

**Joint ICTP-IAEA Workshop on Monte Carlo Radiation Transport
and Associated Data Needs for Medical Applications**

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Lecture 17

DOSXYZnrc dose calculations in a phantom

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Government
of Canada

Gouvernement
du Canada



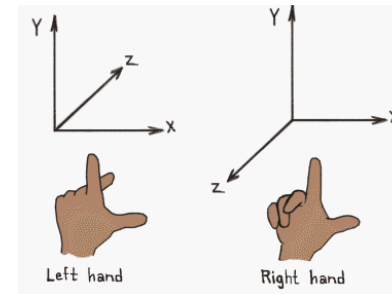
DOSXYZnrc History

- DOSXYZ, for use with EGS4, coded by DWOR in 1987 to show that specialized coding of HOWFAR for rectilinear voxels faster than using generalized macros
- Became basis for a MC timing benchmark in 1992
- Released with BEAM as part of the OMEGA project in 1995
- Updated to incorporate new physics in EGSnrc in 2001: DOSXYZ → DOSXYZnrc
- Became an EGSnrc application in mid 00's
- Remains a workhorse for efficient dose calculations in phantoms with rectilinear voxels, including CT-based phantoms

DOSXYZnrc

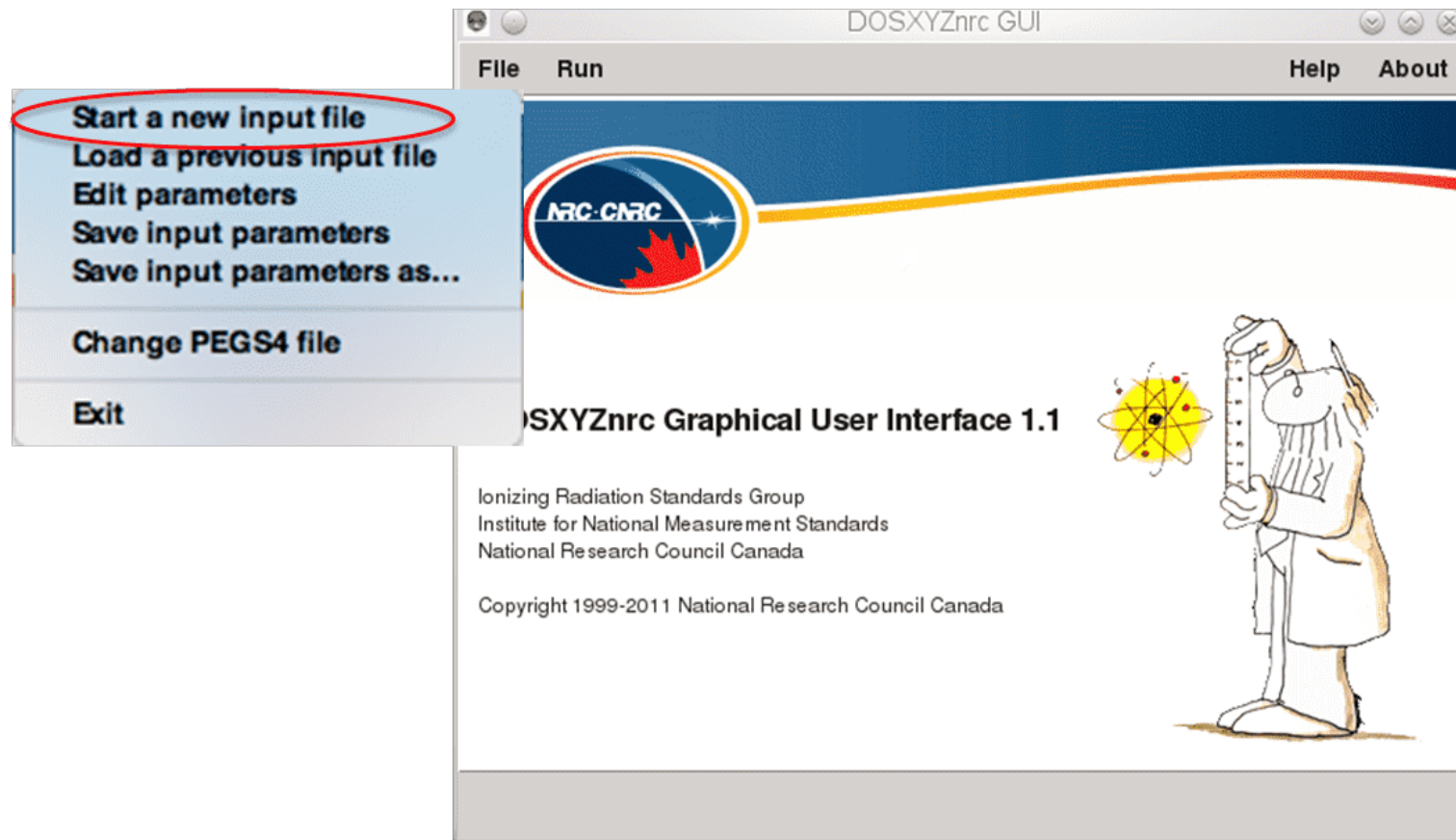
Geometry is a rectilinear volume with X-Y plane on the page, X to the right, Y down the page, and the Z-axis into the page (right-handed coordinate system). Voxels can have variable dimensions and material composition.

- Dose components based on where particles have passed through or interacted in, or whether the particle is a primary or secondary particle, etc.
- Uses several calculation-efficiency-increasing techniques for fast dose calculations



GUI

- type “dosxyz_gui” or “dosxyznrc_gui”



- option to open with: “dosxyz_gui inputfile pegsfile”

Defining geometry

The screenshot shows the 'Inputs' dialog box for DOSXYZnrc. It is divided into three main sections: Phantom definition, Source parameters, and Simulation parameters.

Phantom definition

If you are using source 2 or 4, you must define the materials in the phantom here first before defining the source.

☒ non-CT data input ☐ phantom created from CT data

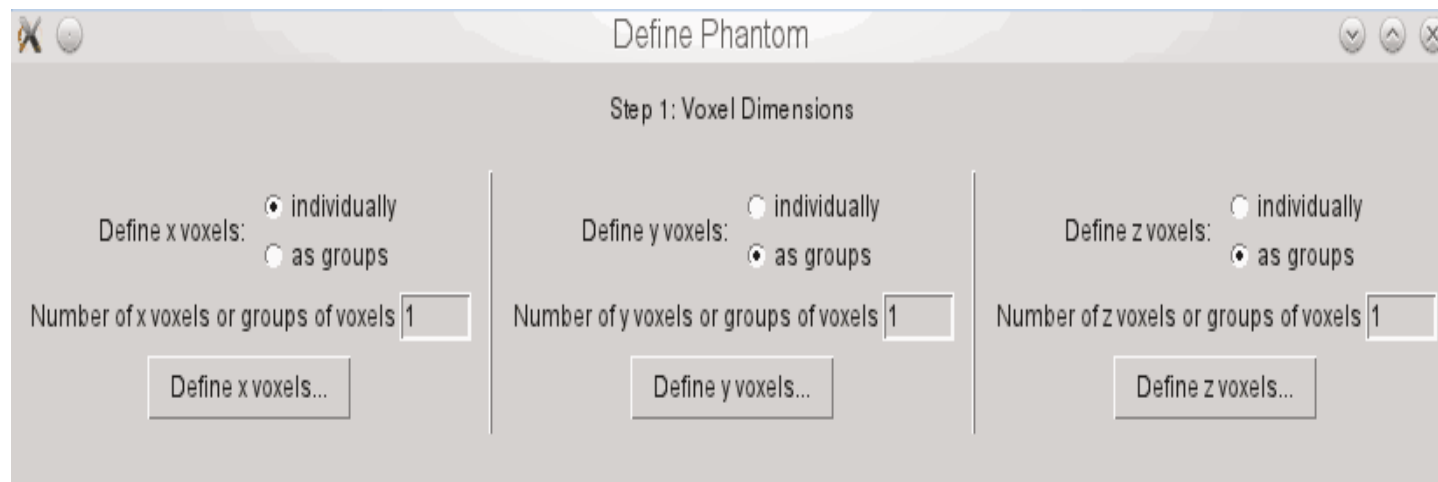
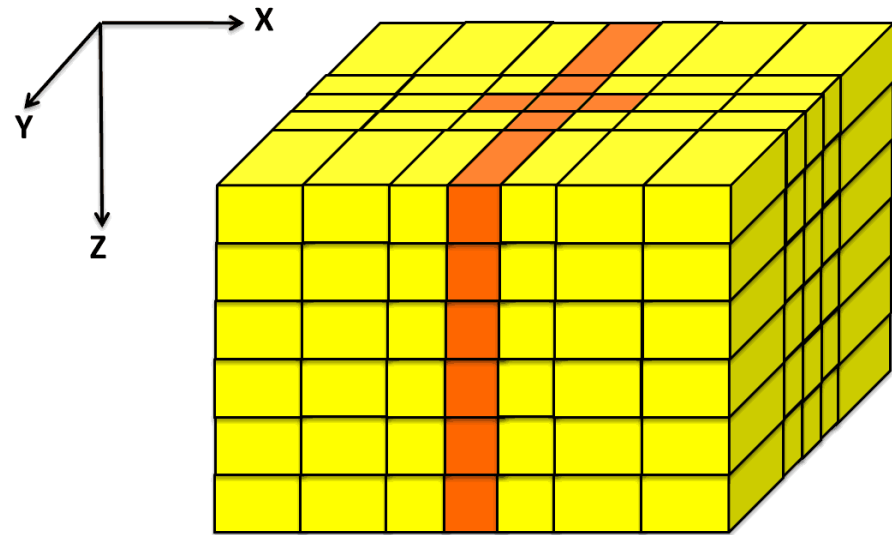
Source parameters

Simulation parameters

<input type="button" value="Number of histories"/> <input type="text" value="100"/>	<input type="button" value="Thickness of region outside phantom is"/> <input type="text" value="uniform"/>
<input type="button" value="WATCH Output"/> <input type="text" value="none"/>	<input type="button" value="Medium of region outside phantom"/> <input type="text" value="VACUUM"/>
<input type="button" value="Maximum CPU time (hours)"/> <input type="text" value="0.99"/>	<input type="button" value="Phase space output on exiting phantom"/> <input type="text" value="none"/>
<input type="button" value="RNG seed 1"/> <input type="text" value="33"/>	<input type="button" value="Output restart data"/> <input type="text" value="after every batch"/>
<input type="button" value="RNG seed 2"/> <input type="text" value="97"/>	<input type="button" value="Range rejection"/> <input type="text" value="off"/>
<input type="button" value="Incident beam size (source 2, 4 or 8)"/> <input type="text" value="100.0"/>	<input type="button" value="ESAVE: range rejection done only below this energy (MeV)"/> <input type="text" value=""/>
<input type="button" value="Run option"/> <input type="text" value="first time"/>	<input type="button" value="Photon splitting number"/> <input type="text" value="1"/>
<input type="button" value="HOWFARLESS"/> <input type="text" value="off"/>	<input type="button" value="# times to recycle each particle in phase space source"/> <input type="text" value=""/>
	<input type="button" value="Run job in parallel"/> <input type="text" value="no"/>

Phantom definition: non-CT input

- Individual voxel definition
- Voxel definition by group



Phantom definition: individual vs groups

group

Define y voxels

Enter the minimum y-value, then for each group enter the width (in cm) of the voxels in this group and the number of voxels which have this y-width.

