), IAPRIM(IM)
2         FORMAT(5A1,5X,F11.0,4X,I2,26X,I1,9X,I1,9X,I1)
        ENDIF
```

solves the problem in a fashion that is not compiler dependant.

References

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