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Teaching Session

Transport Parameter Selection in EGSnrc

D. W. O. Rogers

Carleton Laboratory for Radiotherapy Physics
Physics Dept., Carleton University, Ottawa

This lecture gives a brief discussion of the various transport parameter and cross section options available in EGSnrc. While specific to EGSnrc, these considerations affect almost all Monte Carlo simulations in medical physics.

Overview

- talk is specifically about parameter selection for EGSnrc
  - similar considerations apply to many other general codes
  - different terminology and or algorithms
- I will not discuss variance reduction techniques (VRTs)
  - these are code specific, even within the EGSnrc system
  - this would take several days
- I am assuming some knowledge of the EGSnrc system
  - this is not for absolute beginners
- I will start with the most important issues first and see how far we get

Acknowledgments

Iwan Kawrakow, then at NRC, now at ViewRay, was the main developer of EGSnrc. We all owe him a debt of gratitude for making the code what it is today.

Ernesto Mainegra-Hing, Blake Walters and Frederic Tessier of NRC play major roles in maintaining the system today.

Parts of this talk have been used at EGSnrc/BEAMnrc courses and all of the above have contributed in one way or another.

My work is supported by NSERC, the CRC program, CFI and OIT.

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, The EGSnrc User's Manual.

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 sets with AE=AP=1 keV, and set ECUT=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 (electron impact ionization)
- 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 accuracy

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

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

Understanding AE, AP

Recall: energy lost in processes below AE,AP deposited locally (restricted stopping powers), this must make sense i.e.

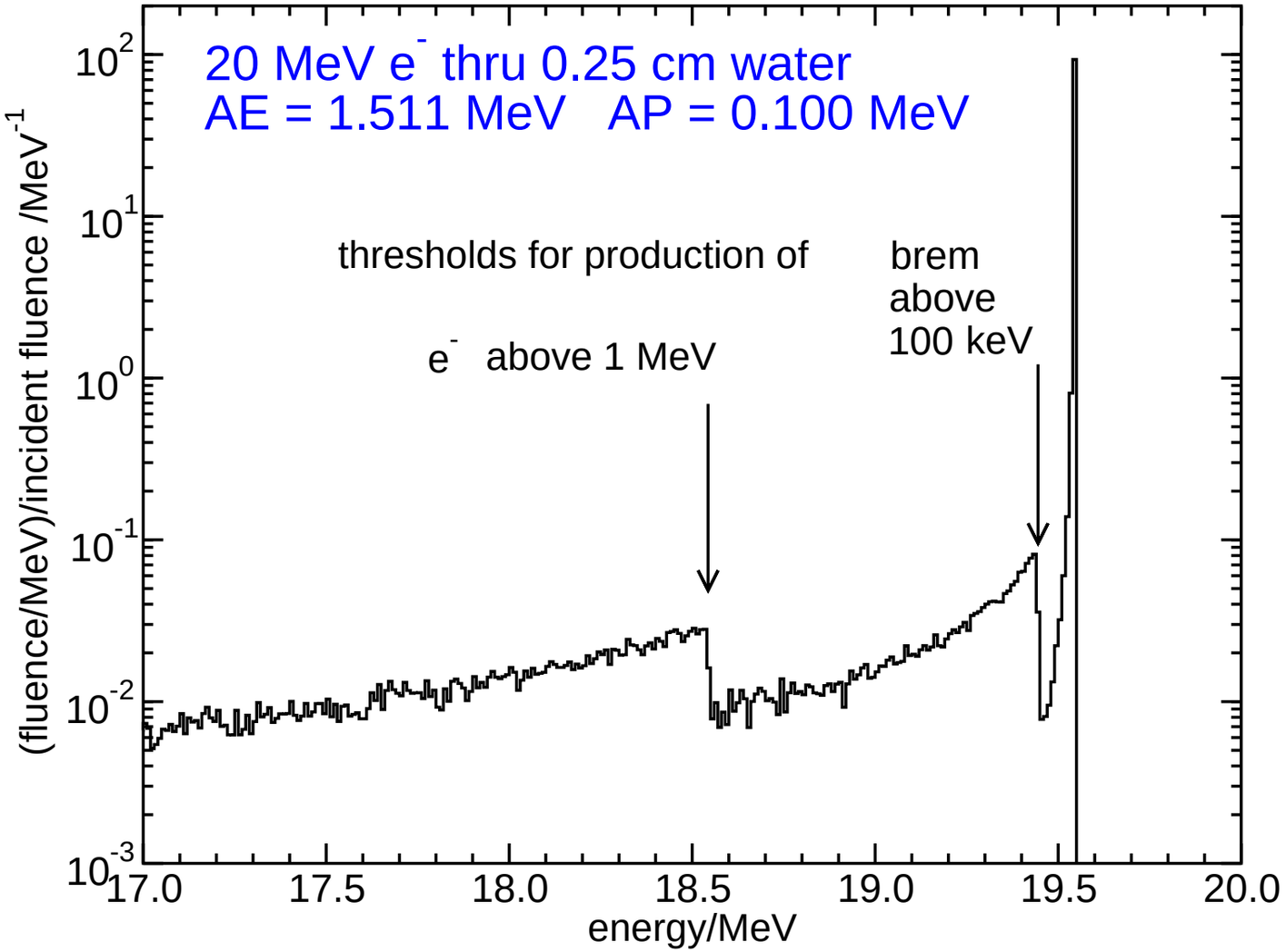
$$\begin{aligned}\text{Range of AE electrons} &\ll \text{geometry scale}\\ \text{Range of AP photons} &\ll \text{geometry scale}\end{aligned}$$

Second condition usually difficult to satisfy. If so, it is also sufficient that

$$\text{Energy lost to sub-AP photons} \ll \text{other energy loss}$$

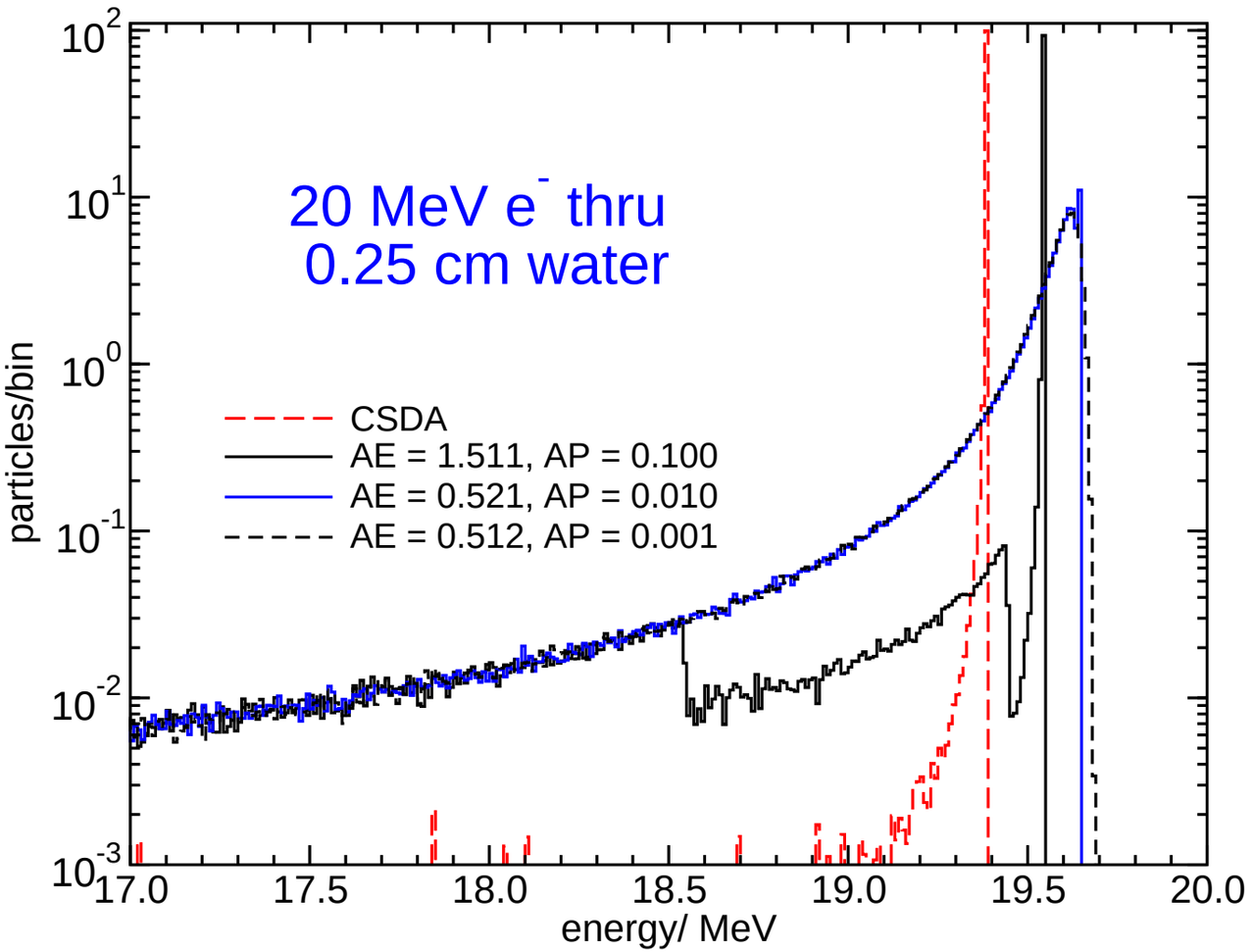
Generally, when AE,AP decrease, accuracy and CPU time increase