Minimum y-boundary (cm)

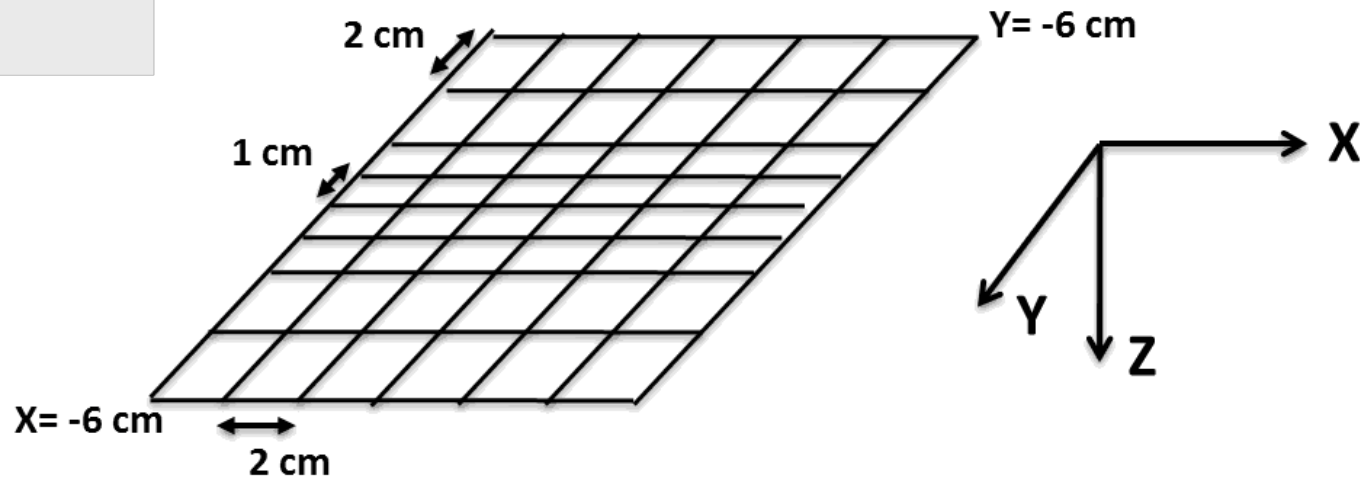
	y-width	Number in group
Group 1	<input type="text" value="2.0"/>	<input type="text" value="2"/>
Group 2	<input type="text" value="1.0"/>	<input type="text" value="4"/>
Group 3	<input type="text" value="2.0"/>	<input type="text" value="2"/>

individual

Define x voxels

Enter the x-voxel spacing in cm; $x(i-1)$ is the x-coordinate of the start of voxel i .

x_0	x_1	x_2	x_3	x_4	x_5	x_6
<input type="text" value="-6"/>	<input type="text" value="-4"/>	<input type="text" value="-2"/>	<input type="text" value="0"/>	<input type="text" value="2"/>	<input type="text" value="4"/>	<input type="text" value="6"/>



Phantom media definition: non-CT input

Define Phantom

Step 1: Voxel Dimensions

Define x voxels: ☒ individually ☐ as groups
Number of x voxels or groups of voxels: 6
Define x voxels...

Define y voxels: ☐ individually ☒ as groups
Number of y voxels or groups of voxels: 3
Define y voxels...

Define z voxels: ☒ individually ☐ as groups
Number of z voxels or groups of voxels:
Define z voxels...

Step 2: Define Media (include medium for region surrounding phantom)

Number of media: 3 Define media...

Step 3: Output

☐ Output .egsphant file Select the voxels for which to list the dose...

Done

- input no. of different media for entire simulation (including surrounding air)

Phantom media definition (cont.)

Media

Select every medium you would like to use in this simulation (including that surrounding the phantom, for phase space beam input) and enter the ESTEPE value that you wish to use for each medium. Any voxel for which the medium is not explicitly declared will be assumed to be the first medium selected here, with its default density.

	Medium
1	H2O700ICRU
2	ICRPBONE700ICRU
3	AIR700ICRU

Set media of voxels...

OK Help

Media of voxels

Define a group of voxels by entering the voxel indices, then set the medium and medium density for the group. Any voxel for which the medium is not explicitly declared will be assumed to be the first medium selected in the Define Media window (currently H2O700ICRU), with its default density. The default density of a selected material will be used if it is not overridden in the space provided. Click 'Add a group' to define a new group, 'Remove last group' to remove the last group.

from x	to x	from y	to y	from z	to z	medium	density
3	4	3	6	10	10	ICRPBONE700ICRU	

Remove last group Add a group OK

Annotations:

- Default medium:** Points to the first medium (H2O700ICRU) in the 'Media' window.
- Drop down menus list all media available in pgs data file or, if running pgsless, all media defined in .egsinp file and material data file:** Points to the medium selection dropdowns in the 'Media' window.
- leave blank to use density in pgs(less) definition:** Points to the empty density field in the 'Media of voxels' window.
- voxel indices:** Points to the 'from x' and 'to x' fields in the 'Media of voxels' window.

Phantom output control

Define Phantom

Step 1: Voxel Dimensions

Define x voxels: ☒ individually ☐ as groups
Number of x voxels or groups of voxels:

Define y voxels: ☐ individually ☒ as groups
Number of y voxels or groups of voxels:

Define z voxels: ☒ individually ☐ as groups
Number of z voxels or groups of voxels:

Step 2: Define Media (include medium for region surrounding phantom)
Number of media:

Step 3: Output
☐ **Output .egsphant file**

format readable by
dosxyz_show

- controls output to .egslst file
- might want to have no output for phantom with many voxels

IZSCAN of voxels

Define a group of voxels by entering the voxel indices, then set the direction of the the scan per page. Unless declared here, the default is no output. Click 'Add a group' to define a new group.

from x	to x	from y	to y	from z	to z	scan
<input type="text" value="1"/>	<input type="text" value="6"/>	<input type="text" value="1"/>	<input type="text" value="8"/>	<input type="text" value="1"/>	<input type="text" value="10"/>	<input type="button" value="z-scan per..."/> ▾

Built-in sources

The screenshot shows the 'Inputs' window for DOSXYZnrc. The 'Incident particle' is set to 'photon'. The 'Source type' dropdown menu is open, showing a list of 22 options. A red bracket highlights the first five options: 0, 1, 2, 3, and 4. A tooltip is visible over the 'Source type' dropdown, listing 'electron', 'photon', 'positron', and 'all'.

Phantom definition

If you are using source 2 or 4, you must define the materials in the phantom here first before defining the source.

Define phantom materials: ☐ non-CT data input ☐ phantom created from CT data

Global electron cutoff energy - ECUT (MeV)

Global photon cutoff energy - PCUT (MeV)

Print summary of highest 20 doses

Source parameters

Incident particle:

Source type:

Source type options:

- 0 - Parallel beam from the front
- 1 - Parallel beam from any direction with rectangular collimation
- 2 - Full phase-space source file
- 3 - Point source from the front with rectangular collimation
- 4 - Beam characterization model
- 6 - Uniform isotropically radiating parallelepiped within DOSXYZnrc phantom
- 7 - Parallel rectangular beam from multiple directions
- 8 - Phase-space source from multiple directions
- 9 - BEAM treatment head simulation
- 10 - BEAM simulation source from multiple directions
- 20 - Phase-space source through dynamic library with multiple variable geometry settings
- 21 - Dynamic BEAM simulation source with multiple variable geometry settings

Other parameters:

Noml:

IWAT:

Maxi:

RING:

RING seed 2:

Incident beam size (source 2, 4 or 8):

Run option:

HOWFARLESS:

ESAVE: range rejection done only below this energy (MeV)

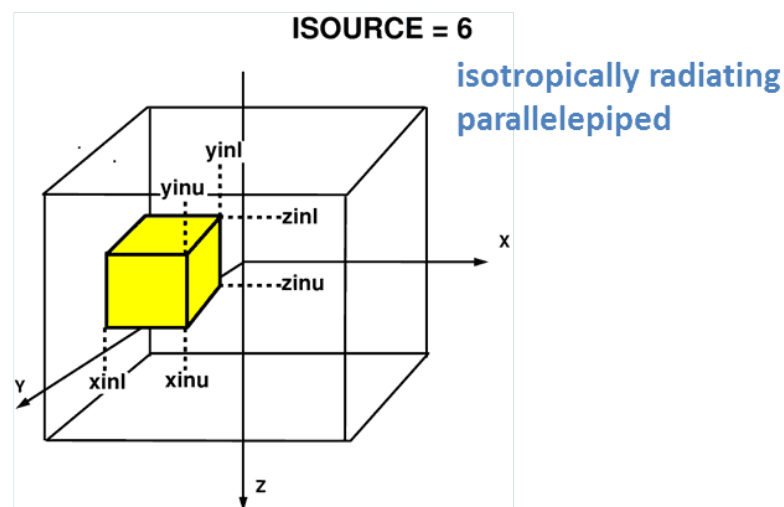
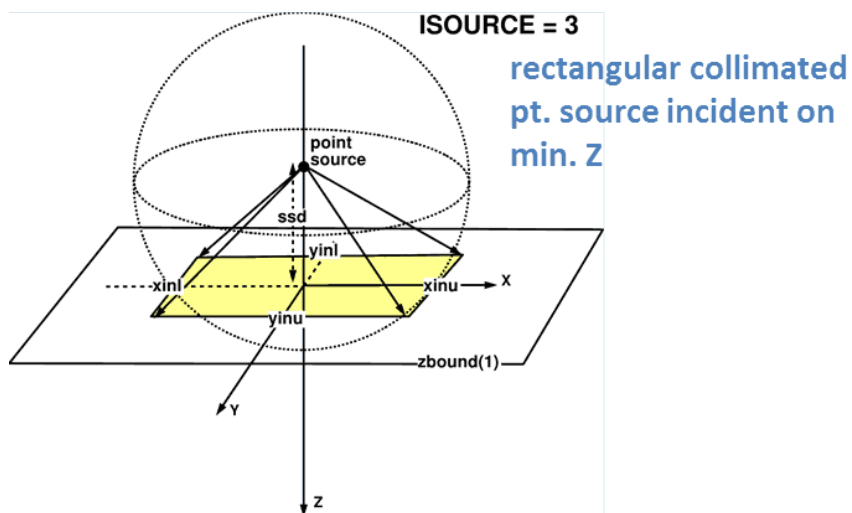
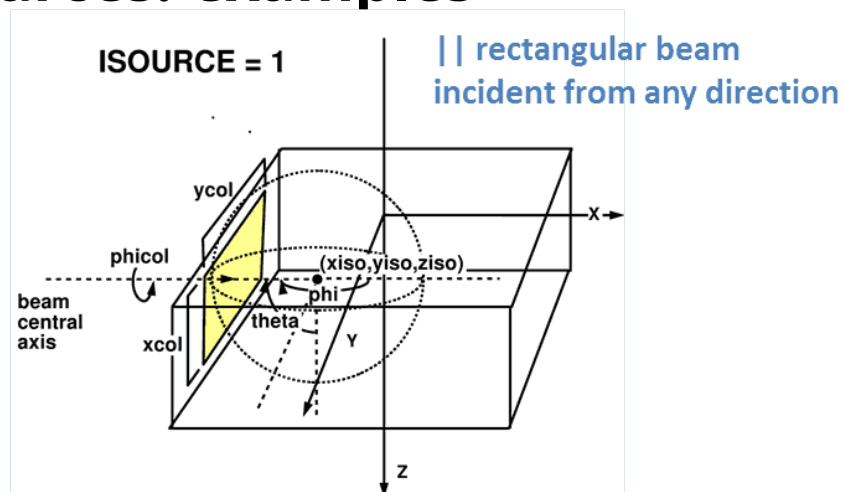
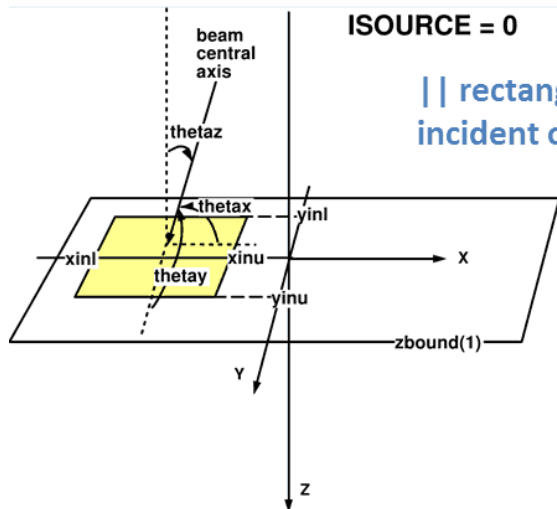
Photon splitting number:

