SIMULATION WITH TOPAS
PRACTICAL WORKSHOP

LIP Internship Program 2024 - Lectures and Tutorials Week

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LABORATÓRIO DE INSTRUMENTAÇÃO
E FÍSICA EXPERIMENTAL DE PARTÍCULAS

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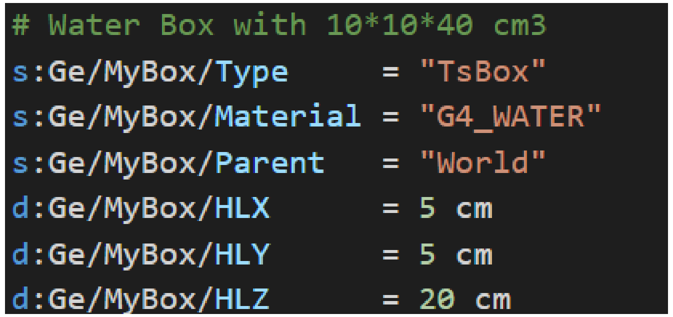
TOol for PArticle Simulation

- A Geant4-based Monte Carlo simulation.
- Easy-to-use:
  - The simulation is controlled by a parameter file.
  - It is possible assemble and control a rich library of simulation objects (geometry components, particle sources, scorers, etc.) with no need to write C++ code.
- Focus on medical applications.
- The users can implement their own simulation objects in C++ code and add them to TOPAS via an extension mechanism.
- Userguide: https://topas.readthedocs.io/en/latest/index.html

TOPAS Parameter files



```
# Water Box with 10*10*40 cm3
s:Ge/MyBox/Type       = "TsBox"
s:Ge/MyBox/Material = "G4_WATER"
s:Ge/MyBox/Parent    = "World"
d:Ge/MyBox/HLX        = 5 cm
d:Ge/MyBox/HLY        = 5 cm
d:Ge/MyBox/HLZ        = 20 cm
```

Parameters files are simple text files made up of lines of key/value pairs.

The order of lines within a parameter file does not matter.

```
Parameter_Type : Parameter_Name = Parameter_Value  #Optional comment
```

Tells TOPAS what **type of data** will be in this parameter:

d for Dimensioned Double

u for Unitless Double

i for Integer

b for Boolean

s for String

dv for Dimensioned Double Vector

similarly, for uv, iv, bv and sv

Can be almost any string, but there are **prefix conventions** to keep things clear:

Ma/ for Materials

El/ for Elements

Is/ for Isotopes

Ge/ for Geometry Components

So/ for Particle Sources

Ph/ for Physics

Vr/ for Variance Reduction

Sc/ for Scoring

Gr/ for Graphics

Tf/ for Time Features

Ts/ for TOPAS overall control

Parameter names are not case sensitive.

TOPAS Parameter files

```
d:Ge/Phantom/HLX                = 10. cm     # Dimensioned Double
i:Sc/DoseScorer/ZBins           = 100        # Integer
b:Sc/DoseScorer/Active          = "True"     # Boolean
s:Ge/Phantom/Material           = "G4_WATER" # String

dv:Ge/RMW_Track1/Angles         = 4 69.1 92.2 111.0 126.0 deg     # Dimensioned Double Vector
uv:Ma/Phantom_Plastic/Fractions = 3 0.05549 0.75575 0.18875       # Unitless Double Vector
iv:Gr/Color/yellow              = 3 225 255 0                     # Integer Vector
bv:Tf/ScoringOnOff/Values       = 4 "true" "false" "true" "false" # Boolean Vector
sv:Ma/MyPlastic/Components      = 3 "Hydrogen" "Carbon" "Oxygen"  # String Vector
```

Relative Parameters

- TOPAS supports “relative parameters”, wherein one parameter may be set relative to another:

```
s:Ge/Phantom/Material = SomeOtherParameterName
```

- With relative dimensioned double parameters, we must insist that a unit be included on the right side of the expression:

```
d:Ge/Phantom/HLX = SomeOtherParameterName cm
```

- TOPAS has a grammar for operations such as adding or multiplying parameters:

```
d:Ge/Compensator/TransZ = Ge/Aperture/DistalEdge + Ge/Compensator/HLZ mm
```

Note that there must be a space before and after the plus sign.
The complete set of allowed syntax for any one parameter line is shown here.

TOPAS Parameter files

GEOMETRY

SOURCE

PHYSICS

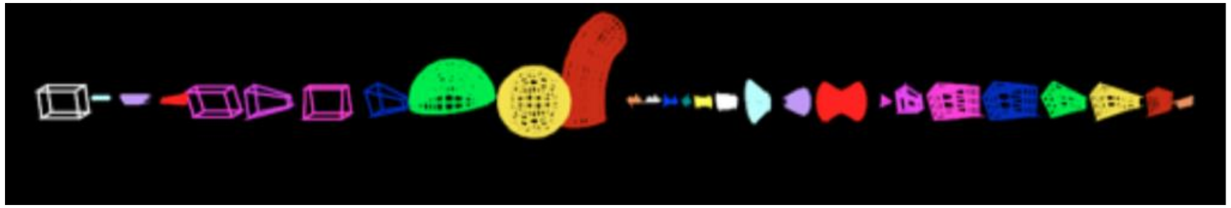
SCORER

VISUALIZATION

Geometry Components

- TOPAS includes all the **standard Geant4 solids**

TsSphere, TsBox, TsCylinder, G4CutTubs, G4Cons, G4Para, …



- Each one of them has its own set of required parameters:

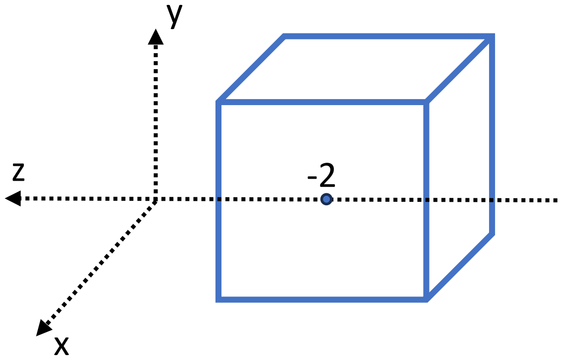
TsBox	TsSphere	TsCylinder
HLX, HLY and HLZ*	RMin, RMax, DPhi and SPhi	HL, RMin, RMax, DPhi and SPhi

All parameters, including optional ones, for all the Geant4 solids, can be found in this example.

