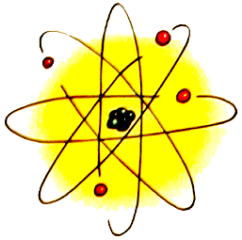

EGSnrc/BEAMnrc Monte Carlo simulation toolkit course

ICTP, Trieste, Italy

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Lecture 9

Monte Carlo transport parameters

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Available parameters

- AE,AP (PEGS data)
- Transport cutoff energies ECUT, PCUT
- Spin effects for elastic scattering on/off
- Bremsstrahlung cross sections BH *vs* NIST *vs* NRC
- Bound Compton scattering *vs* Klein-Nishina
- Rayleigh scattering on/off/custom
- Relaxations on/off
- Bremsstrahlung angular distribution
- Pair angular distribution
- Photo-electron angular distribution
- Electron impact ionization Off/On/casnati/kolbenstvedt/gryzinski/penelope

Available parameters (cont'd)

- Transport algorithm: EGSnrc default *vs* PRESTA-I
- Boundary crossing algorithm: exact *vs* PRESTA-I
- skin_depth_for_bca
- estepe, ximax
- Pair production energy distribution: BH *vs* NRC
- Triplet production on/off
- Photon cross sections: SI/XCOM/EPDL

For details of where to find specific parameters and how to select them, see Chapter 3 of PIRS701.

Parameter selection scenarios

Two possible scenarios:

- Don’t care about CPU time, need the best possible answer

- CPU time is essential (*e.g.* because of repetitive calculations under varying conditions)

Don’t care about CPU time

- Use pegs data with $\mathrm{AE}{=}\mathrm{AP}{=}1$ keV, and set $\mathrm{ECUT}{=}\mathrm{PCUT}{=}1$ keV
- Use default EGSnrc settings except as noted below
- Turn on Rayleigh scattering, use custom (molecular) form factors if available
- Set bremsstrahlung cross sections to NRC
- Set bremsstrahlung angular distribution to KM
- Turn on EII
- Set pair cross sections to NRC
- Set photon cross sections to XCOM

This will give the most accurate answer EGSnrc can produce

CPU time is essential

- Usually the appropriate **selection of AE, ECUT is the most critical choice**
- In general, options related to photon interactions have a very small impact on CPU time, unless you are running a photon-only simulation
- Using certain parameter selections is important for some energy/material combinations but entirely irrelevant for others
- Choice depends on the desired precision

$\Rightarrow$ Need to understand the effect of each parameter!

The following material gives quick (cook book fashion) guidelines.

Remember: use of appropriate VRTs is often a much more important factor!

Understanding ECUT, PCUT

This is covered in lecture 5 in detail, but it is very important

Use $\mathrm{ECUT} = \mathrm{AE}$, $\mathrm{PCUT} = \mathrm{AP}$, unless there is a clear reason not to do so.

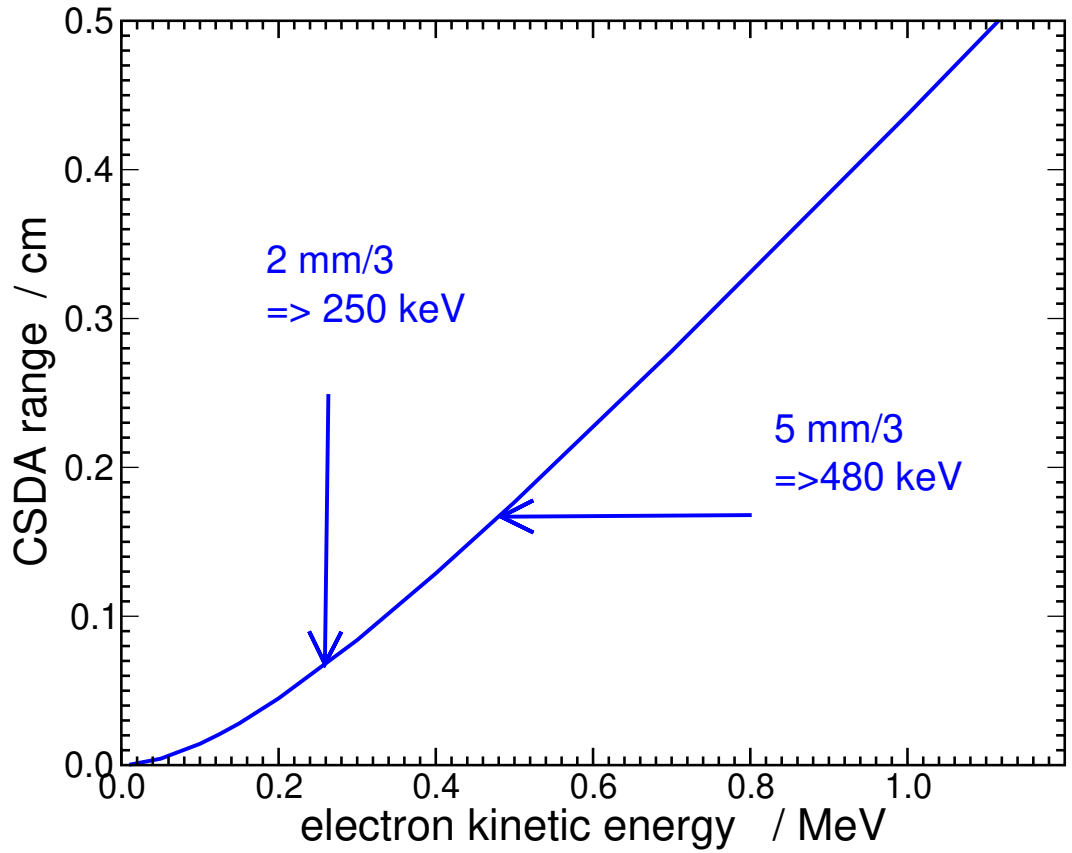
Examples where ECUT $\neq$ AE is useful:

- The calculation of energy spectra as in lecture 5 thru 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 $\mathrm{ECUT} > \mathrm{AE}$.

How do we select ECUT?

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



But in most cases, if doing many such calculations you need to check by using a lower ECUT for a representative case.