Understanding AE, AP



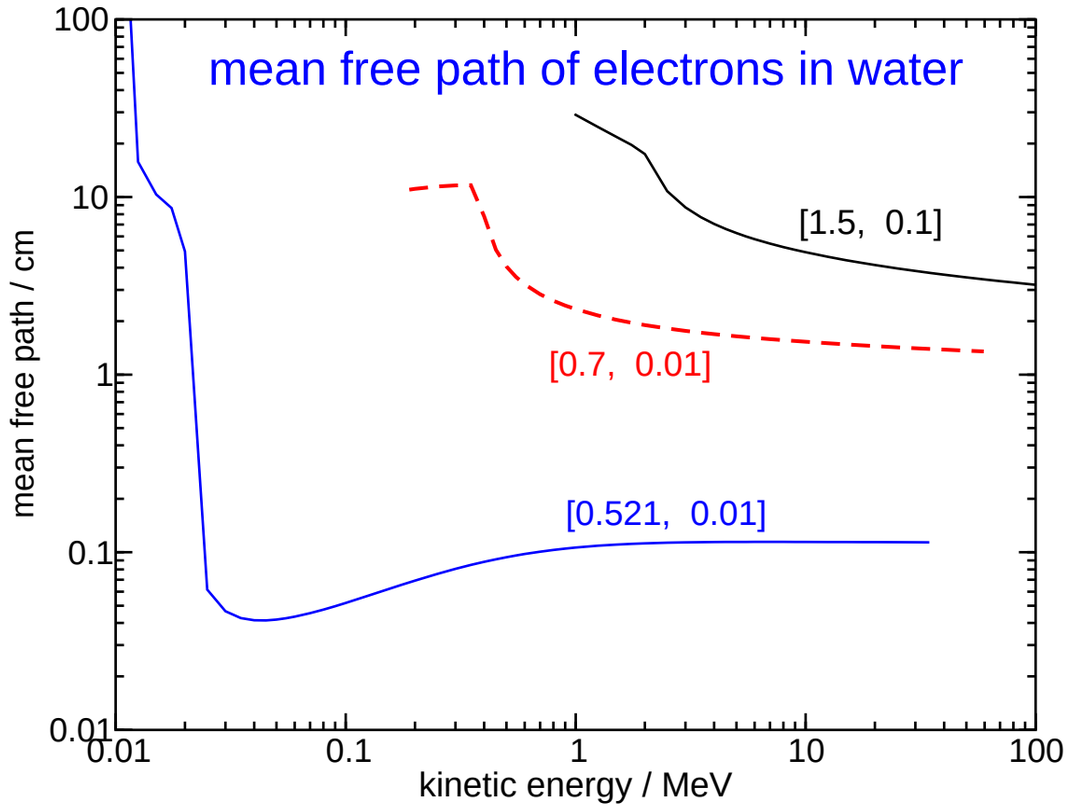
Emerging e– spectrum depends crucially on AE,AP

Understanding AE, AP



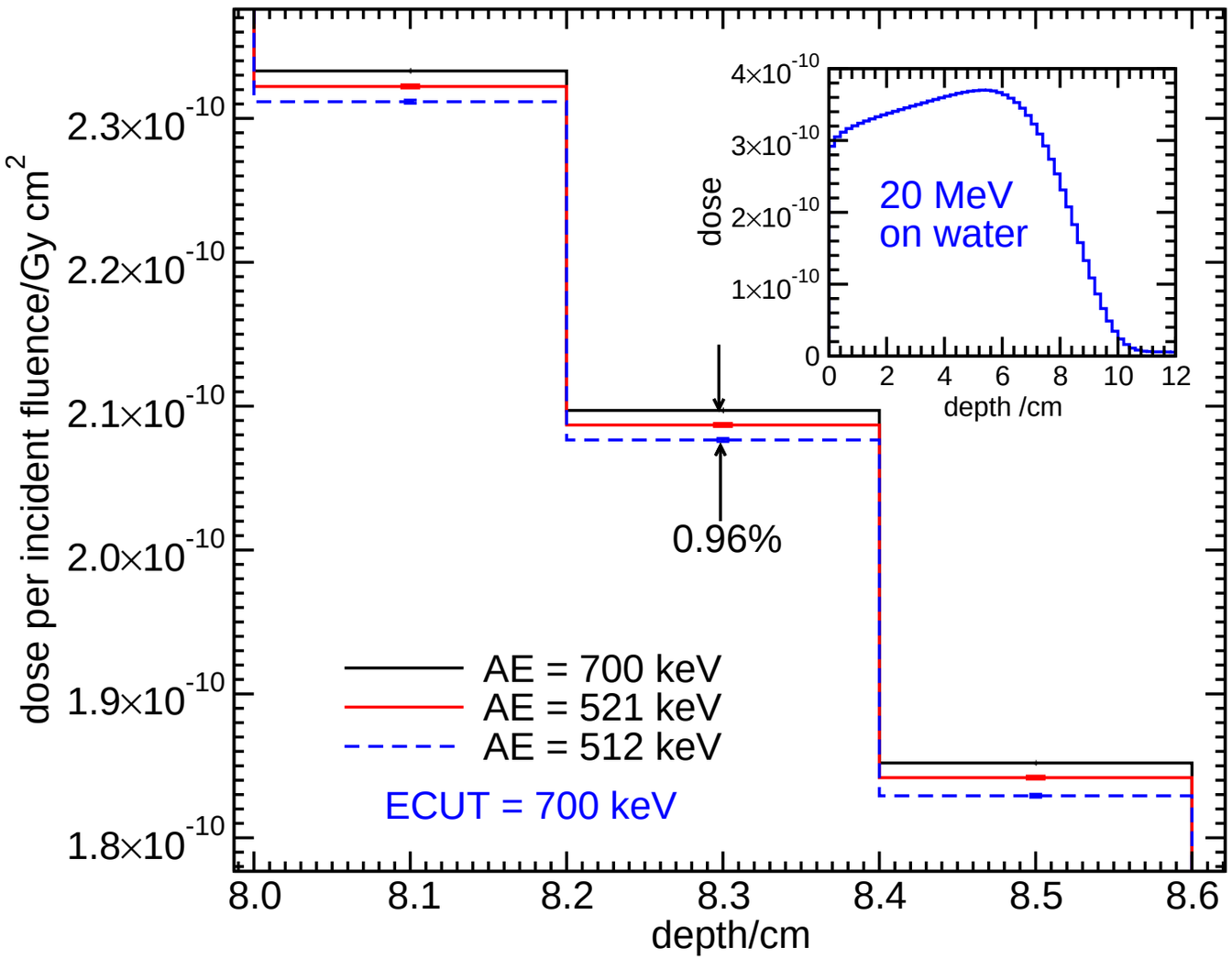
Emerging e- spectrum depends crucially on AE,AP
But mean energy is same 618 keV in all cases

