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Monte Carlo simulations

Eirik Malinen

MC simulations 1

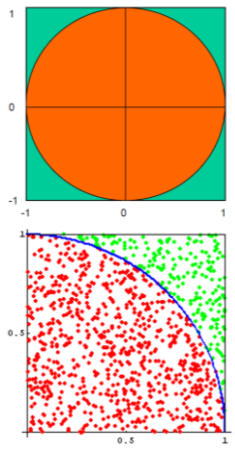
- Simulations of stochastic processes
- Interactions are stochastic: the path of a single ionizing particle may not be predicted
- Interactions are quantified by probabilities (cross sections)
- Random numbers and cross sections may be used to simulate single events
- Better than analytical methods, but requires CPU-time

MC simulations 2

- Photons give rise to electrons and vice versa; coupled energy transport
- Analytic methods are suboptimal for:
  - Modeling of scatter
  - Generating electron- and photon spectra
  - Modeling interface effects
  - Calculating energy dependence of dosimeter response

MC simulation - example

- Use random numbers to estimate π



Ratio of areas: π/4

Draw random numbers;

Sample points so that $x^2 + y^2 \leq 1$

Here, Ratio = 787/1000 = 0.787

$\rightarrow \pi \approx 4 \times 0.787 = 3.148$

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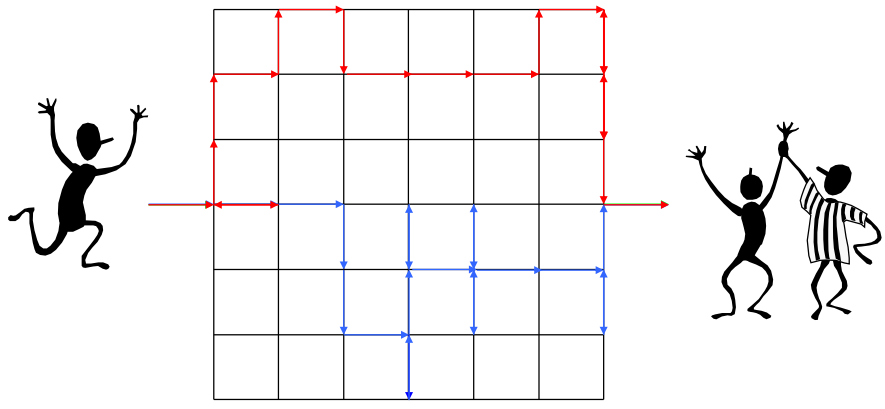
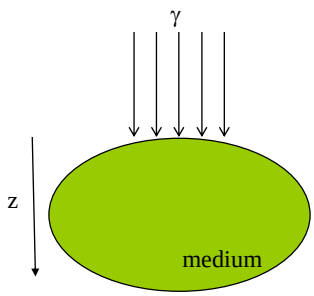
Random walk



Photon MC

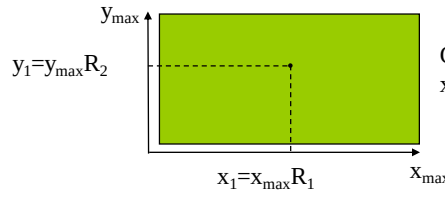


Description of photons and their energy depositions:

1. Position
2. Pathlength
3. Interaction
4. Secondary photon?

} Depends on photon energy

1: Draw two random numbers; $0<R<1$



Cross section of field: $x_{max} \times y_{max}$

Photon pathlength

- Photon attenuation:

$$N = N_0 e^{-\mu z}$$

- Describes the number of photons at depth z – is a type of *frequency distribution*:

$$f(z) = Ce^{-\mu z} \quad , \quad \int_0^\infty f(z)dz \overset{!}{=} 1 \Rightarrow C = \mu$$

$$\Rightarrow \langle z \rangle = \int_0^\infty z f(z)dz = \frac{1}{\mu}$$

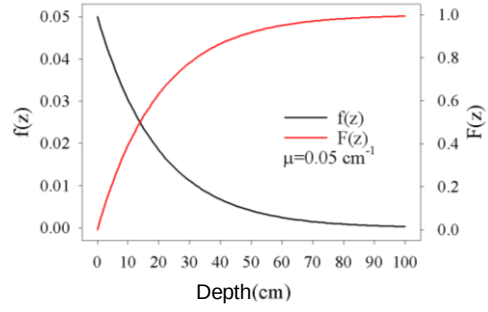
- Expected pathlength: $1/\mu$

Photon interaction point 1

- At what depth does an event (interaction) take place?
- Need a cumulative distribution with respect to depth:

$$F(z) = \int_0^z f(z')dz' = \int_0^z \mu e^{-\mu z'} dz' = 1 - e^{-\mu z}$$

F(z): probability that a photon has interacted between 0 and z



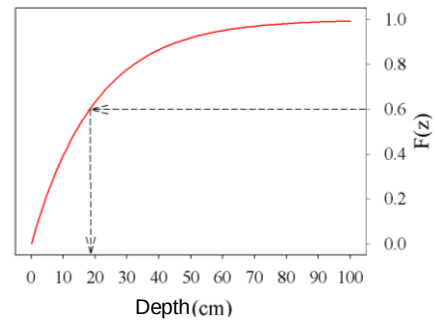
Photon interaction point 2

- Draw a random number R_1 – what is the corresponding pathlenght for this photon?

