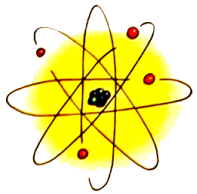




Joint ICTP-IAEA Workshop on Monte Carlo Radiation Transport and Associated Data Needs for Medical Applications
28 October – 8 November 2024
ICTP, Trieste, Italy

Lecture 8

Efficiency-increasing techniques in BEAMnrc

D. W. O. Rogers

Carleton Laboratory for Radiotherapy Physics
Physics Department, Carleton University

Definition of simulation efficiency

$$\varepsilon = \frac{1}{T\sigma^2}$$

- σ is an estimate of the uncertainty of the quantity of interest, e.g., the
  - uncertainty of the photon fluence at the phantom surface around the central axis;
  - uncertainty of the dose at $d_{\max}$;
  - average uncertainty squared in all voxels along the central axis;
  - etc.
- T is the total CPU time required for the calculation.
- As $\sigma^2 \propto 1/N$ and $T \propto N$, the efficiency is independent of the number of histories N used to determine it (except when the uncertainty on the uncertainty is large, which is typically the case for poor statistics).
- Efficiency comparisons only make sense for the same scenario, on the same hardware.

AEIT *vs* VRT

- Both, **A**pproximate **E**fficiency **I**mproving **T**echniques (AEIT) and **V**ariance **R**eduction **T**echniques (VRT) aim to increase the efficiency of a simulation, i.e., to reduce the time needed to obtain a certain statistical uncertainty.

- With **AEIT** the goal is achieved by **using approximations** and therefore the result is not guaranteed to be correct.

  Examples: use of high transport cutoffs and range rejection.

- **VRTs** improve the efficiency **without changing the physics.** When implemented correctly, they are guaranteed to yield the same result as without using these VRTs.

  Examples: photon forcing, particle and interaction splitting, Russian Roulette.

Which type of user are you?

1. I just want to learn how to setup my EGSnrc simulations and I don't care how long they take.
   - I will buy more computers or use a high performance computing facility. Or I will simply wait for my results.

2. Learning how to setup my EGSnrc simulations is my immediate concern, but knowing how to make them run faster is a nice bonus.

3. Life is too short to spend even a minute waiting for Monte Carlo simulation results.

Types 2 and 3 users will benefit greatly from the reminder of this lecture.

Which type of user are you? Redux

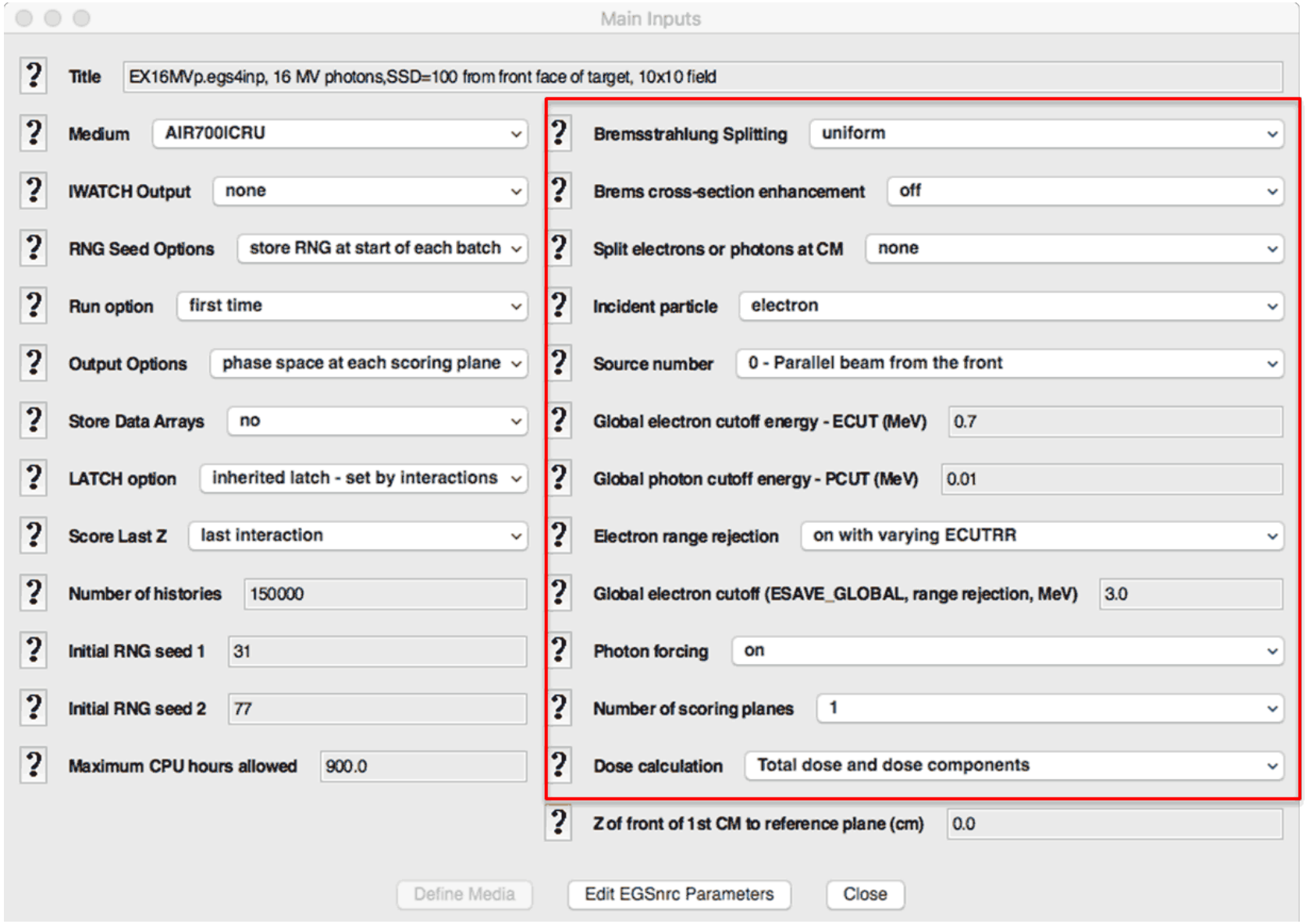
Even for user type 1, who doesn't care about saving time, VRTs might still be necessary:

- Scatter contribution to CBCT scans is a very small portion of the signal. Yet it has a negative impact on the signal's quality, especially in regions of large attenuation. Using a `splitting + RR` technique can give gains of up to 20×10^4 times.
- x-ray production on a W target is very inefficient as less than 1 % of the interactions are bremsstrahlung events. `Directional Bremsstrahling Splitting` allows efficiency gains of up to several 10^6 times.
- Energy deposition in an EBT film's sensitive volume ($\sim$ 30 μm thick) is a very rare event. `Bremsstrahlung Cross section Enhancement` can increase efficiency up to 200 times.

VRT and AEIT in BEAMnrc

- high transport cutoffs and range rejection: **AEIT**
- bremsstrahlung splitting: **VRT**
- particle splitting: **VRT**
- bremsstrahlung cross section enhancement: **VRT**
- forcing photon interactions: **VRT**
- directional source biasing: **VRT**
- compiler choice, optimization options, buy more and faster computers (very cost effective), and use parallel processing

VRT and AEIT in BEAMnrc: GUI inputs



Electron beams *vs.* photon beams

For electron beam simulations, careful selection of transport cutoffs (ECUT,PCUT) and particle production thresholds (AE,AP) and use of range rejection are the only options available to make the simulation run faster.

For photon beam simulations these techniques are less important (compared to DBS), but still significant.

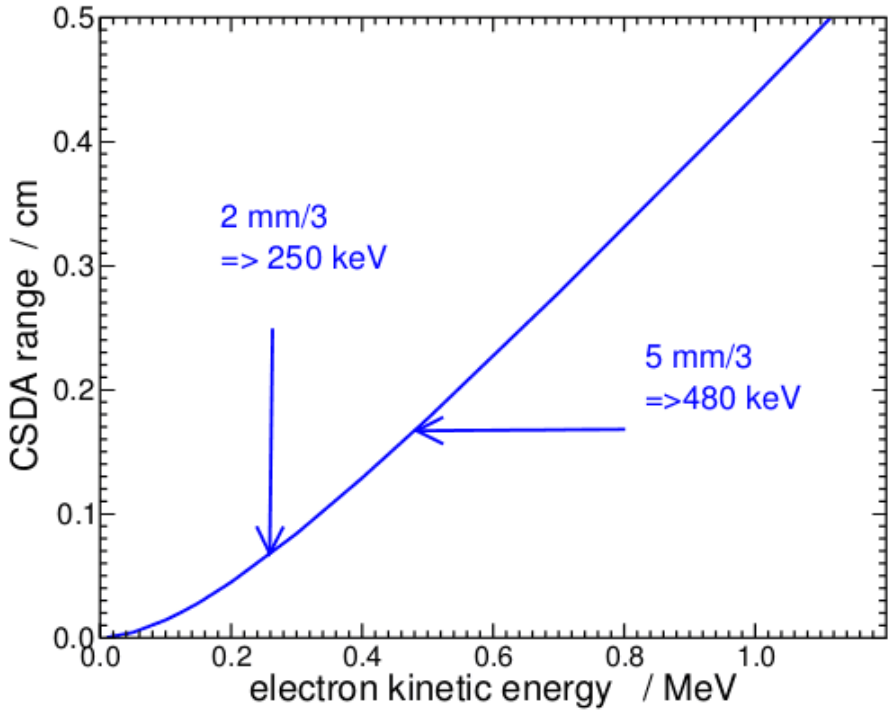
Transport thresholds

The energy at which the transport of an electron is terminated is called ECUT. Same but for photons: PCUT. Note difference to AE, AP.

- **Example 1:**
  - Assume we are interested in 10 keV electrons in the phase space file (cannot imagine why!?)
  - Say there is 50 cm of air below the jaws.
  - e^- needs 200 keV as it leaves the jaws to reach the patient plane.
  - No need to transport e^- with E<721 keV in the the JAWS $\Rightarrow$ set ECUT to 721 keV
- **Example 2:**
  - Say mirror and monitor chamber are thick.
  - e^- in collimator needs > 1 MeV to reach patient plane $\Rightarrow$ set ECUT to 1.5 MeV in flattening filter and above

How do we select ECUT?

Rule of thumb (ROT): range at ECUT should be less than 1/3 dimension of interest.



Good starting point, but in most cases you need to check by using a lower ECUT for a representative case.

Understanding ECUT and PCUT

Use `ECUT = AE, PCUT = AP` , unless there is a clear reason not to do so.

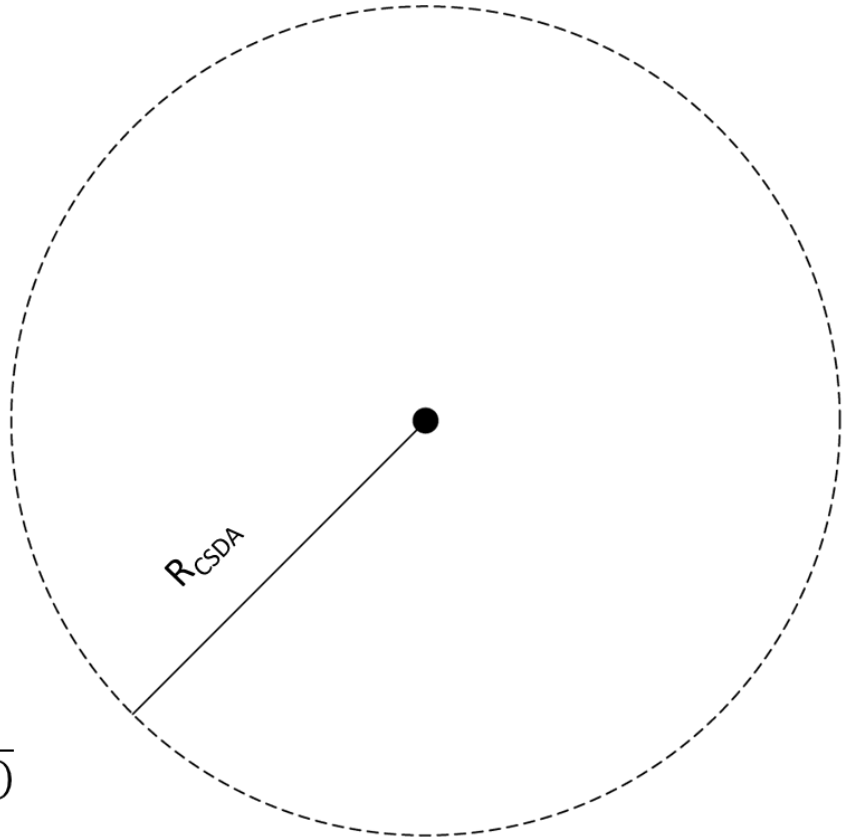
Examples where ECUT $\neq$ AE is useful:

- The calculation of energy spectra through a thin slab (because interested only in the leading portion of the spectrum).
- Want to force all energy that reaches certain region(s) to be deposited locally

For electrons, a better way to terminate a particle's history is to use range rejection, if speed is the only purpose of ECUT > AE .