Effect of AE,AP on step size



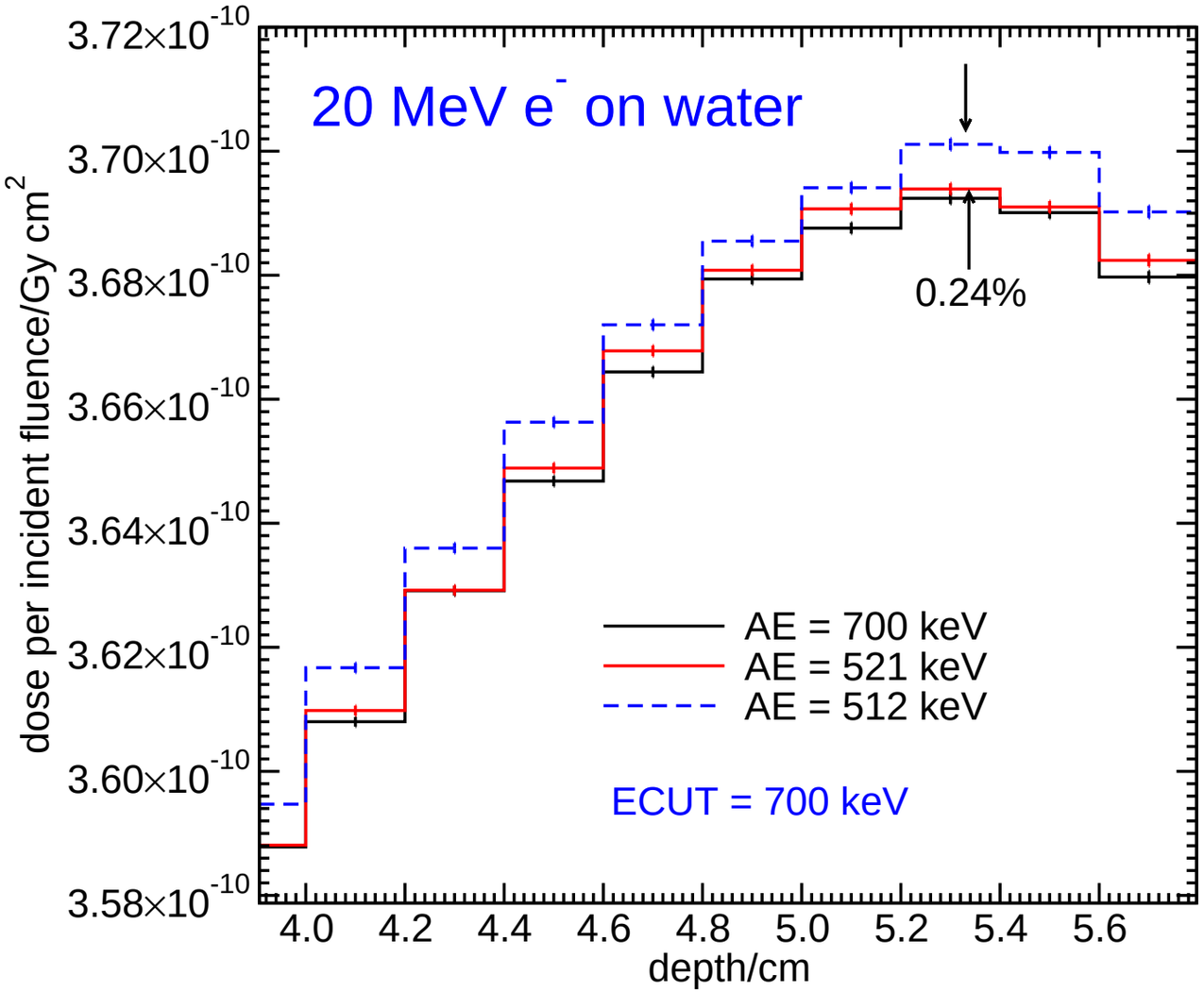
Threshold for producing secondaries affects step sizes dramatically.
Step sizes do not affect EGSnrc transport but may affect other codes.
But changes in energy loss straggling can affect transport.

What is effect of different spectra/energy loss-straggling/AE?



Effect may be very small in many situations.

What is effect of different spectra/energy loss-straggling/AE?



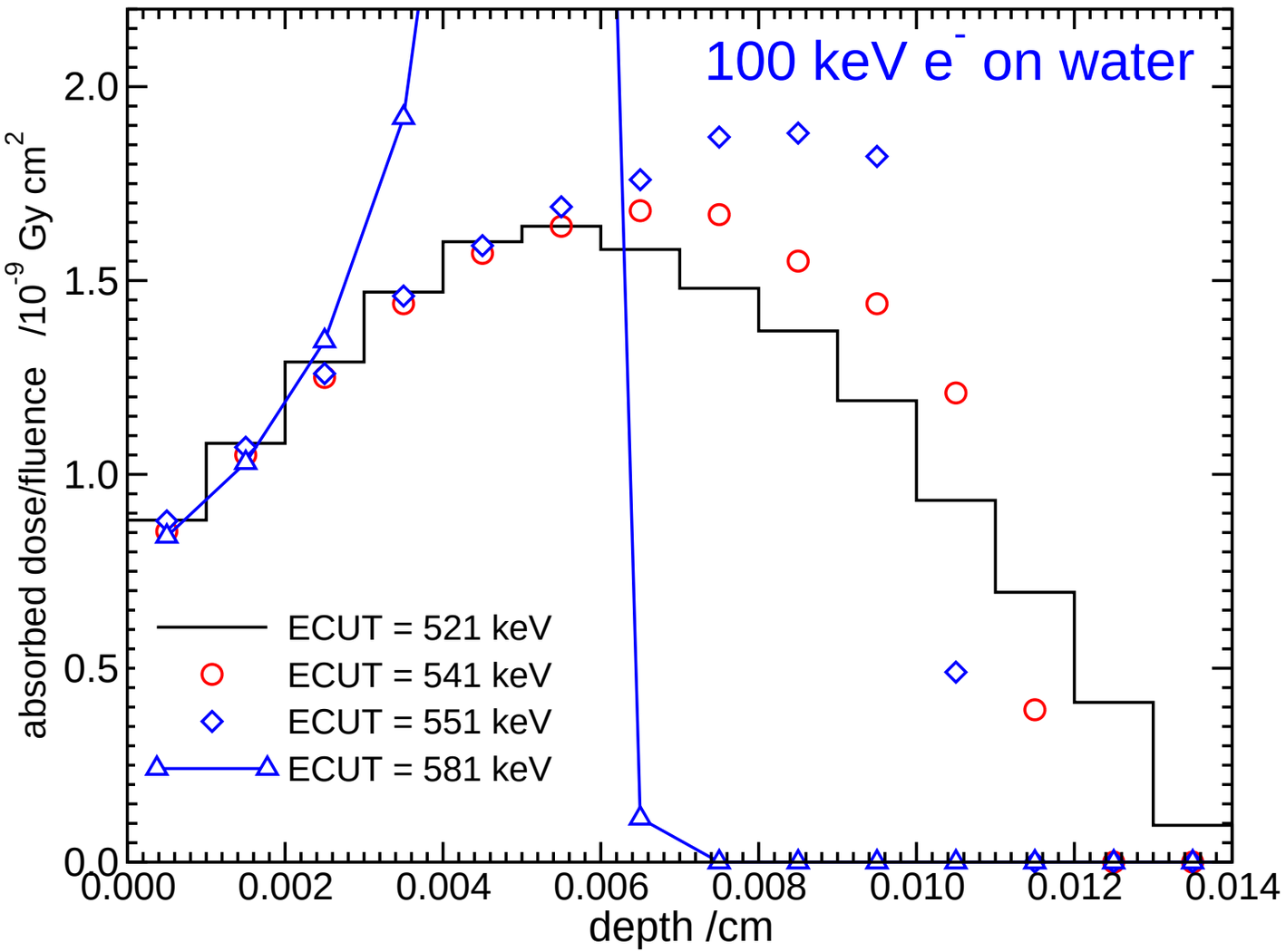
Effect may be very small in many situations: Higher AE is OK often.