$$F(z_1) = R_1 = 1 - e^{-\mu z_1} \quad \Rightarrow \quad e^{-\mu z_1} = 1 - R_1$$

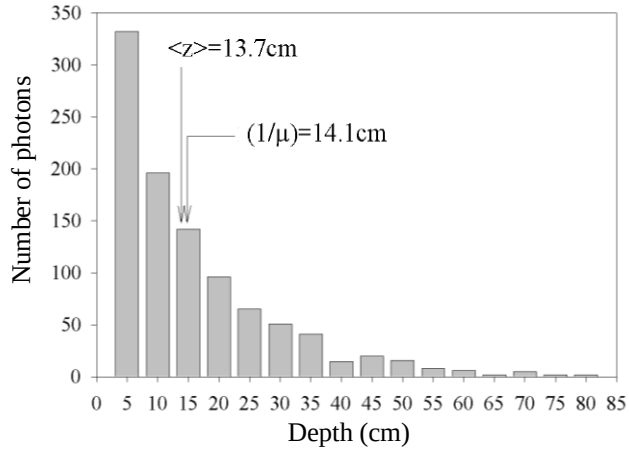
$$z_1 = -\frac{\ln(1-R_1)}{\mu}$$

Example: R_1=0.6 → z_1=18.3 cm



Pathlength sampling

- Sampled pathlength of 1000 photons (1 MeV):



Interaction sampling

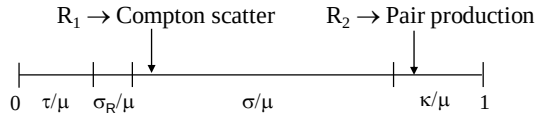
- What interaction occur at given depth?
- Total probability:

$$\mu = \tau + \sigma_R + \sigma + \kappa$$

- Probability for e.g. Compton scatter:

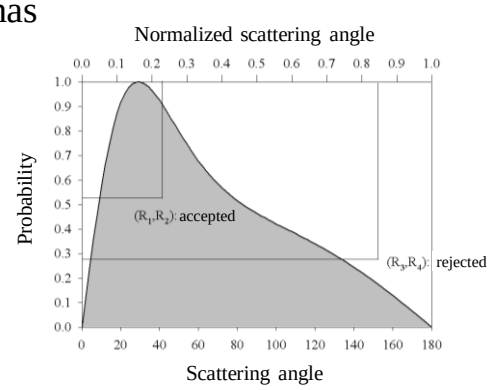
$$p_{Compton} = \frac{\sigma}{\mu}$$

- Draw random number:

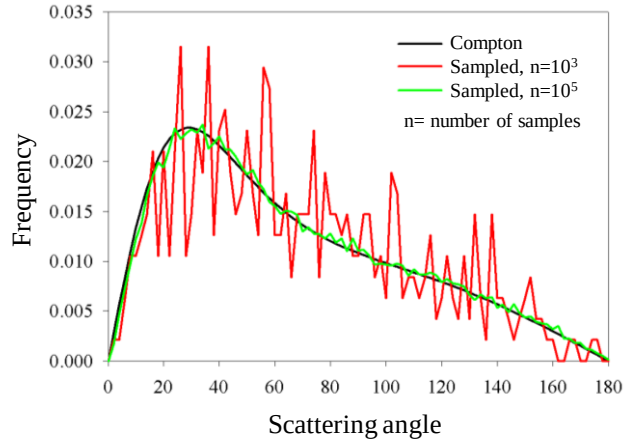


Sampling of scattered photons

- Is the photon scattered? In what direction?
- Angular distribution follows Compton cross section:
- Compton distribution has no analytic cumulative
- Must draw *two* random numbers



Sampling Compton scatter



Electron MC 1

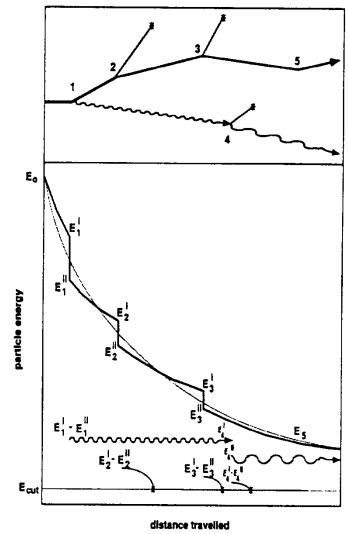
- Simulations of electrons and positrons are more complicated
- A 0.5 MeV electron interacts ~10000 times when slowing down to 1 keV in aluminium!
- Number of calculations $\rightarrow \infty$
- *Macroscopic* Monte Carlo: Evaluate the electron after a given steplength – several interactions included in one step (simulations of every interaction: *microscopic* Monte Carlo)