times to recycle each particle in phase space source:

Run job in parallel:

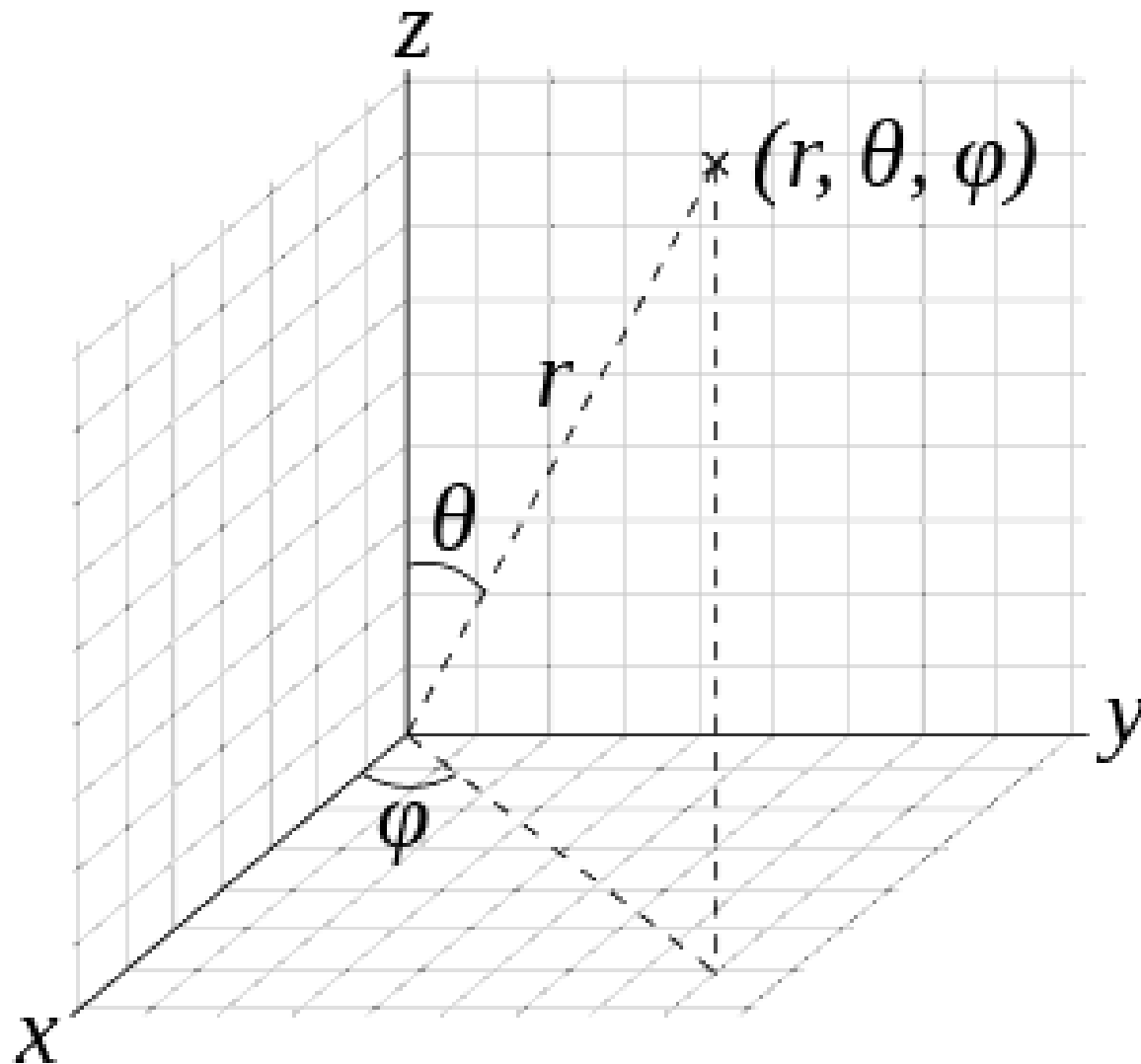
Buttons: Define Media, Edit EGSnrc Parameters, Close

Built-in sources: examples



See DOSXYZnrc manual (PIRS-794) for more details on all these sources!

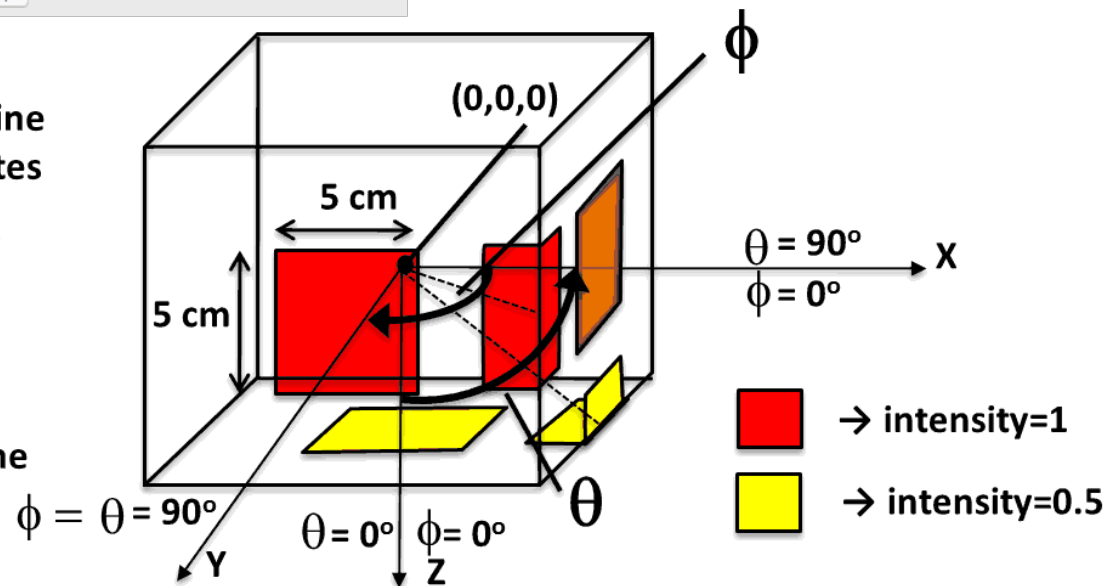
Polar coordinate system



isource=7: parallel beam incident from multiple angles



- isocentre, theta, phi define points in polar coordinates
- theta = angle wrt +Z axis
- phi = angle wrt +X axis
- collimator angle (phicol) rotates the source clockwise in its own plane



Built-in sources (energy spectra)

Set source options

Source 7 - Parallel rectangular beam from multiple directions

x-coordinate of the isocenter: 0
y-coordinate of the isocenter: 0
z-coordinate of the isocenter: 0
Total beam x-width (cm): 5
Total beam y-width (cm): 5
Collimator angle (degrees): 0

☐ theta-phi pairs
☒ theta-phi groups
define theta-phi groups

Specify source beam energy or energy spectrum filename:

☐ monoenergetic
Kinetic energy of beam (MeV):
OR
☒ spectrum

Spectrum filename (complete):
/Users/blakewalters/EGSnrc/HEN_HOUSE/spec
Browse current directory
Browse HEN_HOUSE spectra