* Half length

- It is possible built some complex things just from combinations of the Generic Components.
- TOPAS also has more specialized Components as a Range Modulator Wheel and a Multi Leaf Collimator. Usage is best learned by studying the relevant examples parameter files included in TOPAS.

Geometry Components



- All Geometry Components must have at least the following parameters:

```
s:Ge/MyComponent/Type   = "TsBox"
s:Ge/MyComponent/Parent = "World"
d:Ge/MyComponent/TransX = 0.0 cm  #defaults to 0
d:Ge/MyComponent/TransY = 0.0 cm  #defaults to 0
d:Ge/MyComponent/TransZ = -2. cm  #defaults to 0
d:Ge/MyComponent/RotX   = 0.0 deg #defaults to 0
d:Ge/MyComponent/RotY   = 0.0 deg #defaults to 0
d:Ge/MyComponent/RotZ   = 0.0 deg #defaults to 0
s:Ge/MyComponent/Material = "Air"
```

Translation Parameters

Rotation Parameters

Position of the component in the coordinate system of its parent component.

When building geometry, activate overlap checking. It has a speed cost at initialization, so if you're confident there are no overlaps, you can turn it off.

```
b:Ge/CheckForOverlaps = "False"
```

Materials and Isotopes

- Pre-defined materials: Vacuum, Nickel, Aluminum, … (list in here)

- You are free to define additional materials:

```
sv:Ma/Air/Components = 4 "Carbon" "Nitrogen" "Oxygen" "Argon" #names of elements
uv:Ma/Air/Fractions = 4 0.000124 0.755268 0.231781 0.012827   #fractions of elements
d:Ma/Air/Density = 1.2048 mg/cm3
d:Ma/Air/MeanExcitationEnergy = 85.7 eV
```

- You can also create a new mixture from a combination of other materials.

```
b:Ma/MyMixture/BuildFromMaterials = "True"
sv:Ma/MyMixture/Components = 2 "G4_WATER" "Air"
uv:Ma/MyMixture/Fractions = 2 .5 .5
d:Ma/MyMixture/Density = .5 g/cm3
```

- To define an isotope you must specifying Z, N and A:

```
i:Is/U235/Z = 92
i:Is/U235/N = 235
d:Is/U235/A = 235.01 g/mole
```

Particle Sources

- Different types of particle sources, each with many options:

```
s:So/MySource/Type = "Beam" #Beam, Isotropic, Distributed, Volumetric or PhaseSpace
```

- The source position can be defined by the user, and it must be associated with a geometry component.

```
s:So/MySource/Component = "BeamPosition“
```

- Particle names can take the following forms (case does not matter):

```
s:So/MySource/BeamParticle = "proton"
```

  - A simple string such as “proton”, “e-”, “gamma”, “He3”;
  - A string describing an ion with arguments Z, A, and optionally Charge, such as: “GenericIon(6,12,6)”;
  - An integer PDG ID code;

Particle Sources

Beam Source

- You must define the beam energy and spread:

```
d:So/MySource/BeamEnergy = 169.23 MeV
u:So/MySource/BeamEnergySpread = 0.757504
```

- You can provide an energy spectrum instead of a fixed energy, by defining the energies and weights:

```
s:So/MySource/BeamEnergySpectrumType = "Continuous" # or "Discrete"
dv:So/MySource/BeamEnergySpectrumValues = 3 50. 100. 150. MeV
uv:So/MySource/BeamEnergySpectrumWeights = 3 .20 .60 .20
```

- The beam shape can be further described by a set of parameters that control the **position distribution** of the start of the beam and by a set of parameters that control **how the beam spreads out** from that start position.

`BeamAngular`

`Distribution, CutoffX, CutoffY, SpreadX and SpreadY`

`BeamPosition`

`Distribution, CutoffShape, CutoffX, CutoffZ, SpreadX and SpreadY`

- To define how many particles are generated, you must do:

```
i:So/MySource/NumberOfHistoriesInRun = 100
```

Particle Sources

Isotropic, Distributed and Volumetric Sources

- **Isotropic** sources emit particles uniformly from the center of the specified component.
- **Distributed** source represents radioactive material randomly distributed within other material.

```
s:So/MySource/Component = "DemoSphere"
i:So/MySource/NumberOfHistoriesInRun = 5
i:So/MySource/NumberOfSourcePoints = 4
```

- **Volumetric** source emit particles from randomly sampled starting positions from within the radioactive volume of a given component. This source type has been designed for Brachytherapy applications.

```
s:So/MySource/Type = "Volumetric"
s:So/MySource/Component = "ActiveSource"
s:So/MySource/ActiveMaterial = "G4_Ir"
```

The energies and species of the emitted particles can be specified using the usual parameters as BeamParticle, BeamEnergy and BeamEnergySpread.

Scorers

- There are two basic classes of scorers: Volume and Surface Scorers

You must indicate the relevant Component

```
s:Sc/MyScorer/Component = "Phantom"
```

Quantity	
DoseToMedium	EnergyFluence
DoseToWater	StepCount
DoseToMaterial	OpticalPhotonCount
TrackLengthEstimator	OriginCount
AmbientDoseEquivalent	Charge
EnergyDeposit	EffectiveCharge
Fluence	ProtonLET

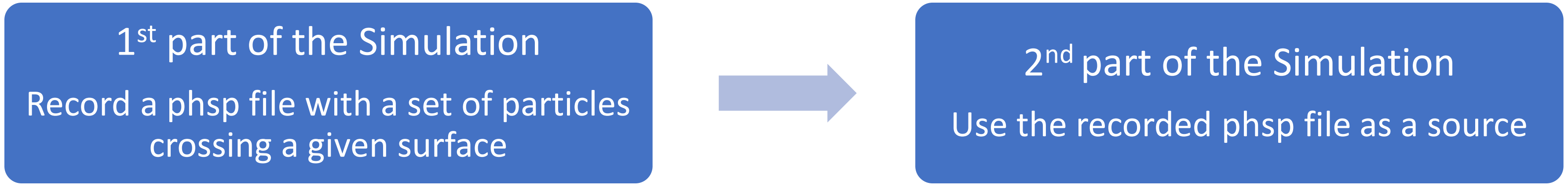
You must indicate the relevant Component and Surface name

```
s:Sc/MyScorer/Surface="Phantom/ZMinusSurface"
```

Quantity	
SurfaceTrackCount	SurfaceCurrent
PhaseSpace	

Phase Space

- This type of scorer enables separating two parts of a simulation and can be used to transfer sets of particles among different codes.