Electron MC 2

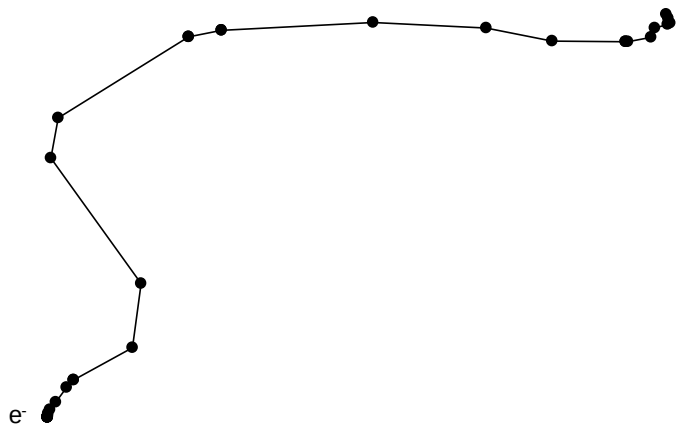
- Relative energy loss per step, η:

$$\eta = \frac{T_{k+1} - T_k}{T_k} = \frac{\Delta T}{T_k}$$

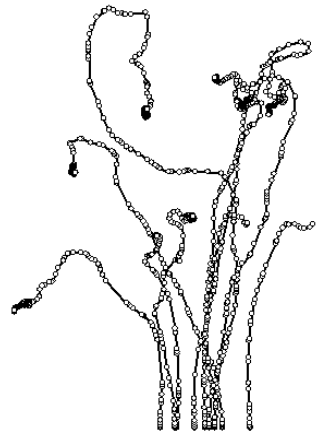
- T_k: electron energy in interaction point k
- η is set by user
  – may be sampled: η'= ηR
- Step length: $\Delta s = \eta \frac{T_k}{\left(\frac{dT}{dx}\right)_{k,k+1}}$



Electron 'walk'

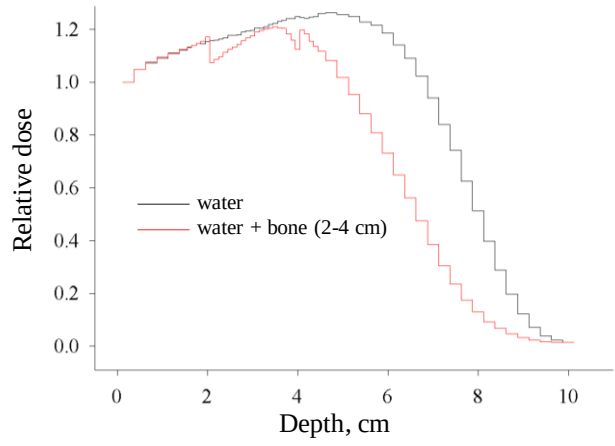


Electron 'tree'



Electron MC, example

- 18 MeV electrons in water/bone



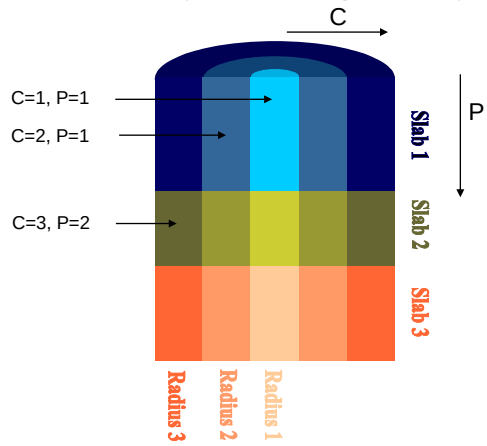
EGSnrc

- EGSnrc is a widely used MC code for e.g. simulations of photon- and electron beams
- Complicated programming, but simplified, user-friendly interface available: egs_inprz

http://nrc-cnrc.github.io/EGSnrc/

EGSnrc/DOSRZ

- DOSRZ: MC in cylindrical geometry



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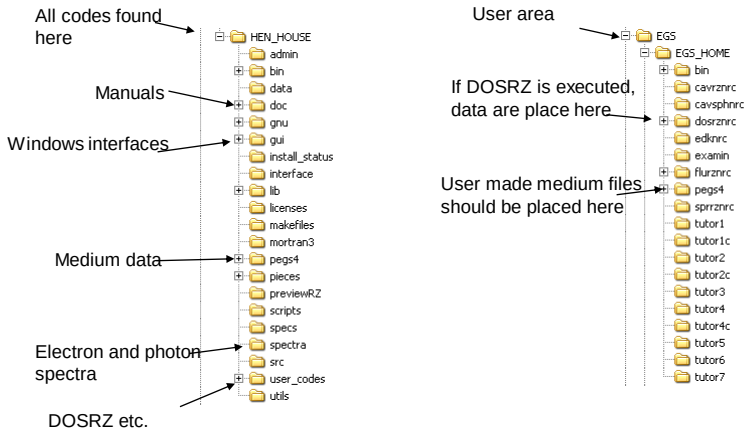
DOSRZ