Bound Compton scattering

- Sampling bound Compton events $\sim 1.5 \cdots 2$ times slower than Klein-Nishina
- Negligible impact on CPU time with e-transport, 1–2 times increase in CPU time for γ-only simulations
- Exception: linac simulations with DBS(see VRT lecture) are $\sim$3 times slower with bound Compton! (since some sampling tricks cannot be used with bound Compton).
- Effect of using Bound Compton usually completely negligible for energies above a few hundred keV

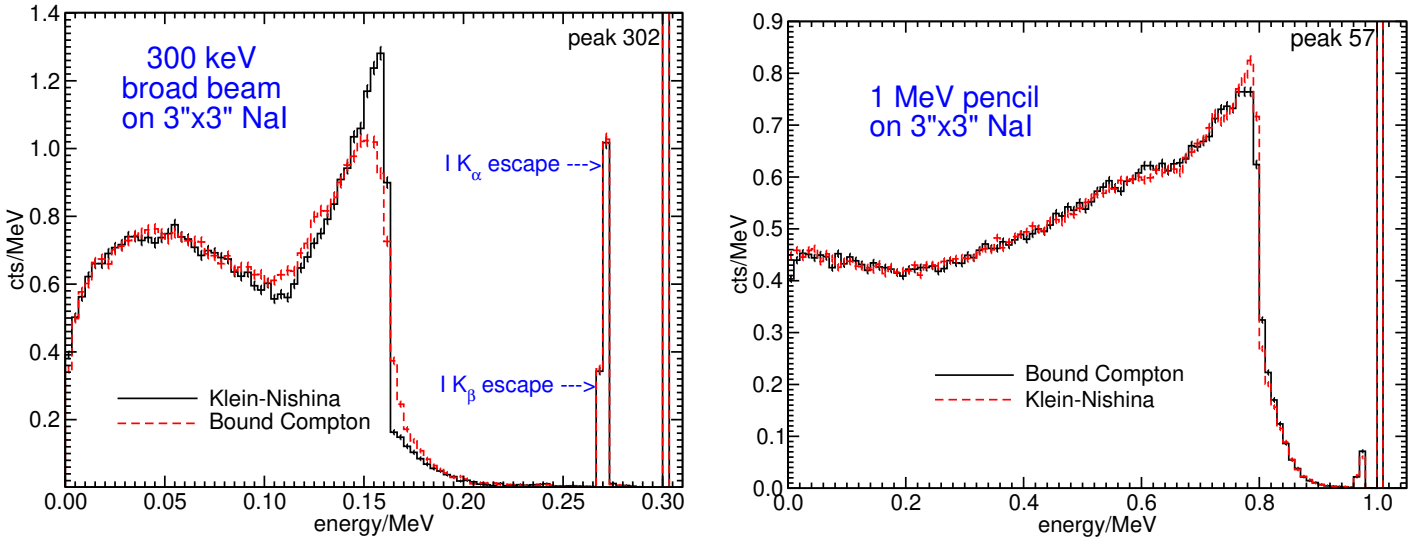
Bound Compton scattering

- Electron binding reduces the total cross section
- Scattering is most strongly suppressed for forward angles
- Doppler broadening increases the average energy transfered to electrons per collision $\Rightarrow$ average energy per unit length transfered via Compton scattering (mass energy transfer coefficient) is quite well reproduced with Klein-Nishina
- Binding effects and Doppler broadening only important at low energies where photo-electric absorption rather than Compton dominates

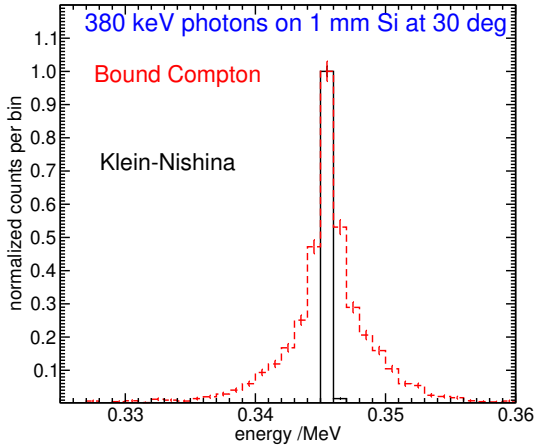
$\Rightarrow$ Very small effect for dose calculations.

- Can be important for detector response function calculations, simulations related to imaging, etc.!

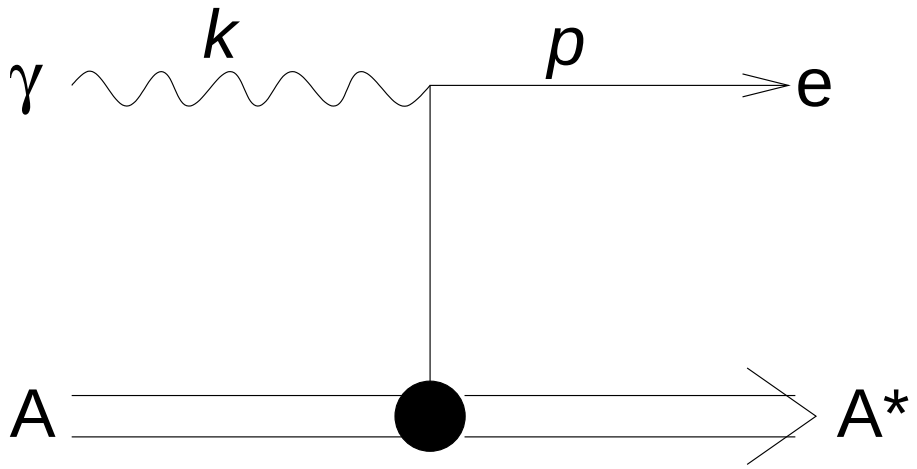
BC vs KN in detector response



Bound Compton is more important at lower energies as are escape peaks. Bound Compton brings with it Doppler broadening of the scattered photons.