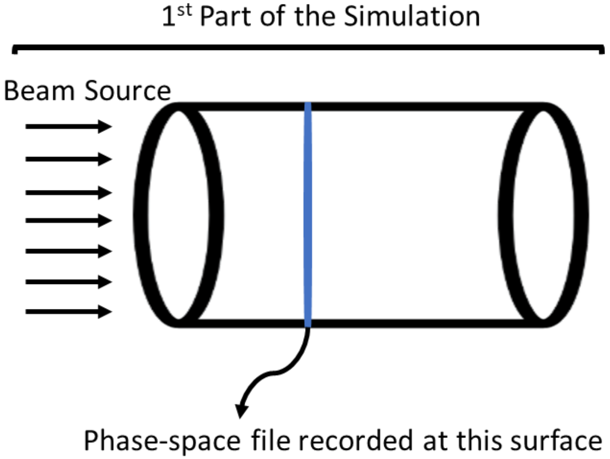


1st part of the Simulation

Record a phsp file with a set of particles crossing a given surface

2nd part of the Simulation

Use the recorded phsp file as a source


1st Part of the Simulation
Beam Source
Phase-space file recorded at this surface

- Four formats for Phase Space are supported: Binary, ASCII, Limited or ROOT.

Phase Space

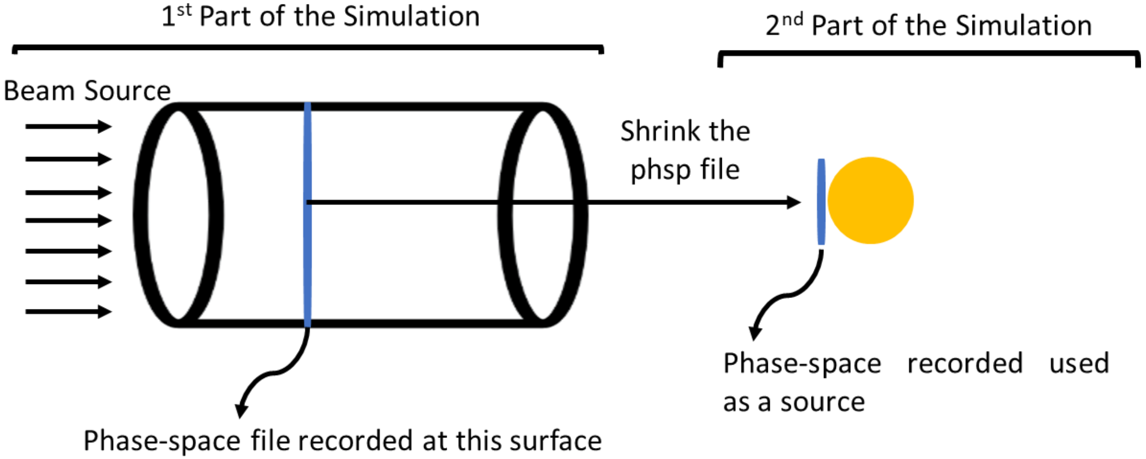
- This type of scorer enables separating two parts of a simulation and can be used to transfer sets of particles among different codes.

1st part of the Simulation

Record a phsp file with a set of particles crossing a given surface

2nd part of the Simulation

Use the recorded phsp file as a source


1st Part of the Simulation
2nd Part of the Simulation
Beam Source
Shrink the phsp file
Phase-space recorded used as a source
Phase-space file recorded at this surface

A Phase Space as a particle source

It is possible scale the phsp position and invert any of the phase space axes.

More details about how to use a phsp file as a source here.

- Four formats for Phase Space are supported: Binary, ASCII, Limited or ROOT

Physics

- A physics list specifies what particles and physics processes are defined, plus various cuts and options.
- You can choose from two general types of physics lists:
  - Reference Physics Lists are pre-made, complete lists provided by Geant4.
  - **Modular Physics Lists** are lists where you mix and match a set of modules to create a customized complete list.

```
sv:Ph/MyPhysics/Modules = 1 "g4em-livermore"
d:Ph/MyPhysics/CutForAllParticles = 0.05 mm
b:Ph/MyPhysics/Fluorescence = "True"
b:Ph/MyPhysics/Auger = "True"
b:Ph/MyPhysics/AugerCascade = "True"
b:Ph/MyPhysics/PIXE = "True"
```

TOPAS Module Name	Geant4 Class Name
g4em-livermore	G4EmLivermorePhysics
g4em-penelope	G4EmPenelopePhysics
g4radioactivedecay	G4RadioactiveDecayPhysics
g4em-dna*	G4EmDNAPhysics

List of Available Modules

*Only for water
Goes down to 10. eV

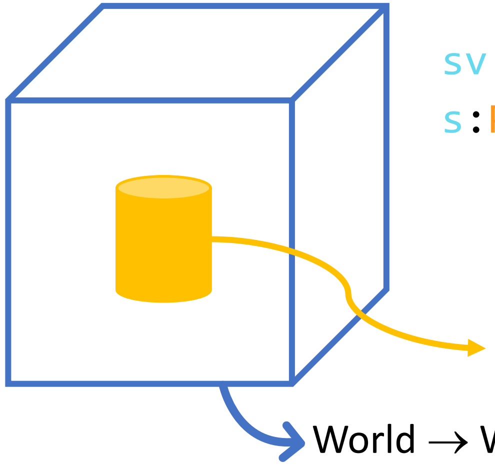
Physics

- By default, cuts affect the entire world, but you can optionally divide the world into several regions and can specify different physics modules and cuts in each region.
- First, specify which components belong to a given region:

```
s:Ge/MyComponent/AssignToRegionNamed = "MyRegion"
```

- Then assign cuts and physics modules per region by including the region name in the parameter name as in:

```
sv:Ph/MyPhysics/Modules = 1 "g4em-dna"
s:Ph/MyPhysics/ForRegion/MyRegion/ActiveG4EmModelFromModule = "g4em-livermore"
```



MyComponent → Other material → Livermore physics list

World → Water → G4DNA physics list

References

Perl J, Shin J, Schumann J, Faddegon B, Paganetti H. TOPAS: an innovative proton Monte Carlo platform for research and clinical applications. Med Phys. 2012; 39(11):6818-37.

Faddegon B, Ramos-Mendez J, Schuemann J, McNamara A, Shin J, Perl J, Paganetti H, The TOPAS Tool for Particle Simulation, a Monte Carlo Simulation Tool for Physics, Biology and Clinical Research, Physica Medica, doi:10.1016/j.ejmp.2020.03.019

Questions?

