Topas Monte-Carlo modelling: Guide and simple techniques

Claus E. Andersen
Technical University of Denmark
Department of Health Technology
clan@dtu.dk
www.mrdc.dtu.dk

Created: January 3, 2023

Revised: January 25, 2023 + March 6, 2023

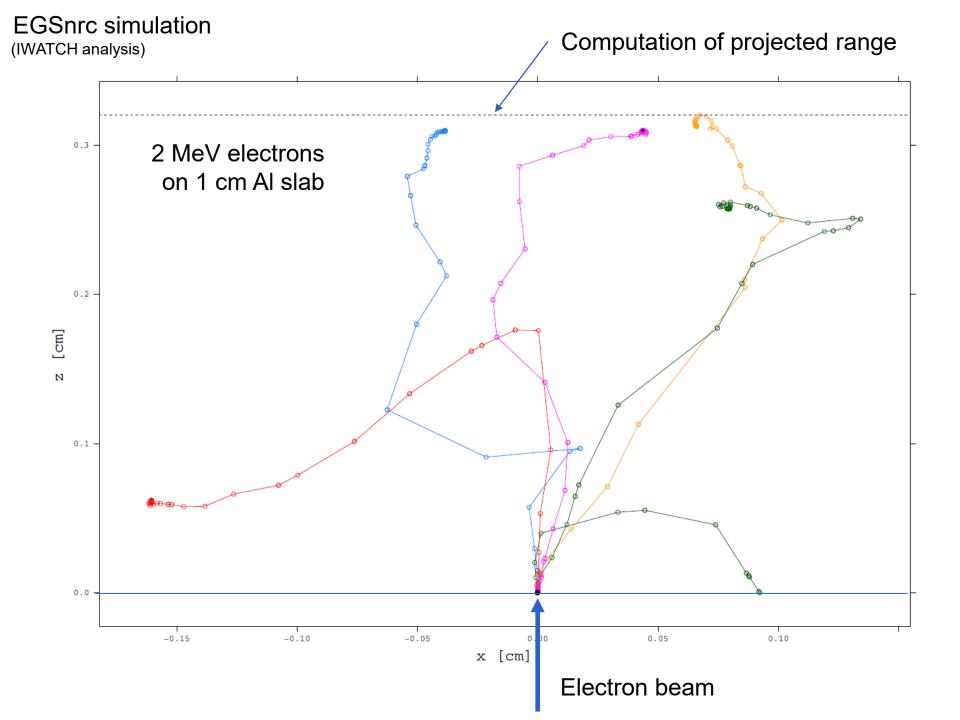


DTU Health Tech

IMPORTANT

Topas is a research tool.

It cannot be used directly for clinical work.



What types of sections do we have in Topas parameter files?

Topas Documentation, Release 3.8 by Topas MC Inc:

8.6.5 Quick Ways to Deactivate Parts of the Parameters Files

For most parameter categories, there is one key kind of parameter that triggers creation:

Parameter object type	Triggering pattern	
Element	El//Symbol =	
Material	Ma//Components =	
Component	Ge//Parent =	
Particle Source	So//Type =	
Physics setup	Ph//Type =	
Scorer	Sc//Quantity =	
Graphic	Gr//Type =	
Variance Reduction	Vr//Type =	
Time Feature	Tf//Function =	

How to refer to particle types in Topas?

Particle names used in parameter files

(e.g. for particle sources or filters)

```
gamma
e-
e+
neutron
proton
```

Main particle codes used in output

(defined by the Particle Data Group, PDG)

```
22 = photon

11 = electron

-11 = positron

2112 = neutron

2212 = proton
```

What processes do Topas know about?

What physics is applied?

Selection of physics lists

1. The default, built-in physics list is:

```
sv:Ph/Default/Modules 6 g4em-standard_opt4 g4h-phy_QGSP_BIC_HP g4decay g4ion-binarycascade g4h-elastic_HP g4stopping

This is what you get if, you do not specify anything.
```

2. Just electromagnetic interactions:

```
s:Ph/ListName = "MyList"
sv:Ph/MyList/Modules = 1 "g4em-standard_opt4"
```

To obtain extra accuracy, one can specify that even very low-energetic electrons should be produced and transported. The energy cut is specified as a range in the local material. For example:

```
d:Ph/MyList/CutForElectron = 0.001 mm  # High accuracy
d:Ph/MyList/CutForElectron = 10 mm  # Low accuracy
```

3. Hadronics, radioactive decay etc. :

```
s:Ph/ListName = "MyList2"
sv:Ph/MyList2/Modules = 7 "g4em-standard_opt4"
"g4h-phy_QGSP_BIC_HP" "g4decay" "g4ion-binarycascade"
"g4h-elastic HP" "g4stopping" "g4radioactivedecay"
```

Process names (examples)

These names can, e.g., be used by filters to score particles from processes.

Name	Description		
"annihil"	Annihilation		
"compt"	Compton		
"eBrem"	Bremsstrahlung produced by electron		
"Decay"	Decay (of sub-atomic particle)		
"eIoni"			
"hadElastic"	Hadronic elastic scattering		
"hIoni"			
"neutronInelastic"			
"nCapture"	Neutron capture		
"phot"	Photoelectric effect		
"primary"			
"protonInelastic"			
"RadioactiveDecayBase"	Radiation from radioactive decay		
"Rayl"	Rayleigh scattering (photons)		

To see what processes you have use: b:Ph/ListProcesses = "TRUE" and b:Ts/DumpParameters = "True"

Registered Physics Processes for "g4em-standard_opt4":

Transportation, StepLimiter, UserSpecialCut, phot, compt, conv, Rayl, msc, eIoni, eBrem, ePairProd, CoulombScat, annihil, muIoni, muBrems, muPairProd, hIoni, hBrems, hPairProd, ionIoni, nuclearStopping

Registered Physics Processes for the default built-in physics list (6 modules):

Transportation, StepLimiter, UserSpecialCut, phot, compt, conv, Rayl, msc, eIoni, eBrem, ePairProd, CoulombScat, annihil, muIoni, muBrems, muPairProd, hIoni, hBrems, hPairProd, ionIoni, nuclearStopping, neutronInelastic, nCapture, nFission, protonInelastic, pi+Inelastic, pi-Inelastic, kaon+Inelastic, kaon-Inelastic, kaon0LInelastic, kaon0SInelastic, lambdaInelasticanti-lambdaInelastic, sigma-Inelastic, anti sigma-Inelastic, sigma+Inelasticanti sigma+Inelastic, xi-Inelastic, anti xi-Inelastic, xi0Inelastic, anti xi0Inelastic, omega-Inelastic, anti omegaInelastic, anti protonInelastic, anti neutronInelastic, anti deuteronInelastic, anti tritonInelastic, anti He3Inelastic anti alphaInelastic, Decay, dInelastic, tInelastic, He3Inelastic, alphaInelastic, ionInelastic, hadElastichFritiofCaptureAtRest, hBertiniCaptureAtRest, muMinusCaptureAtRest

How to estimate the "statistical" uncertainty of a result?

Examples of what we can request Topas to report

Statistics for a scorer

```
sv:Sc/MyScorer/Report = 1 "Sum"
sv:Sc/MyScorer/Report = 4 "Count_In_Bin" "Sum" "Mean" "Standard_Deviation"
Histories, Count In Bin,
Sum, Mean,
Variance, Standard Deviation,
Second Moment,
Min, Max
Histories = total number of histories (N) that were simulated
Count In Bin = number of histories that contributed to the bin
                (i.e. excluding histories for which no particles hit this bin).
If we call
 Standard Deviation = SD
then
 u(mean) = SD/sqrt(N) = the statistical uncertainty of the mean value
```

u(sum) = u(mean * N) = u(mean) * N = SD/sqrt(N) * N = SD * sqrt(N)

Sample output and uncertainty statement

```
# TOPAS Version: 3.7
# Parameter File: sandbox-10011.txt
# Results for scorer clanScorer1
# Scored in component: centerrod
# X in 1 bin of 1 cm
# Y in 1 bin of 1 cm
# Z in 200 bins of 0.15 cm
# DoseToMedium (Gy): Count_in_Bin Sum Mean Standard_Deviation
0, 0, 0, 429, 1.478240250207818e-07, 1.478240269572828e-13, 9.802415598904964e-12
0, 0, 1, 403, 1.445507535891011e-07, 1.445507558951234e-13, 9.149940147400391e-12
...
0, 0, 5, 444, 1.635282558254403e-07, 1.635282491183899e-13, 1.000433808080876e-11
0, 0, 6, 449, 1.670288014565813e-07, 1.670288067970067e-13, 1.056387068426724e-11
```

Sum Mean Standard deviation

```
result. What is the statistical uncertainty? D = 1.670288067970067e-13 \text{ Gy} u(D) = 1.056387068426724e-11 \text{ Gy/sqrt(N)} = 1.1 \text{ E-14 Gy} So, we could write: D = (1.67 + / - 0.11) \text{ E-13 Gy (k=1)}
```

So, assume the mean dose for the z=6 voxel is our key

The uncertainty u(D) tells us how well we think we know the result D. The "k = 1" implies that the uncertaity is a standard uncertainy (i.e. expressed as one standard deviation).

Can I have more than one scorer in a file?

"Multiple scorers" mean "multiple files"

No, there can only be one scorer per output file.

It may therefore be useful to let the names of output files consist of two parts: (1) a first part common for the given parameter file, and (2) a second part which is specific for each scorer.

One can realize the "common part" by using the "message parameter" as shown below:

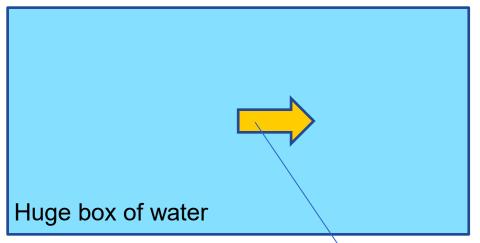
```
s:Ge/World/Message = "flatpanel-10002-"
s:Sc/clanScorer1/OutputFile = Ge/World/Message + "DoseScorer1"
s:Sc/clanScorer2/OutputFile = Ge/World/Message + "DoseScorer2"
s:Sc/clanScorer3/OutputFile = Ge/World/Message + "Phasespace1"
```

which produces output files:

```
flatpanel-10002-DoseScorer1 flatpanel-10002-DoseScorer2 flatpanel-10002-Phasespace1
```

Can Topas measure dose? Let's make a simple test.

Box of water.



All particle energy stays within the huge box of water, so we know the mean dose!