Range rejection: Saving CPU time during e- transport

region 1



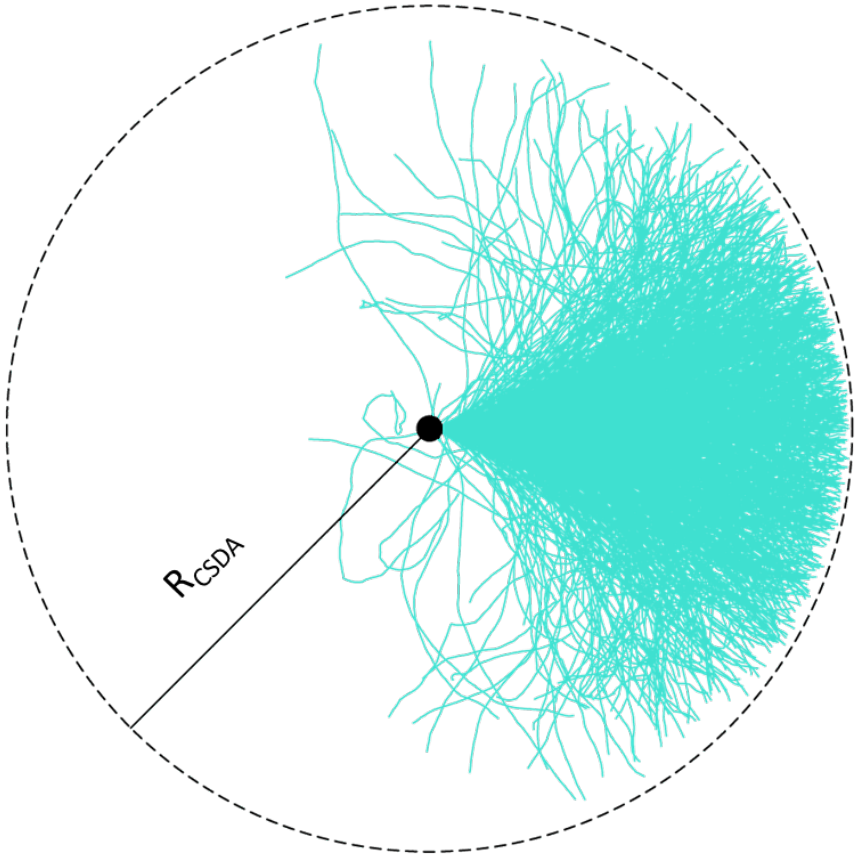
$$R_{CSDA} = \int_{AE}^{E} \frac{dE'}{L(E')}$$

AE ≡ secondary e- creation threshold

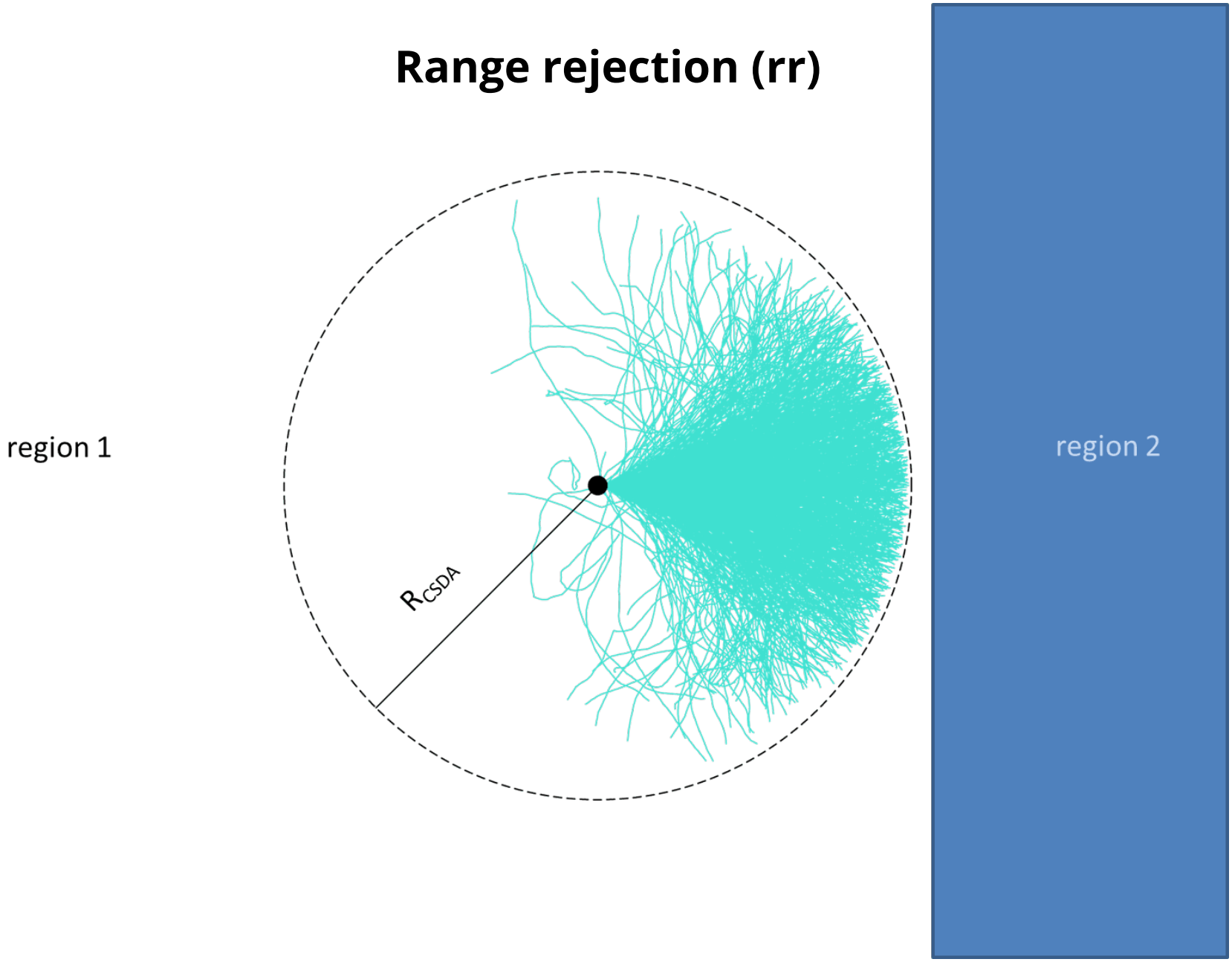
R_{CSDA} ≡ Continuous Slowing Down Approximation e^- Range (longest possible path)

Range rejection (rr)

region 1

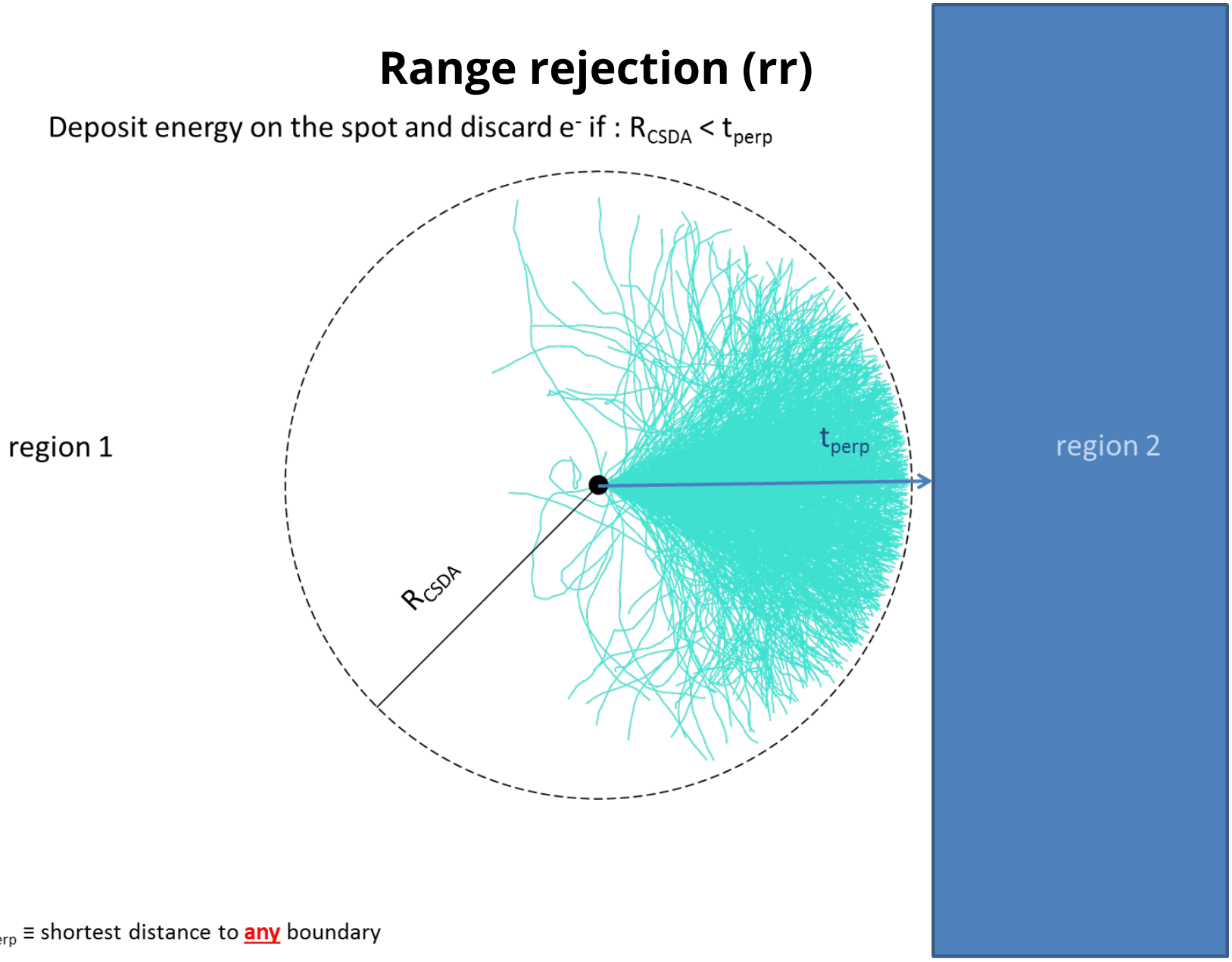


Range rejection (rr)



Range rejection (rr)