Choice of AE

- AE has a major effect on energy loss-straggling
  - So if calculating a spectrum, it may be important to have low AE values
- But little effect on average energy loss and in many cases has a small effect on dose deposition
  - above assumes a fixed ECUT value (more coming)
- lower AE values for a fixed ECUT take longer
  - 10s of percent effect

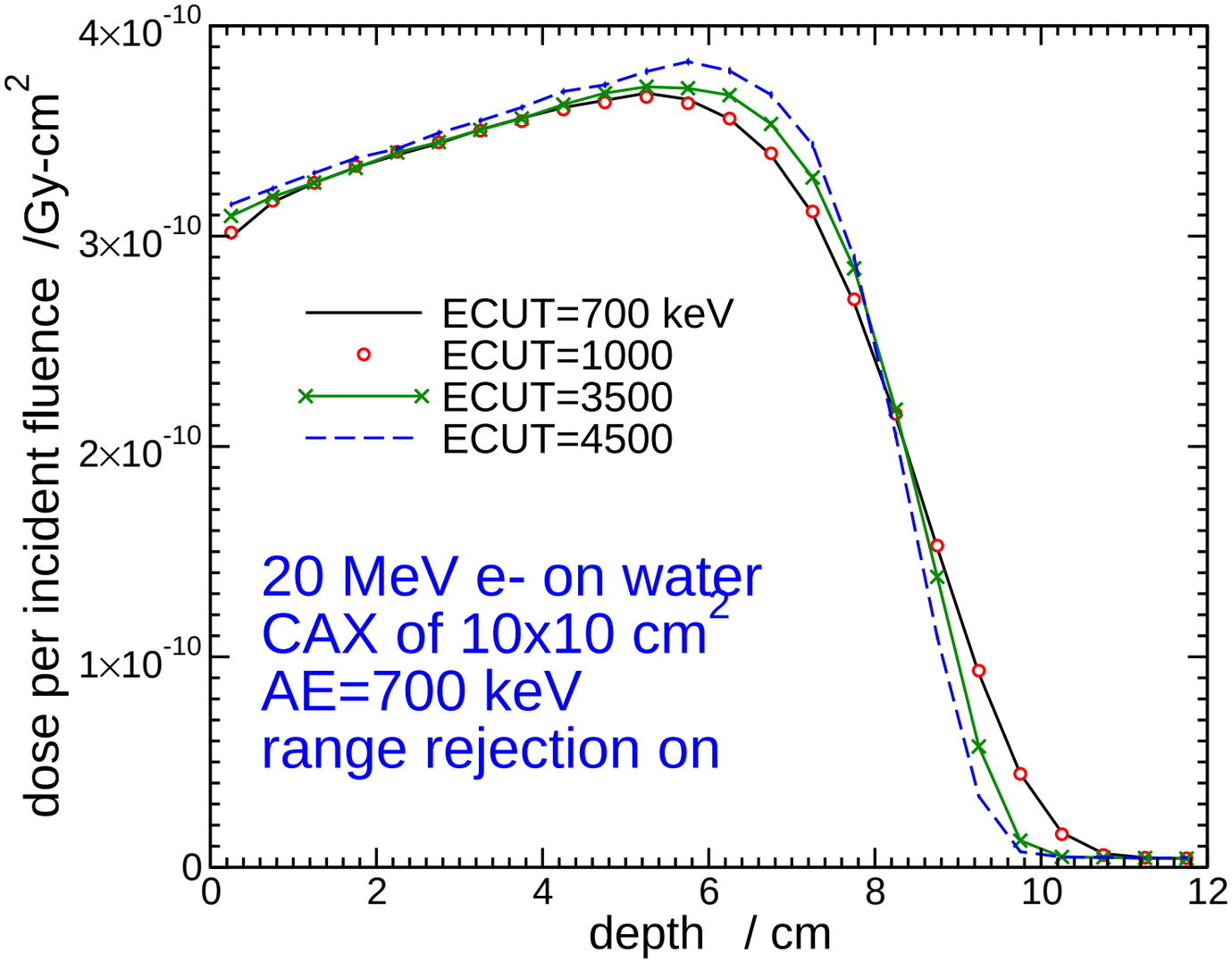
Effect may be very small in many situations: Higher AE is OK often.

Understanding ECUT, PCUT: energies to terminate histories



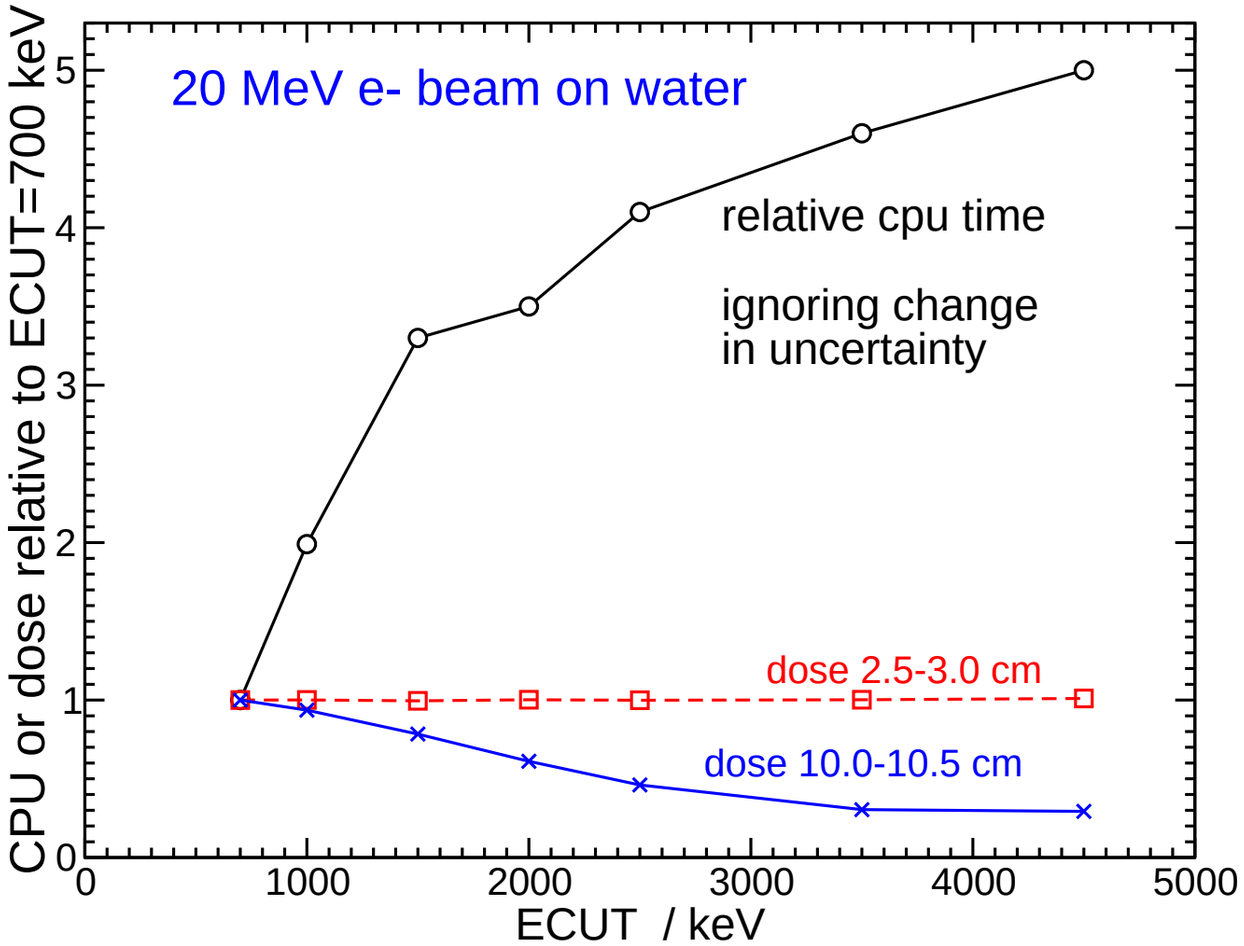
When the energy of a particle falls below ECUT,PCUT it is deposited locally.