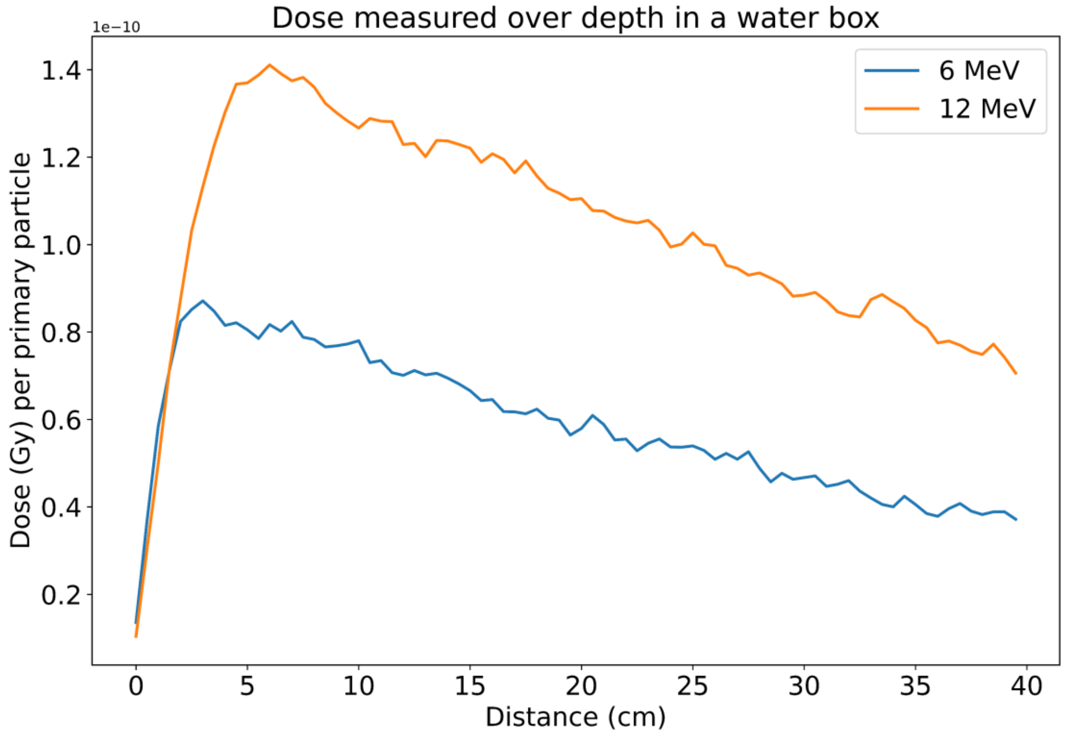
Hands-on session

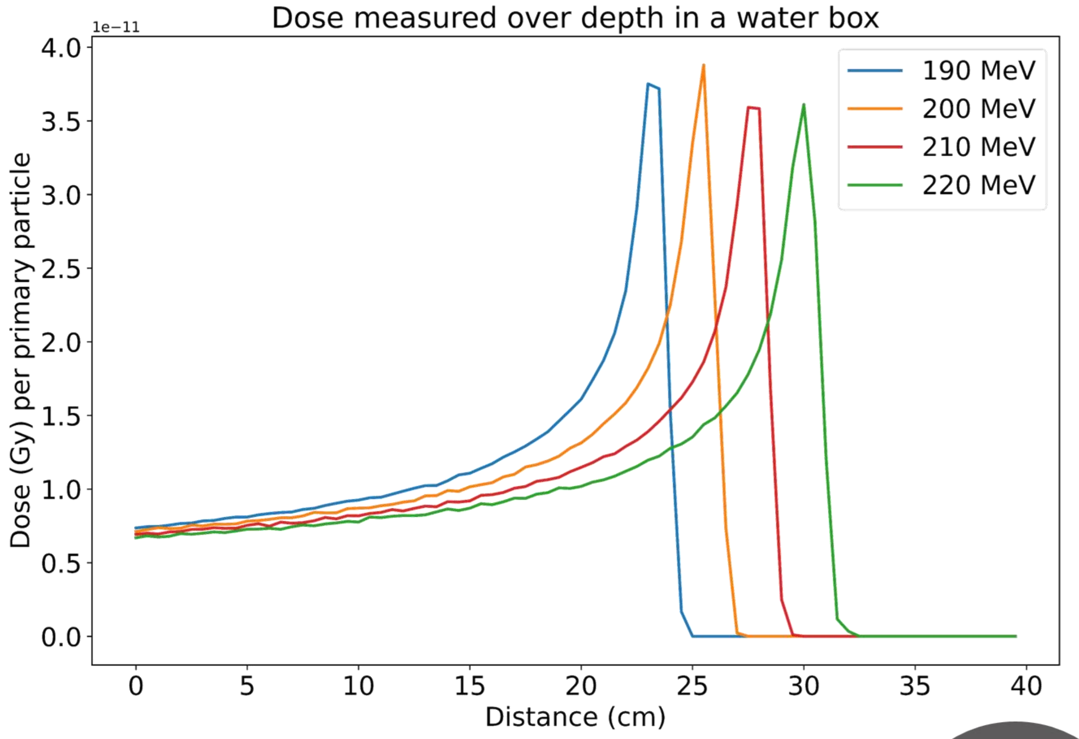
Example 1 – Dose measured over depth in a water box

Example 2 – Radial Dose: Deposited dose as a function of the distance from the AuNP surface.