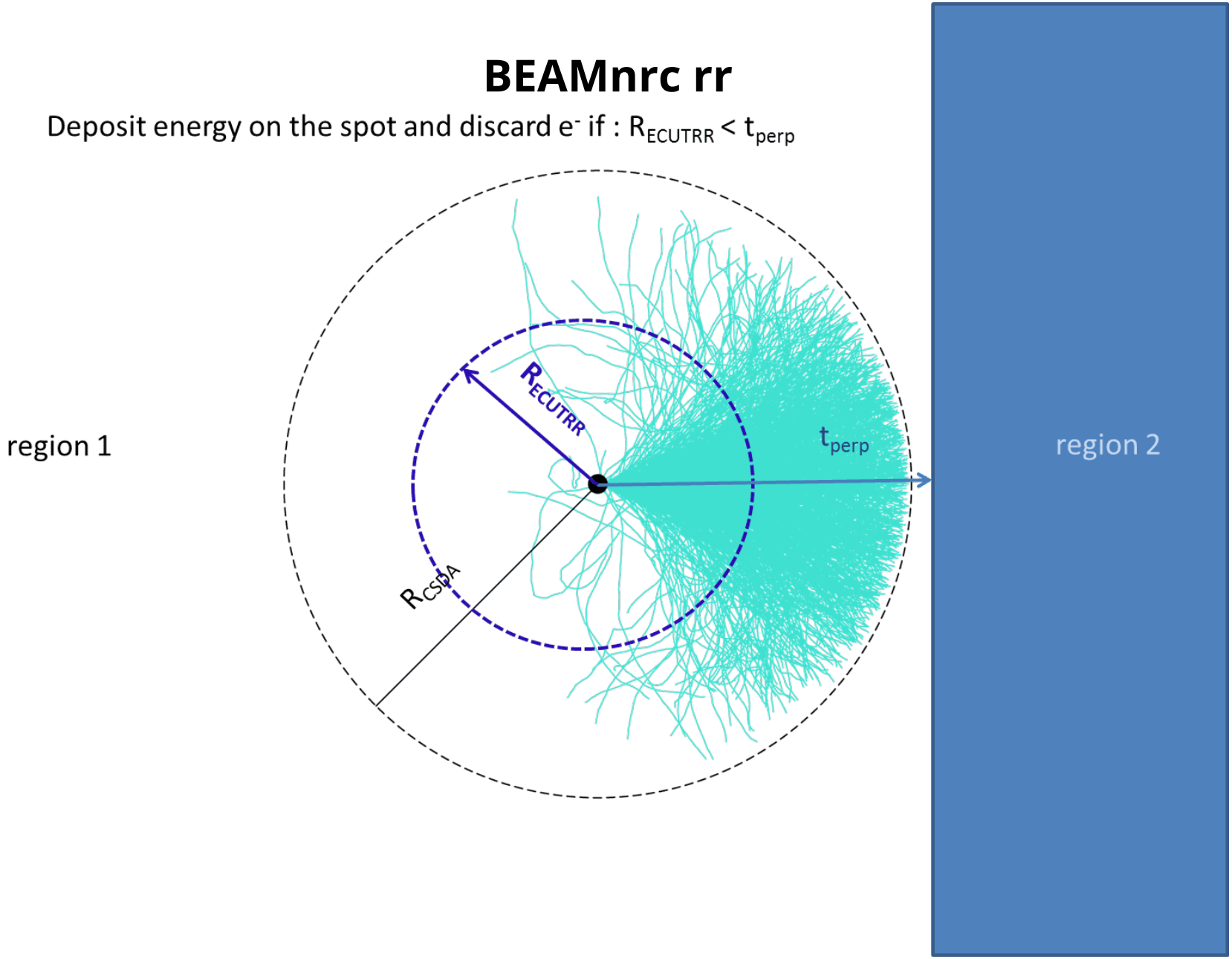
Deposit energy on the spot and discard e^- if : $R_{CSDA} < t_{perp}$



t_{perp} ≡ shortest distance to **any** boundary

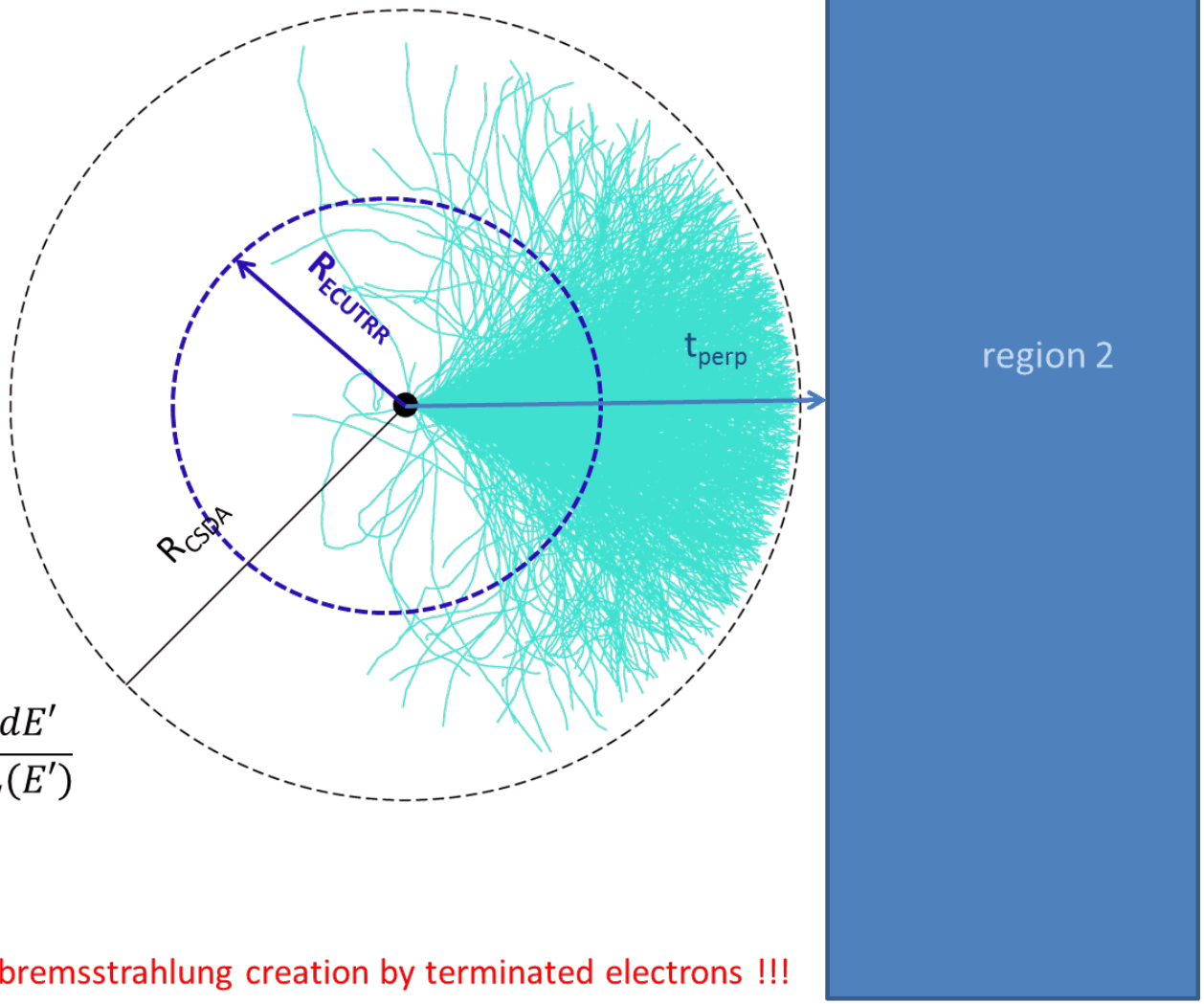
BEAMnrc rr

Deposit energy on the spot and discard e^- if : $R_{ECUTRR} < t_{perp}$



BEAMnrc rr

Deposit energy on the spot and discard e^- if : $R_{ECUTRR} < t_{perp}$

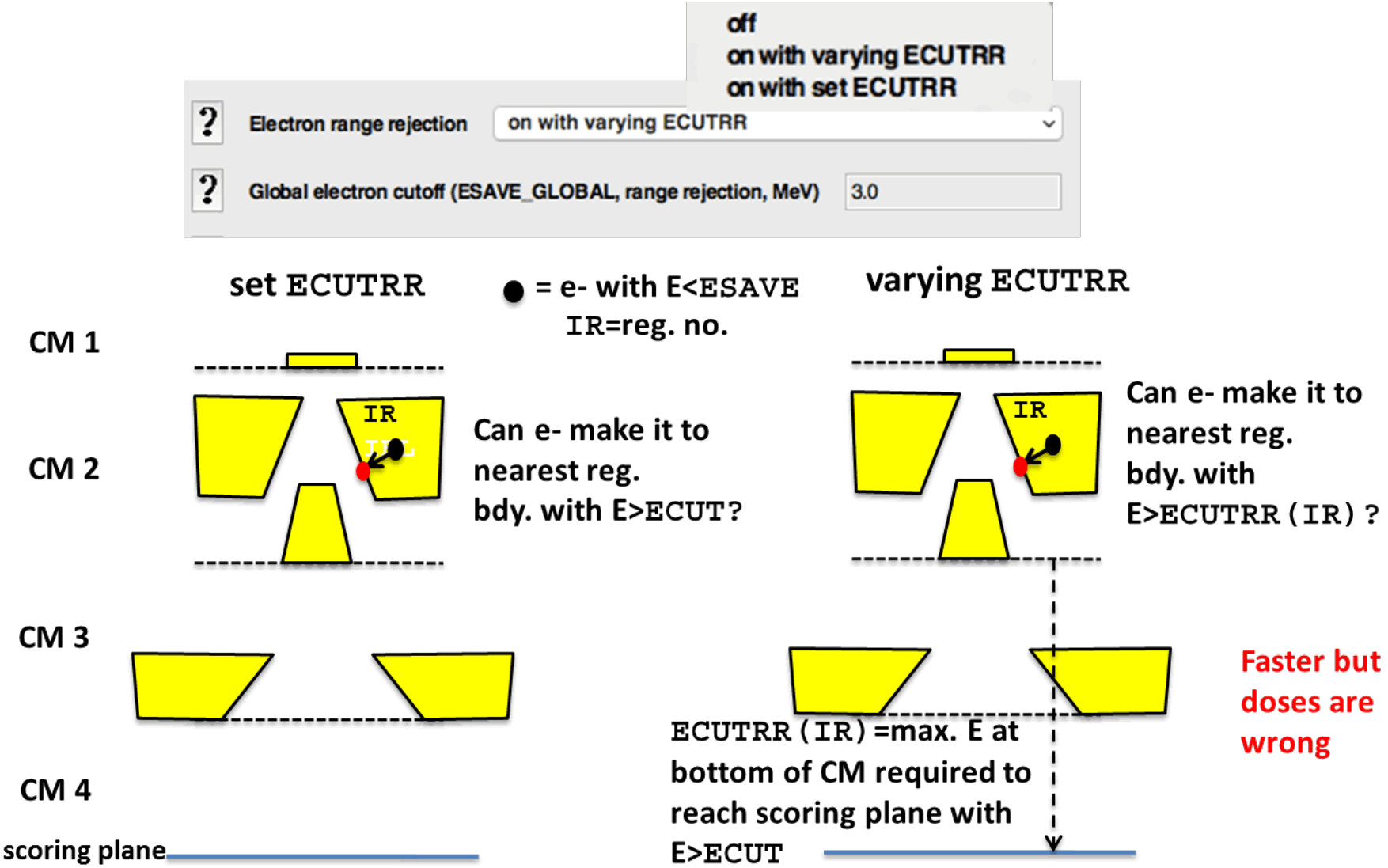


$$R_{ECUTRR} = \int_{ECUTRR}^{E} \frac{dE'}{L(E')}$$

ECUTRR ≥ AE

Approximation: Ignores bremsstrahlung creation by terminated electrons !!!

Range Rejection (rr)



Range Rejection (rr)

Terminate the history of any electron with energy below ESAVE which cannot escape from the current region with an energy above ECUTRR for that region.

Approximation:
Ignores the possibility of bremsstrahlung photon creation by terminated electrons.

Example 1: 20 MeV e^- impinging on tungsten

11% of bremsstrahlung photons are from $E < 5$ MeV, and 2% are from $E < 2$ MeV.

Example 2: 10 MeV e^- impinging on tungsten

37% of bremsstrahlung photons are from $E < 5$ MeV, and 7% are from $E < 2$ MeV.

ESAVE of 2 MeV and 1 MeV respectively ensures an error below 2%.

Note that this is overly conservative since low energy photons also get absorbed.