OK Help

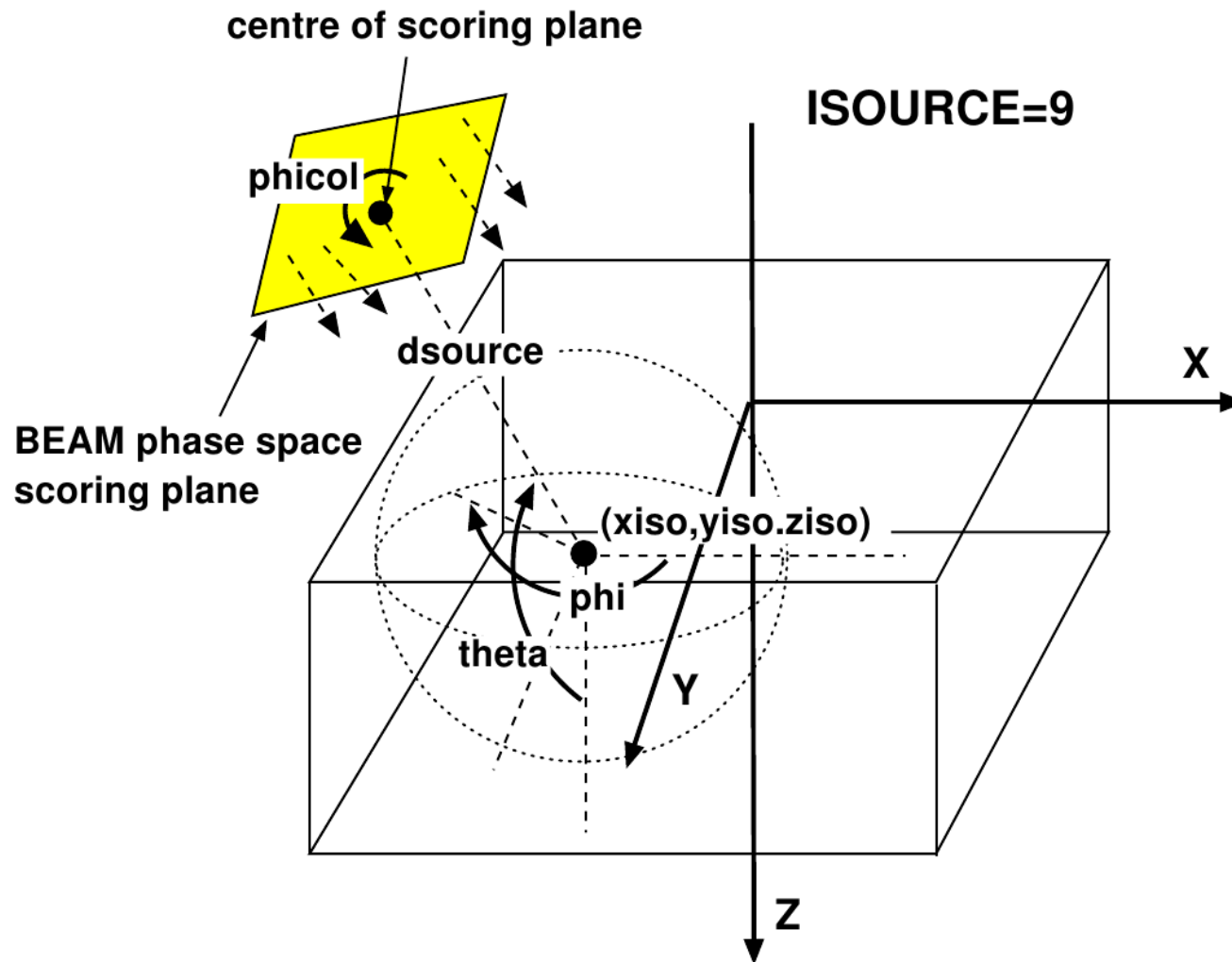
- many sample spectra contained in \$HEN_HOUSE/spectra

spectrum file format:

```
60-Co spectrum Rogers et al 87  
27, 0.01, 0  
0.05, .0000362  
0.10, .00132  
0.15, .01301  
0.20, .02561  
0.25, .03763  
0.30, .03554
```

← title (80 char)
← nbin, Emin, mode (0=cts/bin, 1=cts/MeV)
← Emax(1), prob(1)
← Emax(2), prob(2)

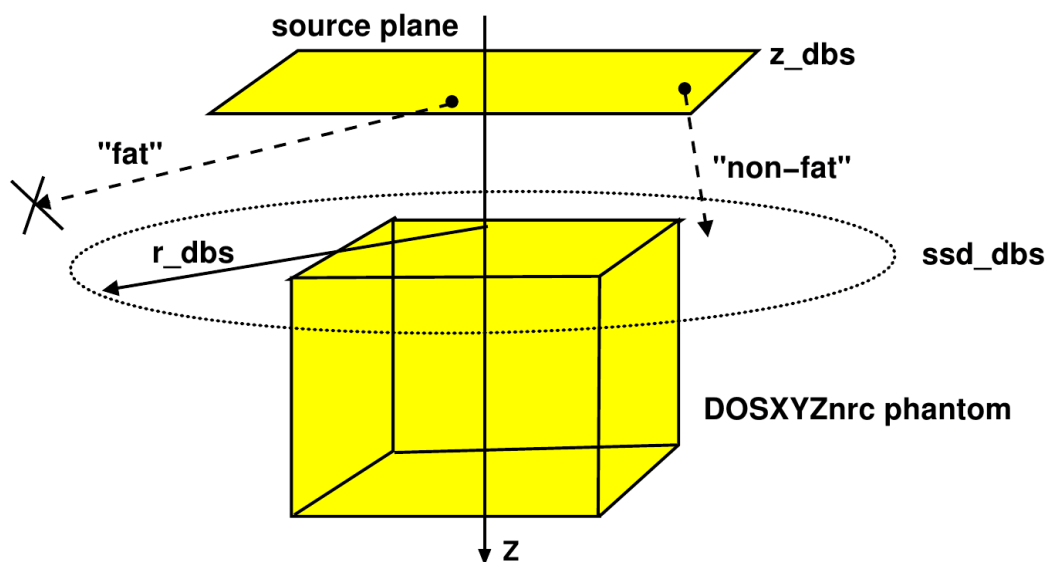
Phase space and BEAM Sources



Other Inputs for Phase Space Sources

Rejecting “fat” photons if DBS used to generate phase space source

- “fat” particles will compromise statistics
- $i_dbs=1$
- r_dbs =DBS splitting radius
- ssd_dbs =SSD at which splitting radius was defined
- $z_dbs=Z$ (in accelerator frame) where phase space file was scored



Other Inputs for Phase Space Sources (cont.)

splitting charged particles (**e_split**)

- Only used with photon splitting **n_split** > 1
- Charged particles split **e_split** times (with weight reduced by $1/\mathbf{e_split}$) as soon as they enter the phantom geometry
- Prevents high-weight contaminant e-'s from compromising dose statistics
- For maximum efficiency, set **e_split=n_split**

Reduce uncertainty by particle redistribution (**ISMMOOTH**)

- On re-use, each particle's (X,Y) and (U,V) are shifted to:
 1. (-X,Y) with (-U,V)
 2. (X,-Y) with (U,-V)
 3. (-X,-Y) with (-U,-V)

Accurate as long as the simulated linear accelerator geometry is symmetric, and the treatment field is centred on the beam axis!

Other Inputs for Phase Space Sources (cont.)

Number of times to recycle each particle before moving on to the next one (NRCYCL)

- avoids restarts \Rightarrow **essential for accurate statistics if no. of histories > no. of particles in phase space source!**
- if set to 0 (and not using only positrons OR filtering incident particles based on LATCH), automatically calculated using:

$$\text{NRCYCL} = \text{INT}\left[\frac{\text{no. of histories}}{\text{no. of particles with selected charge}}\right]$$

- if source restarted more than once or more than 50% of source gets resampled in a restart (particles miss geometry, or are rejected because they are multiple passers or outside BEAM_SIZE), recalculate NRCYCL using formula in manual PIRS-794.

Other inputs for BEAM simulation source

Rejecting “fat” photons if DBS used to generate phase space source

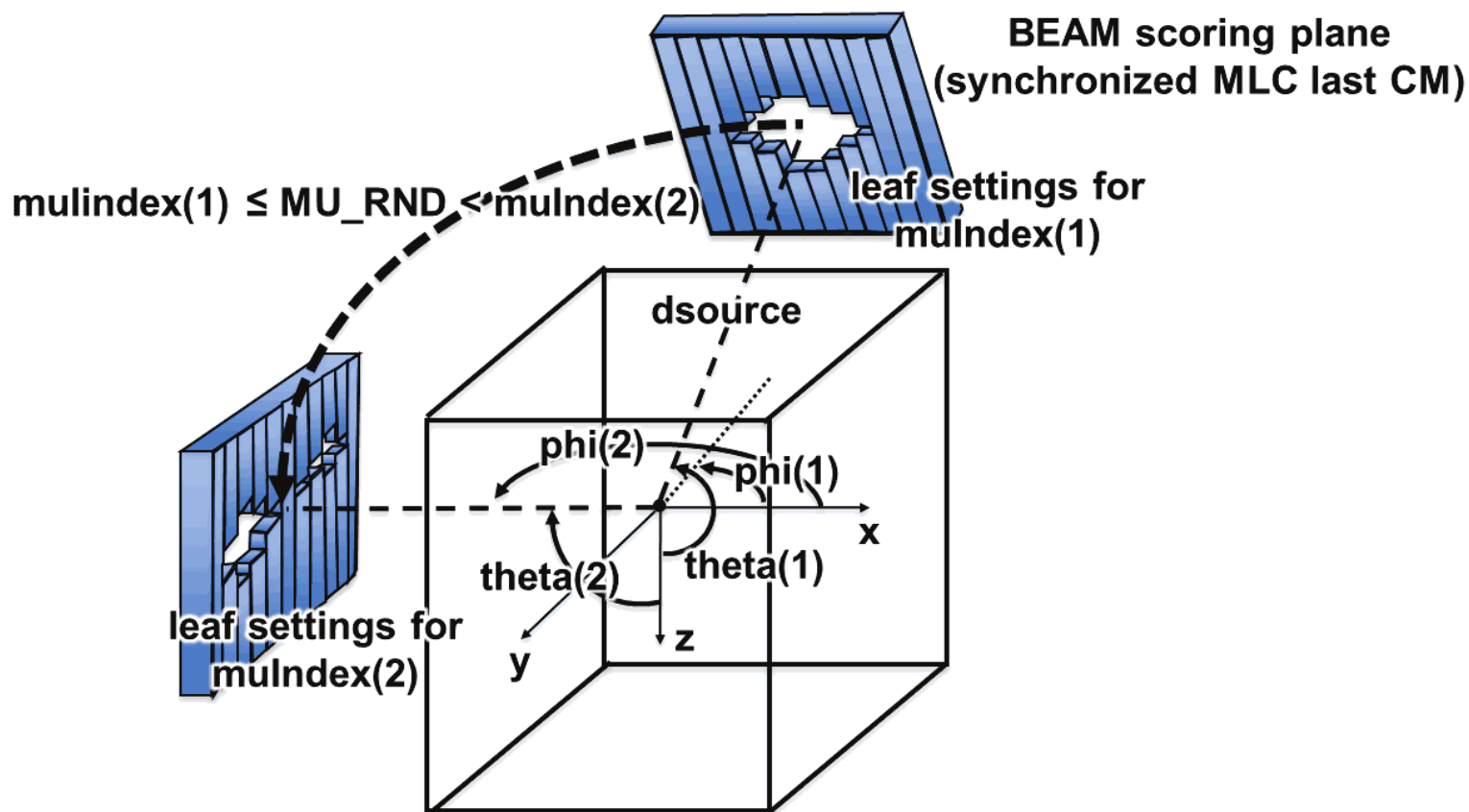
- `i_dbs=1`
- Particle still carries flag indicating if it’s “fat” or not, so this is all we need

Splitting charged particles (`e_split`)

- Same as for phase space source

Synchronized phase space and BEAM sources

- Simulate continuous motion of the source plane between user-defined control points.
- Developed by Tony Popescu and Julio Lobo (PMB 55 (2010) 4431–4443)



Efficiency Increasing Techniques

- Range rejection ([IREJECT](#)): Can save 10 % to 17 % on computing time but for smaller voxels it saves less time (3 % to 4 % for 2.5 mm^3 voxels). For phantoms with some large voxels, the savings will be larger, especially using the [dsurround](#) option.
- Photon splitting ([n_split](#)): Up to $6.5 \times$ efficiency increase depending on energy, field size, and voxel size. Potentially *eliminates need to use phase space files*.
- HOWFARLESS mode ([i_howfarless](#)): improves efficiency by 50 % – 90 % for BEAMnrc photon beams and by a factor of 3 – 5 for monoenergetic electron beams.