Atomic relaxations

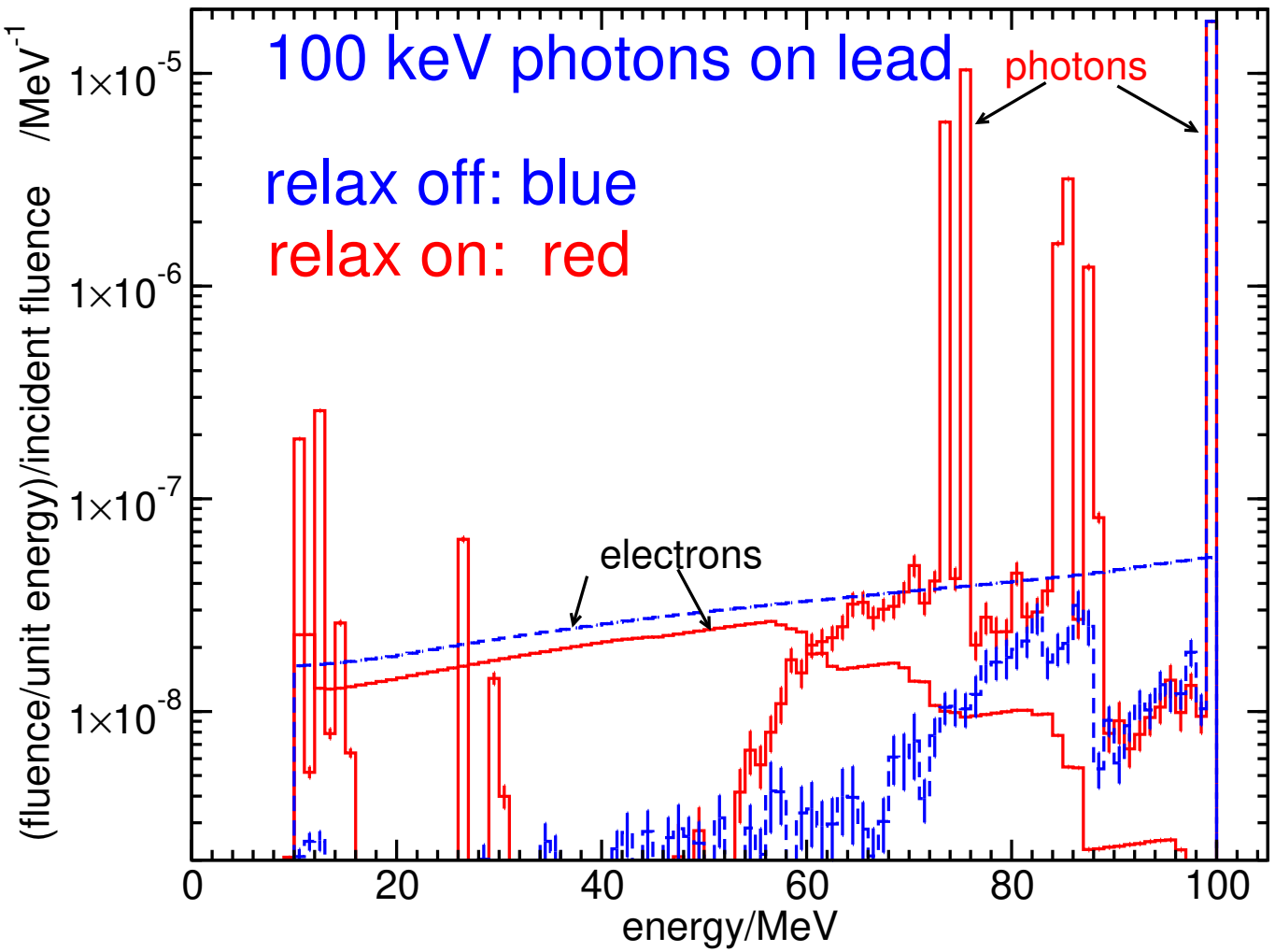


Creation and transport of relaxation particles(fluorescent photons and Auger electrons) from an excited atom is important if their ranges are not small compared to the geometrical scale of the problem.

Be aware: relaxation in high-Z materials produces lots of particles $\Rightarrow$ a lot of overhead.

- relaxation on: photoelectron has photon's energy less shell's binding energy
- relaxation off: photoelectron has photon's energy and there are no relaxation particles

Atomic relaxations on or off in lead



Atomic relaxations: EADL option

Mainegra-Hing added an option to use more detailed information about individual M and N shell enegies rather than averaged values as in the EGSnrc default (as of 2013).

To turn this on, in egsnrc.macros change .false. to .true. in

REPLACE $EADL_RELAX WITH {.false.}

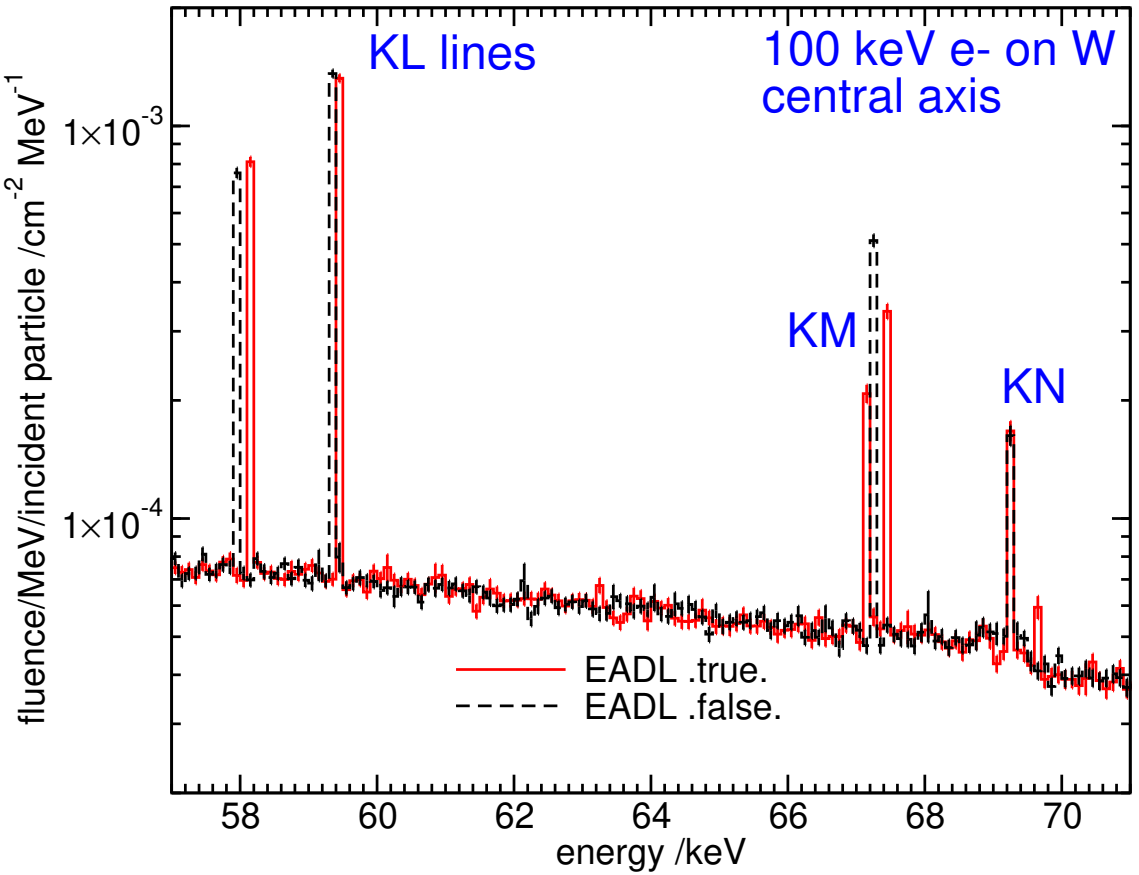

KL lines
100 keV e- on W
central axis
KM
KN
EADL .true.
EADL .false.
fluence/MeV/incident particle /cm-2 MeV-1
1×10-3
1×10-4
58
60
62
64
66
68
70
energy /keV

Photo-electron angular distribution

- Photo-electric absorption is important only at low energies

- Elastic electron scattering at low energies is very strong, the angular distribution of photo-electrons rapidly becomes uniform due to MS

$\Rightarrow$ In most cases turning on photo-electron angular deflections does not make any difference

On the other side the increase in CPU time due to $\mathrm{iphter} = 1$ is negligible $\Rightarrow$ could be used even if not necessary.