Understanding ECUT



Curves with ECUT = 700 or 512 keV are identical (both AE=512 keV)

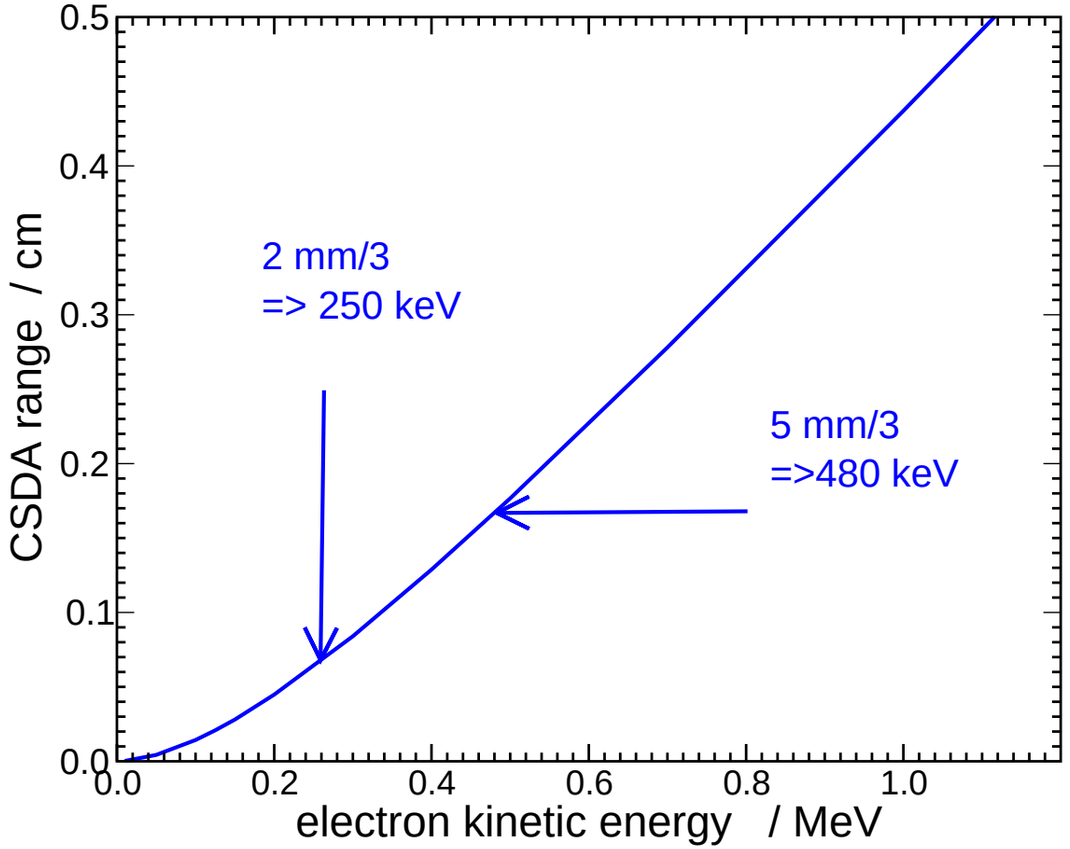
How does ECUT affect the calculation?



Major effect on CPU time and only a small effect on accuracy in some cases. Step sizes roughly equal fractional energy loss per step so 1000 to 100 takes as long as 100 to 10 or 10 to 1 keV.

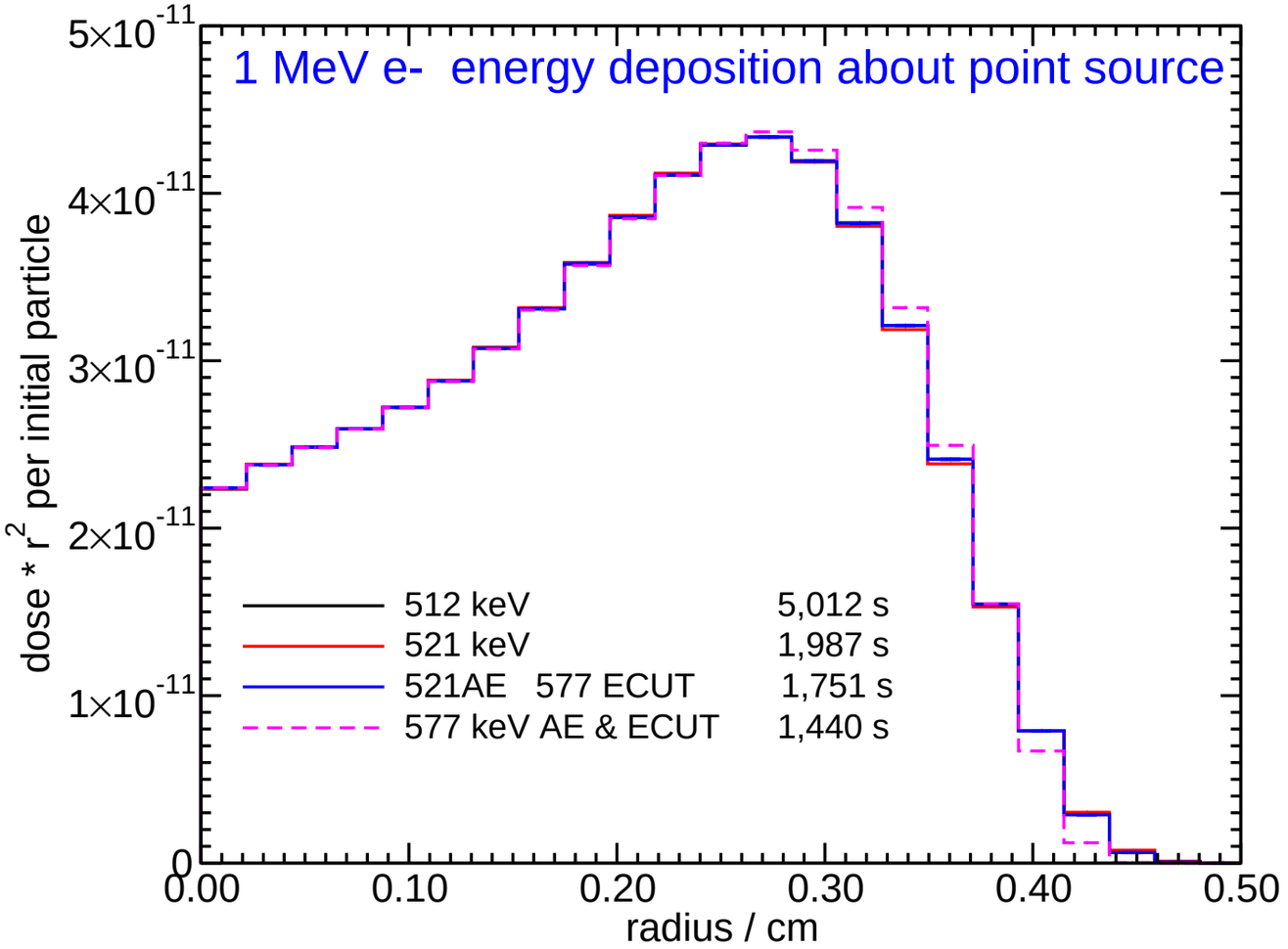
How do we select ECUT?

- 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.