Efficiency Increasing Techniques: GUI

The screenshot shows the 'Inputs' window of the DOSXYZnrc GUI. It contains the following sections and parameters:

- Phantom definition**
 - Global electron cutoff energy - ECUT (MeV): []
 - Global photon cutoff energy - PCUT (MeV): []
 - Print summary of highest 20 doses: no
- Source parameters**
 - Incident particle: photon
 - Source type: 2 - Full phase-space source file
- Simulation parameters**
 - Thickness of region outside phantom is: uniform
 - Medium of region outside phantom: AIR700ICRU
 - Phase space output on exiting phantom: none
 - Output restart data: after every batch
 - Range rejection: on
 - ESAVE: range rejection done only below this energy (MeV): []
 - Photon splitting number: 1
 - # times to recyle each particle in phase space source: []
 - Run job in parallel: no

Red arrows point to the following parameters:

- HOWFARLESS: off
- Photon splitting number: 1
- Range rejection: on
- ESAVE: range rejection done only below this energy (MeV): []

Buttons at the bottom: Define Media, Edit EGSnrc Parameters, Close.

dsurround (region surrounding phantom)

- phase space and BEAMnrc simulation sources only

? Thickness of region outside phantom is

? Medium of region outside phantom

VACUUM
H2O700ICRU
ICRPBONE700ICRU
AIR700ICRU

menu contains all media defined with phantom + vacuum

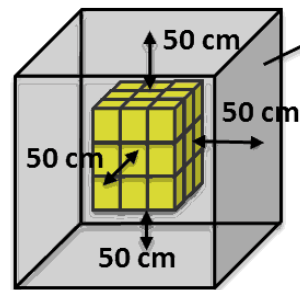
uniform

Region surrounding phantom

Enter the thickness of the surrounding material, in cm.

Thickness

OK



medium surrounding phantom

nonuniform

Region surrounding phantom

Enter the thickness of the region surrounding the phantom in the x, y and z dimensions, in cm.

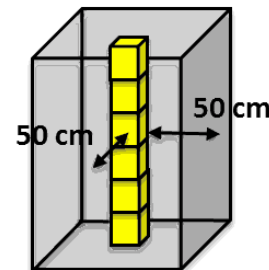
x thickness

y thickness

bottom z thickness

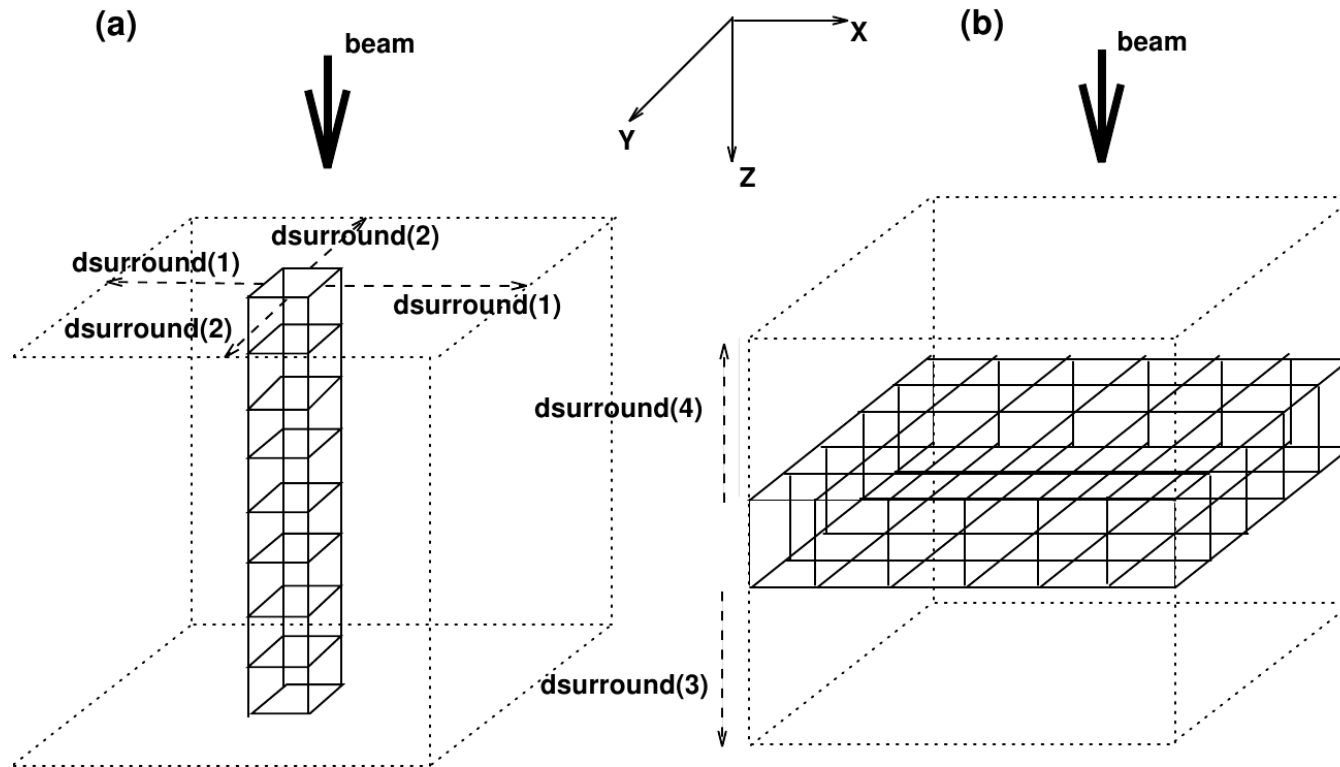
top z thickness

OK



- range rejection can be very efficient

Using non-uniform region surrounding phantom (**dsurround**,**df1ag**)



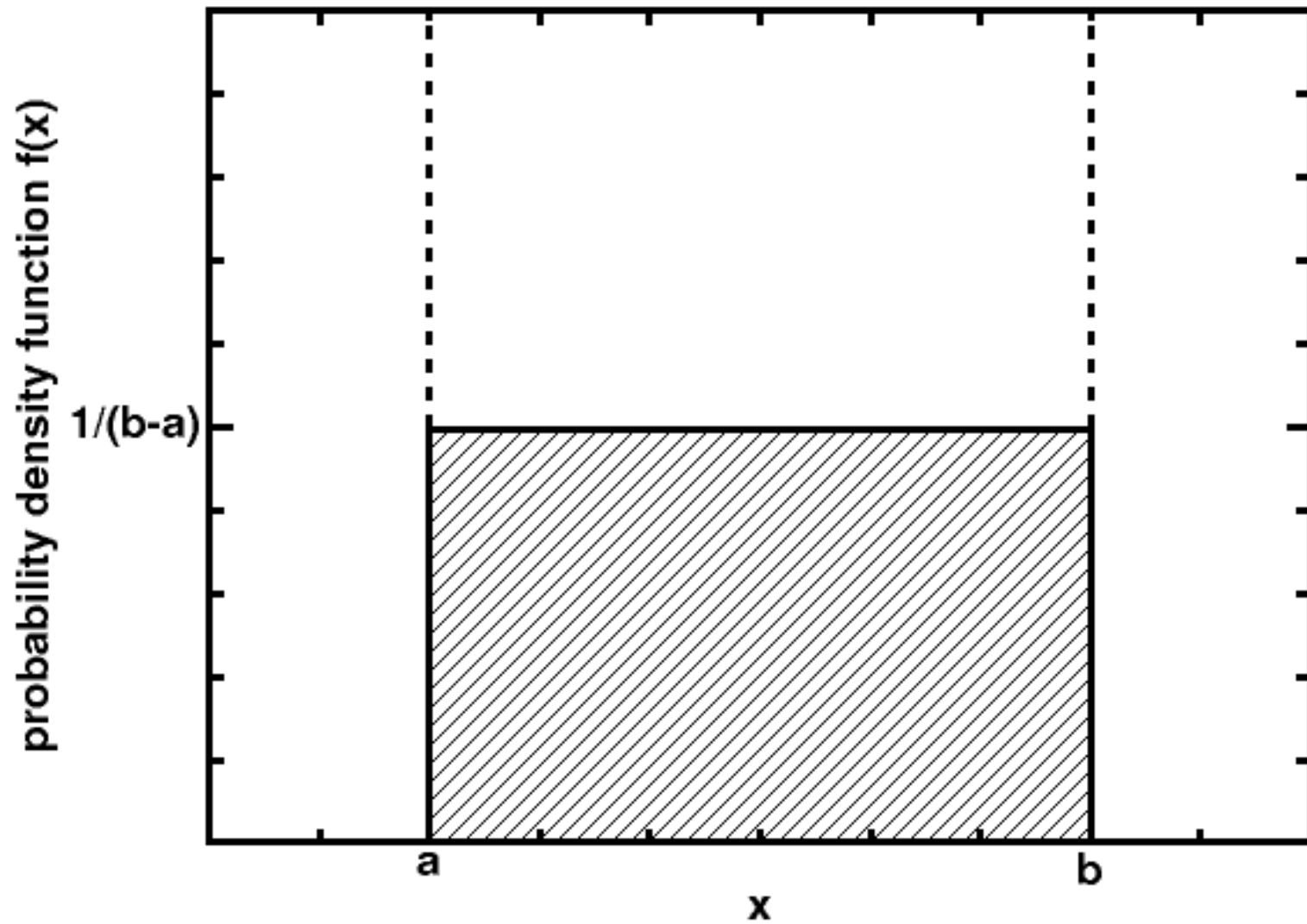
- For phase space source or full BEAM simulation. Makes electron range rejection really effective
- Can decrease simulation time by a factor of 5.5 for electron beams and of 3 for photon beams