Internal source of 1 MeV particles emitted in the z-direction

Dimensions = $10 \text{ m} \times 10 \text{ m} \times 100 \text{ m}$ of water with density 1 g/cm^3

Score the dose in the box: Energy imparted divided by mass of box

Send off N = 80000 1 MeV particles. What will the mean dose in the box be if we assume that no primaries and secondaries escape the box?

$$D = \frac{80000 \cdot 10^{6} \cdot 1.60217649 \cdot 10^{-19} J}{10 \cdot 10 \cdot 100 \text{ m}^{3} \cdot 10^{3} \text{ kg/m}^{3}}$$

$$D = 1.28174119 \cdot 10^{-15} \text{ Gy} \qquad \rho = 1 \frac{g}{\text{cm}^3} = 10^3 \frac{\text{kg}}{\text{m}^3}$$

```
# The slab 1
s:Ge/clanSlab1/Type
                    = "TsBox"
s:Ge/clanSlab1/Material = "Water 75eV"
s:Ge/clanSlab1/Parent
                       = "World"
d:Ge/clanSlab1/HLX
                       = 5 m
d:Ge/clanSlab1/HLY = 5 m
d:Ge/clanSlab1/HLZ
                     = 50 \text{ m}
d:Ge/clanSlab1/TransX = 0. m
d:Ge/clanSlab1/TransY = 0. m
d:Ge/clanSlab1/TransZ = 0. mm
d:Ge/clanSlab1/RotX
                       = 0. deg
d:Ge/clanSlab1/RotY
                       = 0. deq
d:Ge/clanSlab1/RotZ
                       = 0. deq
```

```
# Beam position
s:Ge/clanBeamPosition/Parent = "clanslab1"
s:Ge/clanBeamPosition/Type = "Group"
d:Ge/clanBeamPosition/TransX = 0.0 m
d:Ge/clanBeamPosition/TransY = 0.0 m
d:Ge/clanBeamPosition/TransZ = 0.0 m
d:Ge/clanBeamPosition/RotX = 0.0 deg
d:Ge/clanBeamPosition/RotY = 0.0 deg
d:Ge/clanBeamPosition/RotZ = 0.0 deg
# Beam
s:So/clanBeam/Type
                                = "Beam"
s:So/clanBeam/Component
                                = "clanBeamPosition"
s:So/clanBeam/BeamParticle
                                = "e-"
d:So/clanBeam/BeamEnergy
                                = 1 \text{ MeV}
```

Particle	Energy	Dose [10 ⁻¹⁵ Gy]	Method	
Anything	1 MeV	1.28174119 (hand computation)	Analytical (reference)	
e-	1 MeV	1.28174116	Topas, OK	
gamma	1 MeV	1.28174116	Topas, OK	
proton	1 MeV	1.28174116	Topas, OK	
neutron	1 MeV	4.13712127	Topas, OK?	
neutron	1 eV	2.8540072	Topas	
neutron	1 MeV – 1 eV	1.28311	Difference (probably ok)	

Why did the test apparently fail for neutrons?

Topas measured a dose exceeding 2 MeV per particle even when the neutrons only had 1 eV kinetic energy! This must somehow be related to rest mass changes.

The difference between the dose from 1 eV neutrons and 1 MeV neutrons is about 1 MeV. This indicates that the excess energy is released by a process occurring already at thermal neutron energies.

Further investigation using the 4pi-detector (see later) reveals that thermal neutrons undergo **neutron capture with the emission of a prompt 2.22 MeV gamma**. We transform hydrogen to deuterium, and get heavy water! This explains the excess energy absorption. Deuterium is a stable isotope, so there is no activation. We do not get exactly 2.22 MeV in the computation as activation of oxygen can also happen (see next slide), albeit only with a low probability.

What else to consider with neutron modelling?

We need a physics list that handles hadronics. The Topas 3.9 default physics lists were used for these computations. If the physics list had been set to $g4em-standard_opt4$ (only electromagnetic interactions = em), for example, Topas would not have known how to transport neutrons and the neutron kinetic energy would be dumped on the spot.

Neutron activation of water?

Progress in Nuclear Energy 117 (2019) 10304

Contents lists available at ScienceDirect

Progress in Nuclear Energy

journal homepage: www.elsevier.com/locate/pnucene

Review

On the dose fields due to activated cooling water in nuclear facilities Andrej Žohar, Luka Snoj*

Note that the O-18 reactions are possible at thermal neutron energies

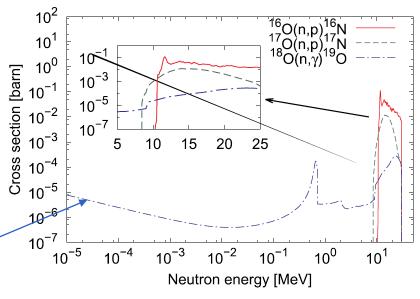


Fig. 1. Cross-section energy dependence for activation of oxygen nuclide taken from the JEFF-3.2 data library (OECD/NEA Data Bank, 2014).

... but it is not very likely

Isotope	Natural abundance [%]	Reaction	Activation product	$t_{1/2}$ [s]	Decay products
¹⁶ O	99.76	(n,p)	¹⁶ N	7.13	2.742 MeV gamma (1 %) 6.129 MeV gamma (67 %) 7.115 MeV gamma (5 %)
¹⁷ O	0.04	(n,p)	¹⁷ N	4.14	0.383 MeV neutron (35 %) 0.884 MeV neutron (1 %) 1.171 MeV neutron (53 %) 1.700 MeV neutron (7 %)
¹⁸ O	0.04	(n,γ)	¹⁹ O	26.9	0.110 MeV gamma (3 %) 0.197 MeV gamma (63 %) 1.357 MeV gamma (33 %) 1.444 MeV gamma (3 %)

How to apply filters to get results for certain particles etc. ?

or

How to find µ for monoenergetic photon beams?

or

What is a primary photon in Topas?

Filters for scorers

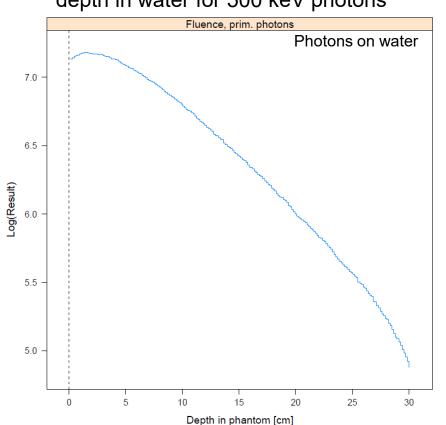
Filters for scorers Example

Fluence of primary photons

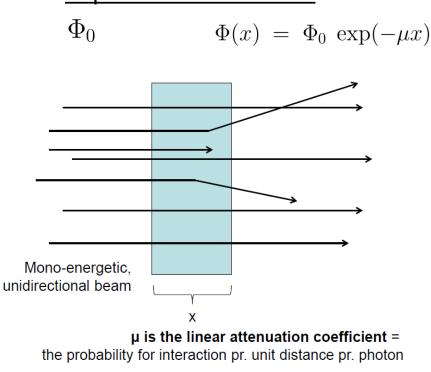
s:Sc/FluenceScorer3/Quantity = "Fluence"

sv:Sc/FluenceScorer3/OnlyIncludeParticlesNamed = 1 "gamma" s:Sc/FluenceScorer3/OnlyIncludeParticlesOfGeneration = "Primary"

Fluence of "Topas primary photons" vs. depth in water for 500 keV photons



Exponential attenuation



Q: Why is the fluence of primary photons **not** governed by exponential attenuation??

A: Because "primary photons" in Topas terminology is not what is primary in the normal sense that they have not undergone any form of interaction.

So, to get truely "primary" photons it is not enough to request Topas to give primaries.

Filters for scorers

Example

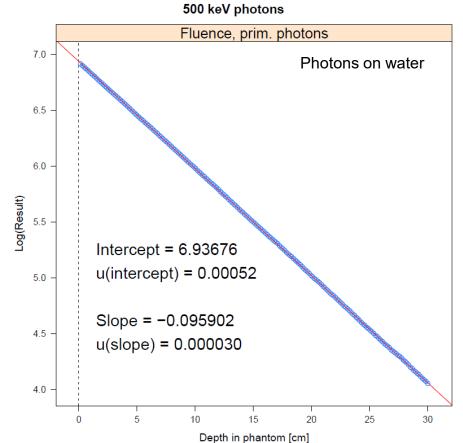
Fluence of primary photons

s:Sc/FluenceScorer3/Quantity = "Fluence"

sv:Sc/FluenceScorer3/OnlyIncludeParticlesNamed = 1 "gamma"

s:Sc/FluenceScorer3/OnlyIncludeParticlesOfGeneration = "Primary"

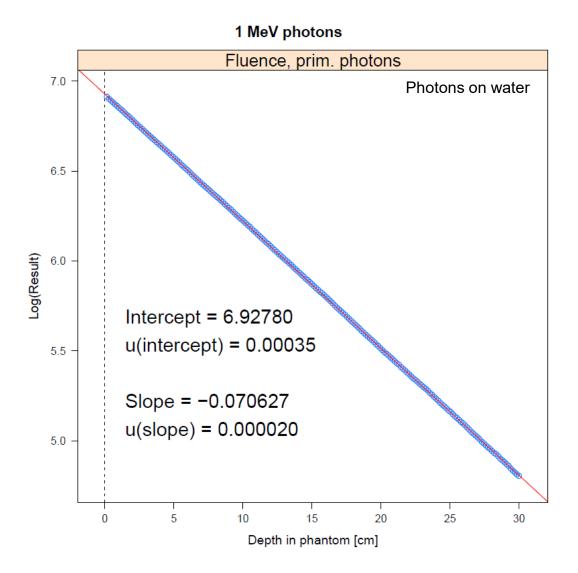
d:Sc/FluenceScorer3/OnlyIncludeIfIncidentParticleKEAbove = 0.495 MeV



We also filter by energy to get the "true" primaries only.

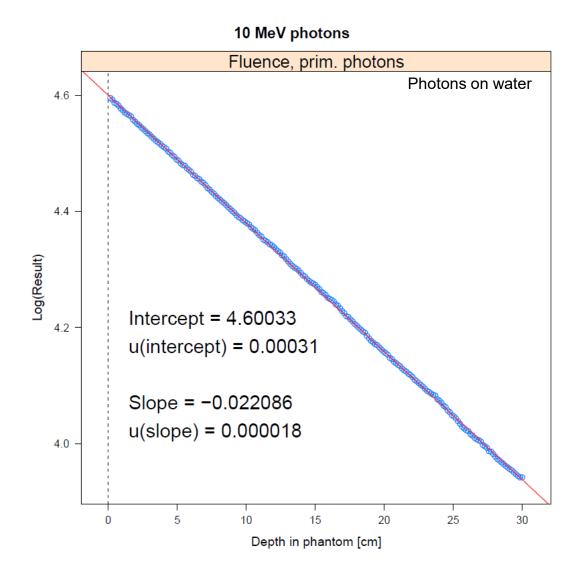
Now, we can confirm exponential attenuation. The mu for 500 keV photons is the negative slope of the semi-log regression: mu = 0.095902 1/cm which is in reasonable agreement with the 0.0966 1/cm given by Attix, Appendix D.

Filters for scorers Example



Good agreement with the 0.0706 1/cm given by Attix, Appendix D.

Filters for scorers Example



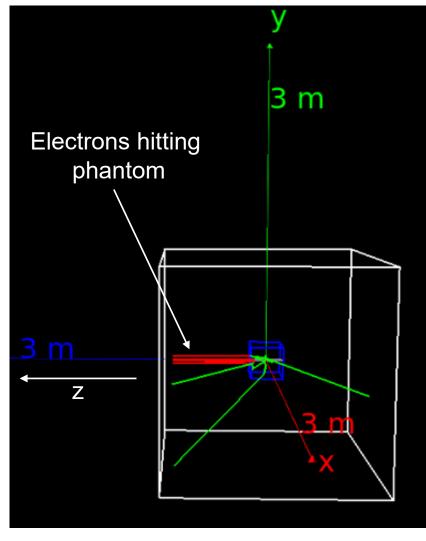
Good agreement with the 0.0222 1/cm given by Attix, Appendix D.