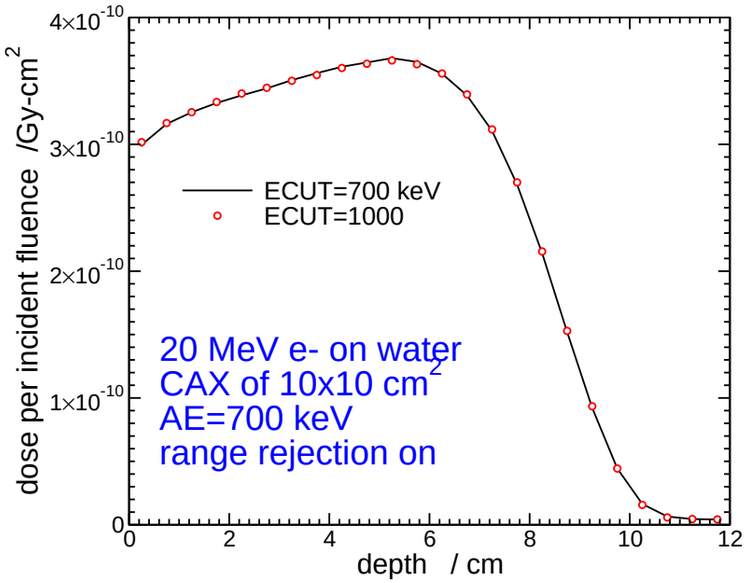
Example: e- energy deposition kernel



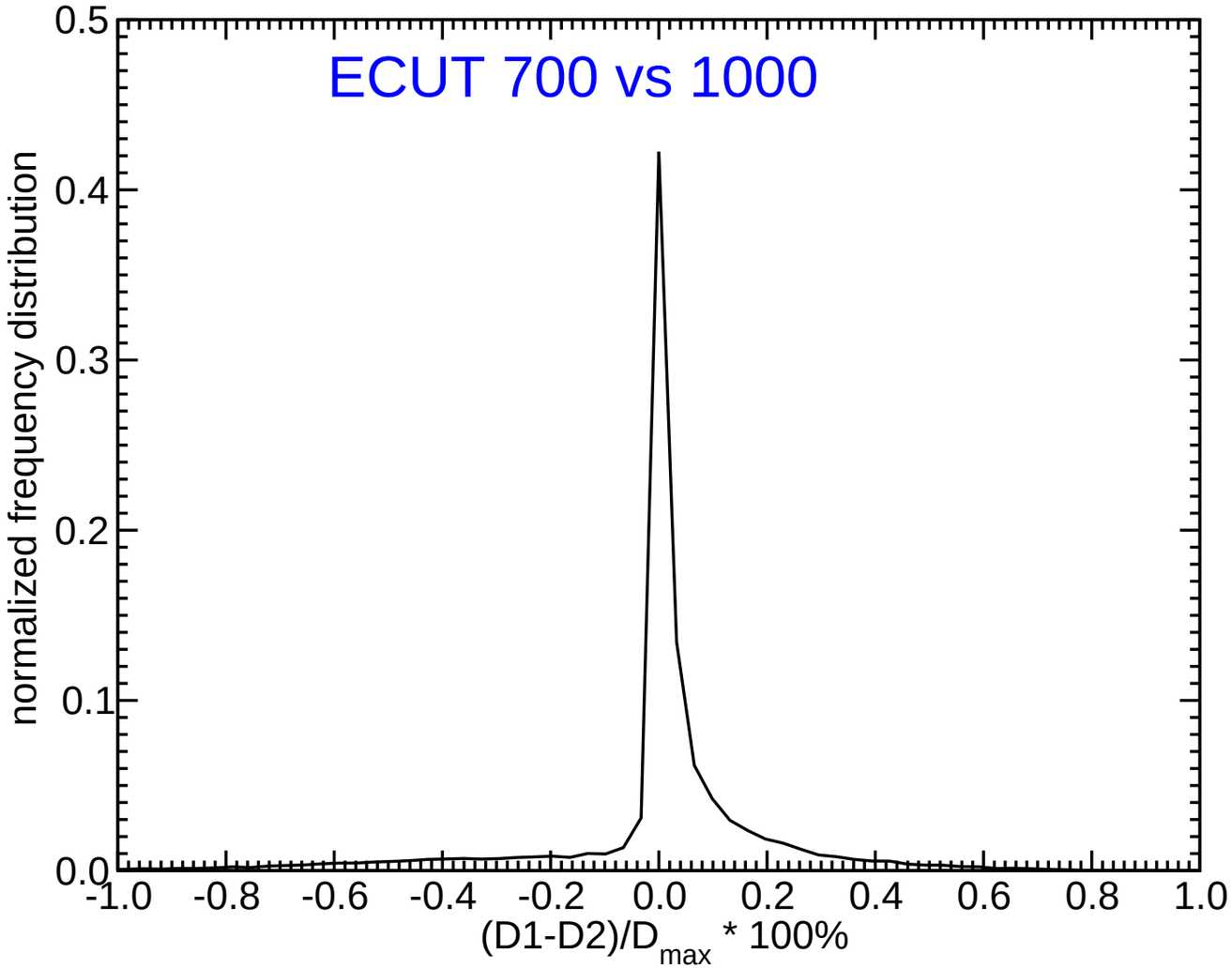
0.022 cm radial bins: CSDA range of 577 keV e- is 0.007 cm.
Here ROT works for ECUT but need a lower AE.

Aside on comparing 3-D dose distributions

- it has become common to use Low et al's gamma function to compare two calculated dose distributions
- this is not appropriate for two MC calculations since there is no uncertainty in the spatial component of the calculation
- there are better approaches
- let's look again at the 20 MeV e- beam



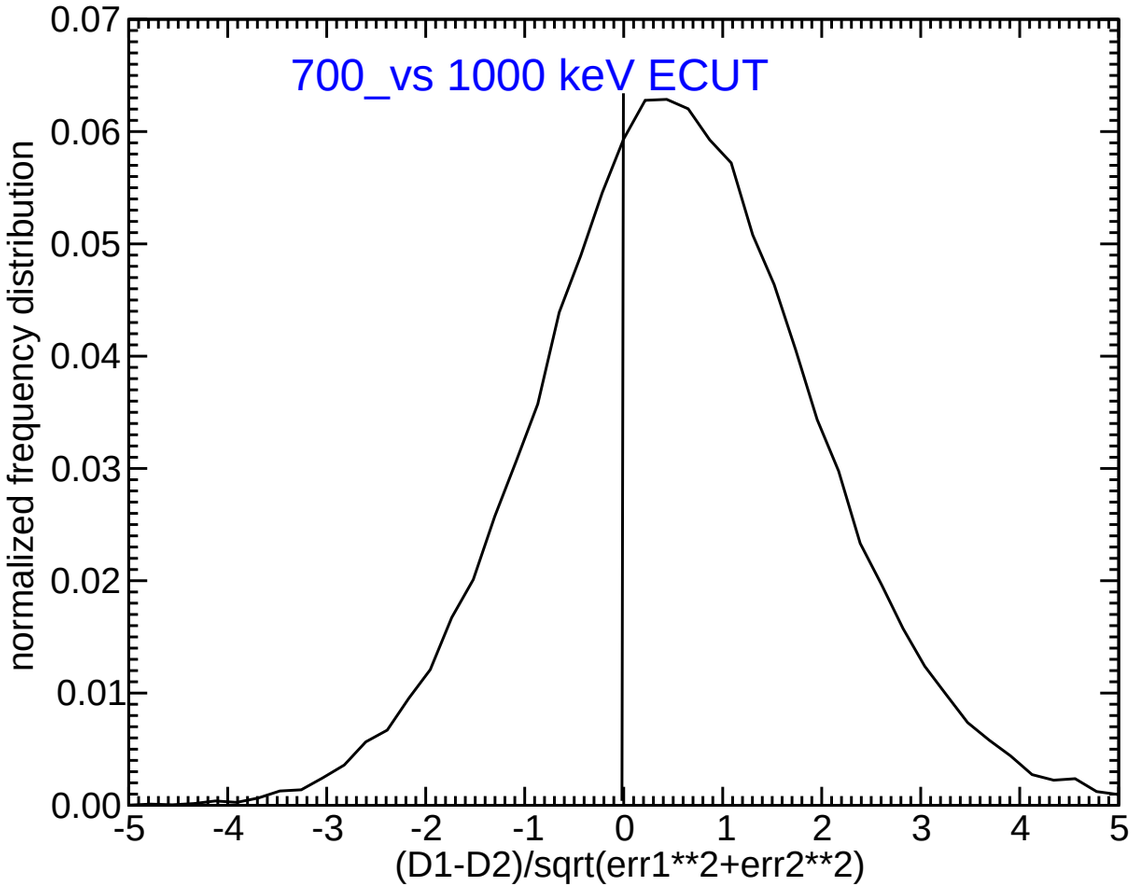
statdose: look at absolute differences



As a fraction of D_{max}, the differences throughout the 3-D dose distribution are small