Photon splitting

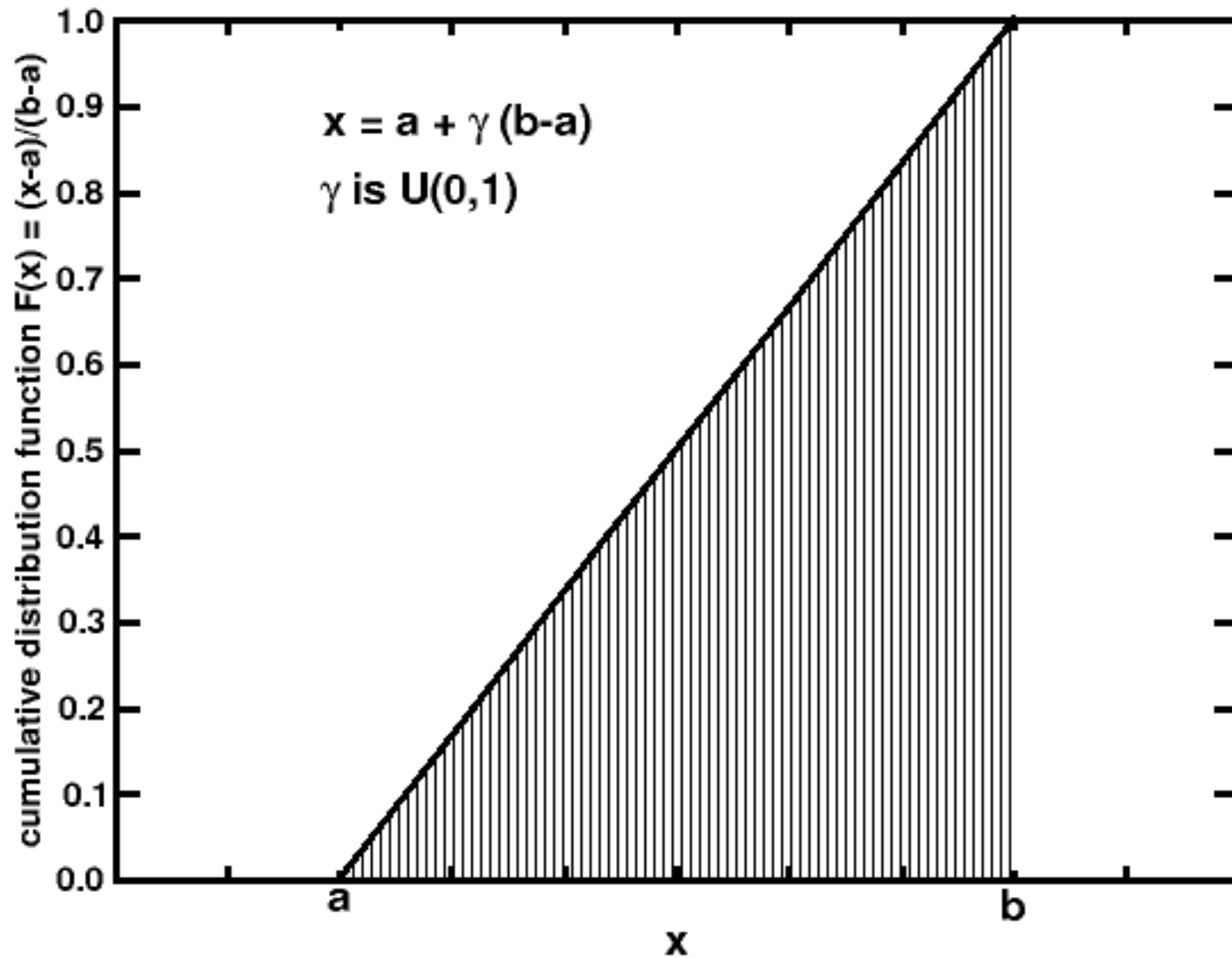
Main ideas:

- **Goal:** Increase efficiency of dose calculations for photon beams
- Split photon into N photons and sample their interaction point from N equidistant intervals of the exponential cumulative distribution function in the interval $(0,1)$
- Transport the N photons simultaneously across the geometry with one geometry tracing
- Play RR with scattered photons and split surviving fat photons
- First introduced for xVMC in Phys. Med. Biol **45** (2000) 2163.
- This technique is used in DOSXYZnrc, CAVRZnrc, and cavity.