- The user sets:
  - Phantom geometry
  - Radiation type- and energy (or spectrum)
  - Source (parallel beam, point source, ...)
  - Number of ”histories”, i.e. number of particles
  - Some MC parameters

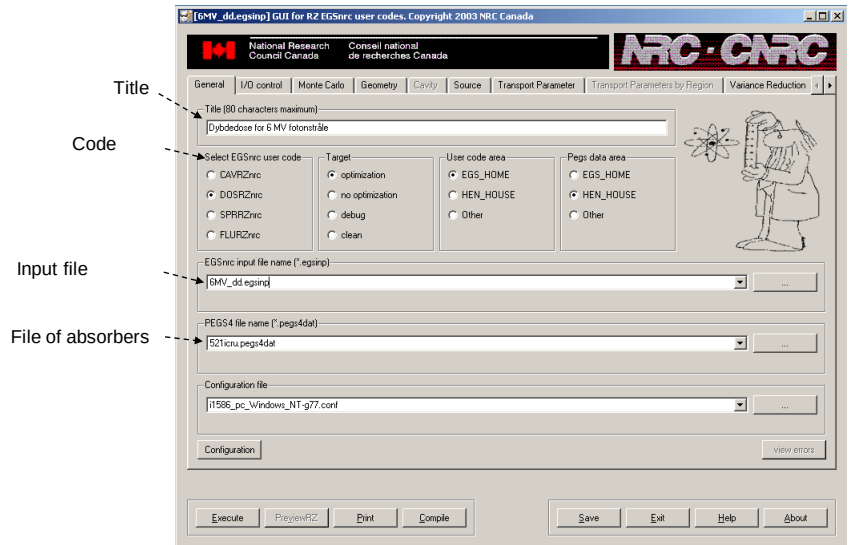
Some important parameters

- ECUT: lower limit for electron transport (includes rest mass of 0.511 MeV)
- PCUT: lower limit for photon transport
- AE: lower limit for generation of electrons
- AP: lower limit for generation of photons
- AE and AP is medium specific and must be set in PEGS (see below)