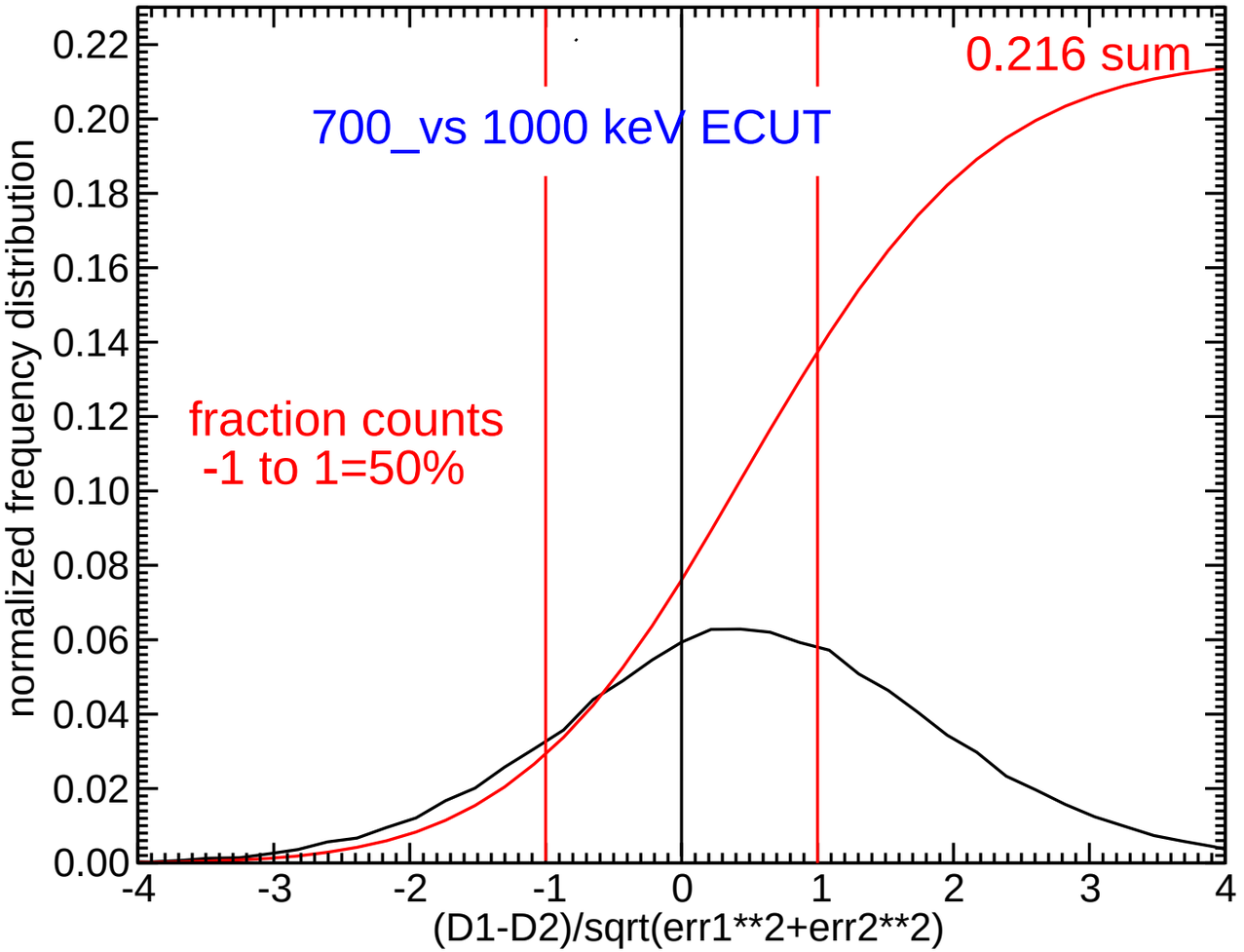
statdose: a statistical approach

- are the differences statistically significant?



$$(D_1 - D_2) \Big/ \sqrt{s_1^2 + s_2^2}$$ Should be centered on 0.0 if completely unbiased.

statdose: a statistical approach (cont)



If the differences were strictly statistical, then 68% of events should be between -1 and 1. Differences here are statistically significant.

Understanding ECUT, PCUT

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

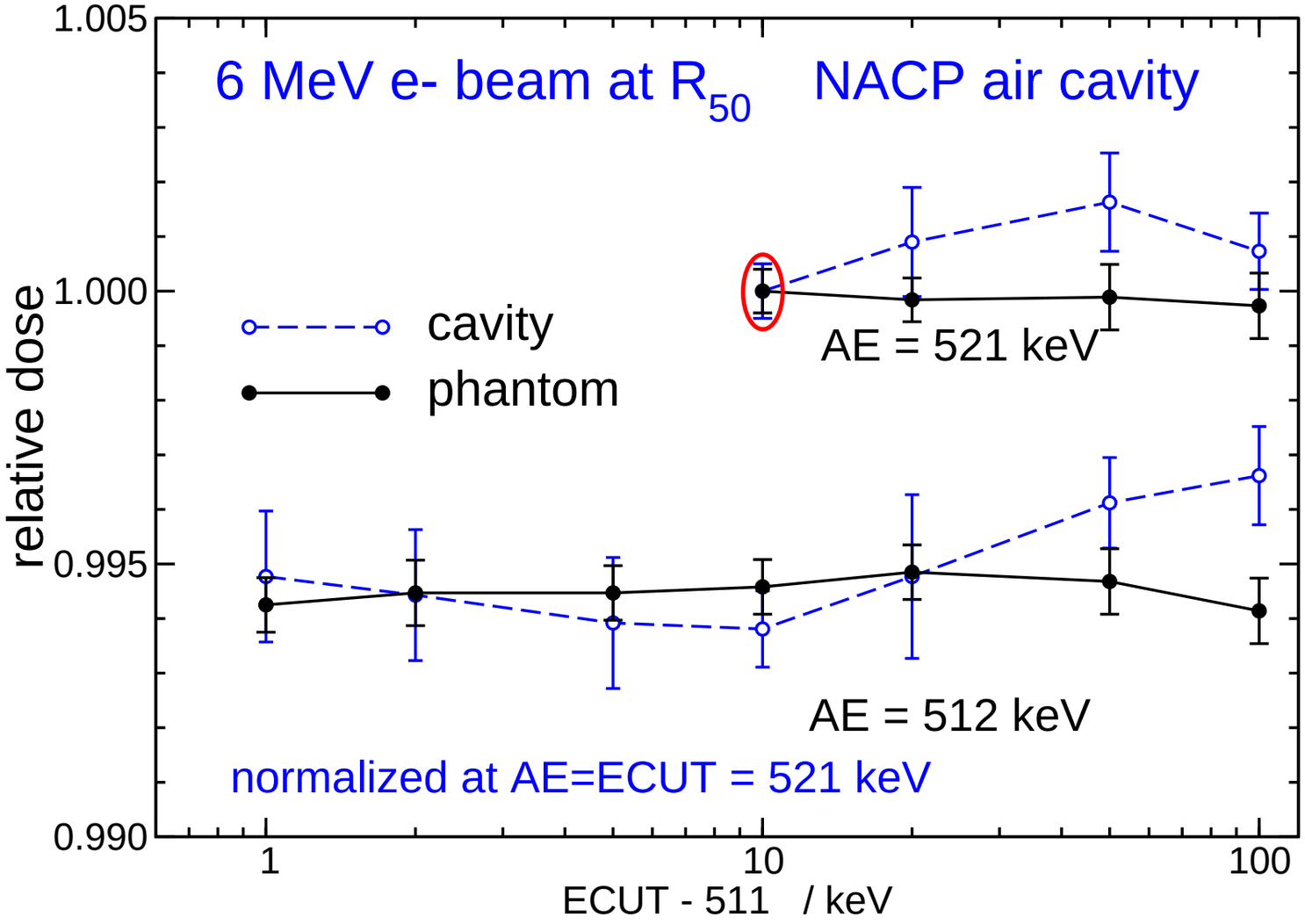
Examples:

- The calculation of energy spectra where low-energy component not of interest.
- Want to force all energy that reaches certain region(s) to be deposited locally

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

But take care.
Sometimes the final quantity sought varies less than individual components.

An example in which things cancel



As seen earlier, at R_{50}, AE has a larger effect than ECUT.