Rayleigh scattering

- May become important for detailed studies only at low energies (say, below 1 MeV for high-Z materials, below 100-200 keV in low-Z materials)

- Note: by default, EGSnrc uses independent atom approximation to calculate form factors for molecules $\Rightarrow$ not good enough for detailed MS investigations of imaging devices
  - there is an option to read in molecular form factors if you want.

- CPU cost negligible (unless running calculation without electron transport)

Recommendation:
Only use Rayleigh scattering when using bound Compton scattering

- there is no such a thing as photon elastic scattering of free electrons

- K-N is more accurate without Rayleigh than with.

Pair angular sampling

- Using the fixed angle approximation (inherited from EGS4) is perhaps never a good idea
- The default selection (leading term of the angular distribution) is most likely good enough for any application. CPU cost compared to fixed angle: negligible
- The more sophisticated distribution from Koch and Motz is derived from an extreme relativistic approximation. It is probably better at high energies (say, above 50 MeV), its outcome at intermediate energies is unclear.
- Have never encountered a situation where the selection of the pair angular sampling scheme made a significant difference on CPU time

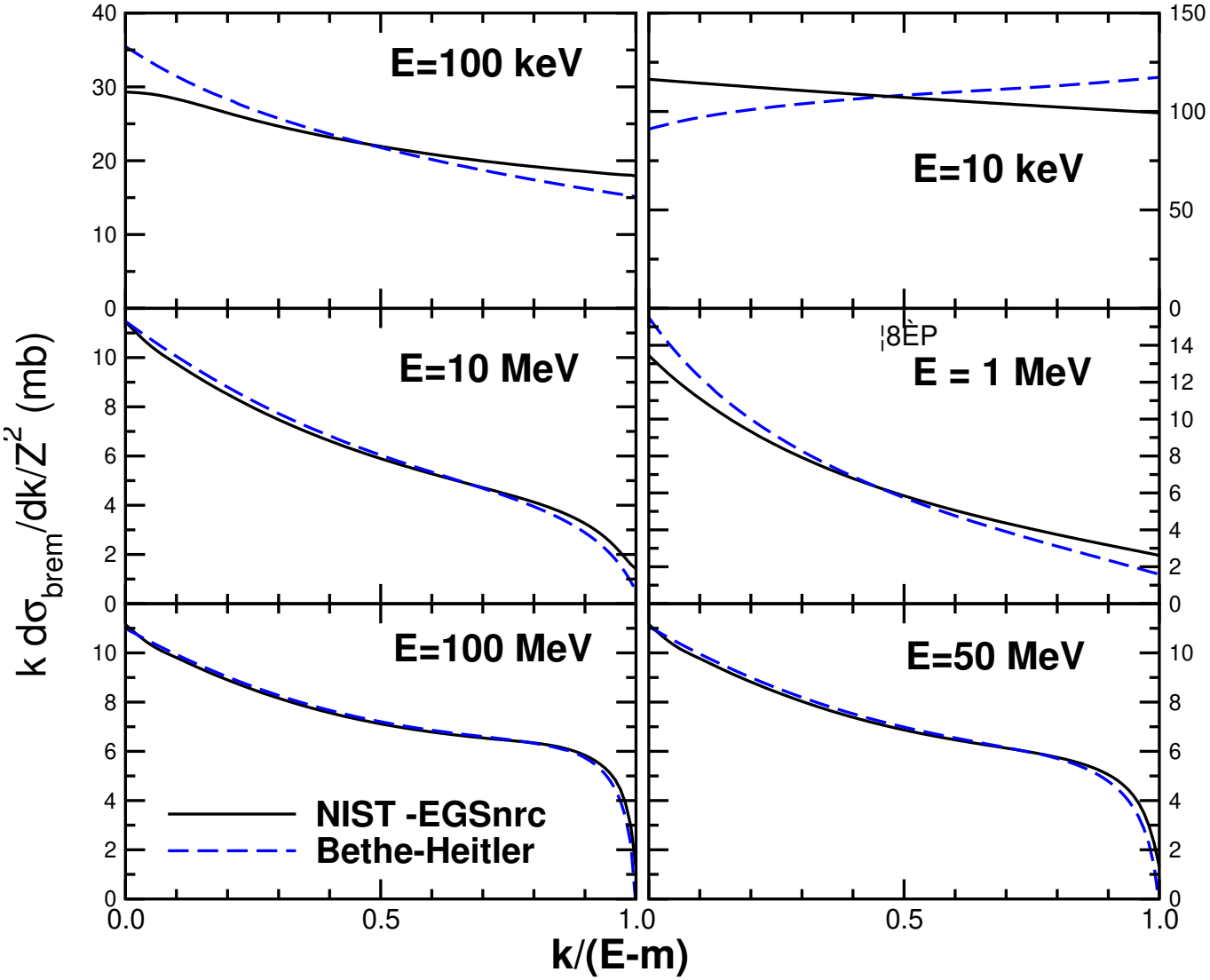
Bremsstrahlung cross sections

- there are three possible differential cross sections to use
- Bethe-Heitler cross section as used in EGS4
- NIST database which is identical to Coulomb corrected Bethe-Heitler above $\sim$ 50 MeV.
- the NIST database for the nuclear bremsstrahlung but with the new electron bremsstrahlung modelled using the work from NRC (F. Tessier and I. Kawrakow, *Calculation of the electron-electron bremsstrahlung cross-section in the field of atomic electrons* , Nucl. Inst. Meth. B **266** (2008)625 –- 634 .)
- There are significant differences at low energies between NIST and Bethe-Heitler (although the radiative stopping powers are forced to be the same).
- Sampling from the NIST or NRC database is faster at low energies but slower at high energies.