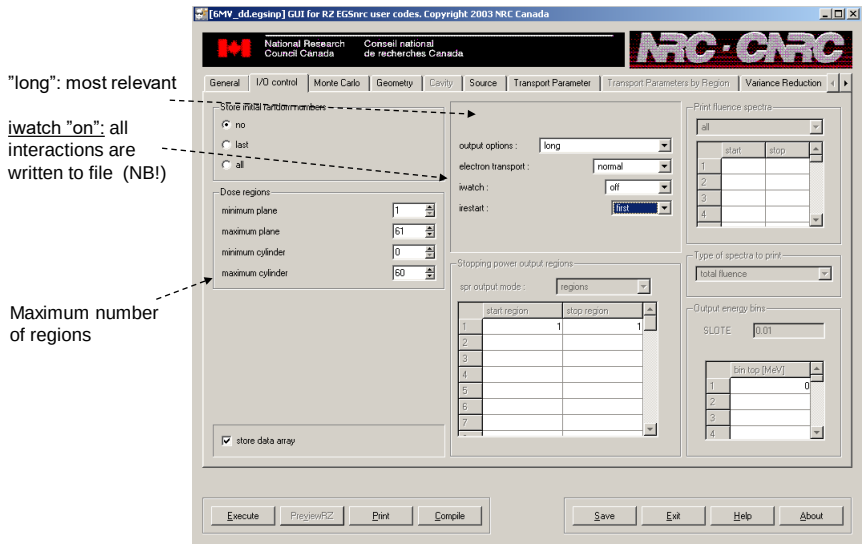
Directories



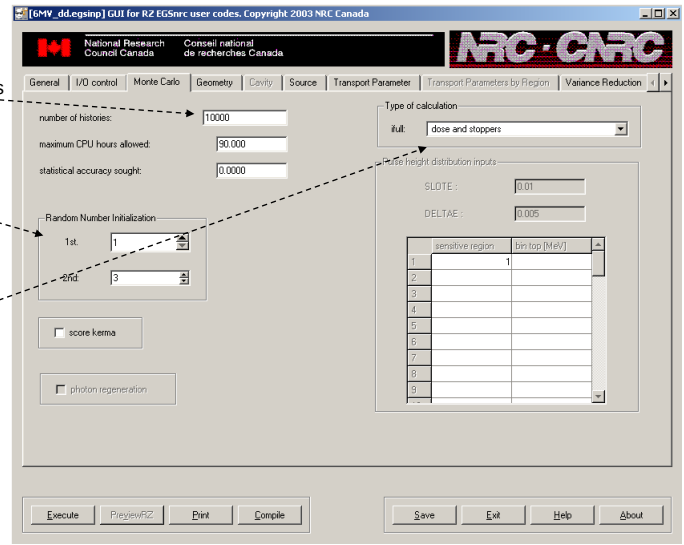
Interface



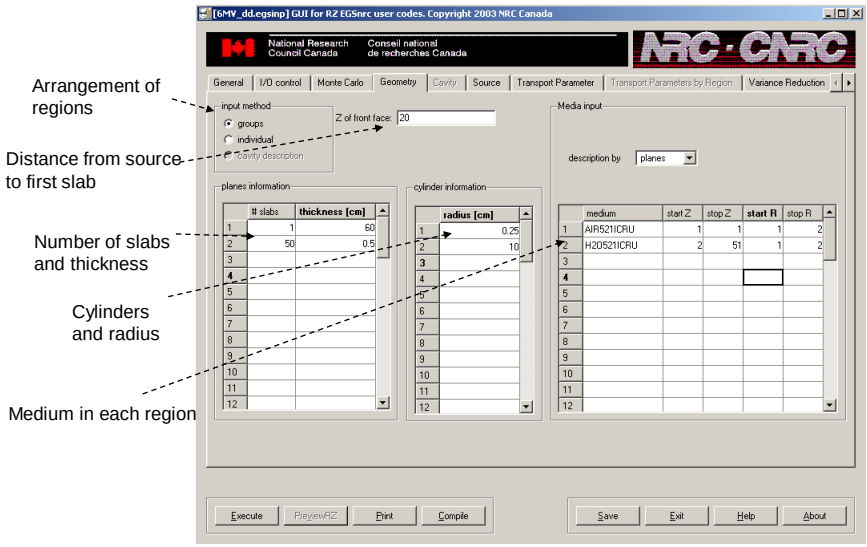
Interface



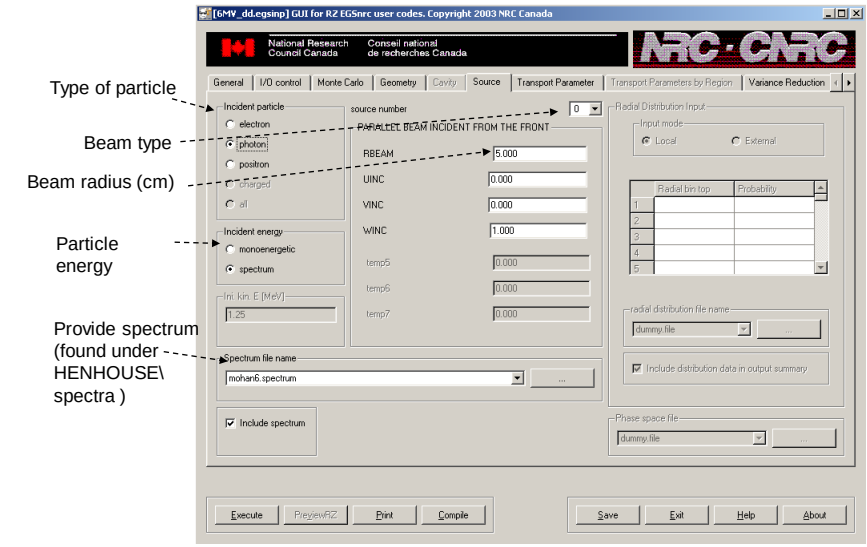
Interface



Interface



Interface

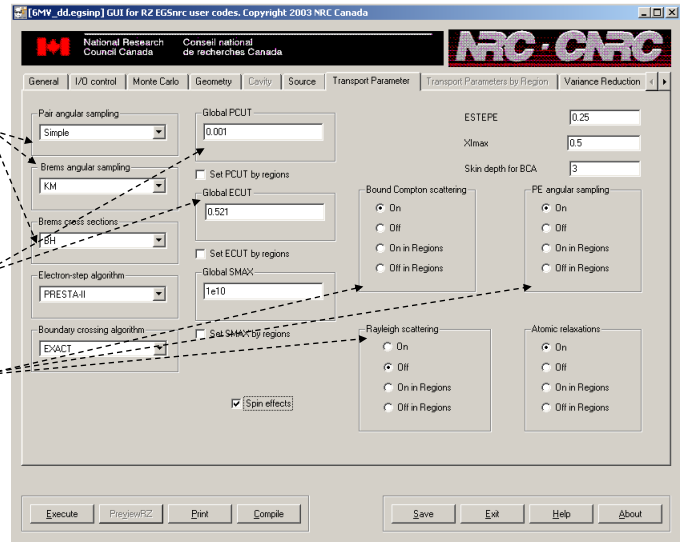


Interface

Methods for calulating pair production and brehmsstrahlung

PCUT and ECUT

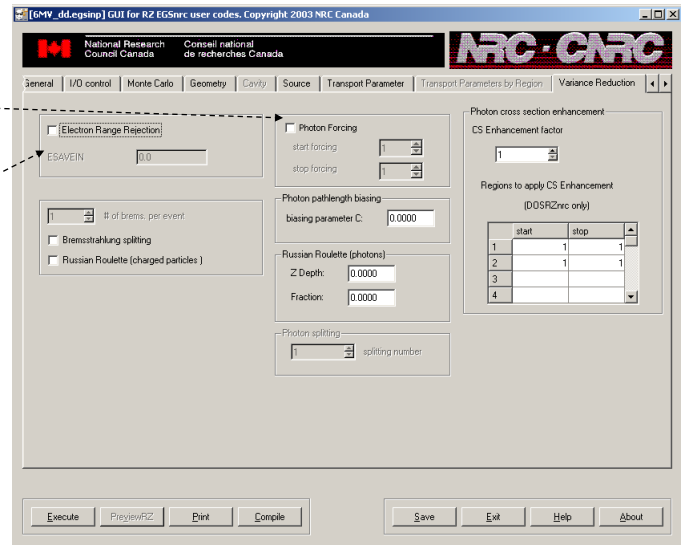
Photon interactions



Interface

Force photon to interact

Stop electron transport if range is short

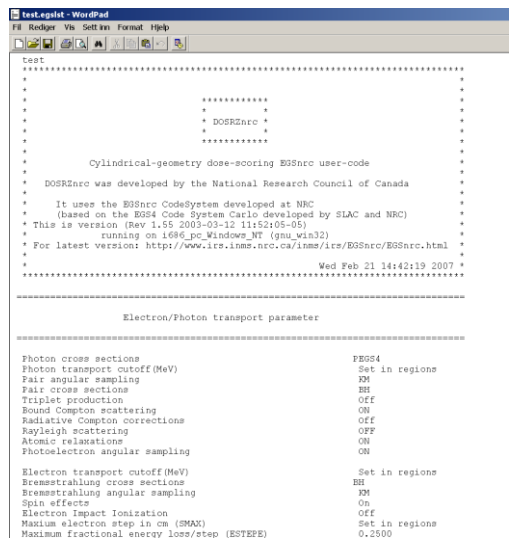


Output - *.egsgph (with IWATCH=graph)

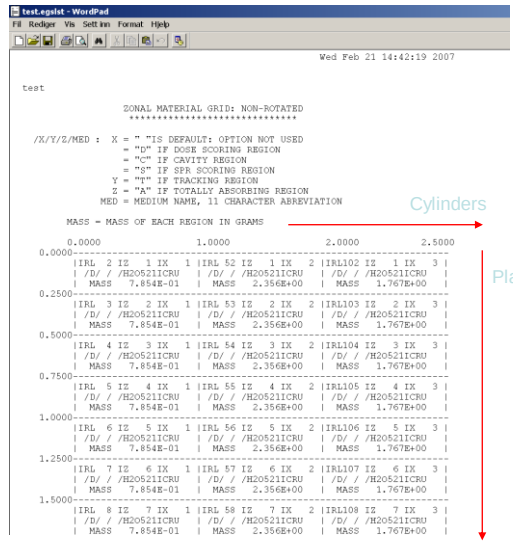
p	q	r	x	y	z	E	
1	0	2	-3.8381002	-2.2746158	0.0000000	0.10000000	
1	0	2	-3.8381002	-2.2746158	1.8895864	0.10000000	
2	-1	2	-3.8381002	-2.2746158	1.8895864	0.52920631	
2	-1	2	-3.8381002	-2.2746158	1.8895864	0.52920631	
2	-1	2	-3.8381002	-2.2746158	1.8895864	0.52920631	
1	0	2	-3.8381002	-2.2746158	1.8895864	0.81773069E-01	
1	0	2	-3.9120636	-3.2345552	1.8234146	0.81773069E-01	
2	-1	2	-3.9120636	-3.2345552	1.8234146	0.52306919	