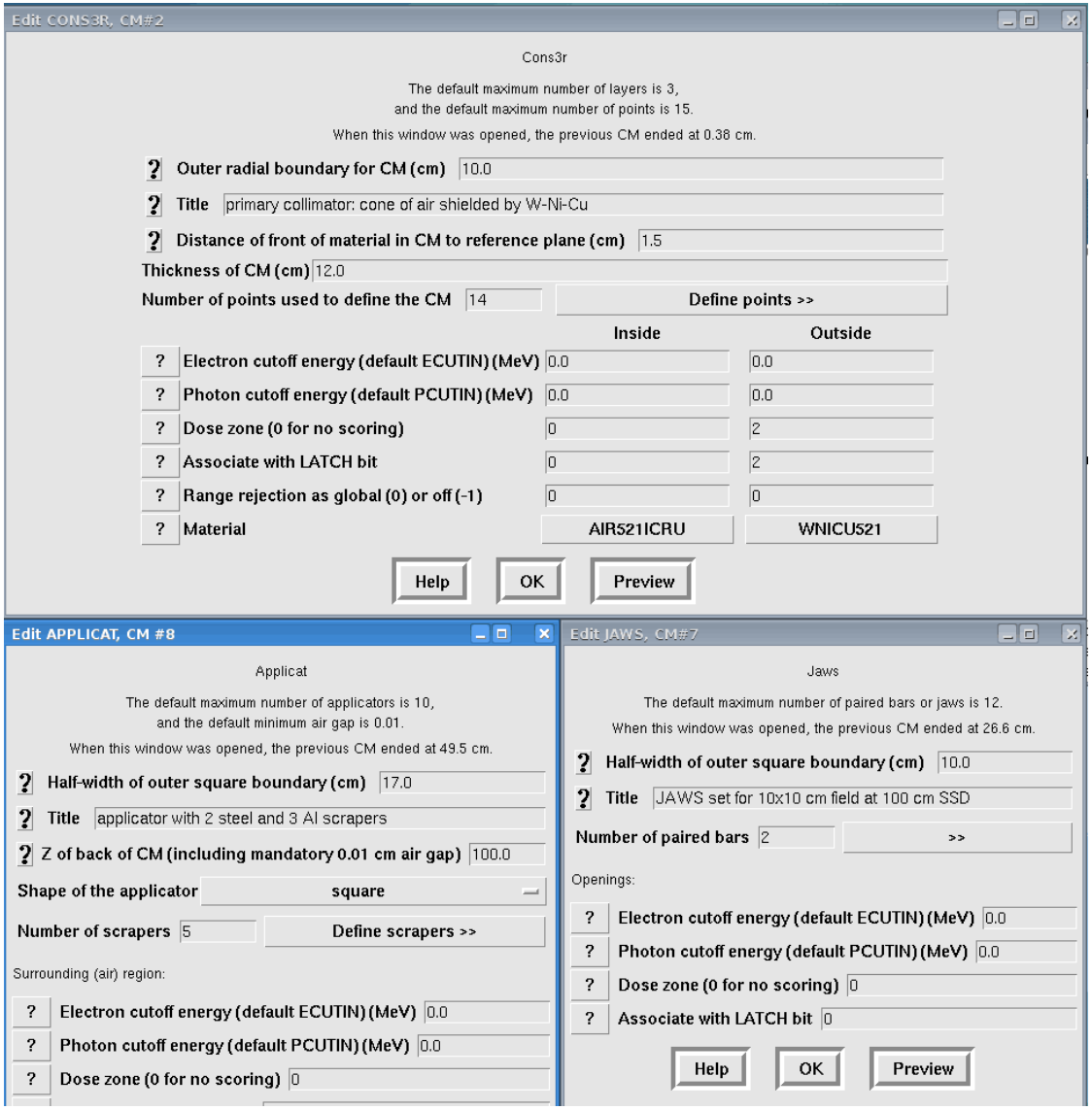
Set ECUTRR Summary (IREJCT_GLOBAL = 2)

- Terminate a charged particle's history (depositing all of its energy at that point) if it cannot leave the current region with an energy larger than ECUT.
- ECUTRR is the electron transport cut-off energy ECUT. For each medium in an accelerator, BEAMnrc calculates a table of ranges to ECUT as a function of electron energy.
- These ranges are calculated using restricted stopping powers and, thus, represent the longest possible paths to cutoff energy.

Varying ECUTRR Summary (IREJCT_GLOBAL = 1)

- Range rejection performed with respect to whether or not a charged particle can reach the bottom of the accelerator and still have energy ECUT at the base of the accelerator.
- ECUTRR is the minimum energy a charged particle can have as it leaves the current region and still reach the bottom of the accelerator with an energy greater than ECUT.
- ECUTRR is calculated for each region; if the range to ECUTRR is less than the distance to the nearest region boundary, the particle is terminated and energy deposited in the current region.
- Can save more time, but can only be used if there is only 1 scoring plane and it is at the very bottom of the accelerator.
- One can approximate `IREJCT_GLOBAL=1` for other situations by carefully selecting ECUT for different regions throughout the accelerator.

GUI: Transport threshold selection (ECUT, PCUT)



ESAVE Variation

CPU times for 18 MeV e$^-$ linac using automatic ECUTRR (BEAM paper).

Case	AE (MeV)	ECUT (MeV)	ESAVE (MeV)	cpu s per history	total to file/inc e$^-$	e$^-$ per 100 inc e$^-$	γ per 100 inc e$^-$
1	0.700	0.700	5.0	**0.0124**	0.417	9.15	32.4
3	0.700	0.700	2.0	**0.0125**	0.420	9.07	32.8
4	0.700	0.700	0.0	**0.0249**	0.421	9.03	33.0
7	0.521	0.521	5.0	**0.0538**	0.414	8.79	32.6
8	0.521	0.521	2.0	**0.0631**	0.416	8.83	32.7
9	0.521	0.521	0.0	**0.300**	0.421	8.94	33.1

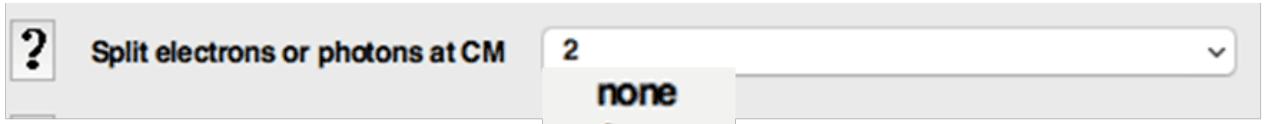
$\Rightarrow$ you must have a very good reason for using AE=521 keV (or a ridiculous amount of computing power).

Examples of very good reasons: you are interested in a very detailed spectrum of the electron emerging from an electron accelerator or you want to calculate the dose to a very thin-walled ion chamber directly at the phantom surface.

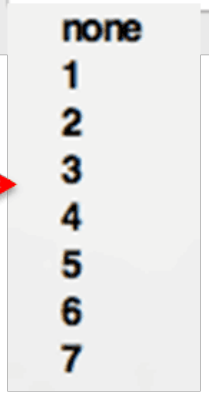
Particle splitting

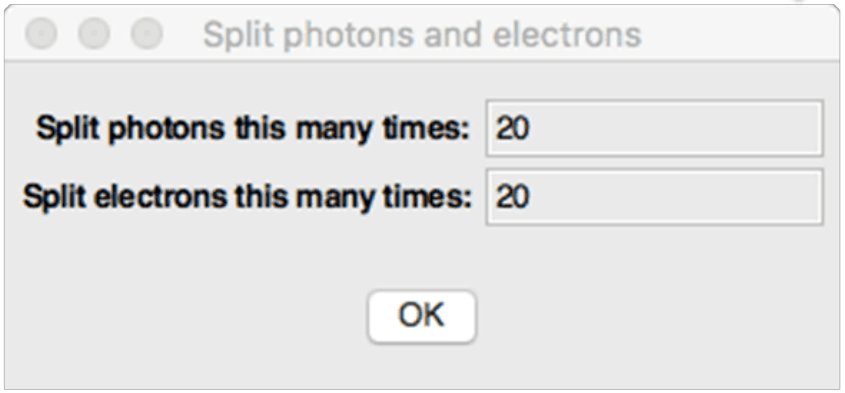
- In Monte Carlo, one can *split* a particle into N identical particles at any time.
- Each of the daughter particles gets $1/N$ of the statistical weight of the original particle, to ensure that the physics remains unaffected.
- Each daughter particle can then be transported separately, thus improving the information gain.
- Typical application: particles arriving in a region that is only rarely visited during a simulation or in combination with Russian Roulette.
- Particle splitting is a **true VRT:** it does not modify the physics in any way (statistically speaking).

Particle splitting: GUI inputs



Split particles on entering this CM no.





- wt of resultant particles = 1/(splitting no.)
- should have e- splitting no. ≈ photon splitting no. to prevent large disparities in particle wt → poor dose statistics

Mainly useful to improve dose statistics in phantoms (CHAMBER)

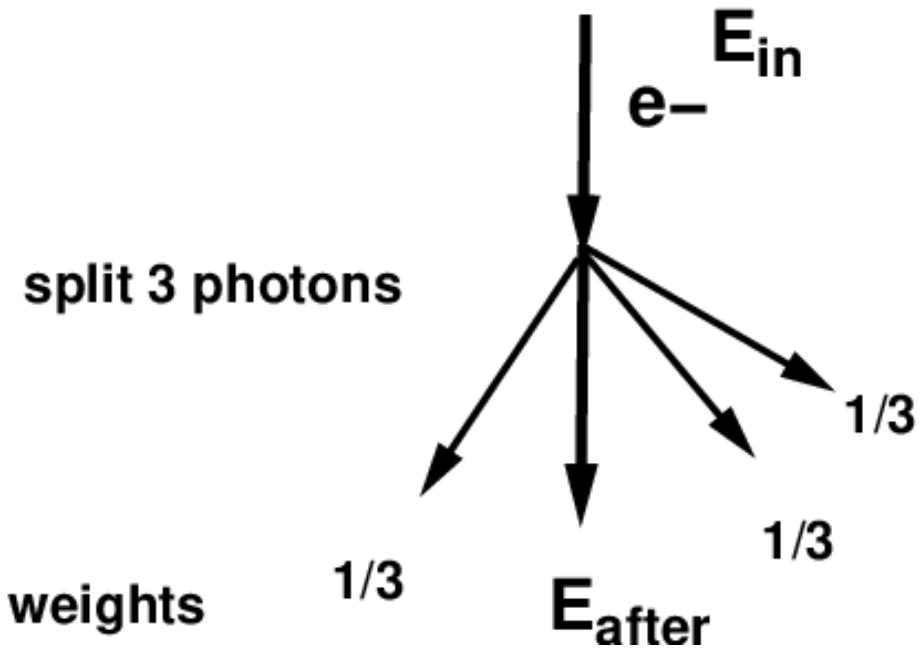
Russian Roulette (RR)

- Russian Roulette (RR) is the "inverse" of particle splitting: at any time one can terminate a particle trajectory with a given probability p (i.e., play a RR game with the particle, where the *survival* probability is p).
- If the particle *survives*, its statistical weight is increased by $1/p$.
- A particle surviving a RR game represents all other particles killed in the game.
- Typical application: avoid transporting particles that contribute nothing or very little to the quantity of interest.
- RR is a **true VRT:** it does not modify the physics in any way.
- Combining RR with rr removes the approximation in rr: play RR rather than terminate history.

Bremsstrahlung splitting

- In a simulation without any VRT most of the time is spent tracking electrons. For a photon beam one is mostly interested in the photons
- By splitting bremsstrahlung interactions the number of γ's reaching the scoring plane per simulated incident e^- can be increased dramatically.
- There are three splitting options available in EGSnrc/BEAMnrc:
  - Uniform Bremsstrahlung Splitting (UBS): $\epsilon \uparrow$ by up to a factor of 25 (with RR on) or 7 (with RR off) compared to no splitting (in EGSnrc and BEAMnrc)
  - Directional Bremsstrahlung Splitting (DBS):
    * Available since BEAMnrc05
    * $\epsilon \uparrow$ by up to a factor of 500 (e-splitting off or 150 (e-splitting on) for MV beams
    * $\epsilon \uparrow$ by up to a factor of 10^6 for kV beams
  - Selective Bremsstrahlung Splitting (SBS): Abandoned.

Bremsstrahlung splitting

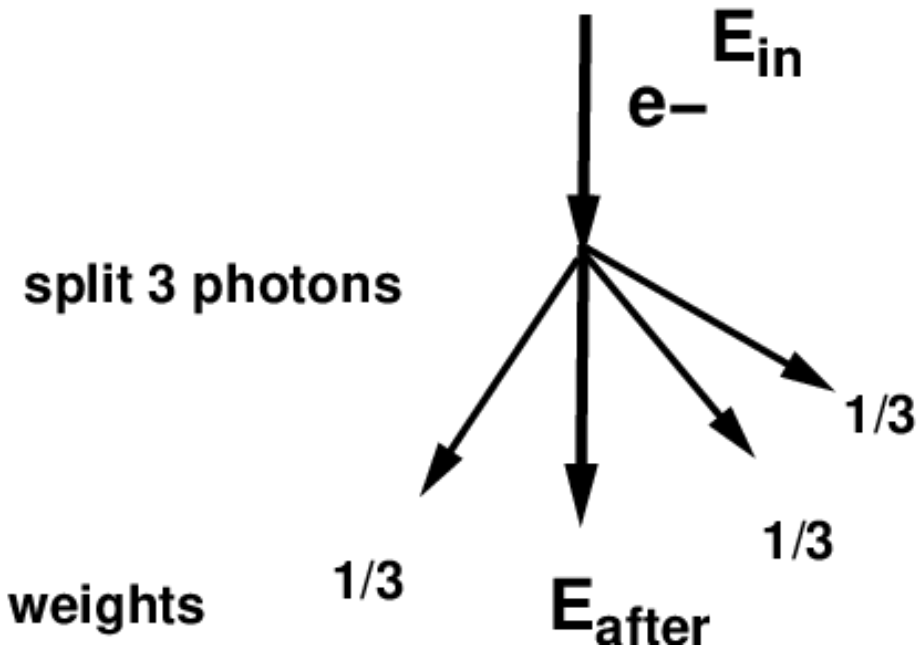


Approach A: $E_{\text{after}} = E_{\text{in}} - E_{\gamma 1}$ (or $E_{\gamma 2}$ or $E_{\gamma 3}$)

Approach B: $E_{\text{after}} = E_{\text{in}} - \overline{E}_{\gamma}$

Which is correct? Why?