Example 1

Dose measured over depth in a water box





Example 1

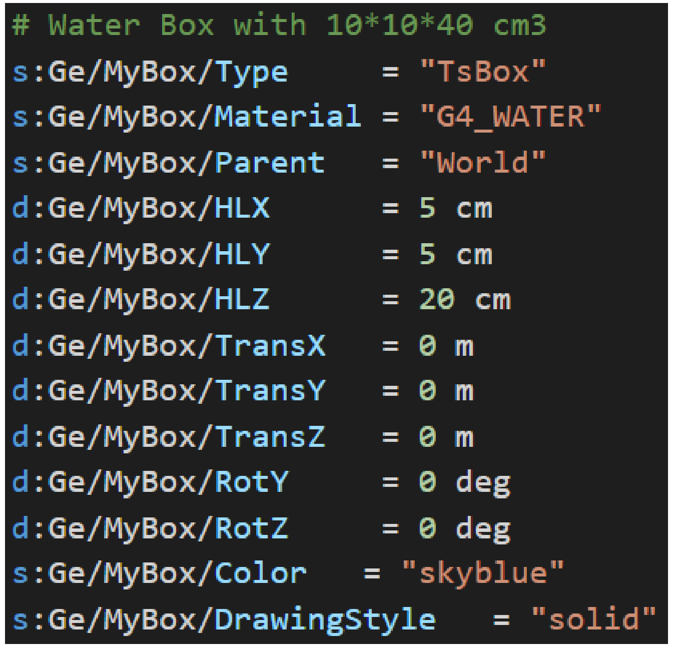
Dose measured over depth in a water box

- Geometry: Water Box (10*10*40 cm3)
- Physics: g4-livermore
  - Cut for gammas and electrons: 5 µm
  - Fluorescence, Auger, Auger Cascade, Deexcitation Ignore Cut and PIXE activated.
- Scorer: `DoseToMedium`
  - Output file name: Dose_###MeV
  - You must indicate how many Zbins do you want
- Source:
  - The source beam direction was chosen to irradiate the box along the z-axis. Particle tracks were originated from a gaussian, and elliptical plane placed at the box begin.
  - Protons: 190, 200, 210 and 220 MeV; 100 histories
  - Gammas: 6 and 12 MeV; 50000 histories
- Results analysis:
  - Example1_Plots.py: Example1_gammas.png and Example1_protons.png

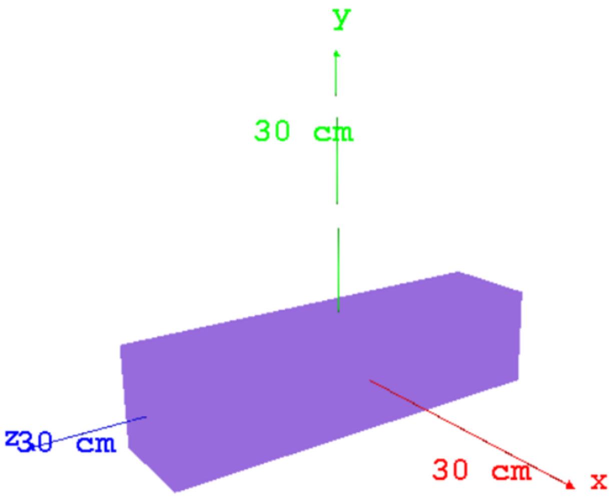
Example 1

Dose measured over depth in a water box

- **Geometry**: Water Box



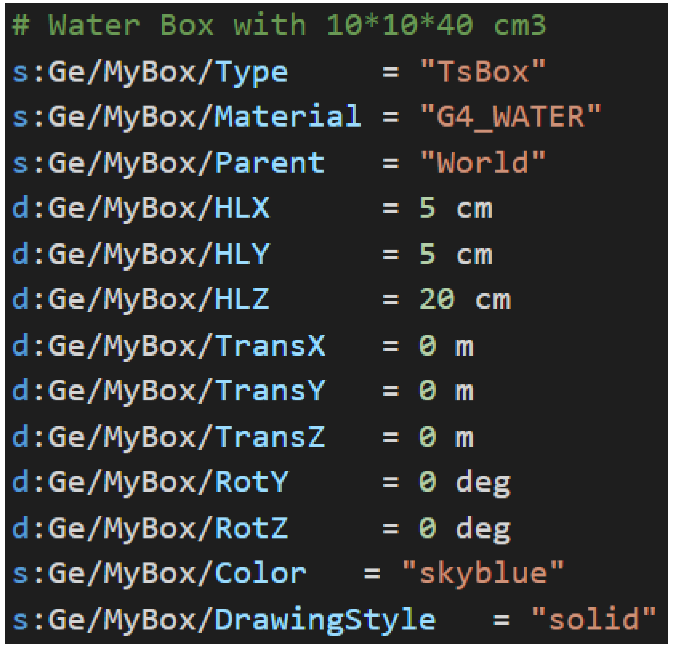
```
# Water Box with 10*10*40 cm3
s:Ge/MyBox/Type      = "TsBox"
s:Ge/MyBox/Material = "G4_WATER"
s:Ge/MyBox/Parent   = "World"
d:Ge/MyBox/HLX      = 5 cm
d:Ge/MyBox/HLY      = 5 cm
d:Ge/MyBox/HLZ      = 20 cm
d:Ge/MyBox/TransX   = 0 m
d:Ge/MyBox/TransY   = 0 m
d:Ge/MyBox/TransZ   = 0 m
d:Ge/MyBox/RotY     = 0 deg
d:Ge/MyBox/RotZ     = 0 deg
s:Ge/MyBox/Color   = "skyblue"
s:Ge/MyBox/DrawingStyle   = "solid"
```