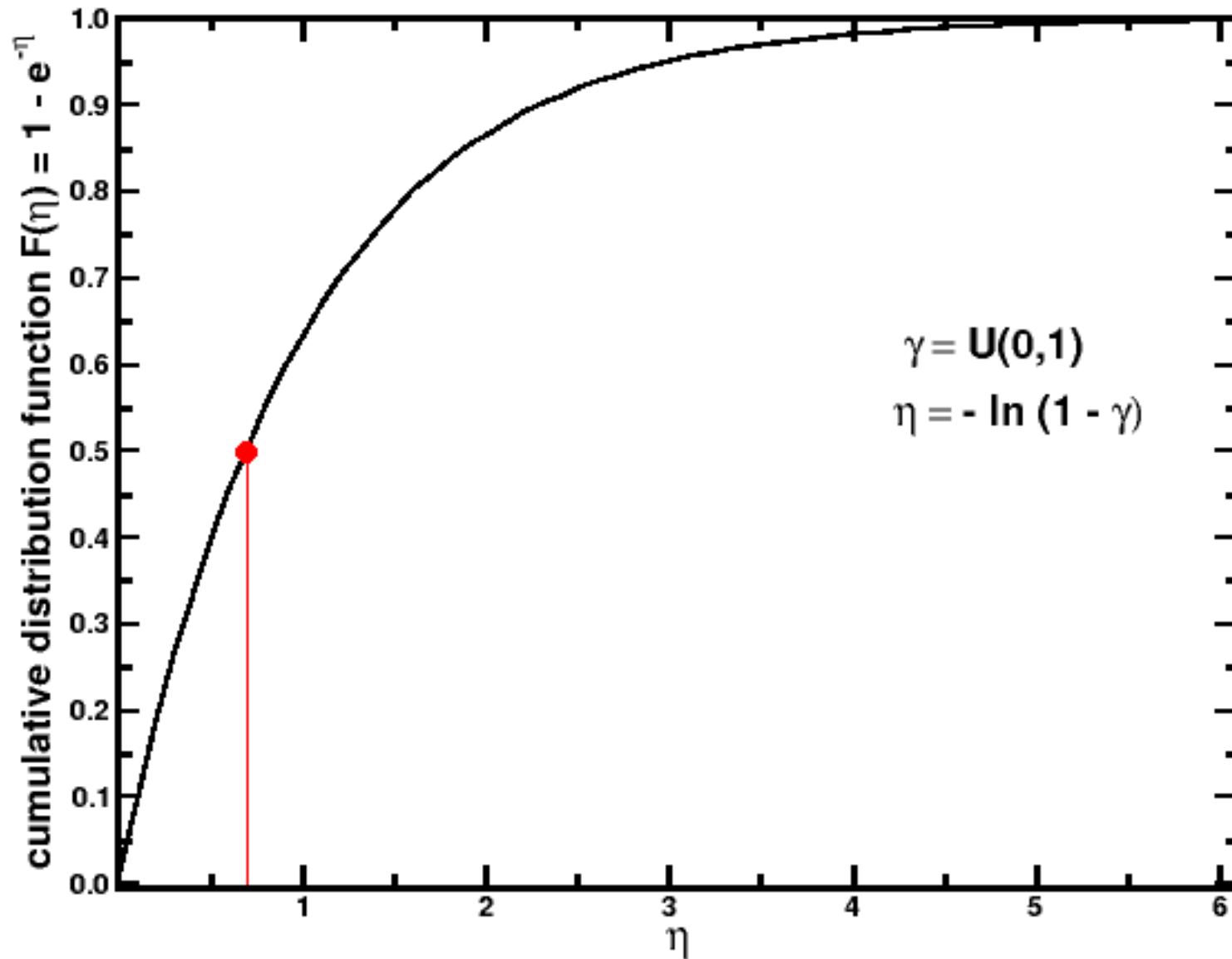
Uniform distribution



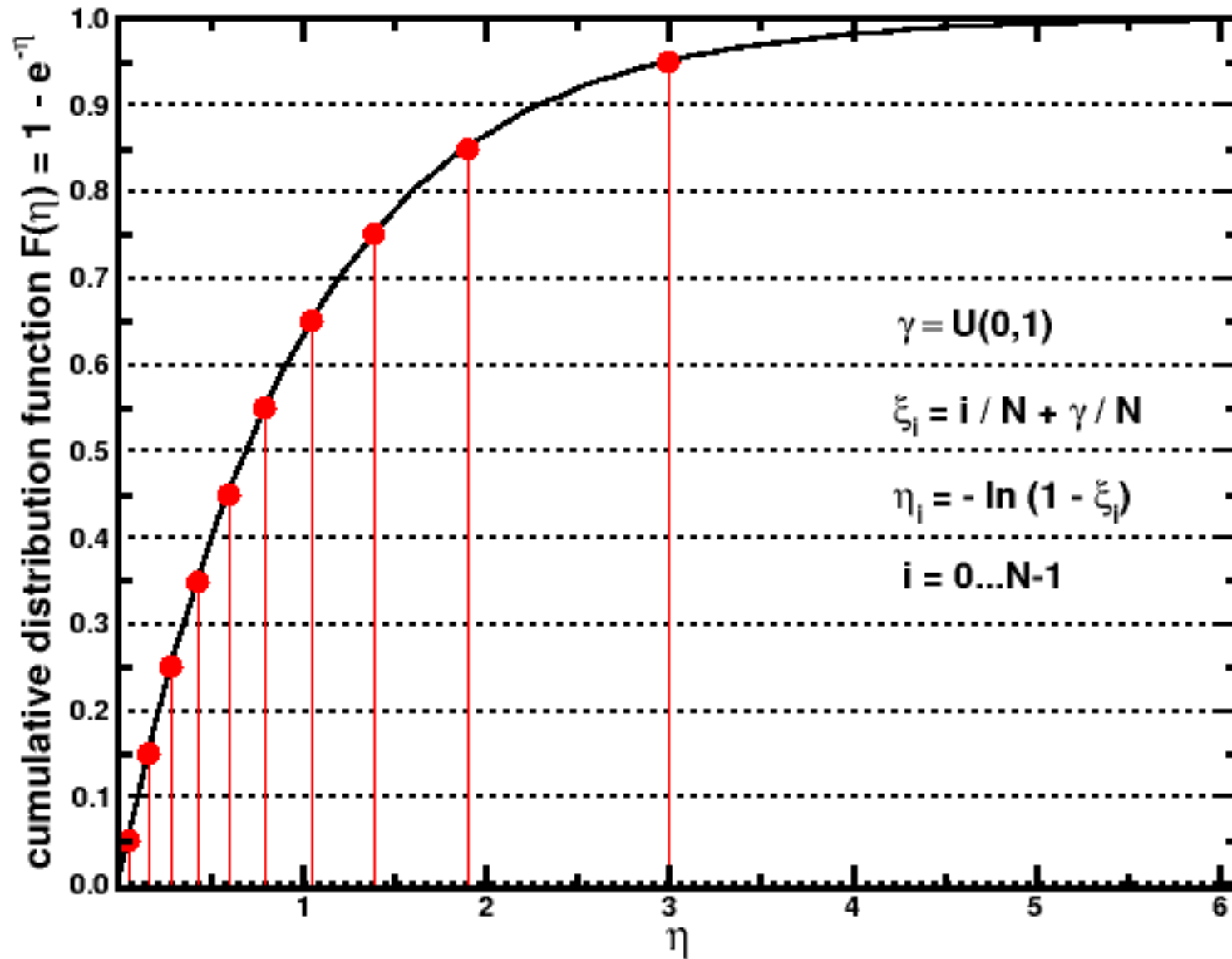
Sampling from the uniform distribution



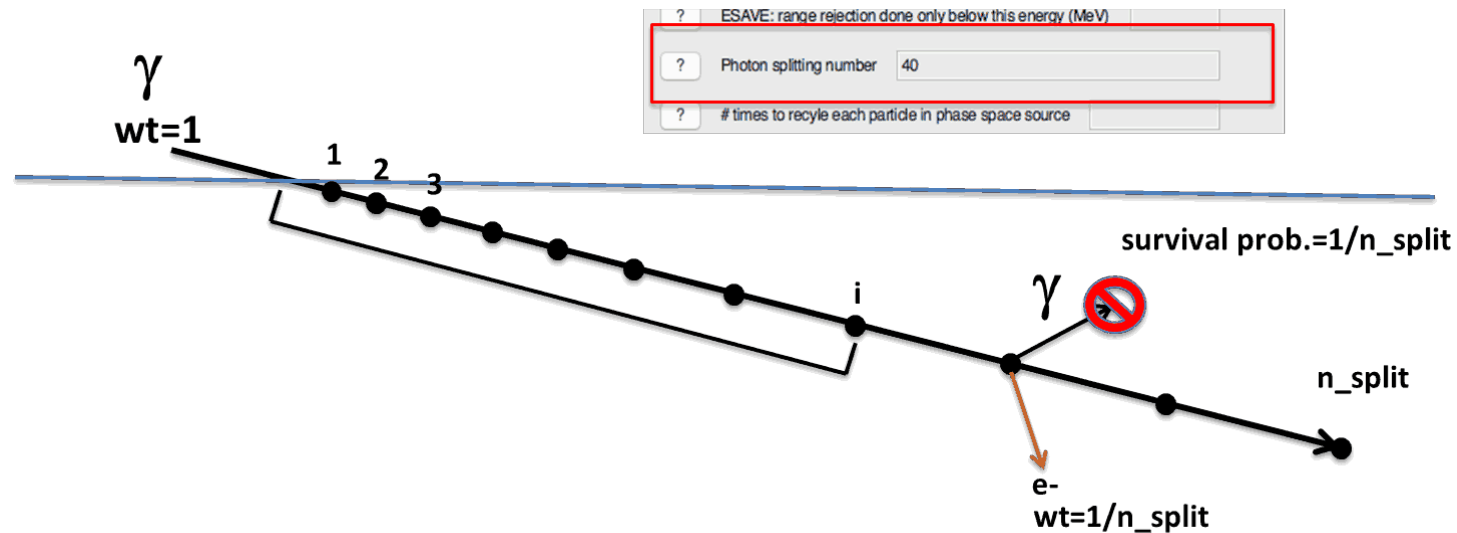
Sampling from the exponential distribution



Photon splitting



Photon splitting: Summary



- We have n_split interactions spread through the phantom and a single photon sets several electrons in motion.
- Electrons have weight $\frac{w_0}{n_split}$, where w_0 is the initial photon's statistical weight.
- RR scattered and bremsstrahlung photons \Rightarrow survivors have weight w_0 and are split again.

Choice of n_split

$$n_{\text{split}} = \frac{n}{1 - e^{-X}}$$

where X is approximately equal to the number of γ -mfp in the geometry of interest and $n \geq 5$. This will increase the number of primary interactions per incident photon by approximately [n_split](#). See also [Kawrakow and Walters, Med. Phys. 33 (2006) 3046–3056]

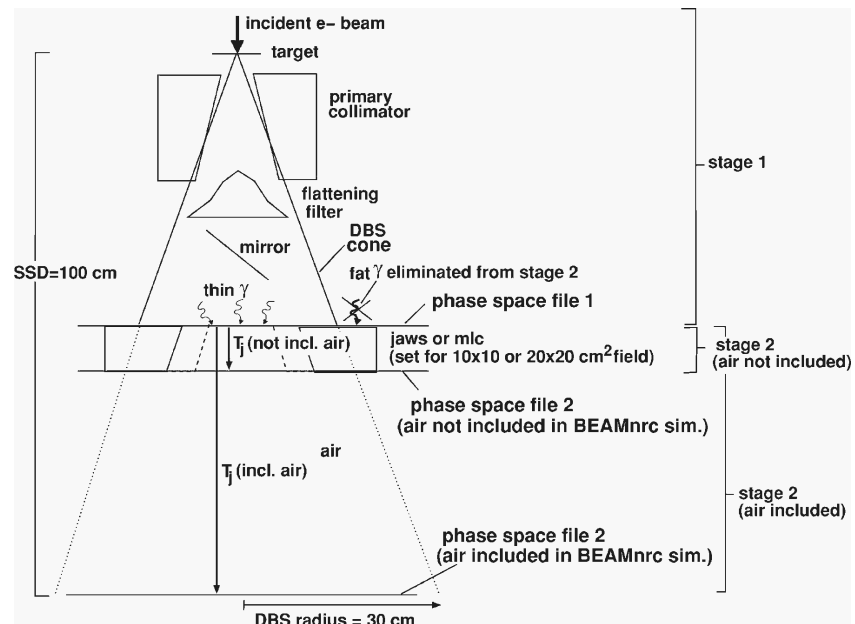
The improvement in efficiency using splitting with photon beams is not great (25%) because photon transport is a relatively small fraction of the computing time, but can become a factor of 6 improvement if electron transport is turned off in the phantom.

Extremely useful if doing a DOSXYZnrc simulation with a BEAMnrc treatment head simulation source or if one includes the time spent for transport through the jaws in the efficiency balance.

Example: Photon splitting in DOSXYZnrc

Approach A

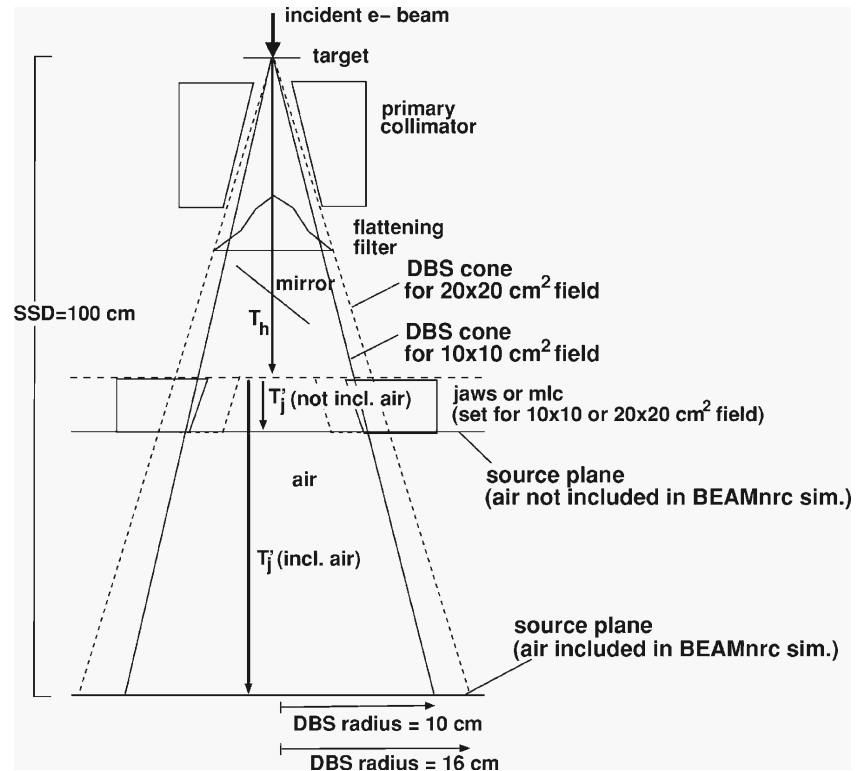
- Create a phase space file above the jaws using BEAMnrc.
- Transport this phase space through the jaws for a given jaws setting and record a second phase space file just above the phantom.
- Use the phase space source in DOSXYZnrc to perform a dose calculation in a water phantom.
- Time to generate phase space above jaws can be excluded because it can be reused.



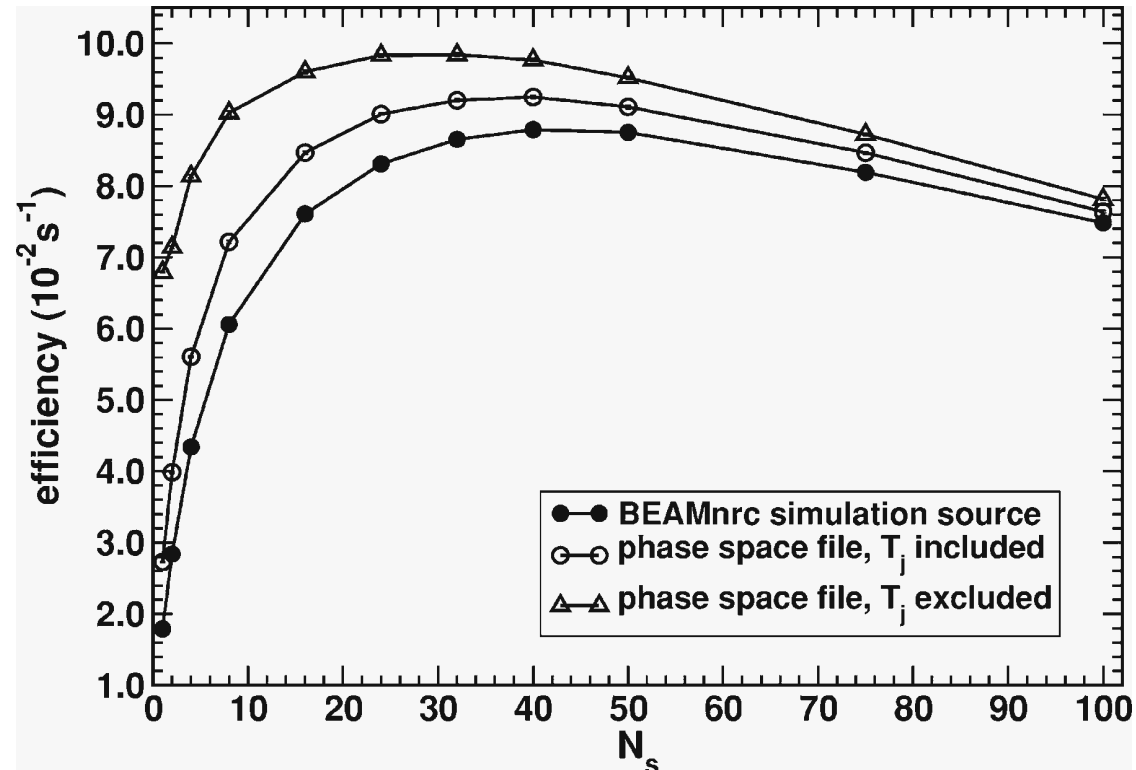
Example: Photon splitting in DOSXYZnrc

Approach B

- Run a DOSXYZnrc simulation using the BEAM simulation source, which performs a full treatment head simulation starting at the bremsstrahlung target.
- The CPU time in this case is the total time (DOSXYZnrc + treatment head simulation).