Bremsstrahlung splitting



Approach A: $E_{\text{after}} = E_{\text{in}} - E_{\gamma 1}$ (or $E_{\gamma 2}$ or $E_{\gamma 3}$)

Approach B: $E_{\text{after}} = E_{\text{in}} - \overline{E}_{\gamma}$

Which is correct? Why?

Hint: Final electrons could be killed with probability 1/3 in a game of Russian Roulette

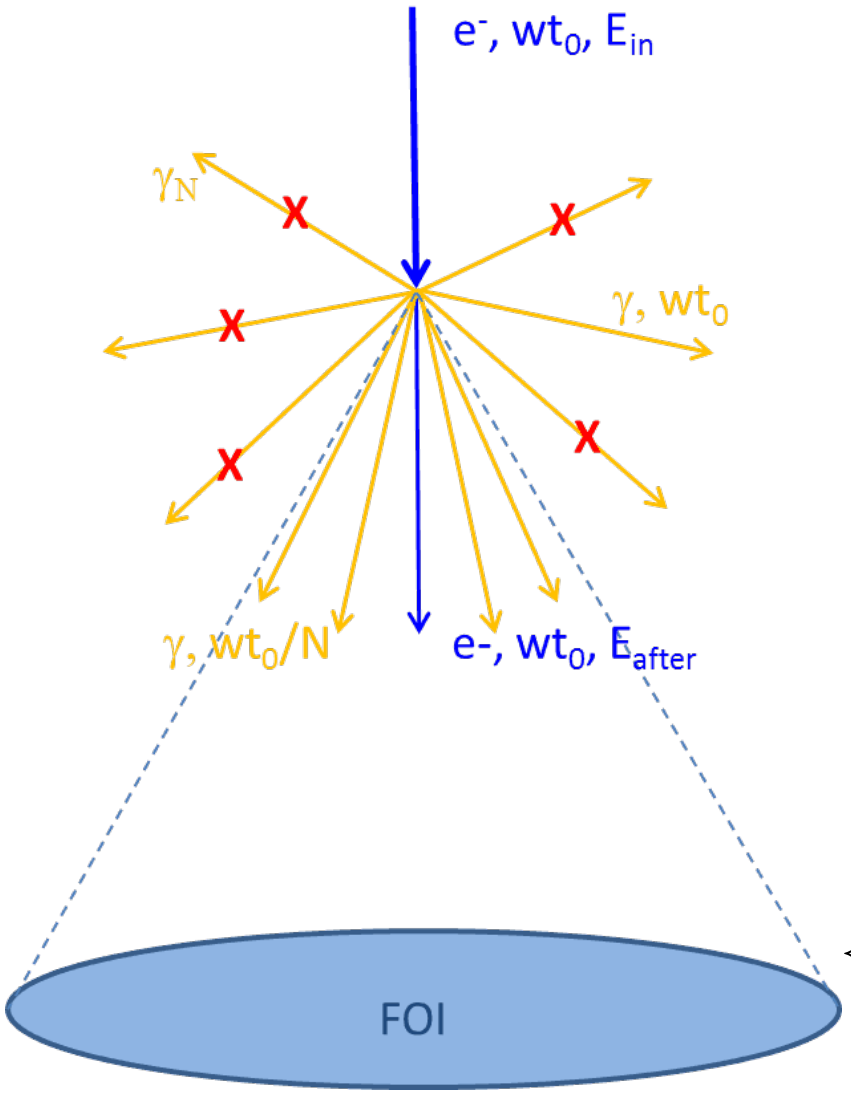
Bremsstrahlung splitting

- Split electron about to interact in 3 electrons. Each gets weight 1/3
- Perform a bremsstrahlung interaction for each electron $\Rightarrow$ 3 gammas and 3 electrons
- Play RR with final electrons with probability 1/3. One out of 3 will survive on average
- This is equivalent to just keeping final electron 1 (or 2 or 3)

$\Rightarrow$ **Approach A** is correct.

$\Rightarrow$ Bremsstrahlung splitting with **Approach A** (or any other interaction splitting) is simply the combination of 2 other true VRTs and therefore is also a true VRT. It preserves energy straggling and energy is conserved on average.

DBS: Radiative events



Bremsstrahlung and positron annihilation

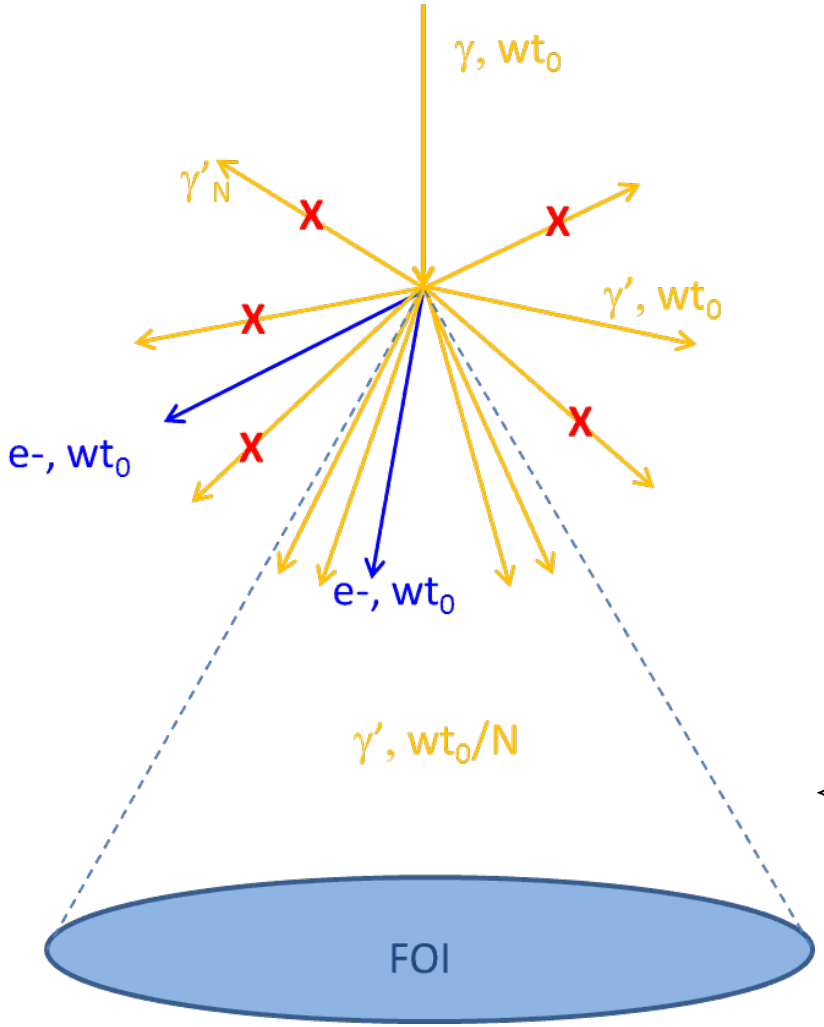
- Define a "field of interest" (FOI), which is a circle around the beam with sufficiently large margin.
- Split interaction N times. N bremsstrahlung or 2N annihilation photons are generated.
- Play RR with all photons not directed towards the FOI. Surviving photons have weight wt_0 and are called `fat`.

⇐ **Example: Bremsstrahlung**

DBS: Photon interactions

- For thin photons (wt = wt_0/N) that are about to undergo an interaction:
  - Play RR if medium's density larger than 0.012 g/cm^3. Surviving photons are fat.
  - Else, assume medium to be a gas and proceed with normal interaction.
- Split interactions of fat photons

DBS: Scattering events

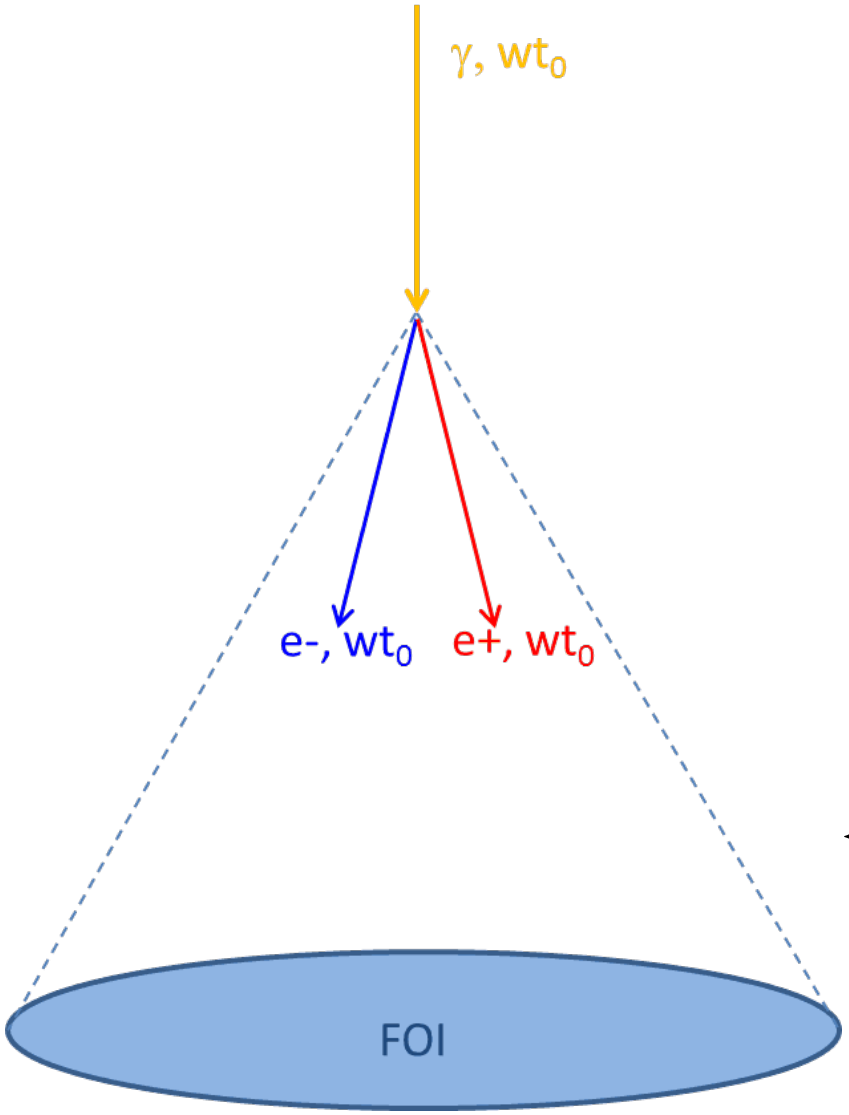


Coherent and incoherent scattering

- If photons are fat, split scatter interactions and play RR with all scattered photons not directed towards the FOI and all Compton electrons.
- If photons are thin, proceed with normal interaction.

⇐ **Example: Compton interaction of fat photons**

DBS: Absorption events



Photoeffect and pair production

- Normal photon interaction regardless of the photon's weight.
- Fat fluorescent photons are isotropically split N times and RR played on those not aimed at the FOI.

⇐ **Example: Pair production event**

DBS: Resultant particles

$\Rightarrow$ All photons directed towards the FOI are “thin” (have weight of 1/N), all other photons and electrons are “fat” (weight of 1)

$\Rightarrow$ Many “thin” photons, only very few “fat” photons and electrons $\Rightarrow$ little time spent to transport these

$\Rightarrow$ Very efficient simulation for photon fluence within FOI but inefficient for contaminant electron calculation

Some special tricks

- Using leading order bremsstrahlung cross-section allows only those photons aimed at the ROI to be created and this saves lots of time (although a recent paper, Ali et al, Med Phys 39(2012) 5990 – 6003 shows that in some extreme cases using leading order vs full KM is not as accurate).