In what direction does the particle source shoot?

Meaning of TransZ and RotX for source components

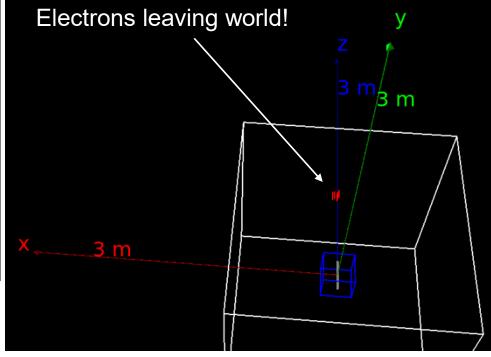
```
# Beam position, With RotX = 180 \text{ deg},
the beam will be in the negative z-axis direction
s:Ge/clanBeamPosition/Parent = "World"
s:Ge/clanBeamPosition/Type = "Group"
d:Ge/clanBeamPosition/TransX = 0. m
                                                      Note the unit
d:Ge/clanBeamPosition/TransY = 0. m
d:Ge/clanBeamPosition/TransZ = 0.9 * Ge/World/HLZ m
d:Ge/clanBeamPosition/RotX = 180. deg
                                            Rotate with x-axis
d:Ge/clanBeamPosition/RotY = 0. deg
                                            as normal vector
d:Ge/clanBeamPosition/RotZ = 0. deg
# Beam
s:So/clanBeam/Type
                                = "Beam"
s:So/clanBeam/Component
                                = "clanBeamPosition"
s:So/clanBeam/BeamParticle
                                = "e-"
d:So/clanBeam/BeamEnergy
                                = 10 MeV
```

Case 1 (ok)
d:Ge/BeamPosition/RotX = 180. deg
Shooting in negative z-direction

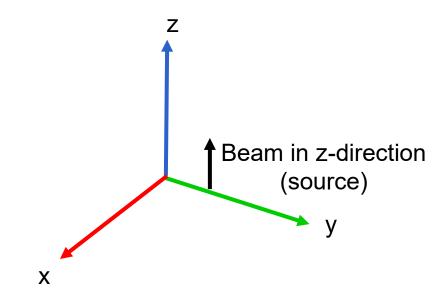


White box = world Source is at $z = 0.9 \times HLZ$ for world

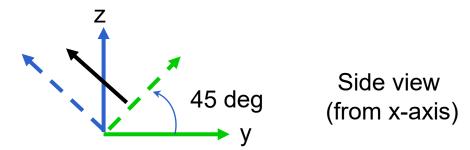
Case 2 (not ok)
d:Ge/BeamPosition/RotX = 0. deg
Shooting in positive z-direction.
Since the source is a bit from
the world edge, we see small
traces of the beam particles
before they leave.



Meaning of RotX = 45.0 deg?



Rotate source 45 deg around the x-axis (i.e. the x-axis as normal vector and then rotate 45 deg following the right-hand-rule).



Rotated beam xrot = 45 deg (still perpendicular with x-axis).

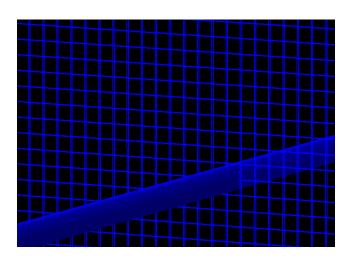
Rotating source RotX = 180 deg means that the source emits in the negative z-direction.

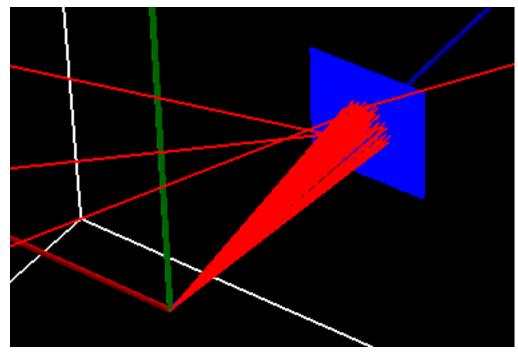
Beam shape parameters

Scoring beam intensity using a 40 cm x 40 cm "flatpanel detector" 1 m from the source

```
# The flatpanel (40 x 40 resoltion)
s:Ge/flatpanel/Type
                         = "TsBox"
s:Ge/flatpanel/Material = "Water 75eV"
s:Ge/flatpanel/Parent
                         = "World"
d:Ge/flatpanel/HLX
                         = 20 \text{ cm}
d:Ge/flatpanel/HLY
                         = 20 \text{ cm}
d:Ge/flatpanel/HLZ
                         = 1 \text{ mm}
d:Ge/flatpanel/TransX
                        = 0. m
                         = 0. m
d:Ge/flatpanel/TransY
d:Ge/flatpanel/TransZ
                         = 1. m
d:Ge/flatpanel/RotX
                         = 0. deq
d:Ge/flatpanel/RotY
                         = 0. deg
d:Ge/flatpanel/RotZ
                         = 0. deg
                         = "blue"
s:Ge/flatpanel/color
i:Ge/flatpanel/XBins = 40
i:Ge/flatpanel/YBins = 40
```

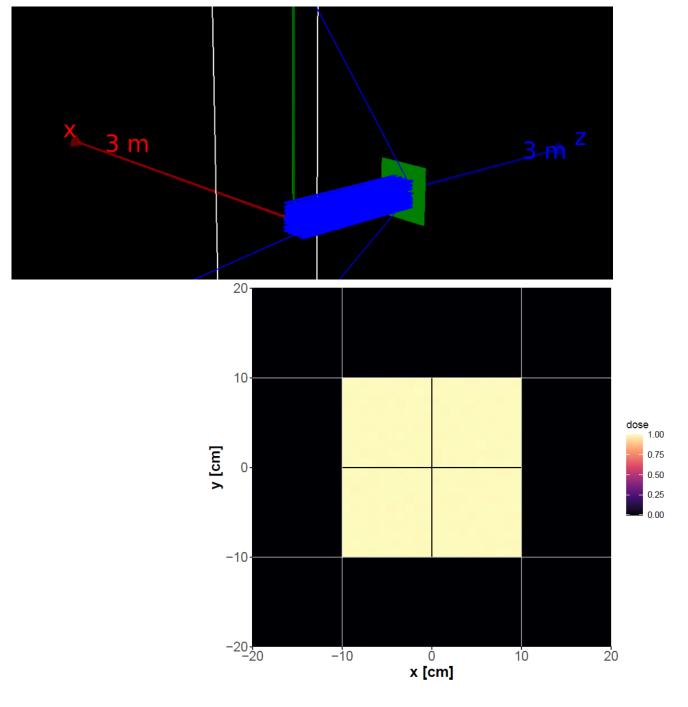
The "flatpanel" scorer will give a 40 x 40 = 1600 (voxels) array of dose values.



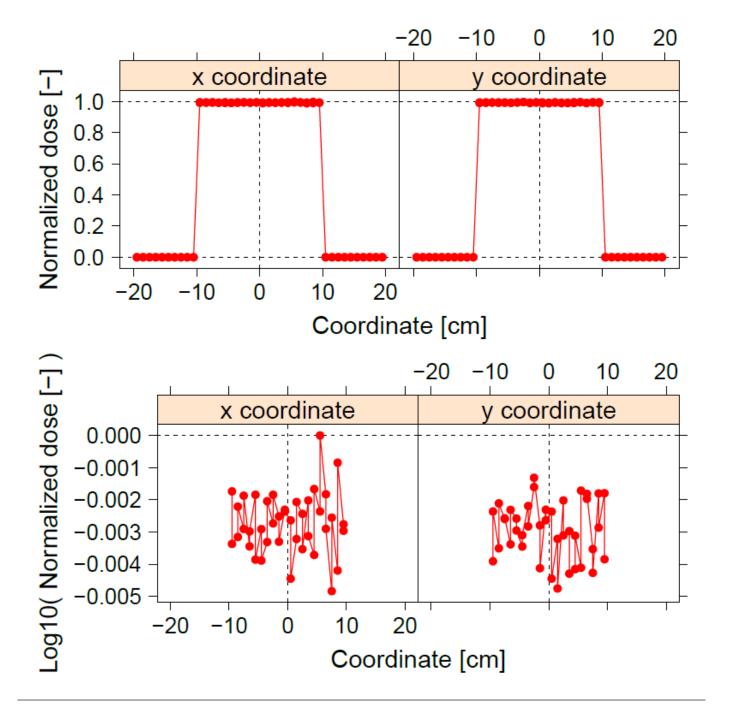


```
s:So/clanBeam/BeamPositionDistribution = "Flat"
# Flat or Gaussian
s:So/clanBeam/BeamPositionCutoffShape = "Rectangle"
# Ellipse, Rectangle
d:So/clanBeam/BeamPositionCutoffX = 100.0 mm
d:So/clanBeam/BeamPositionCutoffY = 100.0 mm
d:So/clanBeam/BeamPositionSpreadX = 0.0 mm
d:So/clanBeam/BeamPositionSpreadY = 0.0 mm
s:So/clanBeam/BeamAngularDistribution = "None"
d:So/clanBeam/BeamAngularCutoffX = 0.0 deg
d:So/clanBeam/BeamAngularCutoffY = 0.0 deg
d:So/clanBeam/BeamAngularSpreadX = 0.0 deg
d:So/clanBeam/BeamAngularSpreadY = 0.0 deg
```