2	-1	2	-3.9120636	-3.2345552	1.8234146	0.52306919	
2	-1	2	-3.9120636	-3.2345552	1.8234146	0.52306919	
1	0	2	-3.9120636	-3.2345552	1.8234146	0.69693251E-01	
1	0	2	-7.7017622	-3.0405600	2.4233341	0.69693251E-01	
2	-1	2	-7.7017622	-3.0405600	2.4233341	0.51507270	
2	-1	2	-7.7017622	-3.0405600	2.4233341	0.51507270	
2	-1	2	-7.7017622	-3.0405600	2.4233341	0.51507270	
1	0	2	-7.7017622	-3.0405600	2.4233341	0.65609927E-01	
1	0	2	-9.9838972	-0.41123173	0.71254671	0.65609927E-01	
1	0	2	-9.9838972	-0.41123173	0.71254671	0.65609927E-01	
1	0	2	-9.9838972	-0.41123173	0.71254671	0.65609927E-01	
1	0	1	-9.9919167	-0.40199202	0.70653480	0.65609927E-01	
0	0	0	0.0000000	0.0000000	0.0000000	0.0000000	1
1	0	2	-0.81262147	-1.4711231	0.0000000	0.10000000	
1	0	2	-0.81262147	-1.4711231	0.17595443	0.10000000	
2	-1	2	-0.81262147	-1.4711231	0.17595443	0.52714602	
2	-1	2	-0.81262147	-1.4711231	0.17595443	0.52714602	
2	-1	2	-0.81262147	-1.4711231	0.17595443	0.52714602	
1	0	2	-0.81262147	-1.4711231	0.17595443	0.83314356E-01	
1	0	1	-7.7556510	-6.3126755	0.52070326	0.83314356E-01	