- Similarly, using Klein-Nishina Compton scattering (free electrons) allows only those photons aimed at the ROI to be generated (this will be accurate in MV simulations)

Improving electron statistics: electron splitting

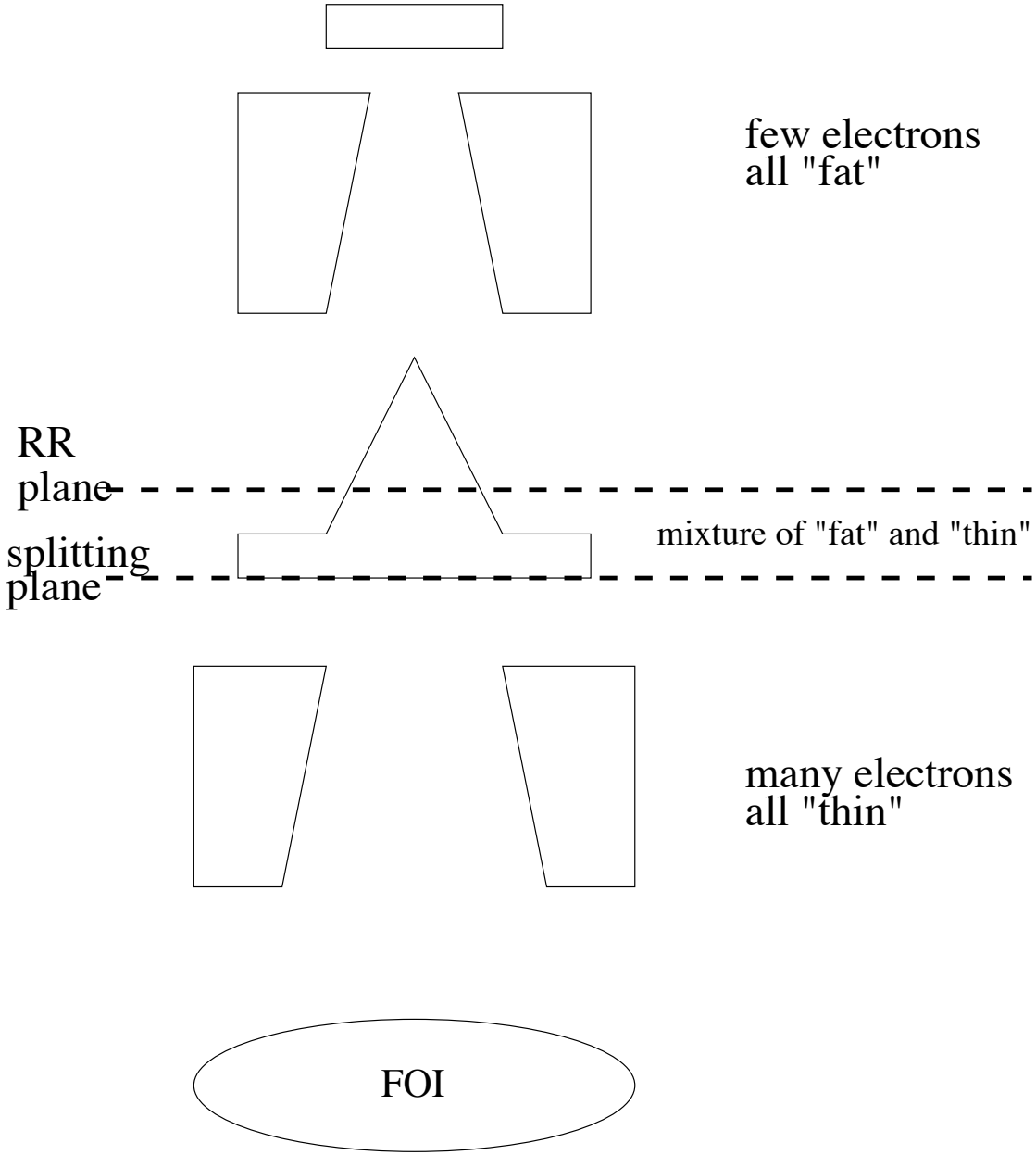
- The vast majority of charged particles arriving at the patient have been created in the lower portion of the flattening filter, the inner faces of the jaws and the air between the treatment head and the patient

$\Rightarrow$ Increase number of created/transported electrons in the lower portion of the treatment head by introducing two planes, the “RR plane” and the “splitting plane”.

- The splitting plane should be near the bottom of the flattening filter
- The RR plane should be slightly above the the splitting plane (a few millimeter)

$\Rightarrow$ The treatment head is divided into 3 distinct regions:(more next slide)

  - Above RR plane: few electrons, all “fat”
  - Below splitting plane: many electrons, all “thin”
  - Between RR and splitting planes: mixture of “fat” and “thin”

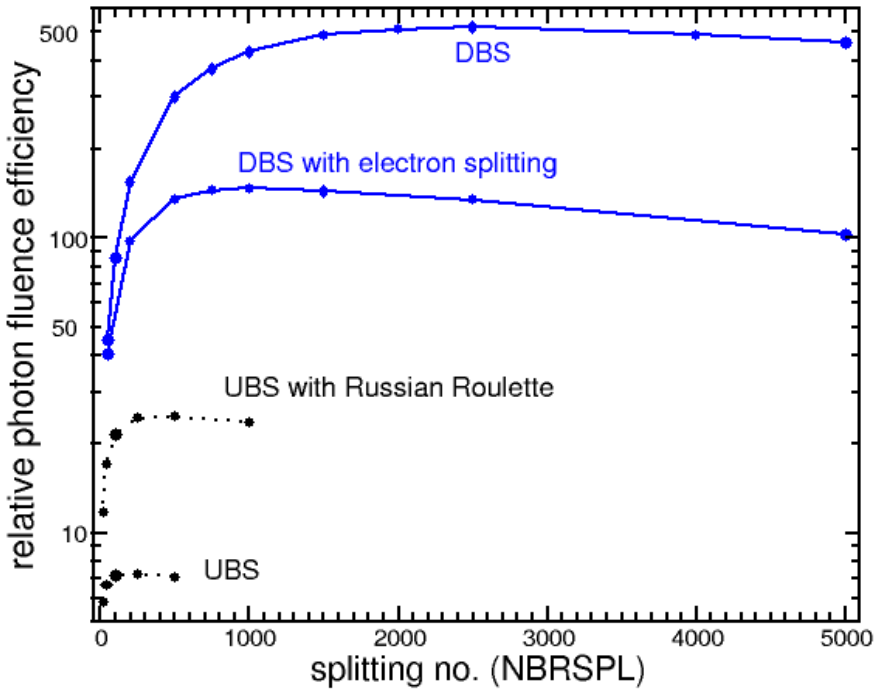

few electrons
all "fat"
RR
plane
splitting
plane
mixture of "fat" and "thin"
many electrons
all "thin"
FOI

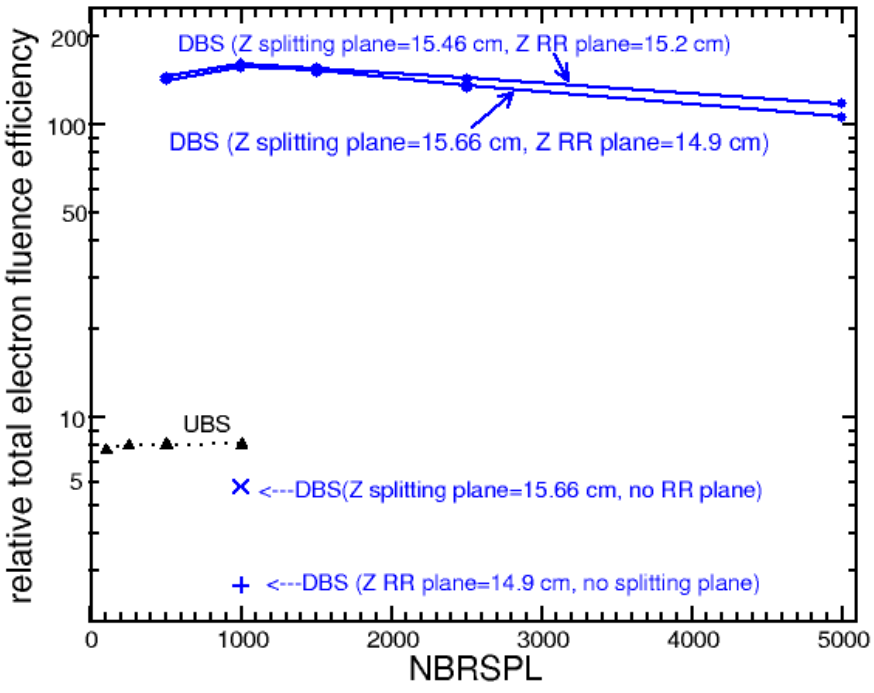
Electron splitting (cont'd)

- Above RR plane transport is done as explained before
- Below RR plane
  - No RR played with interacting "thin" photons
  - Interactions of "fat" photons are split $\Rightarrow$ resulting electrons are "thin" (no RR)
  - RR with scattered photons not directed towards the FOI
- "Fat" electrons crossing the splitting plane are split
  $\Rightarrow$ all electrons below splitting plane are "thin"

$\Rightarrow$ Much better statistics for contaminant electrons

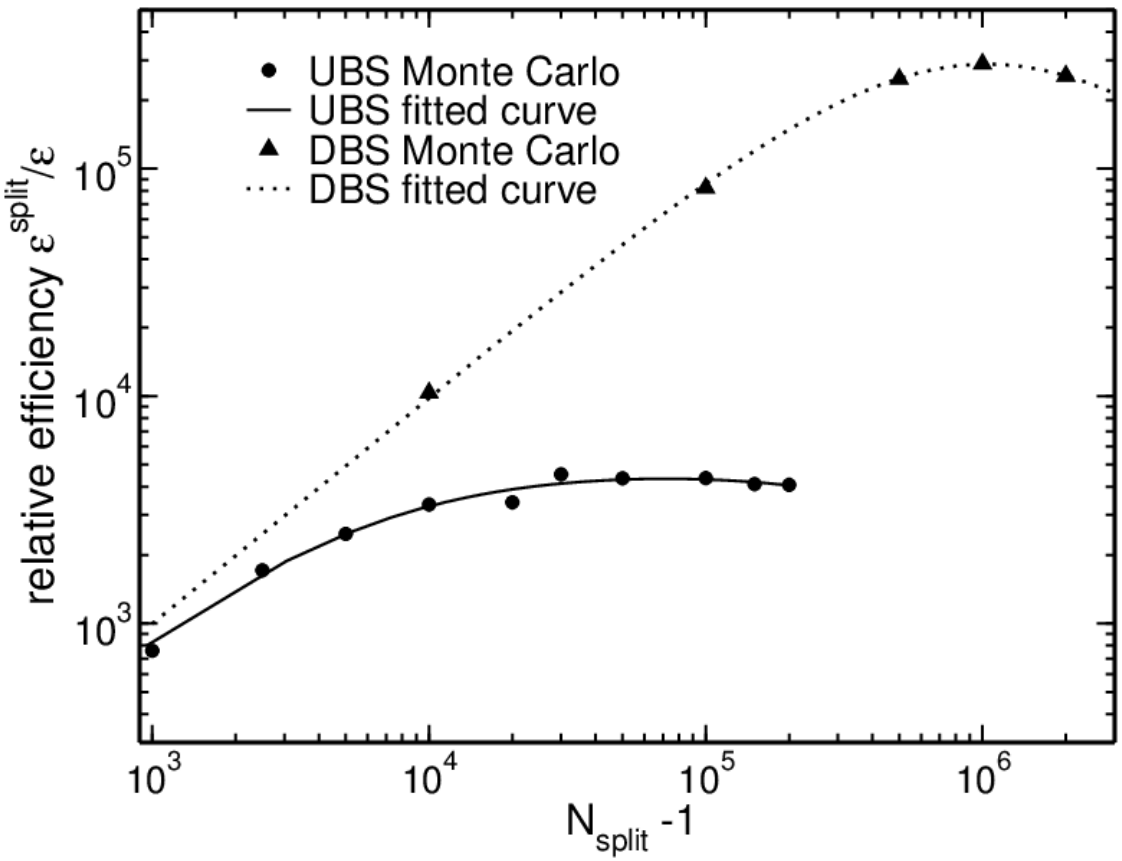
$\Rightarrow$ Longer CPU time because more electrons must be transported





- In MV beams, DBS improves efficiency by up to a factor of 20 compared to UBS and 150 compared to no VRT.
- Good e^- statistics costs a factor of $\sim$3.5 loss in photon fluence efficiency.
- For more details, Kawrakow et al, Med.Phys. **31**(2004)2883 (source of figures).
- For an easy way to find optimum splitting number (NBRSPL), see Kawrakow, Med.Phys. **32** (2005) 2320. Note that optimum splitting numbers can often be 1000 or greater.