Case 1

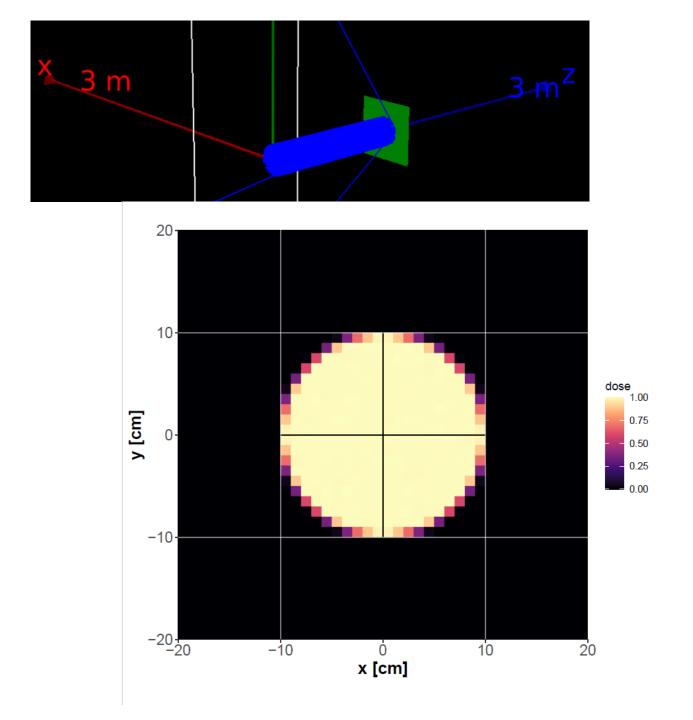


Case 1

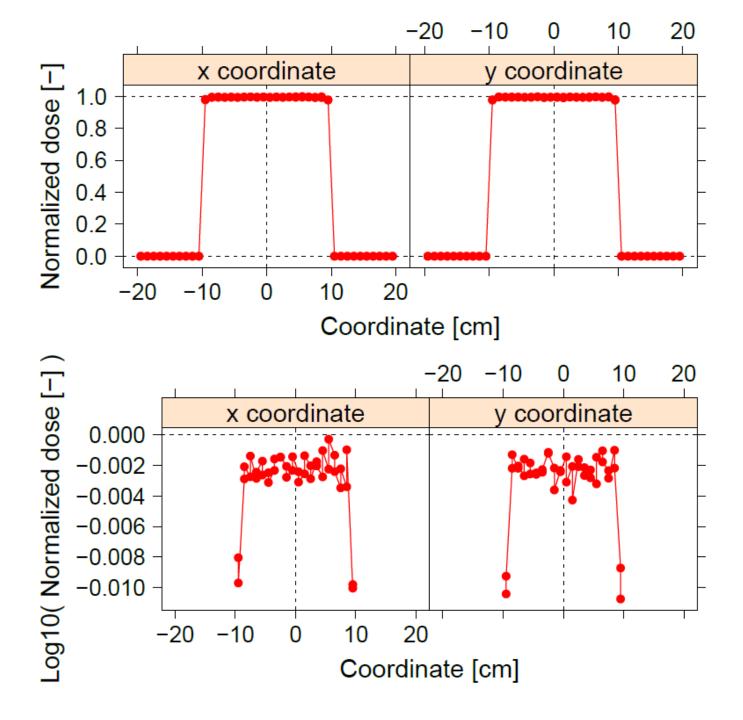


```
s:So/clanBeam/BeamPositionDistribution = "Flat"
# Flat or Gaussian
s:So/clanBeam/BeamPositionCutoffShape = "Ellipse"
# Ellipse, Rectangle
d:So/clanBeam/BeamPositionCutoffX = 100.0 mm
d:So/clanBeam/BeamPositionCutoffY = 100.0 mm
d:So/clanBeam/BeamPositionSpreadX = 0.0 mm
d:So/clanBeam/BeamPositionSpreadY = 0.0 mm
s:So/clanBeam/BeamAngularDistribution = "None"
d:So/clanBeam/BeamAngularCutoffX = 0.0 deg
d:So/clanBeam/BeamAngularCutoffY = 0.0 deg
d:So/clanBeam/BeamAngularSpreadX = 0.0 deg
d:So/clanBeam/BeamAngularSpreadY = 0.0 deg
```

Case 2



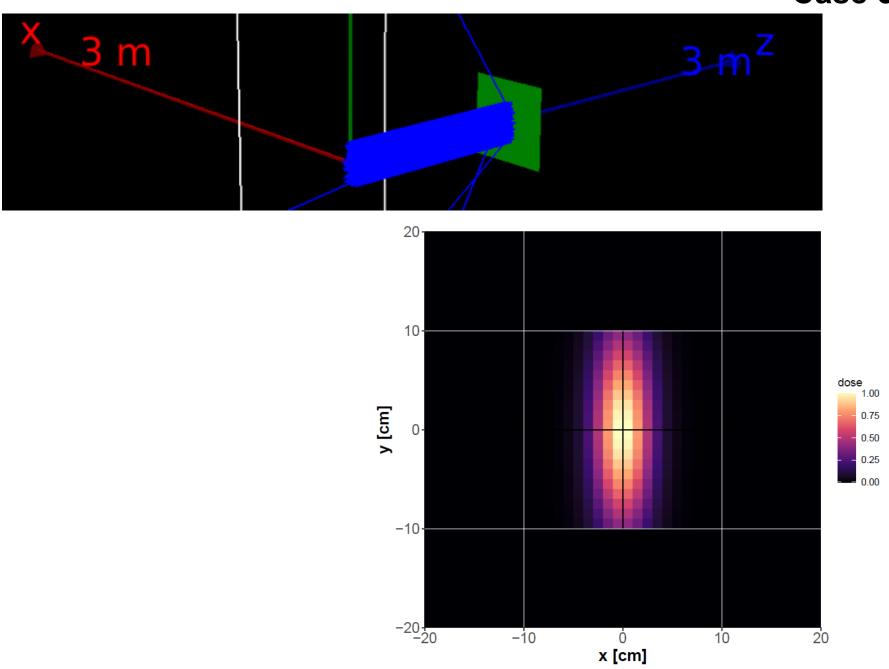
Case 2

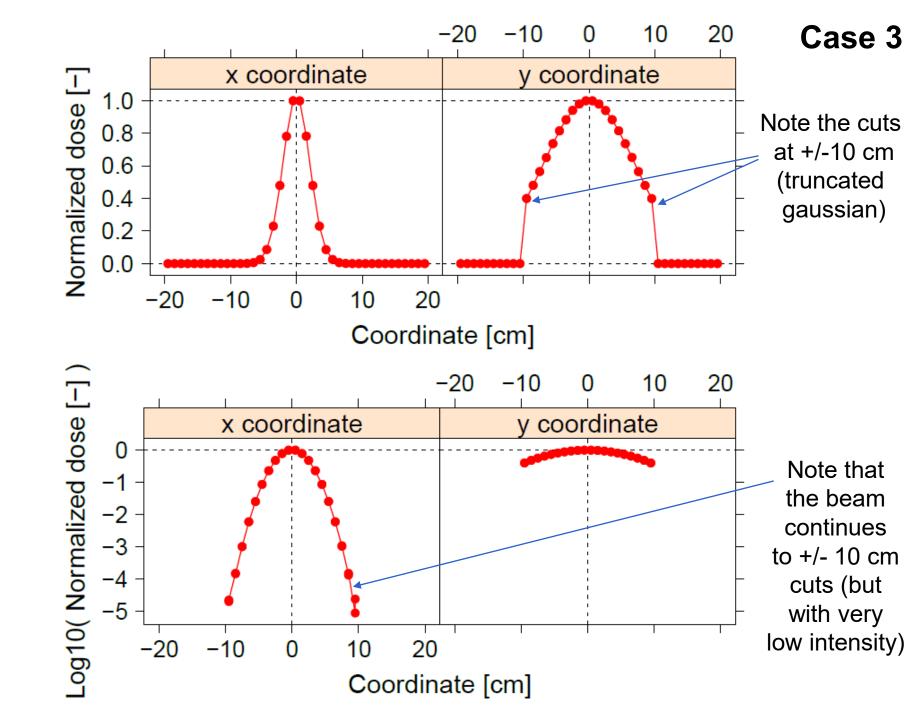


NOTE: Beam intensity described by gaussian parameters

```
s:So/clanBeam/BeamPositionDistribution = "Gaussian"
# Flat or Gaussian
s:So/clanBeam/BeamPositionCutoffShape = "Rectangle"
# Ellipse, Rectangle
d:So/clanBeam/BeamPositionCutoffX = 100.0 mm
d:So/clanBeam/BeamPositionCutoffY = 100.0 mm
d:So/clanBeam/BeamPositionSpreadX = 20.0 mm
d:So/clanBeam/BeamPositionSpreadY = 70.0 mm
s:So/clanBeam/BeamAngularDistribution = "None"
d:So/clanBeam/BeamAngularCutoffX = 0.0 deg
d:So/clanBeam/BeamAngularCutoffY = 0.0 deg
d:So/clanBeam/BeamAngularSpreadX = 0.0 deg
d:So/clanBeam/BeamAngularSpreadY = 0.0 deg
```

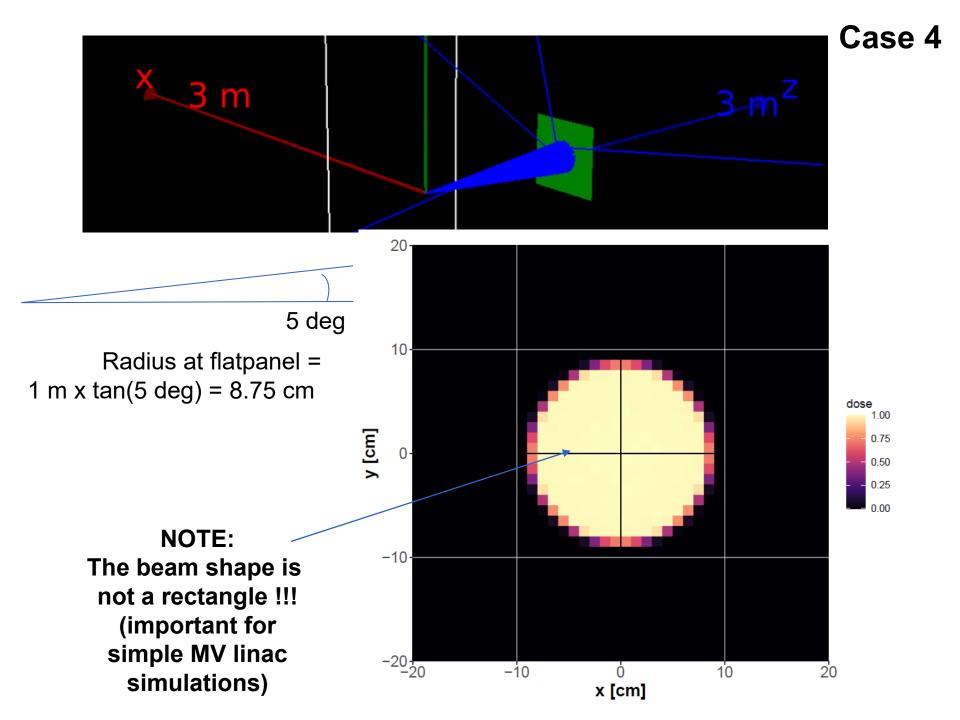
Case 3



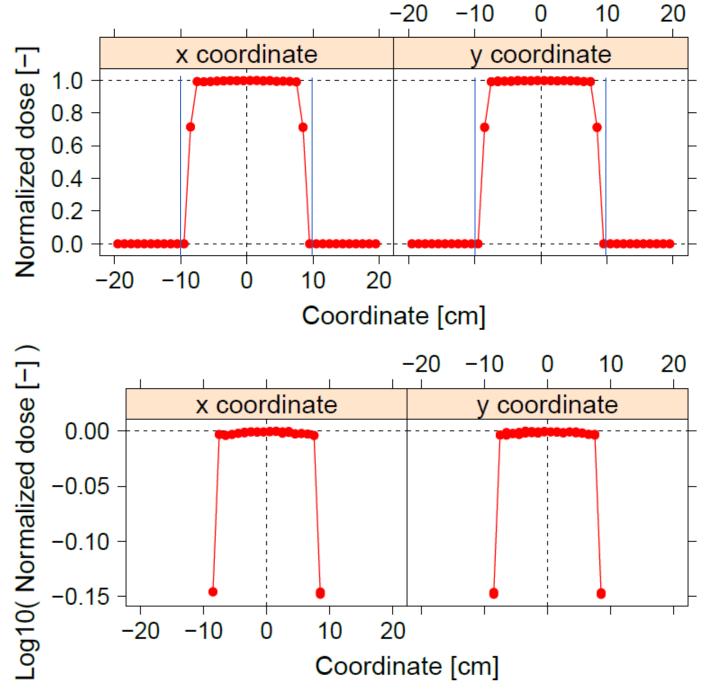


NOTE: Diverting point source

```
s:So/clanBeam/BeamPositionDistribution = "Flat"
# Flat or Gaussian
s:So/clanBeam/BeamPositionCutoffShape = "Rectangle"
# Ellipse, Rectangle
d:So/clanBeam/BeamPositionCutoffX = 0.000001 mm
d:So/clanBeam/BeamPositionCutoffY = 0.000001 mm
d:So/clanBeam/BeamPositionSpreadX = 0.0 mm
d:So/clanBeam/BeamPositionSpreadY = 0.0 mm
s:So/clanBeam/BeamAngularDistribution = "Flat"
d:So/clanBeam/BeamAngularCutoffX = 5.0 deg
d:So/clanBeam/BeamAngularCutoffY = 5.0 deg
d:So/clanBeam/BeamAngularSpreadX = 0.0 deg
d:So/clanBeam/BeamAngularSpreadY = 0.0 deg
```