p: particle q: charge r: region x: x-coord E=energy

Output - *.egslst



Output - *.egslst



test.egslst - WordPad

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test

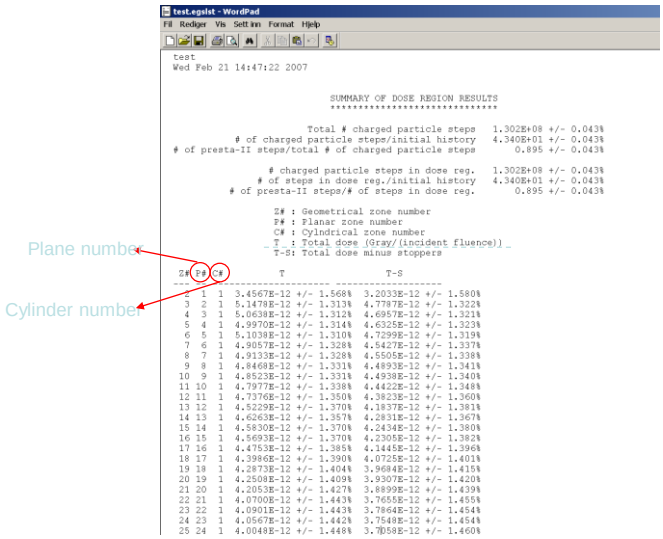
                  ZONAL MATERIAL GRID: NON-ROTATED
                   ****************************

  /X/Y/Z/MED :  X = " "IS DEFAULT: OPTION NOT USED
                  = "D" IF DOSE SCORING REGION
                  = "C" IF CAVITY REGION
                  = "S" IF SPR SCORING REGION
                Y = "T" IF TRACKING REGION
                Z = "A" IF TOTALLY ABSORBING REGION
              MED = MEDIUM NAME, 11 CHARACTER ABBREVIATION