Example: bremsstrahlung splitting in kV beams



- Even more important than in MV beams; DBS is $\sim$60 times better than UBS
- For an easy way to find the optimum N_{split}, see Mainegra-Hing and Kawrakow, Med. Phys. **33**, (2006) 2683

Fat photons

- In a phantom dose calculation fat photons may scatter into the field and may set in motion fat electrons
- These fat electrons will destroy the statistics of the dose calculation

$\Rightarrow$ It is better to ignore fat photons in the phase space file for dose calculations

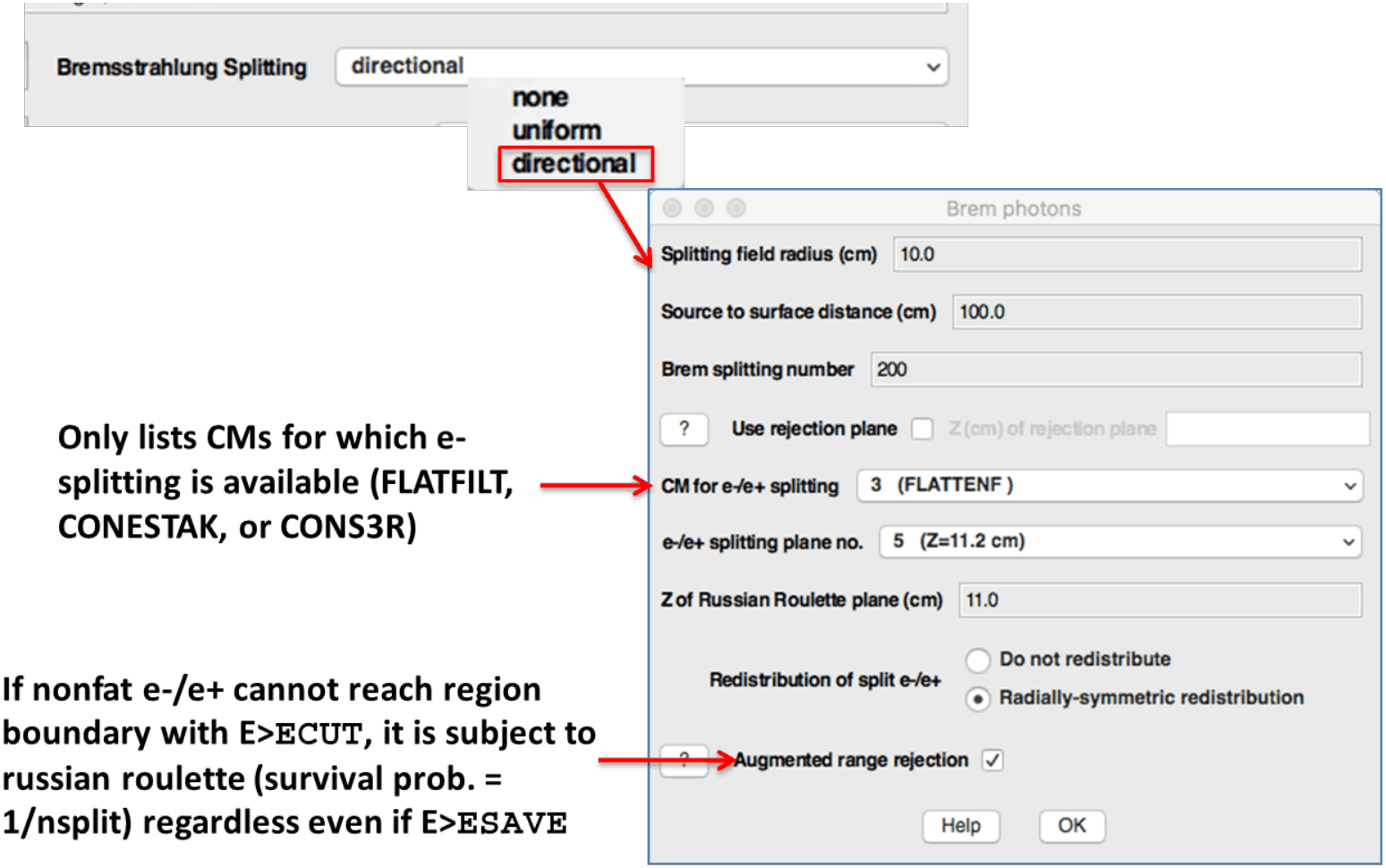
$\Rightarrow$ The contribution of fat photons to the dose region of interest must be negligible

$\Rightarrow$ FOI radius in the DBS BEAM simulation must be made large enough to make this true.

- The efficiency of the DBS BEAMnrc simulations decreases with increasing FOI radius

$\Rightarrow$ The optimum FOI radius is a compromise between efficiency and accuracy

DBS: GUI inputs



Only lists CMs for which e- splitting is available (FLATFILT, CONESTAK, or CONS3R)

If nonfat e-/e+ cannot reach region boundary with E>ECUT, it is subject to russian roulette (survival prob. = 1/nsplit) regardless even if E>ESAVE

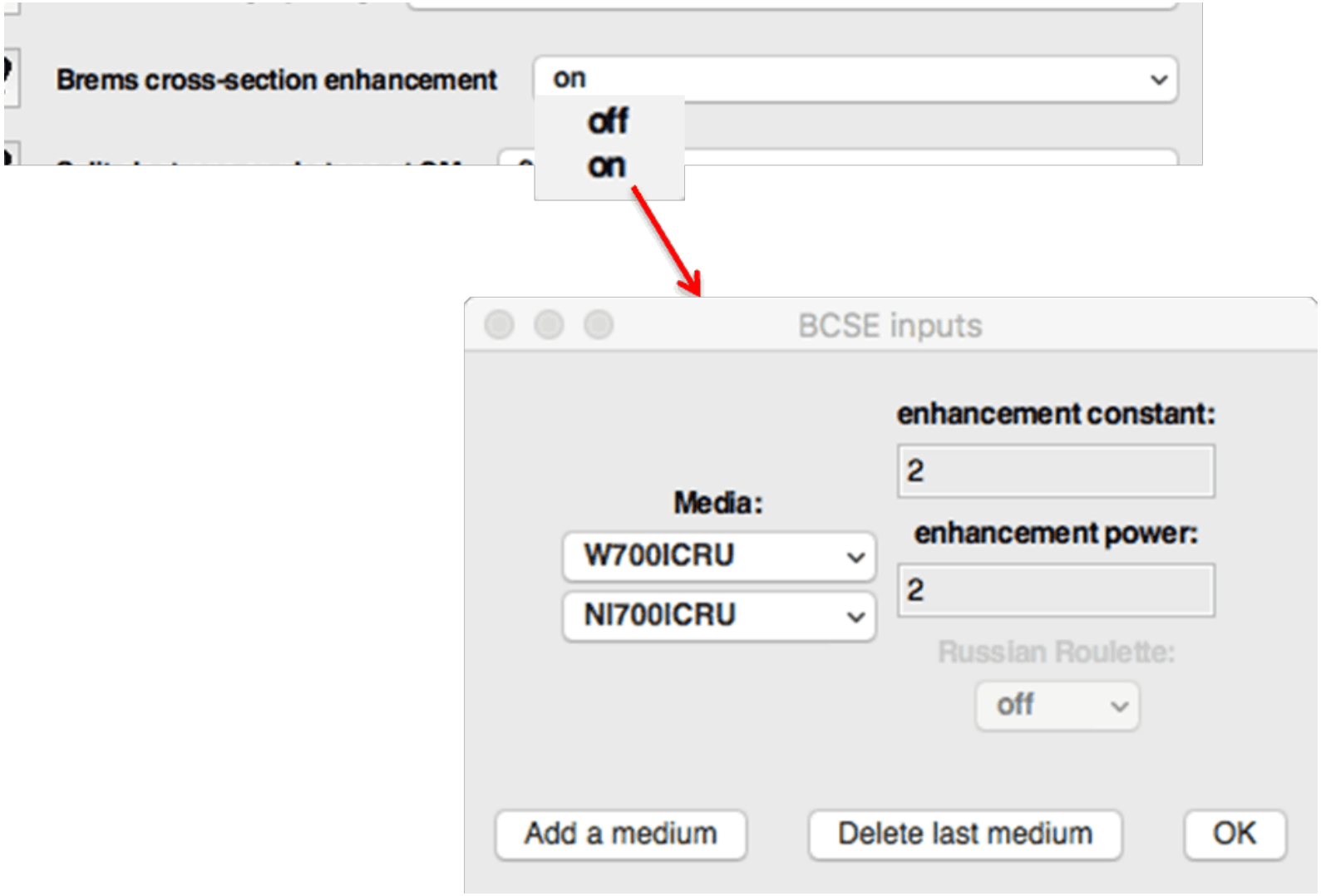
Bremsstrahlung Cross Section Enhancement (BCSE)

- Main idea: increase frequency of bremsstrahlung production by artificially increasing the cross section by an enhancement factor f which can be constant or a function of the particle's energy.

- RR can be used alone or in conjunction with UBS. If used with UBS, the RR setting must mirror that for BCSE. Recommended if the user is only interested in photons.

- Developed by E. Ali and Dave Rogers at Carleton U. For details see chapter 6.4 and [Ali and Rogers, Med. Phys. 34 (2007) 2143–2154]

BCSE: GUI inputs



BCSE:

- Enhancement factor f is constant if BCSE_POWER <= 0, or else a function of the particle's energy E:

$$f = 1 + \mathrm{BCSE\_CONSTANT} \cdot (E)^{\mathrm{BCSE\_POWER}}$$

- Most effective if combined with DBS (MV beams, X-ray tubes) or UBS (4π brachy sources)
- Up to a factor 5 (kV beams) or up to 40% (MV beams) efficiency increase compared DBS or UBS alone

Photon forcing

- Consider a photons passing through a geometry (or region) with a thickness Λ, measured in number of mean-free paths (mfp).
- The fraction of photons interacting in the geometry is $1 - e^{-\Lambda}$.
- The fraction of photons crossing the geometry without interacting is $e^{-\Lambda}$.

$\Rightarrow$ Split photon into an interacting portion (weight $1 - e^{-\Lambda}$) and a non-interacting portion (weight $e^{-\Lambda}$).

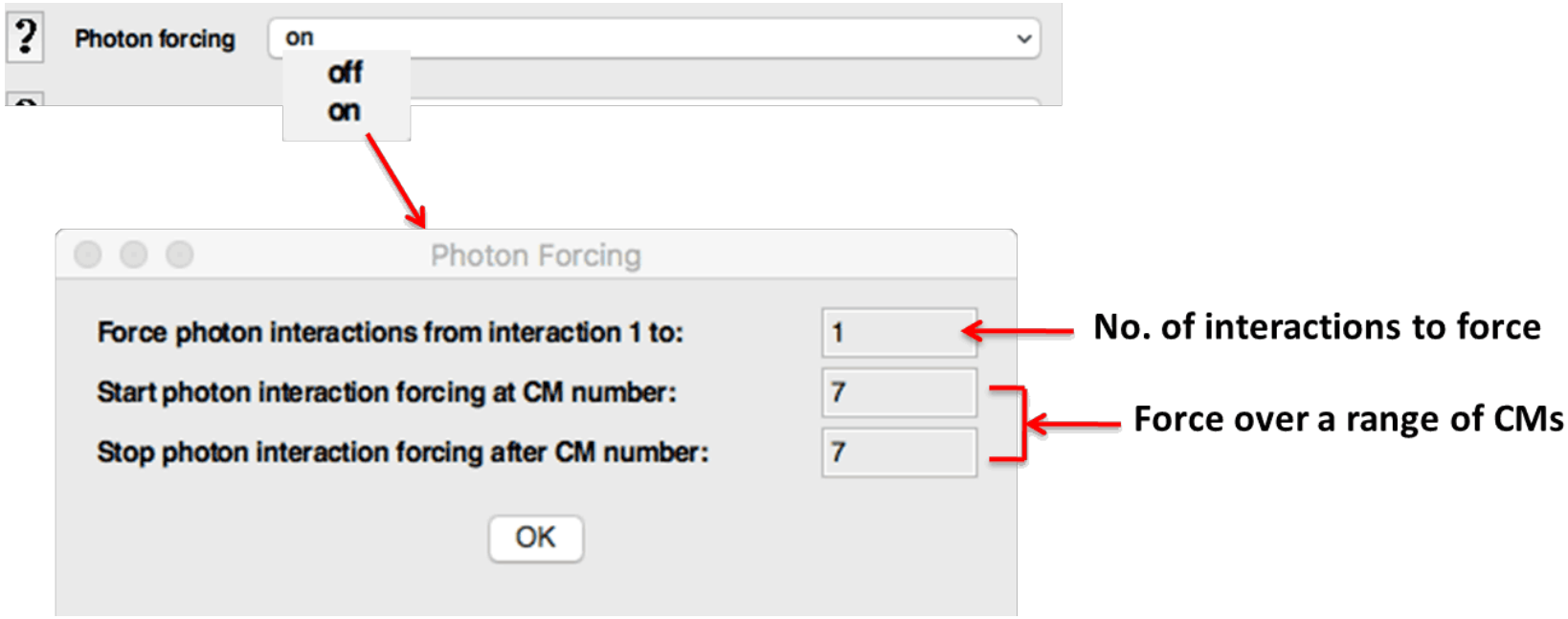
$\Rightarrow$ Ignore, or transport the non-interacting portion to the end of geometry (or region) if necessary.