$\Rightarrow$ Don't use the NIST or NRC option for energies above 100 MeV

$\Rightarrow$ Use of the NRC option is strongly recommended for energies below 1 or 2 MeV.

Bremsstrahlung cross sections (cont)



Bremsstrahlung angular distribution

- Sampling from the leading term of the angular distribution (option simple) is 2-3 times faster than using Eq. 2BS from Koch and Motz (option KM).

- In most cases, this translates into very modest (if not negligible) increase of overall simulation time.

- Experience show that using simple is accurate enough for *e.g.* in phantom dose calculations for RTP or correction factor calculations

- The KM option is recommended for *e.g.* linac simulations using $\mathrm{BEAMnrc}$. Ali's work demonstrated several cases where it appears to be important/more accurate.

- Note, however, that when using DBS, using KM translates into a factor of $\sim$6 penalty in CPU time!

Spin effects

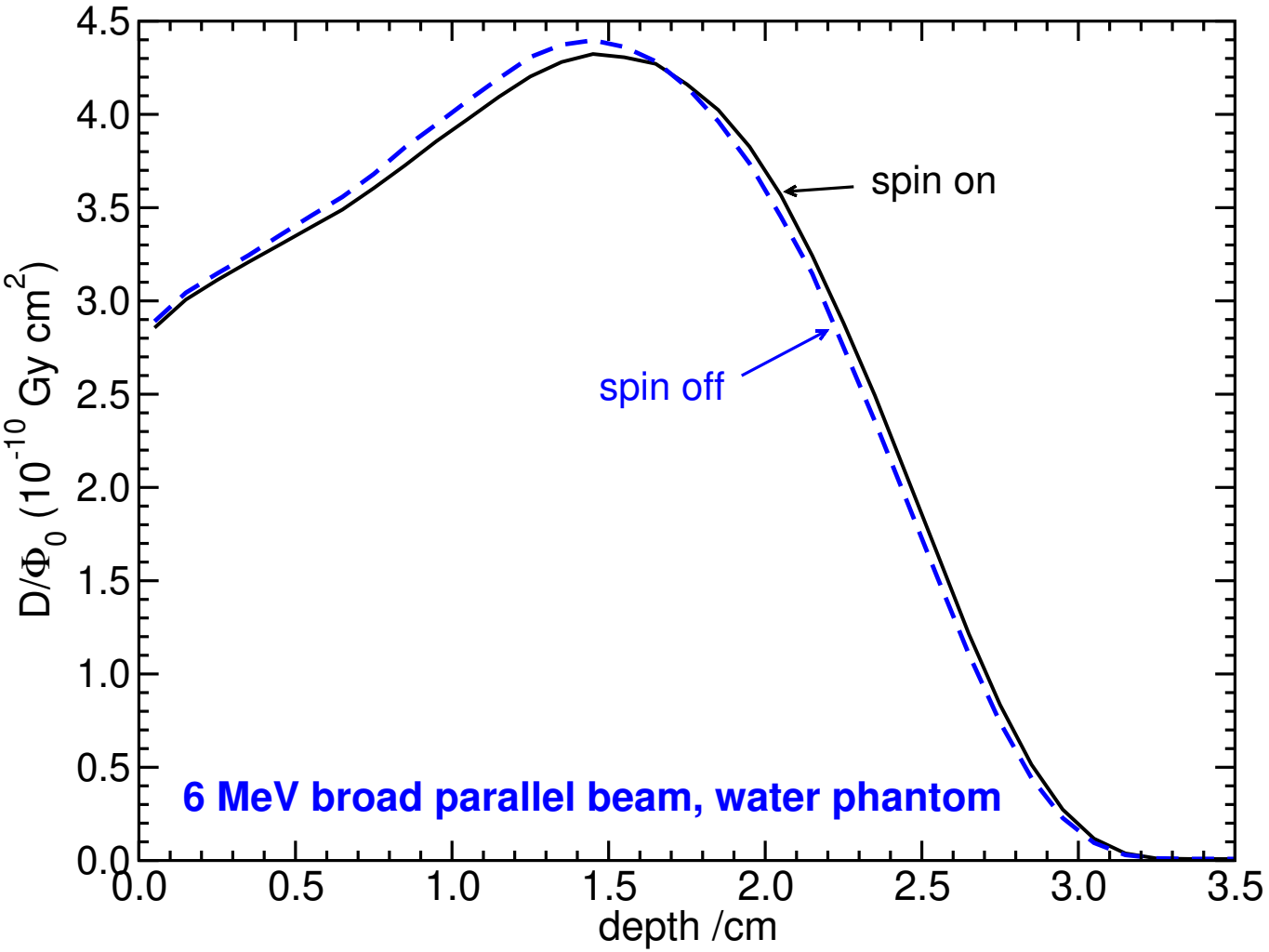
- In electron transport, sampling single scattering and multiple scattering angles from the distributions that take into account spin effects is
  - $\sim$ 2 times slower for high-Z materials
  - $\sim$ 1.3 times slower for low-Z materials

  This translates into $\sim$30-50% (high-Z) or $\sim$10-30% (low-Z) increase in overall simulation time.

- Use of the spin option will **ALWAYS** have an effect on the calculated result! (if electron transport matters)