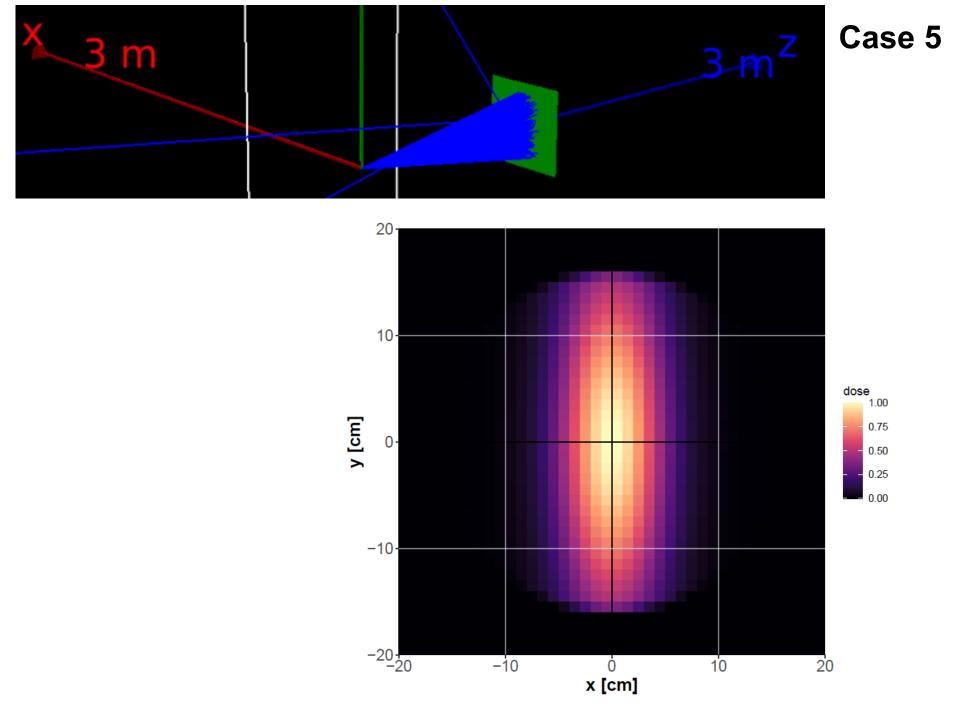


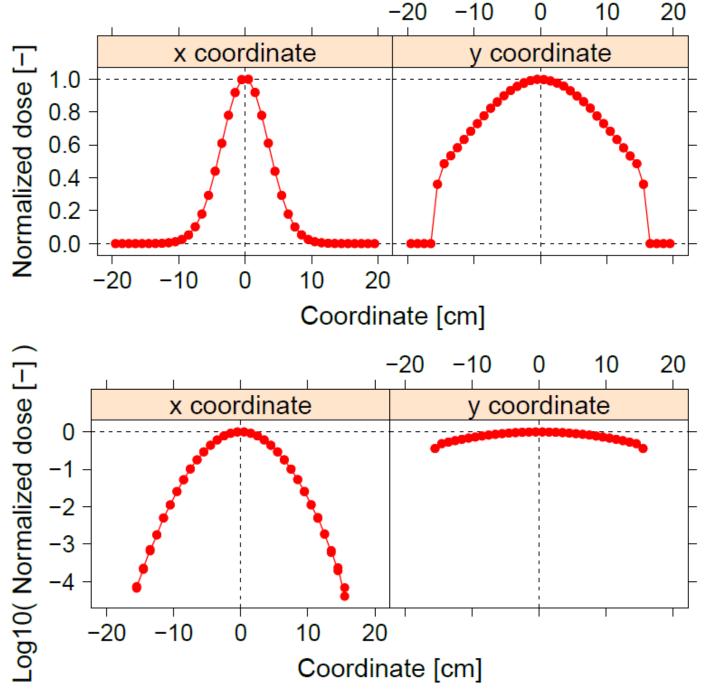
Case 4



NOTE: Diverting point source

```
s:So/clanBeam/BeamPositionDistribution = "Flat"
# Flat or Gaussian
s:So/clanBeam/BeamPositionCutoffShape = "Rectangle"
# Ellipse, Rectangle
d:So/clanBeam/BeamPositionCutoffX = 0.000001 mm
d:So/clanBeam/BeamPositionCutoffY = 0.000001 mm
d:So/clanBeam/BeamPositionSpreadX = 0.0 mm
d:So/clanBeam/BeamPositionSpreadY = 0.0 mm
s:So/clanBeam/BeamAngularDistribution = "Gaussian"
d:So/clanBeam/BeamAngularCutoffX = 9.0 deg
d:So/clanBeam/BeamAngularCutoffY = 9.0 deg
d:So/clanBeam/BeamAngularSpreadX = 2.0 deg
d:So/clanBeam/BeamAngularSpreadY = 7.0 deg
```

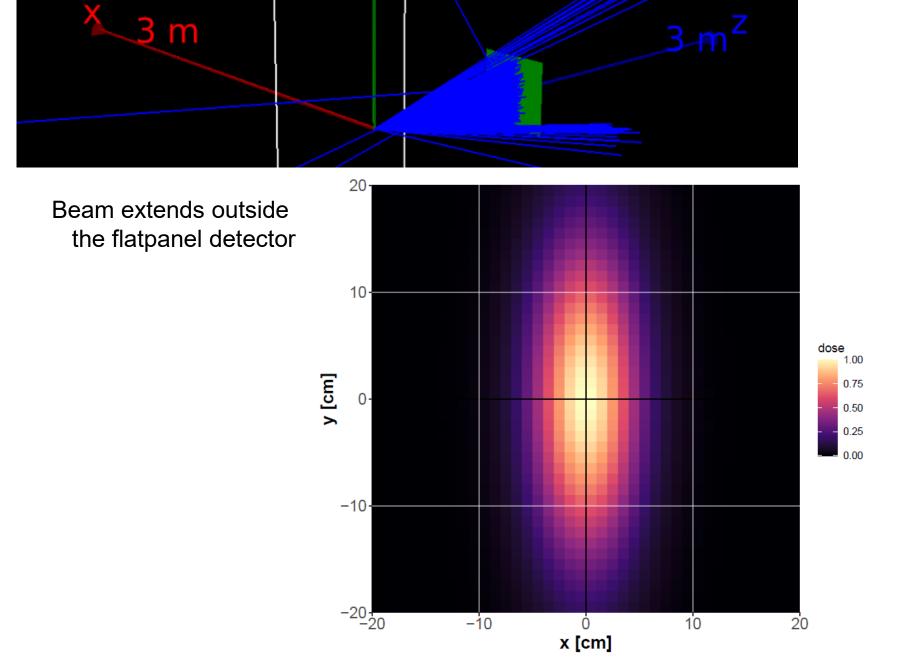




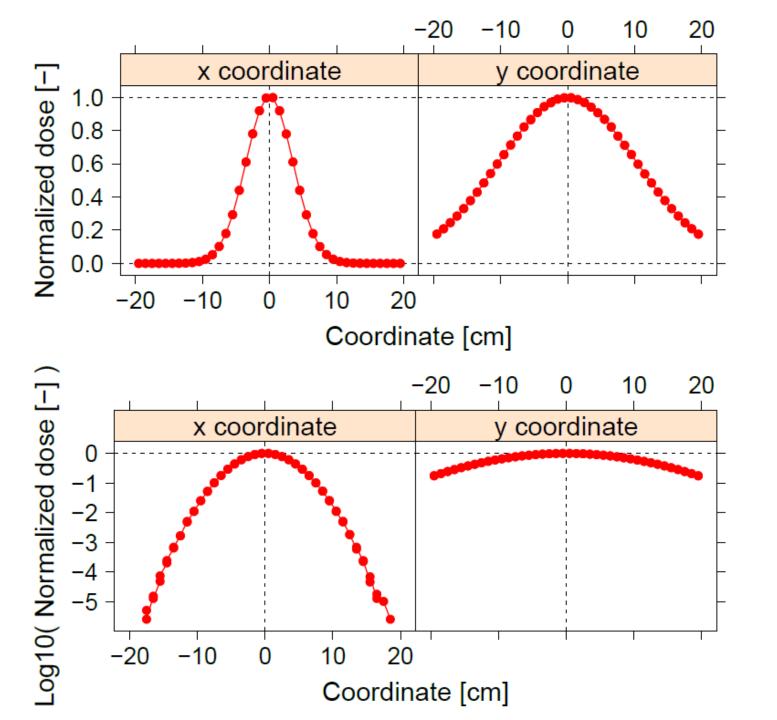
NOTE: Diverting point source

```
s:So/clanBeam/BeamPositionDistribution = "Flat"
# Flat or Gaussian
s:So/clanBeam/BeamPositionCutoffShape = "Rectangle"
# Ellipse, Rectangle
d:So/clanBeam/BeamPositionCutoffX = 0.000001 mm
d:So/clanBeam/BeamPositionCutoffY = 0.000001 mm
d:So/clanBeam/BeamPositionSpreadX = 0.0 mm
d:So/clanBeam/BeamPositionSpreadY = 0.0 mm
s:So/clanBeam/BeamAngularDistribution = "Gaussian"
d:So/clanBeam/BeamAngularCutoffX = 100.0 deg
d:So/clanBeam/BeamAngularCutoffY = 100.0 deg
                                                 Now, essentially
d:So/clanBeam/BeamAngularSpreadX = 2.0 deg
                                                 no truncation
d:So/clanBeam/BeamAngularSpreadY = 6.0 deg
                                                of beam.
```

Case 6



Case 6



Welcome to "parallel worlds"!

You can now score with different resolutions and across components.

Wunderful !!!

How to score multiple quantities in a component using different resolutions?

Answer: Use a parallel-world component without mass or material:

```
# Flatpanel2 (10 x 10 resolution)
b:Ge/flatpanel2/IsParallel = "True"
s:Ge/flatpanel2/Type = "TsBox"
s:Ge/flatpanel2/Parent = "World"
d:Ge/flatpanel2/HLX = 20 cm
d:Ge/flatpanel2/HLY = 20 cm
d:Ge/flatpanel2/HLZ = 1 mm
d:Ge/flatpanel2/TransX = 0. m
d:Ge/flatpanel2/TransY = 0. m
d:Ge/flatpanel2/TransZ = 1. m
d:Ge/flatpanel2/RotX = 0. deg
d:Ge/flatpanel2/RotY = 0. deg
d:Ge/flatpanel2/RotZ = 0. deg
s:Ge/flatpanel2/color = "blue"
i:Ge/flatpanel2/XBins = 10
                                  (The "real-world" flatpanel has
i:Ge/flatpanel2/YBins = 10
                                  40 x 40 resolution)
```

When we make a scorer, we just refer to this "parallel world" componet:

```
s:Sc/SomeScorerName/Component = "flatpanel2"
```

How about time-of-flight?