$\Rightarrow$ Force the distance to the next interaction to be between 0 and Λ for the interacting portion:

$$\eta = -\ln\left[1 - \gamma(1 - e^{-\Lambda})\right] \quad (\gamma \text{ is a uniform random number}).$$

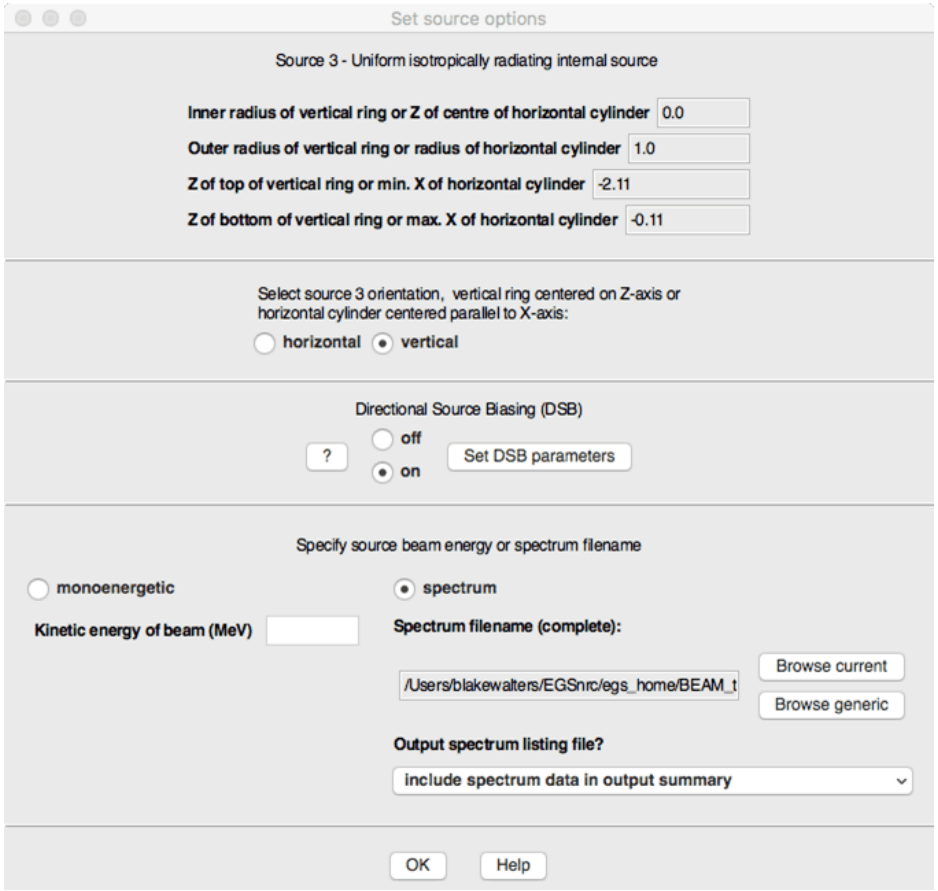
Can be used in BEAMnrc to (slightly) improve the statistics of contaminant electrons by forcing photons to interact in the air between the jaws and the phantom.

Photon forcing: GUI inputs

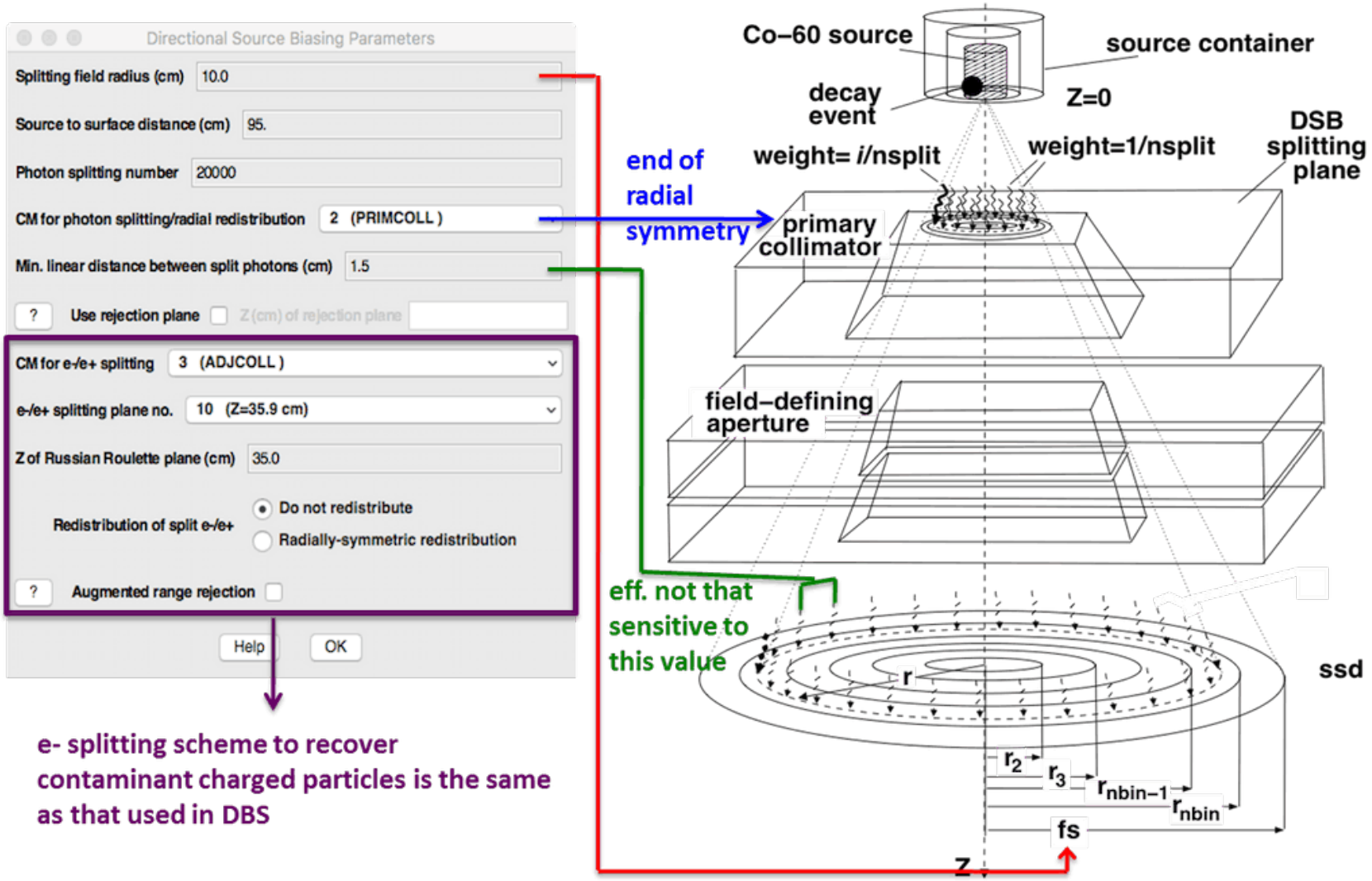


Directional source biasing: DSB

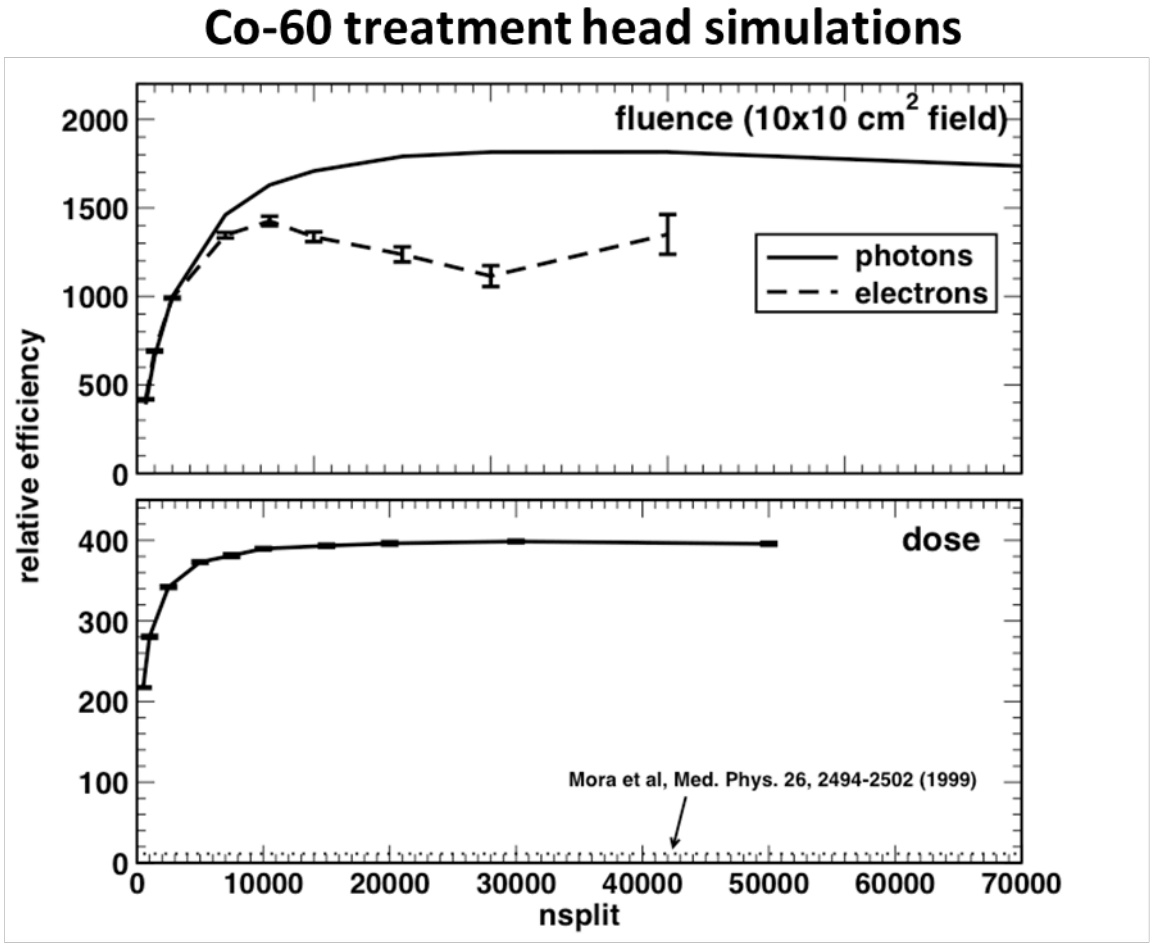
Directional source biasing can be used to increase the efficiency of isotropically radiating photon sources modelled using `ISOURC` = 3.



Directional source biasing: DSB



DSB: Efficiency



- **De-facto requirement for efficient Co-60 beam simulations**
- **Applicable to other isotropically radiating sources**

Further options to increase efficiency

- **Buying computers:** Computers are cheap these days, buy as many as you can and use the parallel processing option (see Chapter 12 of the BEAMnrc manual and Chapter 10 of the DOSXYZnrc manual).

- **Tweak compiler switches:** All modern compilers provide options for optimizing the code. You must read your compiler documentation to find the available options.

- **Use of profiling information:** typically results in a $\sim$10% speed gain and is compiler dependent. For the GNU compilers:
  - Compile with all switches you will be using + `-fprofile-generate`
  - Run a relatively short simulation (not more than 2-3 minutes). This will create a profiling information for the application.
  - Recompile with all switches you will be using + `-fprofile-use`. This will use the profiling information from the previous run to optimize the branching probabilities.

Playing around with compilation options

Not possible within the GUIs. The process is as follows:

1. Open a shell and go to the application directory
2. Delete the fortran file (`application_$my_machine.F`).
3. Type

   ```
   make FOPT="whatever flags you want to try"
   ```

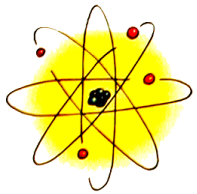
4. Run a simulation and record the CPU time
5. Repeat 2–4 with different compiler switches.

Once you have found the optimum switches for your system, you can edit the EGSnrc config file to define `FOPT` accordingly. From there on you can simply use the GUI's or just type `make` in a shell.

Take-home message

- It is **ALWAYS** worth taking the time to optimize the simulation.
- Even if it takes a day or two, gaining several factors in efficiency could be the difference between months or days of CPU time!!!





Joint ICTP-IAEA Workshop on Monte Carlo Radiation Transport and Associated Data Needs for Medical Applications
28 October – 8 November 2024
ICTP, Trieste, Italy

Lecture 8

Efficiency-increasing techniques in BEAMnrc

D. W. O. Rogers

Carleton Laboratory for Radiotherapy Physics
Physics Department, Carleton University