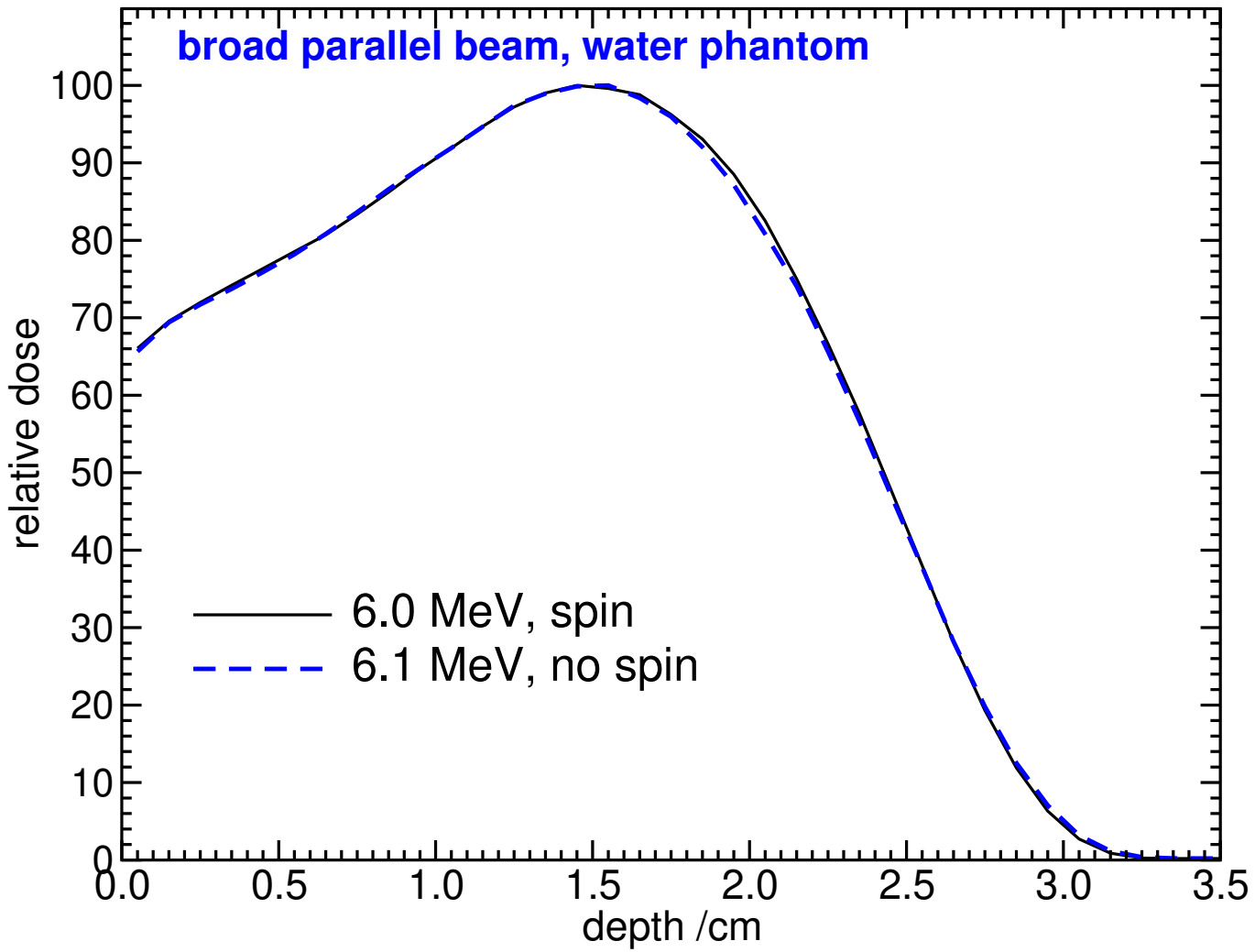
$\Rightarrow$ You must have some very strong arguments to turn the spin off.

Spin effects: example



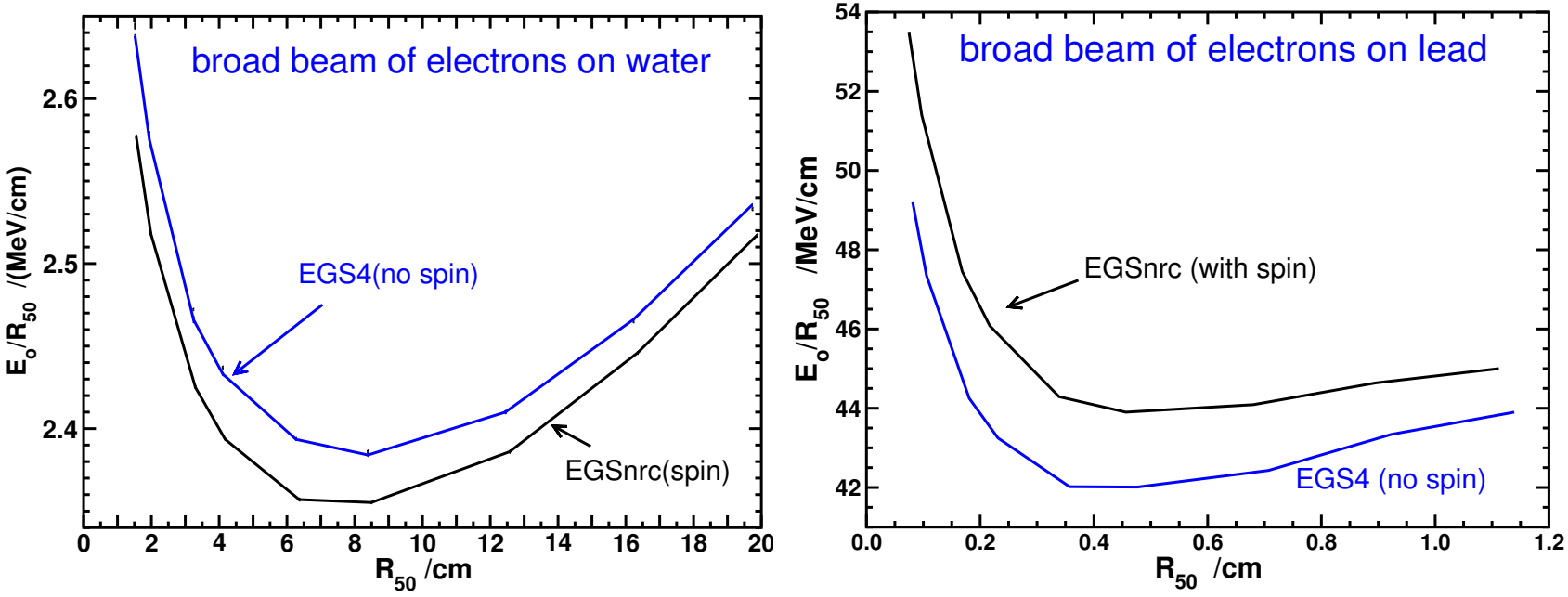
Spin has increased R_{50} for low Z but it is the reverse for high Z.