What is phase-space scoring?

How to score time of flight of particles?

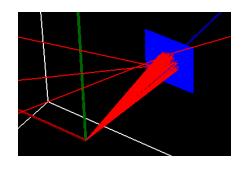
Answer: One possibility is to use a phasespace scorer.

```
s:Sc/clanScorer3/Quantity = "Phasespace"
s:Sc/clanScorer3/Surface= "flatpanel/ZMinusSurface"
b:Sc/clanScorer3/IncludeTimeOfFlight = "True"
b:Sc/clanScorer3/IncludeRunID = "True"
b:Sc/clanScorer3/IncludeEventID = "True"
b:Sc/clanScorer3/IncludeTrackID = "True"
b:Sc/clanScorer3/IncludeParentID = "True"
  # Track ID of parent particle
b:Sc/clanScorer3/IncludeCharge = "True"
b:Sc/clanScorer3/IncludeCreatorProcess = "True"
b:Sc/clanScorer3/IncludeVertexInfo = "True"
  # Initial KE, Position and Momentum
b:Sc/clanScorer3/IncludeSeed = "True"
s:Sc/clanScorer3/OutputType = "ASCII"
b:Sc/clanScorer3/PropagateToChildren = "True"
s:Sc/clanScorer3/Component = "flatpanel2"
s:Sc/clanScorer3/IfOutputFileAlreadyExists = "Overwrite"
b:Sc/clanScorer3/OutputToConsole = "False"
s:Sc/clanScorer3/OutputFile = Ge/World/Message + "Phasespace1"
```

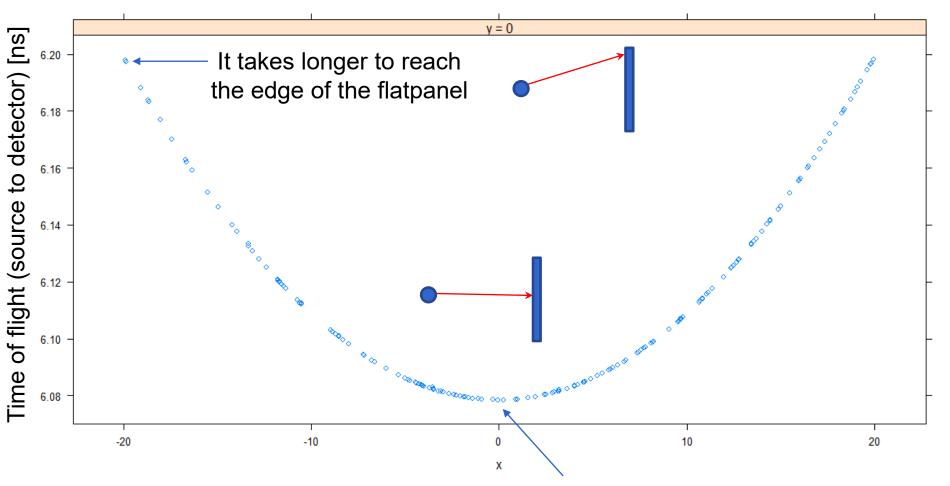
Phasespace file with 28 columns: #1: Position X [cm] #2: Position Y [cm] #3: Position Z [cm] #4: Direction Cosine X #5: Direction Cosine Y #6: Energy [MeV] #7: Weight #8: Particle Type (in PDG Format) #9: Flag to tell if Third Direction Cosine is Negative (1 means true) #10: Flag to tell if this is the First Scored Particle from this History (1 means true) #11: Time of Flight [ns] #12: Run ID #13: Event ID #14: Track ID #15: Parent ID #16: Charge [e+] #17: Creator Process Name #18: Initial Kinetic Energy [MeV] #19: Vertex Position X [cm] #20: Vertex Position Y [cm] #21: Vertex Position Z [cm] #22: Initial Direction Cosine X #23: Initial Direction Cosine Y #24: Initial Direction Cosine Z #25: Seed Part 1 #26: Seed Part 2 #27: Seed Part 3 #28: Seed Part 4

Point source with 15 deg angle (not 5 deg as in the picture)

1m / 6.08 ns = 1.64E8 m/s (approx. 50% speed of light)



Time of flight in ns for point source of 100 keV electrons vs. flatpanel x coordinate at y = 0



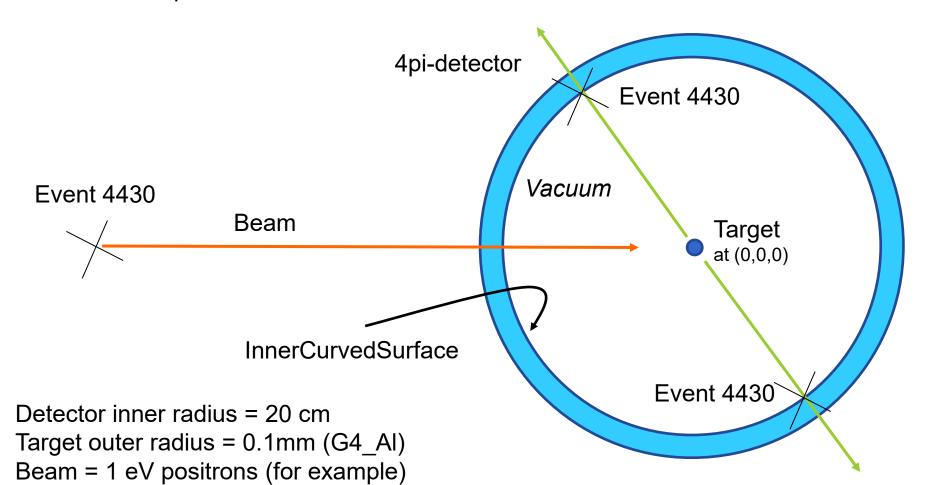
Shorest distance (center of flatpanel) is the fastest.

More about phase-space scoring

Using 4pi detector and phase space scoring

Each particle history from the beam source is associated with an event id. These are unique within each run.

The phasespace scorer can give us detailed information about the recorded hits, for example, at the inner curved surface of the detector.



Results from phasespace scorer in 4pi detector

Beam = positrons, target = Al

Run event												
id	x	Y	z	MeV Part	icle Creater	MeV.sum						
				type	process							
					name							
Shooting 1 eV positrons into target:												
0-0	1.2537300	-5.880420 -19	.07480000	0.510999 22	2 annihil	1.021998						
0-0	-1.2537300	5.880420 19	.07480000	0.510999 22	2 annihil	1.021998						
0-1	6.4156800	-13.075500 13	.70660000	0.510999 22	2 annihil	1.021998						
0-1	-6.4156800	13.075500 -13	.70660000	0.510999 22	2 annihil	1.021998						
0-2	18.1159000	8.357020 1	.40523000	0.510999 22	2 annihil	1.021998						
02	-18.1159000	-8.357020 -1	.40523000	0.510999 22	2 annihil	1.021998						
<i>†</i>	†											
Run 0, e	Run 0, event 2											

Note the perfect symmetry around (0,0,0). These annihilations are perfect back-to-back gammas.

Note, as an example, that the distance from (x,y,z) to (0,0,0):

 $((-18.1159000 \text{ cm})^2 + (-8.357020 \text{ cm})^2 + (-1.40523000 \text{ cm})^2)^0.5 = 20.000 \text{ cm}$ which verifies that these points are actually located on the detector sphere.

Note that the sum of energy for particles hitting the detector is always 1.021998 MeV.

Results from phasespace scorer in 4pi detector

Beam = positrons, target = Al

```
Run event
id
                                           MeV Particle Creater MeV.sum
                       У
             X
                                               type
                                                        proce
Shooting 1 MeV positrons into target:
0-412 \quad -5.4949400
                   7.855230 17.552800 1.2307200
                                                  22
                                                         annihil 2.017131
0-412 9.0652200 -15.725900
                            8.397520 0.7864110
                                                  2.2
                                                         annihil 2.017131
0-882 -3.8491100
                  -7.544530
                             18.118100 1.3963700
                                                  22
                                                         annihil 2.006963
                  18.521900
0-882 -7.3570100
                              1.677870 0.6105930
                                                  2.2
                                                         annihil 2.006963
0-1882 1.3758200 3.614410
                              19.622500 1.5717700 22
                                                         annihil 2.005375
0-1882 -1.6320100 -18.778200
                                                         annihil 2.005375
                              -6.686900 0.4336050 22
```

Note that the sum of energy hitting the detector pr. event (MeV.sum) is now variable and always less than 2.021998 MeV. Why?

Answer: The positron loses a variable amount of energy in the target before annihilation. The secondaries from these interactions stay in the target and the secondaries are therefore not captured by the detector.

Note that the annihilation photons are not back-to-back in the frame of the laboratory coordinate system (lack of symmetry around (0,0,0)).

Results from phasespace scorer in 4pi detector

Beam = positrons, target = Al

Shooting 1 eV positrons into target. Events with 3 detector hits:

Run event id	x	У	z	MeV I	MeV Partio type	cle	Creater process name	MeV sum
0-115 0-115 0-115	-1.54866000 -3.19828000 2.51310000	-19.569600		0.5109990	0.2348890	22	annihil	
0-452 0-452 0-452	8.47510000 -3.49529000 -3.91598000	-18.041100		0.5109990	0.3317510	22	annihil	1.00087
0-947 0-947 0-947	18.88940000 -16.03400000 13.90580000	-5.398080 3.532880 3.755140		0.3074050		11	compt	0.95168

Note that the annihilation photons that underwent Compton scattering are classified as annihilation photons. Only the electrons from the Compton interactions, are classified as being created by the Compton.