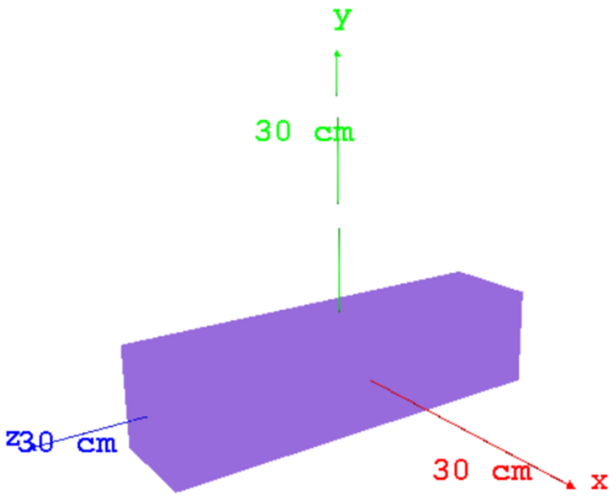
Example 1

Dose measured over depth in a water box

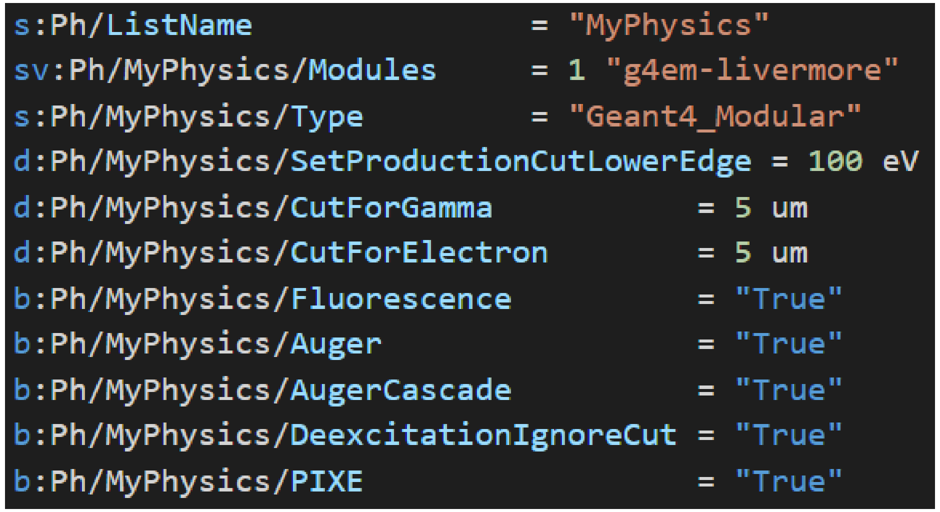
- **Geometry**: Water Box



```
# Water Box with 10*10*40 cm3
s:Ge/MyBox/Type      = "TsBox"
s:Ge/MyBox/Material = "G4_WATER"
s:Ge/MyBox/Parent    = "World"
d:Ge/MyBox/HLX       = 5 cm
d:Ge/MyBox/HLY       = 5 cm
d:Ge/MyBox/HLZ       = 20 cm
d:Ge/MyBox/TransX    = 0 m
d:Ge/MyBox/TransY    = 0 m
d:Ge/MyBox/TransZ    = 0 m
d:Ge/MyBox/RotY      = 0 deg
d:Ge/MyBox/RotZ      = 0 deg
s:Ge/MyBox/Color    = "skyblue"
s:Ge/MyBox/DrawingStyle    = "solid"
```



- **Physics**
  - Cut for gammas and electrons: 5 µm
  - Fluorescence, Auger, Auger Cascade, Deexcitation Ignore Cut and PIXE activated.

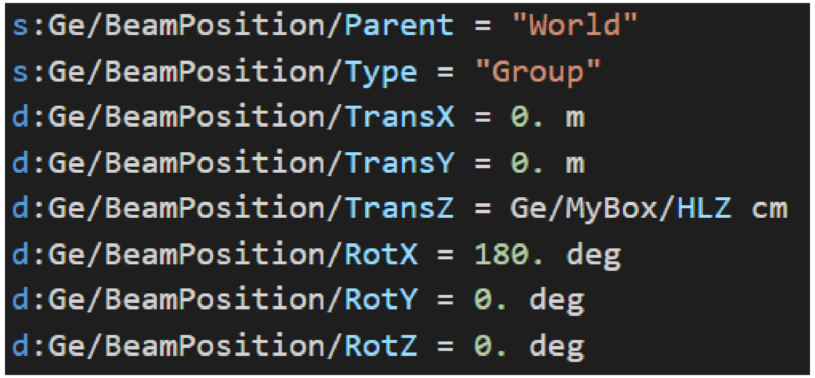


```
s:Ph/ListName                      = "MyPhysics"
sv:Ph/MyPhysics/Modules            = 1 "g4em-livermore"
s:Ph/MyPhysics/Type                = "Geant4_Modular"
d:Ph/MyPhysics/SetProductionCutLowerEdge = 100 eV
d:Ph/MyPhysics/CutForGamma               = 5 um
d:Ph/MyPhysics/CutForElectron            = 5 um
b:Ph/MyPhysics/Fluorescence              = "True"
b:Ph/MyPhysics/Auger                     = "True"
b:Ph/MyPhysics/AugerCascade              = "True"
b:Ph/MyPhysics/DeexcitationIgnoreCut     = "True"
b:Ph/MyPhysics/PIXE                      = "True"
```

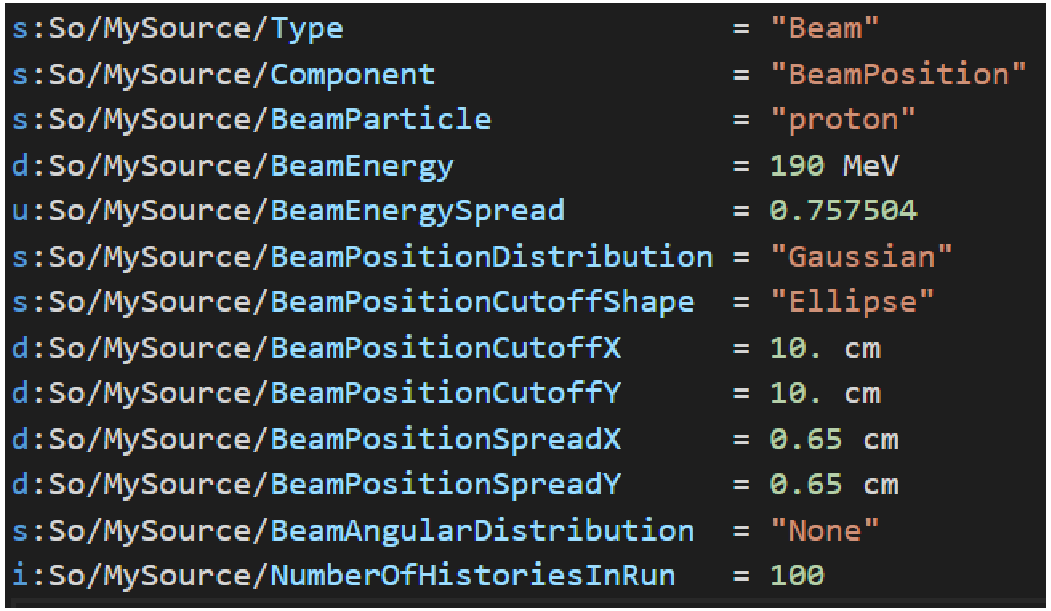
Example 1

Dose measured over depth in a water box

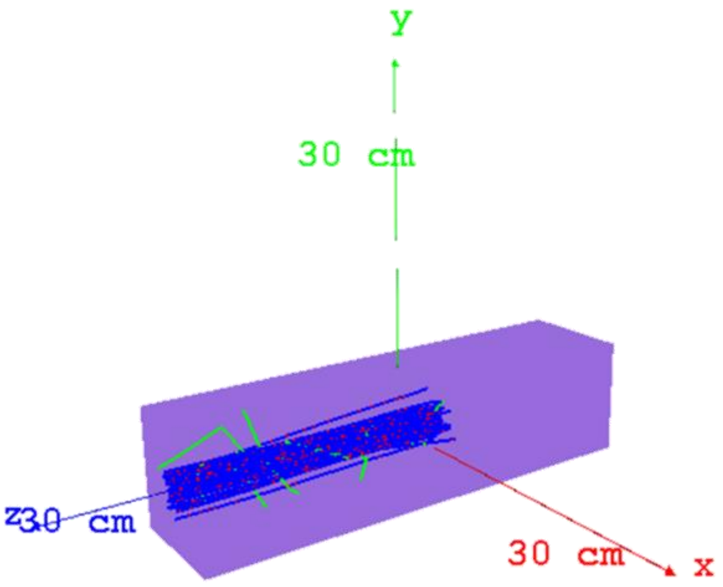
- **Source**:
    - The source beam direction was chosen to irradiate the box along the z-axis. Particle tracks were originated from a gaussian, and elliptical plane placed at the box begin.
    - Protons: 190, 200, 210 and 220 MeV; 100 histories
    - Gammas: 6 and 12 MeV; 50000 histories



```
s:Ge/BeamPosition/Parent = "World"
s:Ge/BeamPosition/Type = "Group"
d:Ge/BeamPosition/TransX = 0. m
d:Ge/BeamPosition/TransY = 0. m
d:Ge/BeamPosition/TransZ = Ge/MyBox/HLZ cm
d:Ge/BeamPosition/RotX = 180. deg
d:Ge/BeamPosition/RotY = 0. deg
d:Ge/BeamPosition/RotZ = 0. deg
```