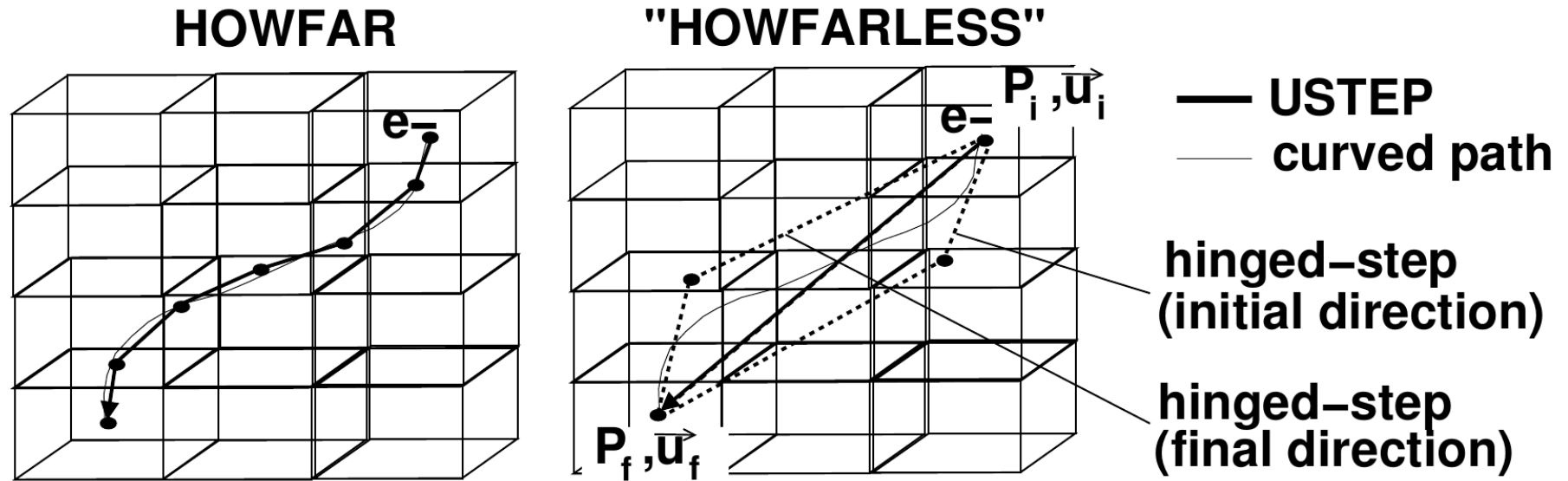
Example: Photon splitting in DOSXYZnrc



- ⇒ With a suitable choice of `n_split` for the DOSXYZnrc simulation and `NBRSPL` for the BEAM simulation the efficiency is comparable for A and B if initial time included in efficiency
- ⇒ Factor of ~ 3 and ~ 5 increase in efficiency by using splitting in DOSXYZnrc with phase-space and BEAMnrc sources, respectively. See [Med. Phys. 33 (2006) 3046–3056] for full details.

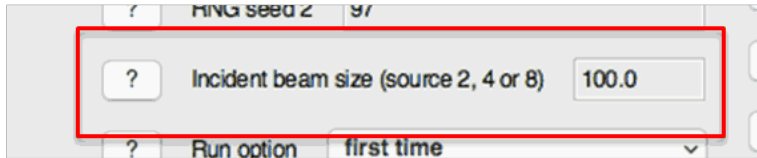
"HOWFARLESS" ($i\text{howfarless}=1$)

Goal: Increase efficiency of *beam commissioning calculations* for homogeneous phantoms

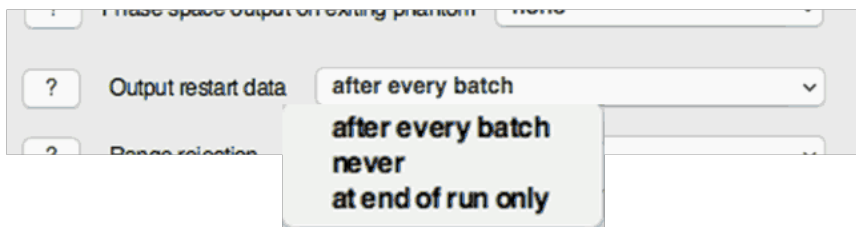
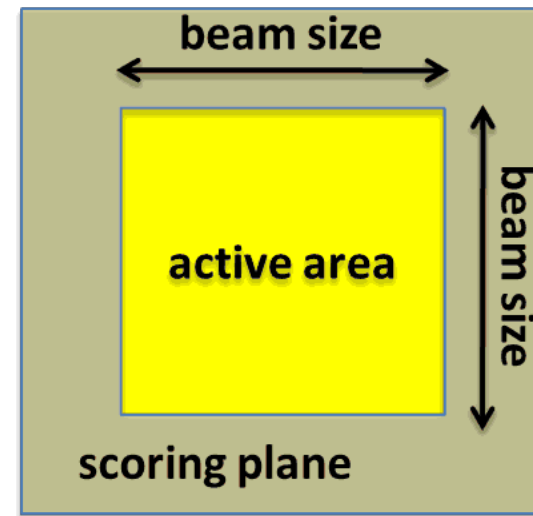


- HOWFAR and HOWNEAR only “consider” the outer boundaries of the phantom when determining step lengths \Rightarrow step length limited by $e\text{step}_{\text{e}}$, max. energy loss/step
- 1:1 ratio of hinged steps based on initial:final direction
- improves efficiency by 50 %–90 % for BEAMnrc photon beams and by a factor of 3-5 for monoenergetic electron beams \Rightarrow highly-recommended

Incident beam size & Output restart data

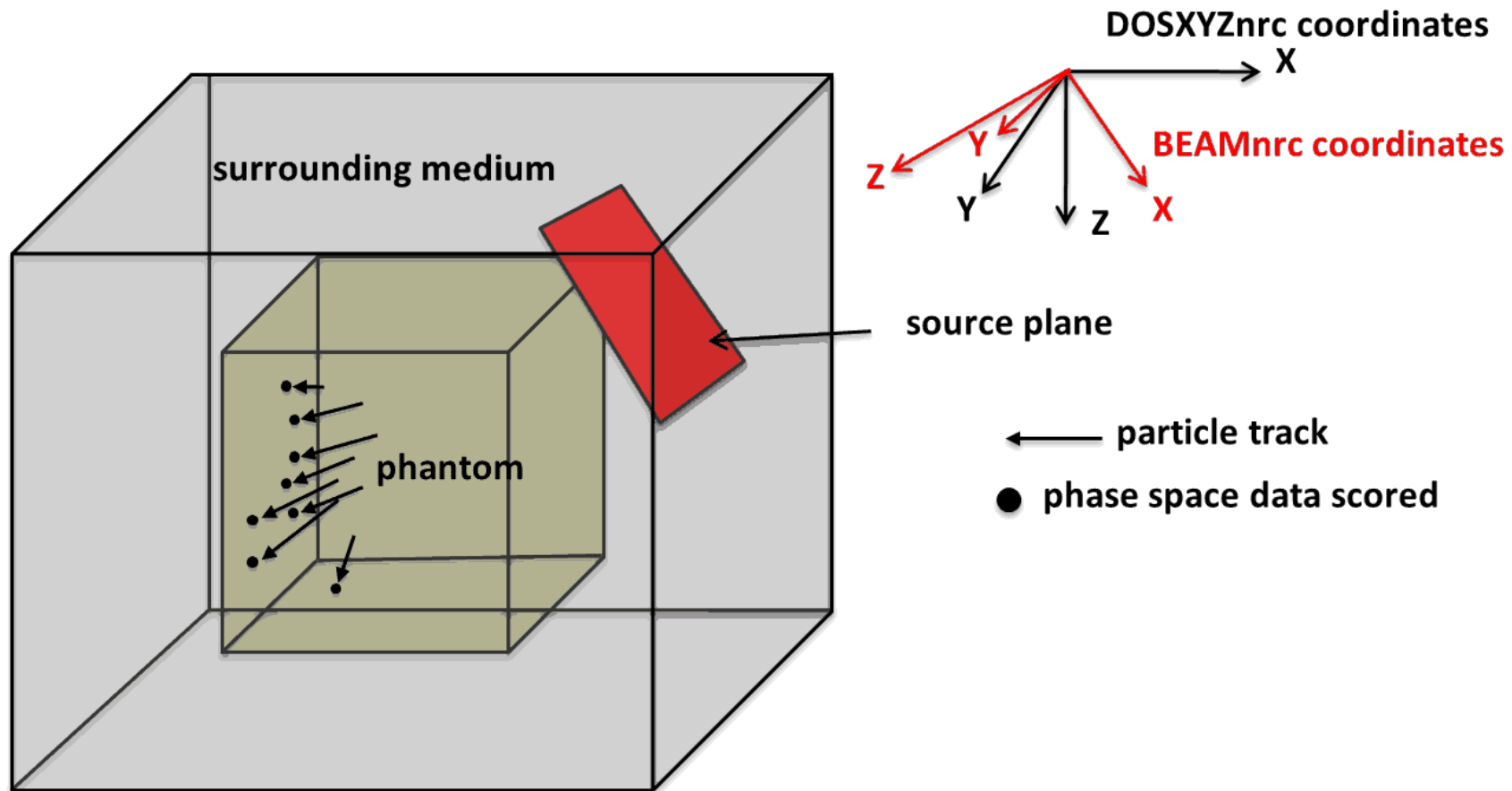


- only for phase space or BEAMnrc simulation source



- binary output to .egsdat file
- necessary for restarts (after crash or to improve statistics)
- but can become CPU time-limiting for phantoms with many voxels → output at end only

Phase space output (BEAMnrc or phase space source)



- can output in DOSXYZnrc or BEAMnrc coordinates
- 3-D phase space (X,Y,Z) scored for each particle → IAEA format only

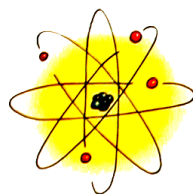
DOSXYZnrc output

- ***3ddose files**: Information about the simulation geometry and the calculation results.
- ***pardose files**: Binary format output for parallel jobs containing enough information to reconstruct a ***.3ddose** file
- ***egslst files**: contain the dose (when asked for) and statistical data but also the information about simulation geometry, number of histories run, CPU time used, etc
- IAEA Phase space files (**i_phsp_out**)
 - **i_phsp_out=1** \Rightarrow particle positions in DOSXYZnrc coordinate system
 - **i_phsp_out=2** \Rightarrow particle positions in BEAMnrc coordinate system
- **STATDOSE**: Reads ***.3ddose** files
 - Visualizes dose profiles using xmgrace plots
 - Dose distributions can be normalized, rebinned
 - Statistical comparisons can be performed if only two or more dose distributions have been read in, and the voxel geometries are identical

DOSXYZnrc output (.3ddose file)

* **.3ddose** files are ASCII files which can be read by [STATDOSE](#) for analysis and plotting

block	data	description
1	nx ny nz	no of voxels in X,Y,Z
2	(xbound(i),i=1,nx+1)	X voxel boundaries
3	(ybound(j),j=1,ny+1)	Y voxel boundaries
4	(zbound(k),k=1,nz+1)	Z voxel boundaries
5	((dose(i,j,k),i=1,nx),j=1,ny),k=1,nz)	Dose in Gy/incident particle or Gy/incident fluence
6	((doseun(i,j,k),i=1,nx),j=1,ny),k=1,nz)	Fractional uncertainty on dose



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Lecture 17

DOSXYZnrc dose calculations in a phantom

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Government
of Canada

Gouvernement
du Canada