Phasespace scorer in 4pi detector

Topas parameters

The 4pi-detector

```
s:Ge/detector/Type
                       = "TsSphere"
s:Ge/detector/Material = "G4 Galactic"
                       = "World"
s:Ge/detector/Parent
d:Ge/detector/RMin
                       = 20.0 \text{ cm}
d:Ge/detector/RMax = 20.1 cm
d:Ge/detector/TransX = 0. m
d:Ge/detector/TransY = 0. m
d:Ge/detector/TransZ
                     = 0. m
d:Ge/detector/RotX
                       = 0. deq
d:Ge/detector/RotY
                       = 0. deq
d:Ge/detector/RotZ
                       = 0. deg
s:Ge/detector/color
                       = "blue"
```

The target

```
s:Ge/target/Type
                      = "TsSphere"
s:Ge/target/Material = "G4 Al"
s:Ge/target/Parent
                      = "world"
d:Ge/target/RMax
                      = 0.01 \text{ cm}
d:Ge/target/TransX
                      = 0. m
d:Ge/target/TransY
                      = 0. m
d:Ge/target/TransZ
                      = 0. m
d:Ge/target/RotX
                      = 0. deq
d:Ge/target/RotY
                      = 0. deg
d:Ge/target/RotZ
                      = 0. deq
s:Ge/target/color
                      = "blue"
```

Phasespace scorer in 4pi detector

Topas parameters

Beam

```
s:So/clanBeam/Type
                              = "Beam"
s:So/clanBeam/Component
                              = "clanBeamPosition"
s:So/clanBeam/BeamParticle
d:So/clanBeam/BeamEnergy
                              = 1 eV
u:So/clanBeam/BeamEnergySpread = 0.0
s:So/clanBeam/BeamPositionDistribution = "Flat"
s:So/clanBeam/BeamPositionCutoffShape = "Rectangle"
dc:So/clanBeam/BeamPositionCutoffX = 0.000001 mm
dc:So/clanBeam/BeamPositionCutoffY = 0.000001 mm
dc:So/clanBeam/BeamPositionSpreadX = 0.000001 mm
dc:So/clanBeam/BeamPositionSpreadY = 0.000001 mm
s:So/clanBeam/BeamAngularDistribution = "Flat"
dc:So/clanBeam/BeamAngularCutoffX = 0.000001 deg
dc:So/clanBeam/BeamAngularCutoffY = 0.000001 deg
dc:So/clanBeam/BeamAngularSpreadX = 0.000001 deg
dc:So/clanBeam/BeamAngularSpreadY = 0.000001 deg
i:So/clanBeam/NumberOfHistoriesInRandomJob = 0
```

Phasespace scorer in 4pi detector

Topas parameters

```
# Phasespace scorer
s:Sc/clanScorer3/Quantity = "Phasespace"
s:Sc/clanScorer3/Component = "detector"
s:Sc/clanScorer3/Surface = "detector/InnerCurvedSurface"
s:Sc/clanScorer3/OnlyIncludeParticlesGoing = "In"
b:Sc/clanScorer3/IncludeTimeOfFlight = "True"
b:Sc/clanScorer3/IncludeRunID
                                     = "True"
b:Sc/clanScorer3/IncludeEventID
                                      = "True"
b:Sc/clanScorer3/IncludeTrackID
                                       = "True"
b:Sc/clanScorer3/IncludeParentID
                                       = "True"
b:Sc/clanScorer3/IncludeCharge
                                       = "True"
b:Sc/clanScorer3/IncludeCreatorProcess = "True"
b:Sc/clanScorer3/IncludeVertexInfo
                                       = "True"
b:Sc/clanScorer3/IncludeSeed
                                       = "True"
s:Sc/clanScorer3/OutputType = "ASCII"
b:Sc/clanScorer3/PropagateToChildren = "True"
s:Sc/clanScorer3/IfOutputFileAlreadyExists = "Overwrite"
b:Sc/clanScorer3/OutputToConsole = "False"
s:Sc/clanScorer3/OutputFile = Ge/World/Message + "Phasespace1"
```

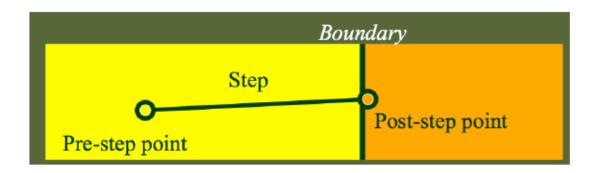
GEANT4 terminology

- Events are the basic units of a simulation (G4Event)
- At the beginning of an event, primary tracks are generated and stored in a stack
- The track is a snapshot of a particle, and it keeps its current information: energy, momentum, etc.
- GEANT4 gets a track from the stack and follows it in the geometry, until it exits the world or stops
 - If secondary tracks are produced in this process, they are also stored in the stack
 - When the stack is empty the event is completed
 - A run is a collection of events all with the same detector setup and physics settings

From: 1st LIP Introductory Course on GEANT4, Feb. 2020, Universidade do Minho

GEANT4 terminology

- Tracks are divided in steps
- A new step occurs every time the particle crosses a border or has an interaction
- A step has two points (pre-step and post-step) and G4Step stores information about both and the deltas (e.g. energy loss in the step)
- If a step is limited by a volume boundary, the post-step point is physically at the border, and associated with the next logical volume



From: 1st LIP Introductory Course on GEANT4, Feb. 2020, Universidade do Minho

How to score a fluence spectrum differential in energy?

Fluence spectra scoring

Unless you score the fluence in vacuum, you normally need to select the "PreStep" energy for binning:

```
i:Sc/MyScorer/EBins = 10
# defaults to 1, that is, un-binned

d:Sc/MyScorer/EBinMin = 0. MeV
# defaults to zero

d:Sc/MyScorer/EBinMax = 100. MeV
# must be specified if EBins is greater than 1

s:Sc/MyScorer/EBinEnergy = "PreStep"
# "IncidentTrack" # "IncidentTrack", "PreStep" or
# "DepositedInStep"
```

Note that if you create particles inside your scoring volume (<u>volume source</u>), then they have no incident energy, and they will not be considered if you select "IncidentTrack" for binning. This is another reason to select "PreStep".

How to score kerma?

Topas manual (3.9) section 12.2.1

Cuts do not affect all processes, but only those listed below:

- Energy thresholds for gamma are used in Bremsstrahlung
- Energy thresholds for electrons are used in ionization and e+e- pair production processes Energy thresholds for positrons are used in e+e- pair production process
- Energy thresholds for gamma and electrons are **used optionally** in all discrete processes
- Photoelectriceffect
- Compton
- gamma conversion
- Energy thresholds for protons are used in processes of elastic scattering for hadrons and ions defining the threshold for kinetic energy of nuclear recoil

Unknown what this means

or how this is controlled

BE CAREFUL HERE: This does not work in general!!!!
We cannot simply force all electrons **not** to be transported if they have an energy below say 10 MeV (specified by an equivalent range in the medium):

d:Ph/Default/cutforelectron = 10 m

So, unfortunately, we cannot score kerma using the dosetomedium scorer by simply stopping electrons from moving after photons have undergone, for example, photoelectric effect or Compton scattering.

Collision-kerma scorer

```
##### Collion-kerma scoring using the TLE (see paper by Berumen et al. (2020))
s:Sc/kerma/Quantity = "TrackLengthEstimator"
b:Sc/kerma/PropagateToChildren = "True"
sv:Sc/kerma/Report = 5 "Count In Bin" "Sum" "Mean" "Standard Deviation" "Histories"
s:Sc/kerma/InputFile
                               = "Muen.dat"
= "centerrod" You need to copy this file from the
s:Sc/kerma/Component
                                                        examples/Brachytherapy folder
                                    = "False"
b:Sc/kerma/OutputToConsole
s:Sc/kerma/IfOutputFileAlreadyExists = "Overwrite"
                                                                (or make a direct link)
                           = "csv"
s:Sc/kerma/OutputType
s:Sc/kerma/OutputFile
                                      = Ge/World/Message + "DoseScorer2"
sv:Sc/kerma/OnlyIncludeParticlesNamed = 1 "gamma"
```

DO NOT FORGET THIS!

Essentially, this is just the photon fluence times the mass energy absorption coefficient (μ_{en}/ρ) from the Muen. dat file.

Berumen et al. (2020):

"Validation of the TOPAS Monte Carlo toolkit for HDR brachytherapy simulations" Medical Physics

The TLE technique approximates the absorbed dose as electronic (collisional) kerma. For a photon traversing a voxel, the absorbed dose is

$$D = \Phi E \frac{\mu_{en}}{\rho} = \frac{L}{V} E \frac{\mu_{en}}{\rho},$$

where L is the track length (the distance traveled in the voxel), V is the voxel volume, E is the photon energy, and μ_{en}/ρ is the mass energy absorption coefficient.

The Muen.dat file contains photon interaction data. The source of data is not clear.

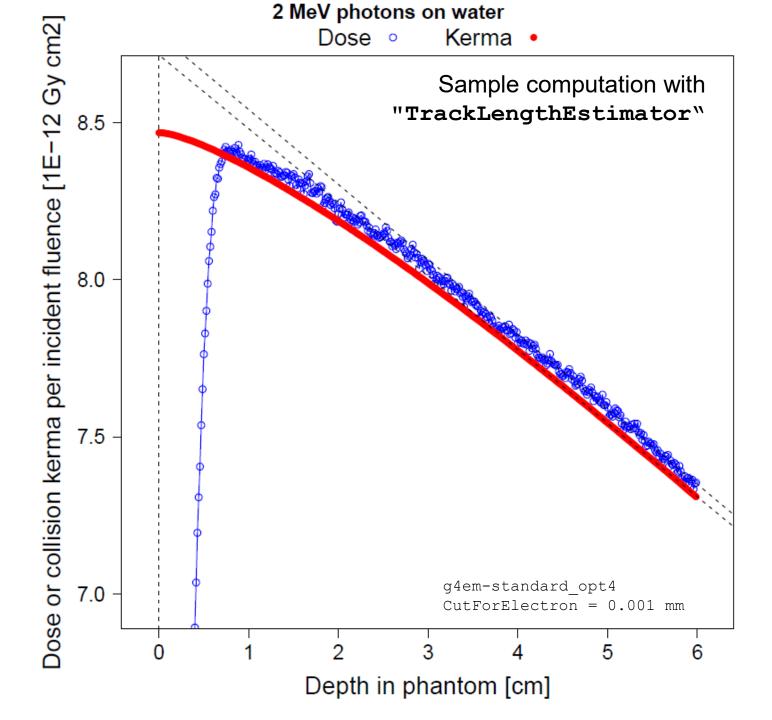
```
1 36
1.00000E-03 7.217E+00 6.820E+00
1.50000E-03 2.148E+00 1.752E+00
2.00000E-03 1.059E+00 6.643E-01
3.00000E-03 5.612E-01 1.693E-01
4.00000E-03 4.546E-01 6.549E-02
5.00000E-03 4.193E-01 3.278E-02
6.00000E-03 4.042E-01 1.996E-02
8.00000E-03 3.914E-01 1.160E-02
1.00000E-02 3.854E-01 9.849E-03
1.00000E-01 2.944E-01 4.063E-02
1.50000E-01 2.651E-01 4.813E-02
2.00000E-01 2.429E-01 5.254E-02
3.00000E-01 2.112E-01 5.695E-02
4.00000E-01 1.893E-01 5.860E-02
5.00000E-01 1.729E-01 5.900E-02
6.00000E-01 1.599E-01 5.875E-02
8.00000E-01 1.405E-01 5.739E-02
1.00000E+00 1.263E-01 5.556E-02
1.25000E+00 1.129E-01 5.311E-02
1.00000E+01 3.254E-02 2.247E-02
1.50000E+01 2.539E-02 1.837E-02
2.00000E+01 2.153E-02 1.606E-02
```