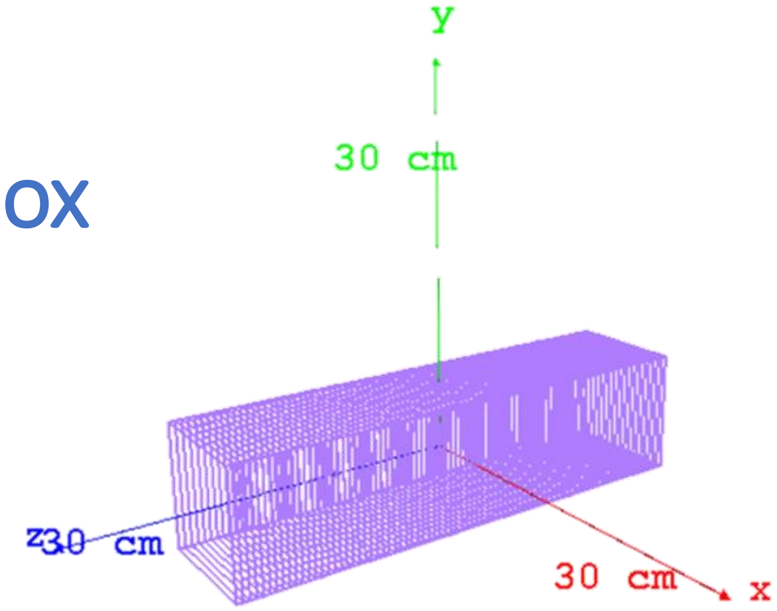


```
s:So/MySource/Type                        = "Beam"
s:So/MySource/Component                   = "BeamPosition"
s:So/MySource/BeamParticle                = "proton"
d:So/MySource/BeamEnergy                  = 190 MeV
u:So/MySource/BeamEnergySpread            = 0.757504
s:So/MySource/BeamPositionDistribution = "Gaussian"
s:So/MySource/BeamPositionCutoffShape     = "Ellipse"
d:So/MySource/BeamPositionCutoffX         = 10. cm
d:So/MySource/BeamPositionCutoffY         = 10. cm
d:So/MySource/BeamPositionSpreadX         = 0.65 cm
d:So/MySource/BeamPositionSpreadY         = 0.65 cm
s:So/MySource/BeamAngularDistribution     = "None"
i:So/MySource/NumberOfHistoriesInRun      = 100
```

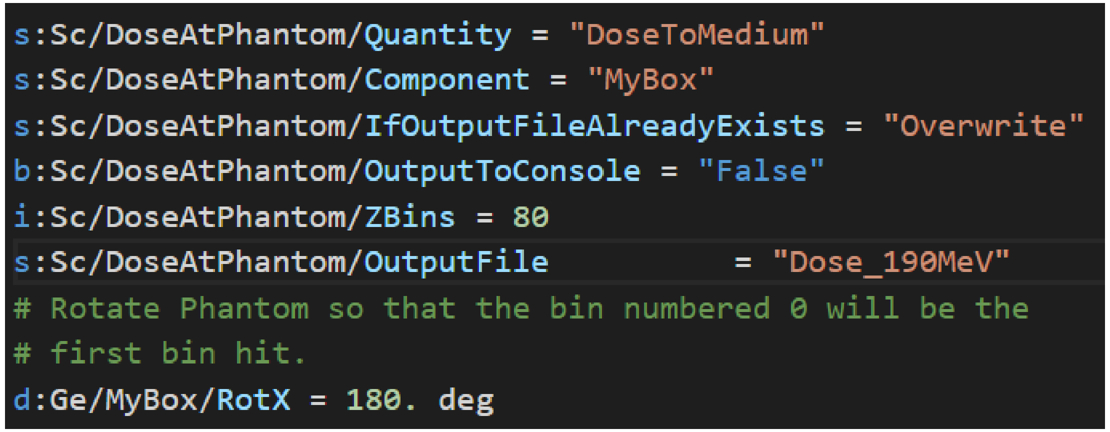


Example 1

Dose measured over depth in a water box



- **Scorer**: DoseToMedium
  - Output file name: Dose_###MeV
  - You must indicate how many Zbins do you want



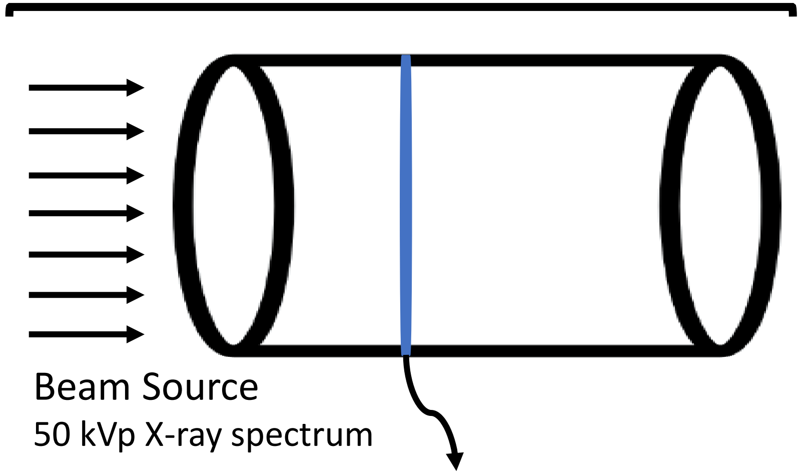
```
s:Sc/DoseAtPhantom/Quantity = "DoseToMedium"
s:Sc/DoseAtPhantom/Component = "MyBox"
s:Sc/DoseAtPhantom/IfOutputFileAlreadyExists = "Overwrite"
b:Sc/DoseAtPhantom/OutputToConsole = "False"
i:Sc/DoseAtPhantom/ZBins = 80
s:Sc/DoseAtPhantom/OutputFile          = "Dose_190MeV"
# Rotate Phantom so that the bin numbered 0 will be the
# first bin hit.
d:Ge/MyBox/RotX = 180. deg
```