Spin effects: example

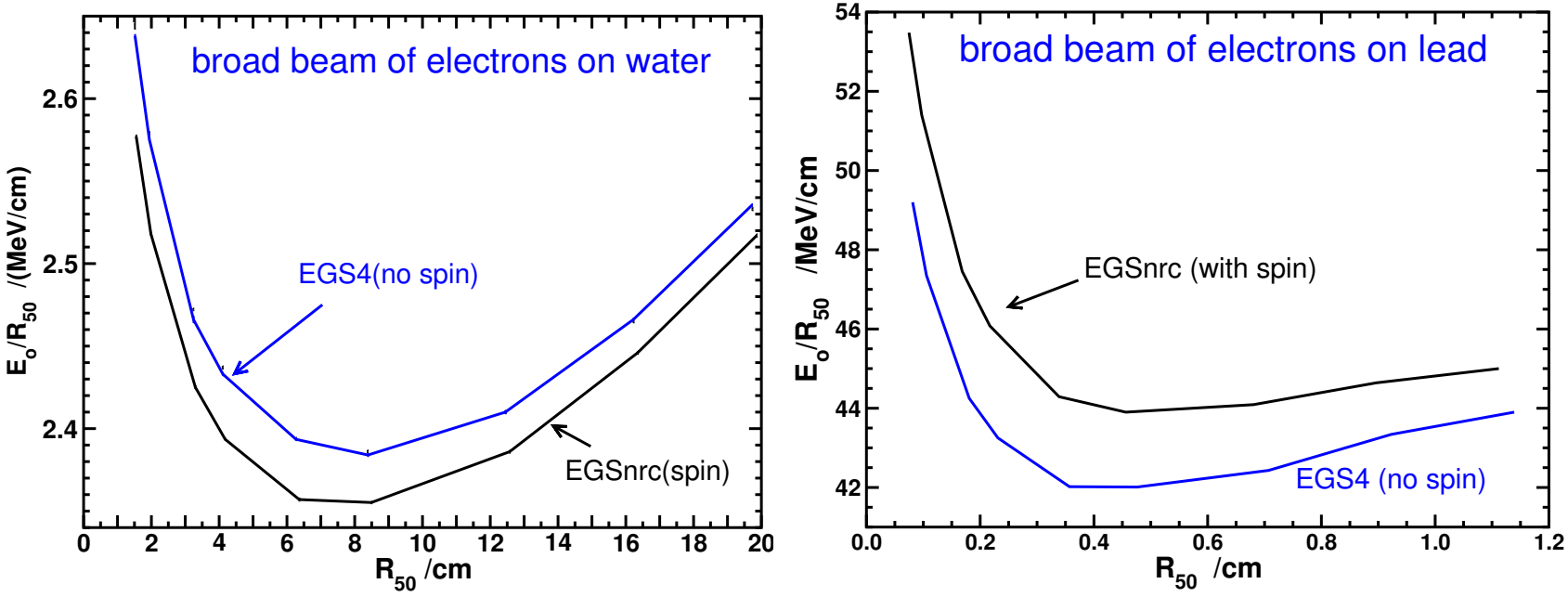


When modelling electron beams, one matches $R_{50} \Rightarrow$ hard to see a problem.

Spin effects on R_{50} for low-Z or high-Z materials



Spin effects on R_{50} for low-Z or high-Z materials



This implies that R_{50} increases for a given E_0 for low-Z materials and the reverse for high-Z materials..

Electron-step (transport) algorithm

- The default EGSnrc algorithm needs $\sim$ 1.7 times longer per step compared to PRESTA ($\mathrm{transport\_algorithm} = 1$)(recall 2 substeps/step).

- It is by an order of magnitude more accurate than PRESTA

$\Rightarrow$ In an infinite geometry (where step sizes are not modified due to boundaries, ...), using EGSnrc default will be

  - $\sim$ 1.5 times slower than using PRESTA with the same step size
  - Much faster to achieve the same precision since it can use much larger step sizes.

- In a geometry with many boundaries, the CPU time is more strongly influenced by the boundary crossing algorithm than by the transport algorithm.

Boundary crossing algorithm

is the most crucial parameter if there are many boundaries in the geometry!

- Using exact boundary crossing is absolutely essential for high accuracy simulations (*e.g.* ion chamber response)

- So for problems with relatively few boundaries one might as well just use the EXACT option.

Step sizes

If you use EGSnrc default electron-step algorithm and BCA, then extra controls on step size such as estepe, ximax and $\mathrm{skin\_depth\_for\_bca}$ are irrelvant since they are automaticallty set for maximum accuracy.

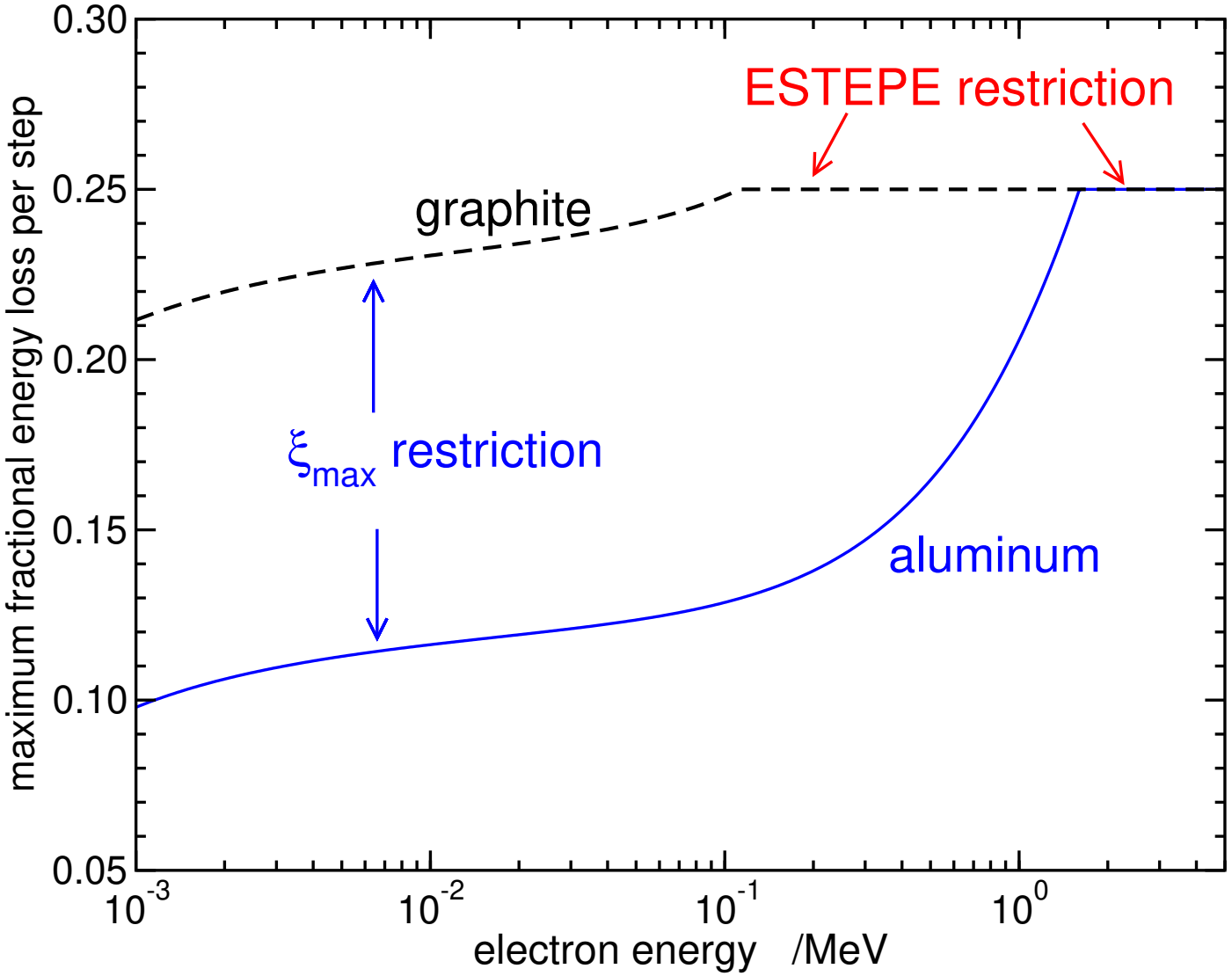
If you find step size dependencies, please let us know!