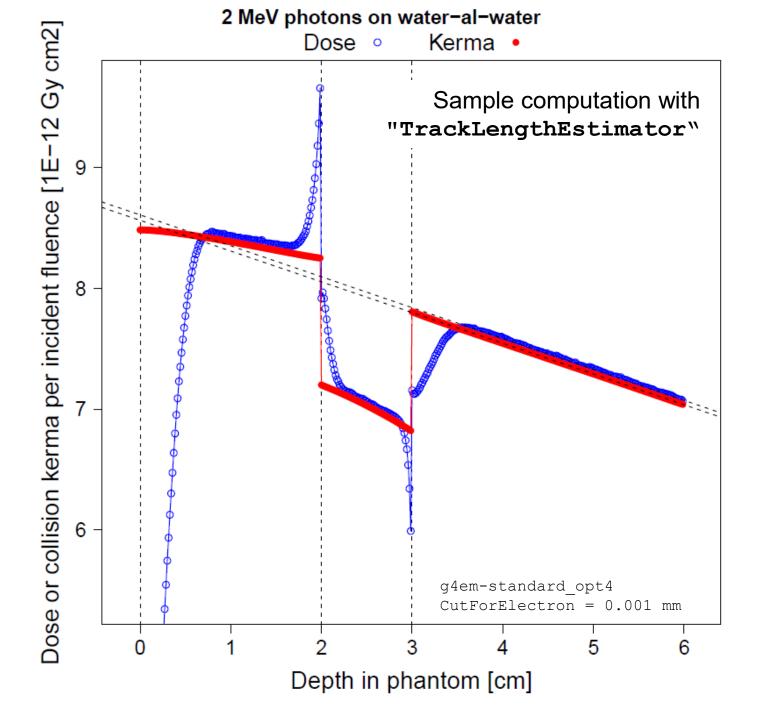
The data to the left is the initial part of the file. The data appears to be in the format:

$$<$$
MeV> $<$ μ/ρ > $<$ μ_{en}/ρ >

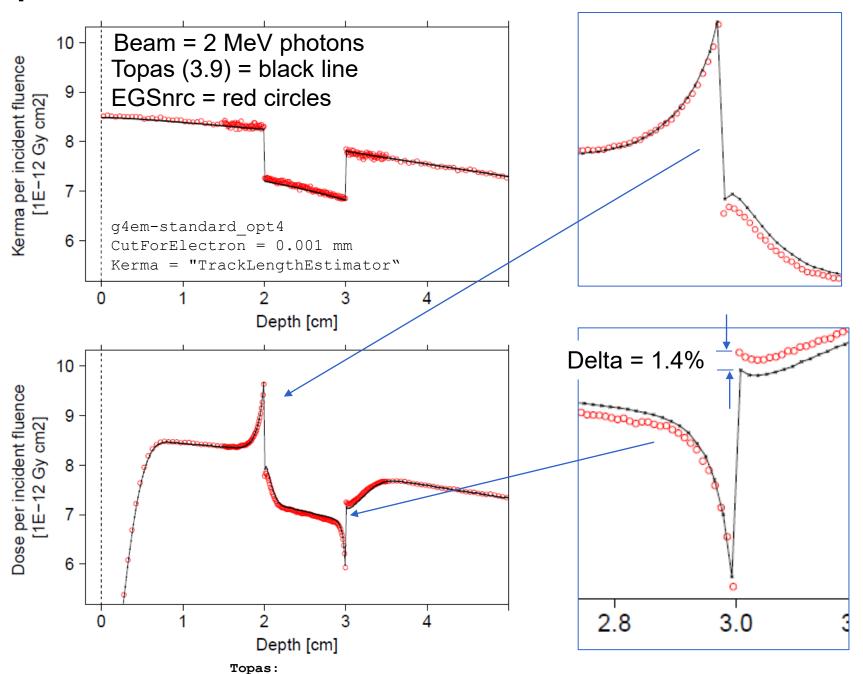
for hydrogen (Z = 1 in the (1, 36) opening line) with 36 data points in the range from 1 keV to 20 MeV.

If, so, then the file contains data for elements 1 to 92.





Topas vs. EGSnrc for the water-aluminium-water interface



How to represent the spectral distribution of photons from a Varian medical linac?

The Topas-VarianBeamAR.txt file on GitHub

Using the data in Table 5 of the Ali & Rogers (2012) paper:

IOP Publishing	PHYSICS IN MEDICINE AND BIOLOGY
Phys. Med. Biol. 57 (2012) 31–50	doi:10.1088/0031-9155/57/1/31

Functional forms for photon spectra of clinical linacs

ESM Ali and DW ORogers

Carleton Laboratory for Radiotherapy Physics, Department of Physics, Carleton University, 1125 Colonel By Drive, Ottawa, ON K1S 5B6, Canada

E-mail: eali@physics.carleton.ca and drogers@physics.carleton.ca

Received 26 May 2011, in final form 18 September 2011 Published 29 November 2011 Online at stacks.iop.org/PMB/57/31

Simple histograms representing the Varian Clinac 4 MV, 6 MV, 10 MV, 15 MV and 18 MV

The spectra are in the file: <u>Topas-VarianBeamAR.txt</u>

availible here:

https://github.com/claus-e-andersen/topas

Use of the Topas-VarianBeamAR.txt file

1. Put the following text in your parameter file.

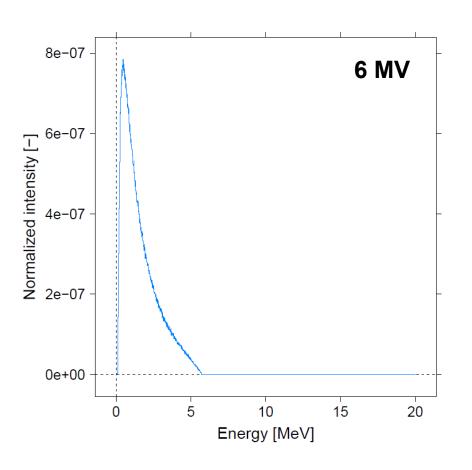
of your gamma source here.

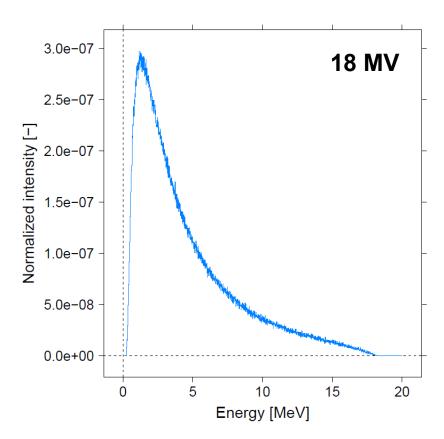
- 2. Copy the Topas-VarianBeamAR. txt file to the folde of your parameter file.
- 3. Modify the source name and select the beam quality as indicated below:

```
includeFile = Topas-VarianBeamAR.txt
s:So/clanBeam/BeamEnergySpectrumType = "Continuous"
# None, Continuous or Discrete
# Code for selection of spectra:
VarianBeamxxMV where xx = 04, 06, 10, 15, or 18
dv:So/clanBeam/BeamEnergySpectrumValues =
                                     So/VarianBeam04MV/BeamEnergySpectrumValues MeV
uv:So/clanBeam/BeamEnergySpectrumWeights =
                                     So/VarianBeam04MV/BeamEnergySpectrumWeights
   Write the specific name
```

This is where you select the beam quality

Topas-VarianBeamAR.txt file examples





How to make radioactivity in Topas?

Radioactive decay

Select a proper physics list:

```
sv:Ph/Default/Modules = 7 "g4em-standard_opt4"
"g4h-phy_QGSP_BIC_HP" "g4decay" "g4ion-binarycascade"
"g4h-elastic_HP" "g4stopping" "g4radioactivedecay"
```

If you shoot neutrons into a big lump of aluminum sitting in a 4pidetector phasespace scorer, you can see if you get any photons out that were created by the process "RadioactiveDecayBase".

If it works, you may want to limit the scorer only to record photons from this process.

From their initial kinetic energy, you can see if they are the same as you measured (1.7 MeV) and from the time-of-flight data, you can see if they arrive at the detector as expected from exponential decay and the half-life specific for Al-28.

How to make Topas do photonuclear reactions?

Photonuclear reactions

Select a proper physics list:

```
sv:Ph/Default/Modules = 8 "g4em-standard_opt4"
"g4h-phy_QGSP_BIC_HP" "g4decay" "g4ion-binarycascade"
"g4h-elastic_HP" "g4stopping" "g4radioactivedecay" "g4em-extra"
```

Add the g4em-extra to your physics list.

Jan Won Shin "A data-based photonuclear reaction model for GEANT4" Nuclear Instruments and Methods in Physics research B (2015) write:

G4EmExtraPhysics: For photonuclear interactions, GEANT4 uses the "G4EmExtraPhysics" class, which include the "G4PhotoNuclearCrossSection" class [47] and the "G4CascadeInterface" [48] class. G4PhotoNuclearCrossSection provides the total inelastic cross-sections for photonuclear interactions with nuclei. For simulating final states for photonuclear reactions, G4EmExtraPhysics uses the Bertini-style cascade model, the" G4CascadeInterface". Even though the Bertini model is available for the region of incident photon energy 0 6 Ec < 3.5 GeV in GEANT4 (v10.1), the model has been tested in a energy range 60 MeV 3 GeV [48].2 The above mentioned classes are described in detail in the Physics Reference Manual [49].

If you run Topas within VirtualBox and need more hard disk space?

How to expand your hard disk in VirtualBox

- 1. Make a clone of your machine (right-click and select clone ctrl+0).
- 2. Expand disk on VB:

Menu: File / Tools / Manage Virtual machine ("Håndtering af virtuel medie") Ctrl-D

Get properties on machine <name... vdi>

Adjust slider to 49.01 Gb or whatever space you want to expand to.

Apply.

3. Open machine in VB.

Open terminal

Run df (to get an overview of your disks.). Typically the disk with data will be /dev/sda3

sudo cfdisk (sudo password = cavity)

Choose partition (e.g. /dev/sda3)

RESIZE

(select new size, e.g. 49.01 Gb)

WRITE

(write new partition to disk)

QUIT (cfdisk)

Sudo reboot

df (new overview, nothing has happened yet)

sudo resize2fs /dev/sda3 (or whatever the name of the disk is) (resize2fs = resize to free space)

df (now something has happended, hopefully)

4. If all is good you can now delete the machine that you cloned.

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IN CIL

Include Topas in you path

(.bashrc changes)

If you run bash under linux

To include topas in your path, do the following:

Add the following lines to .bashrc in your home-folde:

export TOPAS_G4_DATA_DIR=~/G4Data
export PATH=~/topas/bin:\$PATH

(just put them at the end as the last lines).

Close / open terminal to start using your revised bash profile.

Write:

echo \$PATH

from terminal to verify the status of your path or simply write topas.

Ressources

TOPAS MC

http://www.topasmc.org/

TOPAS MC Users - Google Grupper

https://groups.google.com/g/topas-mc-users (require registration)

Geant4 Forum (cern.ch)

https://geant4-forum.web.cern.ch/

List of materials:

<u>Geant4 Material Database — Book For Application Developers 11.1</u> documentation (cern.ch)

https://geant4-

<u>userdoc.web.cern.ch/UsersGuides/ForApplicationDeveloper/html/Appendix/materialNames.html</u>

Ressources on Github

topasmc (github.com)
https://github.com/topasmc

https://github.com/jschuemann/extensions

"Dirty dose extension etc.:"

<u>Villadslj/Topas-Extension: Different kind of TOPAS extensions</u> (github.com)

Varian spectra:

<u>claus-e-andersen/TopasTools: Tools for Topasmc (Topas Monte-Carlo)</u> <u>modelling (github.com)</u>

https://github.com/claus-e-andersen/TopasTools