       MASS = MASS OF EACH REGION IN GRAMS

        0.0000                1.0000                2.0000          2.5000
  0.0000-------------------------------------------------------------------
        |IRL  2 IZ   1 IX   1 |IRL 52 IZ   1 IX   2 |IRL102 IZ   1 IX   3 |
        | /D/ / /H2O521ICRU   | /D/ / /H2O521ICRU   | /D/ / /H2O521ICRU   |
        |  MASS   7.854E-01   |  MASS   2.356E+00   |  MASS   1.767E+00   |
  0.2500-------------------------------------------------------------------
        |IRL  3 IZ   2 IX   1 |IRL 53 IZ   2 IX   2 |IRL103 IZ   2 IX   3 |
        | /D/ / /H2O521ICRU   | /D/ / /H2O521ICRU   | /D/ / /H2O521ICRU   |
        |  MASS   7.854E-01   |  MASS   2.356E+00   |  MASS   1.767E+00   |
  0.5000-------------------------------------------------------------------
        |IRL  4 IZ   3 IX   1 |IRL 54 IZ   3 IX   2 |IRL104 IZ   3 IX   3 |
        | /D/ / /H2O521ICRU   | /D/ / /H2O521ICRU   | /D/ / /H2O521ICRU   |
        |  MASS   7.854E-01   |  MASS   2.356E+00   |  MASS   1.767E+00   |
  0.7500-------------------------------------------------------------------
        |IRL  5 IZ   4 IX   1 |IRL 55 IZ   4 IX   2 |IRL105 IZ   4 IX   3 |
        | /D/ / /H2O521ICRU   | /D/ / /H2O521ICRU   | /D/ / /H2O521ICRU   |
        |  MASS   7.854E-01   |  MASS   2.356E+00   |  MASS   1.767E+00   |
  1.0000-------------------------------------------------------------------
        |IRL  6 IZ   5 IX   1 |IRL 56 IZ   5 IX   2 |IRL106 IZ   5 IX   3 |
        | /D/ / /H2O521ICRU   | /D/ / /H2O521ICRU   | /D/ / /H2O521ICRU   |
        |  MASS   7.854E-01   |  MASS   2.356E+00   |  MASS   1.767E+00   |
  1.2500-------------------------------------------------------------------
        |IRL  7 IZ   6 IX   1 |IRL 57 IZ   6 IX   2 |IRL107 IZ   6 IX   3 |
        | /D/ / /H2O521ICRU   | /D/ / /H2O521ICRU   | /D/ / /H2O521ICRU   |
        |  MASS   7.854E-01   |  MASS   2.356E+00   |  MASS   1.767E+00   |
  1.5000-------------------------------------------------------------------
        |IRL  8 IZ   7 IX   1 |IRL 58 IZ   7 IX   2 |IRL108 IZ   7 IX   3 |
        | /D/ / /H2O521ICRU   | /D/ / /H2O521ICRU   | /D/ / /H2O521ICRU   |
        |  MASS   7.854E-01   |  MASS   2.356E+00   |  MASS   1.767E+00   |
```


Output - *.egslst



test.egslst - WordPad

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                        SUMMARY OF DOSE REGION RESULTS
                        ******************************

                                  Total # charged particle steps   1.302E+08 +/- 0.043%
                      # of charged particle steps/initial history   4.340E+01 +/- 0.043%
 # of presta-II steps/total # of charged particle steps              0.895 +/- 0.043%

                         # charged particle steps in dose reg.     1.302E+08 +/- 0.043%
                       # of steps in dose reg./initial history     4.340E+01 +/- 0.043%
                 # of presta-II steps/# of steps in dose reg.       0.895 +/- 0.043%

                        Z# : Geometrical zone number
                        P# : Planar zone number
                        C# : Cylindrical zone number
                         T  : Total dose (Gray/(incident fluence))
                        T-S: Total dose minus stoppers

  Z#  P#  C#          T                    T-S
 ---------------------------------------------------------------------
   2   1   1  3.4567E-12 +/- 1.568%  3.2033E-12 +/- 1.580%
   3   2   1  5.1478E-12 +/- 1.313%  4.7787E-12 +/- 1.322%
   4   3   1  5.0638E-12 +/- 1.312%  4.6957E-12 +/- 1.321%
   5   4   1  4.9970E-12 +/- 1.314%  4.6325E-12 +/- 1.323%
   6   5   1  5.1038E-12 +/- 1.310%  4.7299E-12 +/- 1.319%
   7   6   1  4.9057E-12 +/- 1.328%  4.5427E-12 +/- 1.337%
   8   7   1  4.9133E-12 +/- 1.328%  4.5505E-12 +/- 1.338%
   9   8   1  4.8468E-12 +/- 1.331%  4.4893E-12 +/- 1.341%
  10   9   1  4.8523E-12 +/- 1.331%  4.4938E-12 +/- 1.340%
  11  10   1  4.7977E-12 +/- 1.338%  4.4422E-12 +/- 1.348%
  12  11   1  4.7376E-12 +/- 1.350%  4.3823E-12 +/- 1.360%
  13  12   1  4.5229E-12 +/- 1.370%  4.1837E-12 +/- 1.381%
  14  13   1  4.6263E-12 +/- 1.357%  4.2831E-12 +/- 1.367%
  15  14   1  4.5830E-12 +/- 1.370%  4.2434E-12 +/- 1.380%
  16  15   1  4.5693E-12 +/- 1.370%  4.2305E-12 +/- 1.382%
  17  16   1  4.4753E-12 +/- 1.385%  4.1445E-12 +/- 1.396%
  18  17   1  4.3986E-12 +/- 1.390%  4.0725E-12 +/- 1.401%
  19  18   1  4.2873E-12 +/- 1.404%  3.9684E-12 +/- 1.415%
  20  19   1  4.2508E-12 +/- 1.409%  3.9307E-12 +/- 1.420%
  21  20   1  4.2053E-12 +/- 1.427%  3.8899E-12 +/- 1.439%
  22  21   1  4.0700E-12 +/- 1.443%  3.7655E-12 +/- 1.455%
  23  22   1  4.0901E-12 +/- 1.443%  3.7864E-12 +/- 1.454%
  24  23   1  4.0567E-12 +/- 1.442%  3.7548E-12 +/- 1.454%
  25  24   1  4.0048E-12 +/- 1.448%  3.7058E-12 +/- 1.460%
```

PEGS

- Preprocessor for EGS
- Medium definition is performed in PEGS
- Have to set AE og AP, in addition to UE og UP (upper limit for for electron- and photon energy)

PEGS