If you decide to use PRESTA-I's transport algorithm and/or BCA, they provide means for varying the step size until the result has converged to the (hopefully) correct answer.

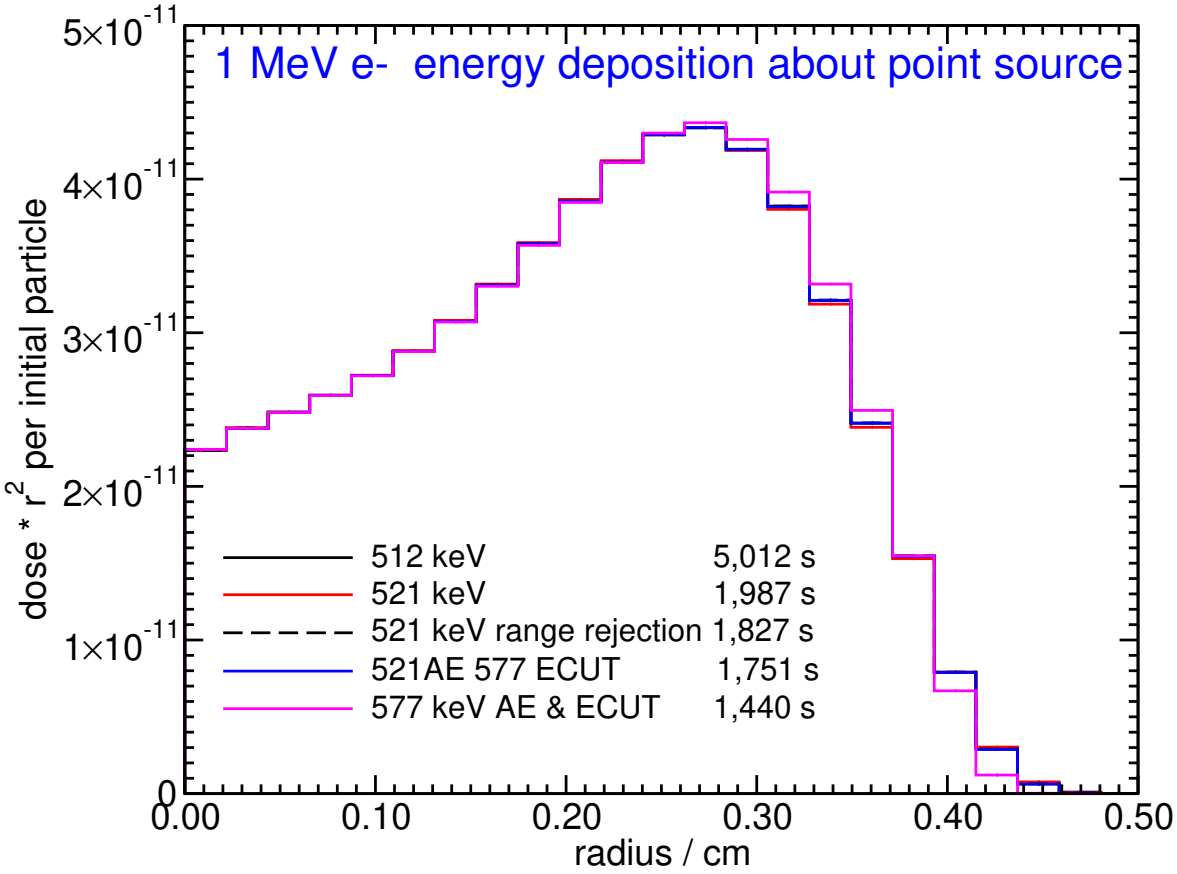
For default EGSnrc (see next slide)

- At low energies the ximax restriction dominates
- At high energies the estepe restriction (=0.25) is more important

Step sizes


0.30
0.25
0.20
0.15
0.10
0.05
maximum fractional energy loss per step
ESTEPE restriction
graphite
ξ_{max} restriction
aluminum
10^{-3}
10^{-2}
10^{-1}
10^{0}
electron energy /MeV

Step size effects on energy deposition kernels



In a timing study of EGSnrc vs GEANT the authors used 1% ESTEPE for EGSnrc and AE=ECUT=512 because that was needed to get the right answer with GEANT. But EGSnrc gets the right answer with much longer steps which allows for higher AE as well.

EII: Electron Impact Ionization

This is the creation of electon vacancies directly by electrons (like an internal bremsstrahlung which undergoes a photoelectric event in the same atom).

- EII “on” is essential for calculation of kilo-voltage X-ray spectra (characteristic X-ray lines are underestimated with EII ”off”)
- Have not seen a situation other than kV spectra where it makes a difference
- CPU time penalty may be not negligible (fractional increase strongly depends on selected AE, AP, ECUT and PCUT)
- Turning EII on automatically turns on atomic relaxations!
- multiple options: Off/On/casnati/kolbenstvedt/gryzinski/penelope
  - Comparison to measured data suggests the Penelope option is the most accurate

NRC pair cross sections and triplet production

- Relatively new option, not much experience
- CPU time penalty is negligible ($\mathrm{pair\_nrc}$ is even more efficient than BH for energies below ~ 10 MeV)
- Default values left to pair a la BH and triplet “off” for now for the sake of compatibility
- Turning triplet production on has a small effect in the build-up region of mega-voltage photon beams
- Using triplet production on makes individual particle histories to be correlated due to the use of a Markov chain technique for sampling
- NRC pair differential cross sections seem to have no effect in all cases studied so far.