- **Results analysis**:
  - Example1_Plots.py: Example1_gammas.png and Example1_protons.png

Example 2

Radial Dose

1st Simulation: Cylinder.txt



Beam Source

50 kVp X-ray spectrum

Phase-space file recorded at this surface

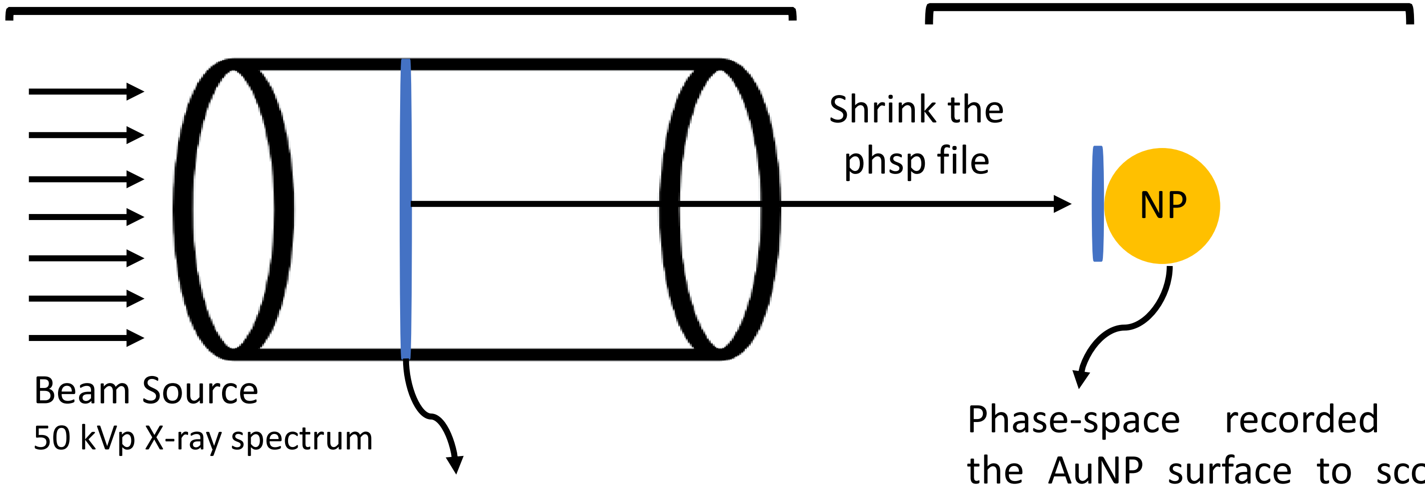
- **Physics**: g4-Livermore or g4-dna
  - Cut for gammas and electrons: 1 nm
  - Fluorescence, Auger, Auger Cascade, Deexcitation Ignore Cut and PIXE activated.

Example 2

Radial Dose

1st Simulation: Cylinder.txt

2nd Simulation: Nanoparticle.txt



Beam Source

50 kVp X-ray spectrum

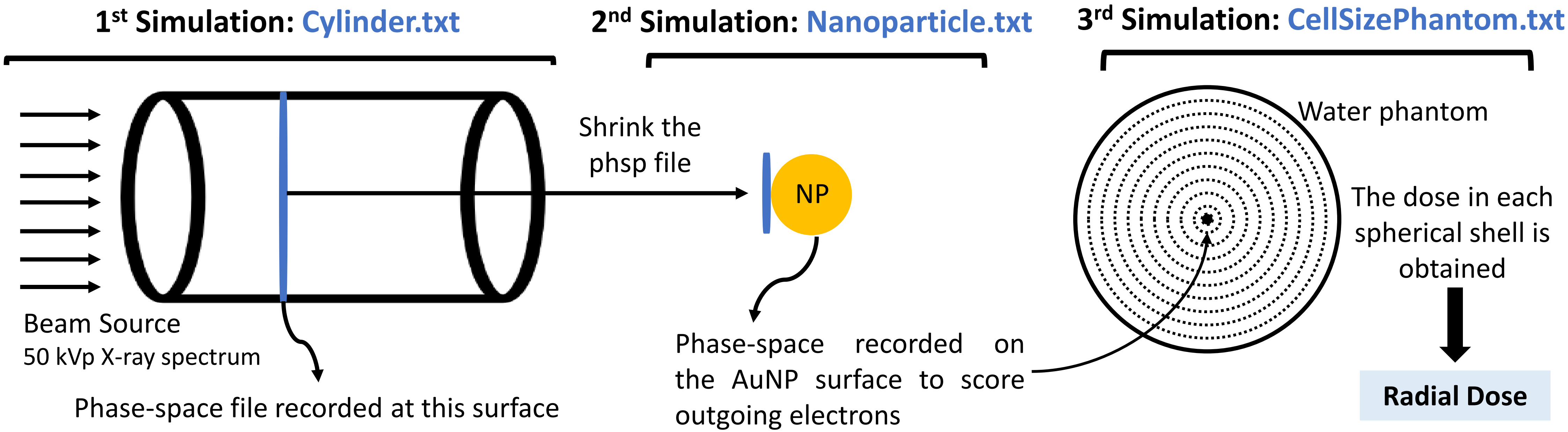
Phase-space file recorded at this surface

Phase-space recorded on the AuNP surface to score outgoing electrons

- **Physics**: g4-livermore
  - Cut for gammas and electrons: 1 nm
  - Fluorescence, Auger, Auger Cascade, Deexcitation Ignore Cut and PIXE activated.

Example 2

Radial Dose



1st Simulation: Cylinder.txt

2nd Simulation: Nanoparticle.txt

3rd Simulation: CellSizePhantom.txt

Beam Source

50 kVp X-ray spectrum

Phase-space file recorded at this surface

Shrink the phsp file

Phase-space recorded on the AuNP surface to score outgoing electrons

Water phantom

The dose in each spherical shell is obtained

Radial Dose

- **Physics**: g4-dna
  - Cut for gammas and electrons: 0.5 nm
  - Fluorescence, Auger, Auger Cascade, Deexcitation Ignore Cut and PIXE activated.
- **Scorer:** DoseToMedium