The ratio of two varying quantities may be steady

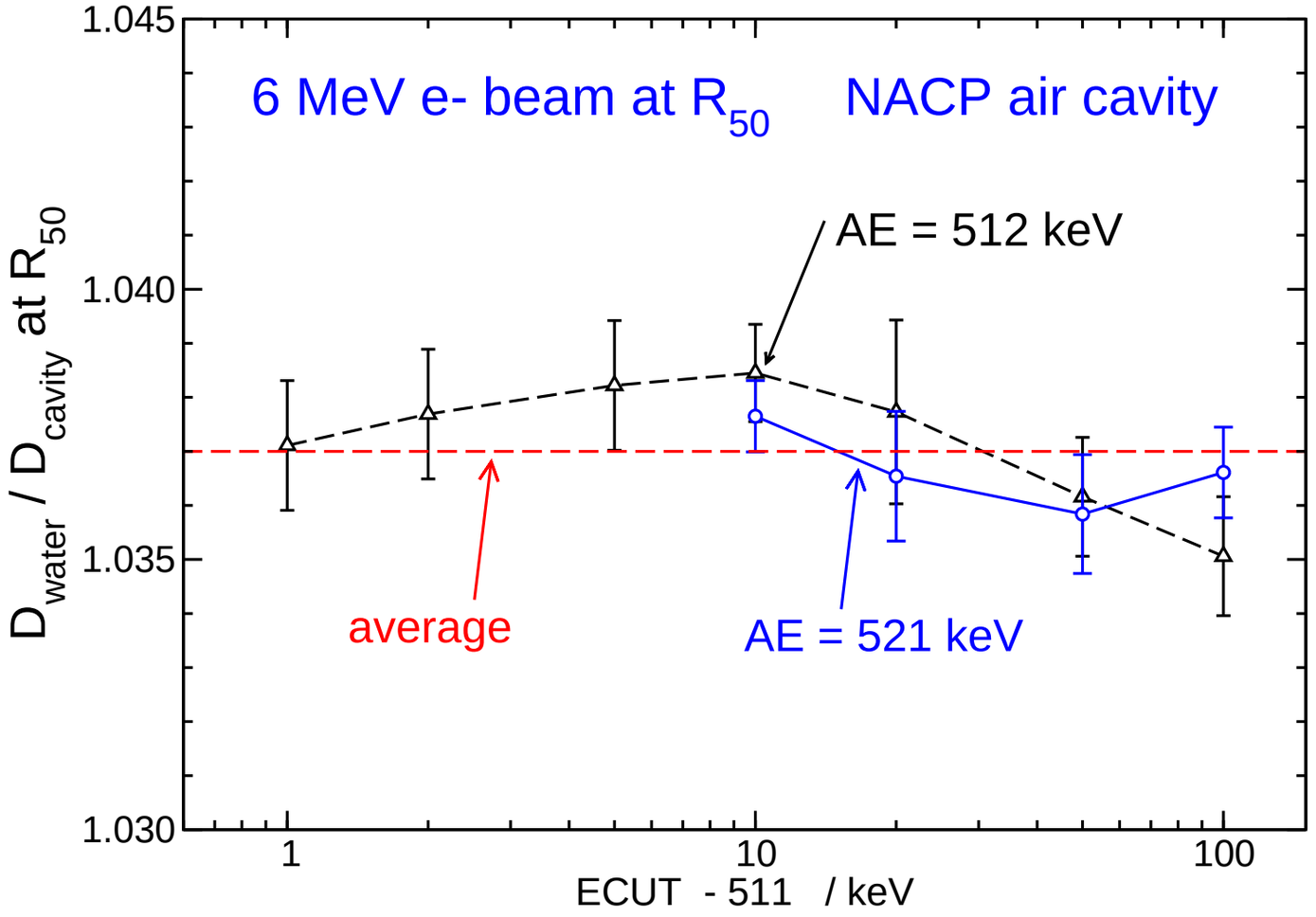


Fig implies one could have used AE=521 keV and ECUT=611 keV but even the more conservative 521/521 saved a great deal of time.

Range Rejection

Terminate history of any electron with energy below ESAVE which cannot get out of current region with an energy above local ECUT.

Approximation involved!

Possibility of brem creation by terminated electrons is ignored.

Example 1: 20 MeV e^- on W
11% of brem yield is from e- with E $<$ 5 MeV and 2% from E $<$ 2 MeV

Example 2: 10 MeV e^- on W
37% and 7% of brem yield is from e- with E $<$5 and $<$2 MeV respectively.

ESAVE of 2 MeV and 1 MeV respectively ensures $<$2% error.

This is overly conservative since low-energy photons absorbed in the target.

ESAVE Variation

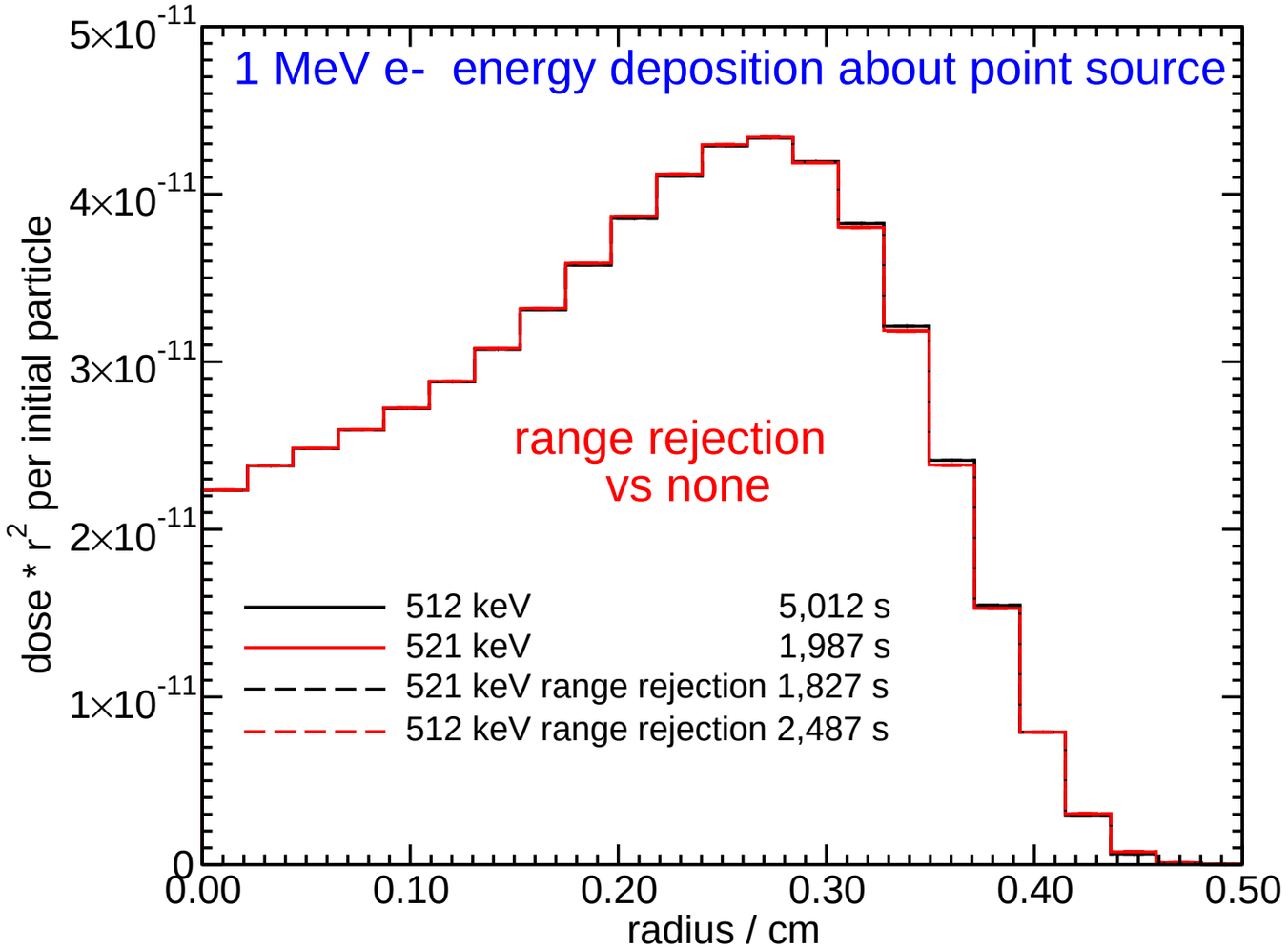
CPU times for 18 MeV e– linac using automatic ECUTRR (BEAM paper).

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

$\Rightarrow$ have a very good reason for using AE=521 keV (or too many computers).

e.g.: calculating dose to very thin-walled ion chamber at phantom surface.

Range rejection is important



At 1 keV saves $>$ factor 2, 10 keV 8%. More important for low ECUT since low energy e- take time to transport but short range means rejected often.

Photon cross sections

- options are SI/XCOM/EPDL or user supplied
  - Storm and Israel as per original EGS4
  - NIST's XCOM data set (now the default)
  - Evaluated Photon Data Library from Lawrence Livermore National Laboratory (1997)
- EGSnrc no longer uses the photon data in the PEGS4 data set

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 can be $\sim$3 times slower with bound Compton!
  (special tricks on sampling cannot be used with bound Compton).
- Effect usually completely negligible for energies above a few hundred keV

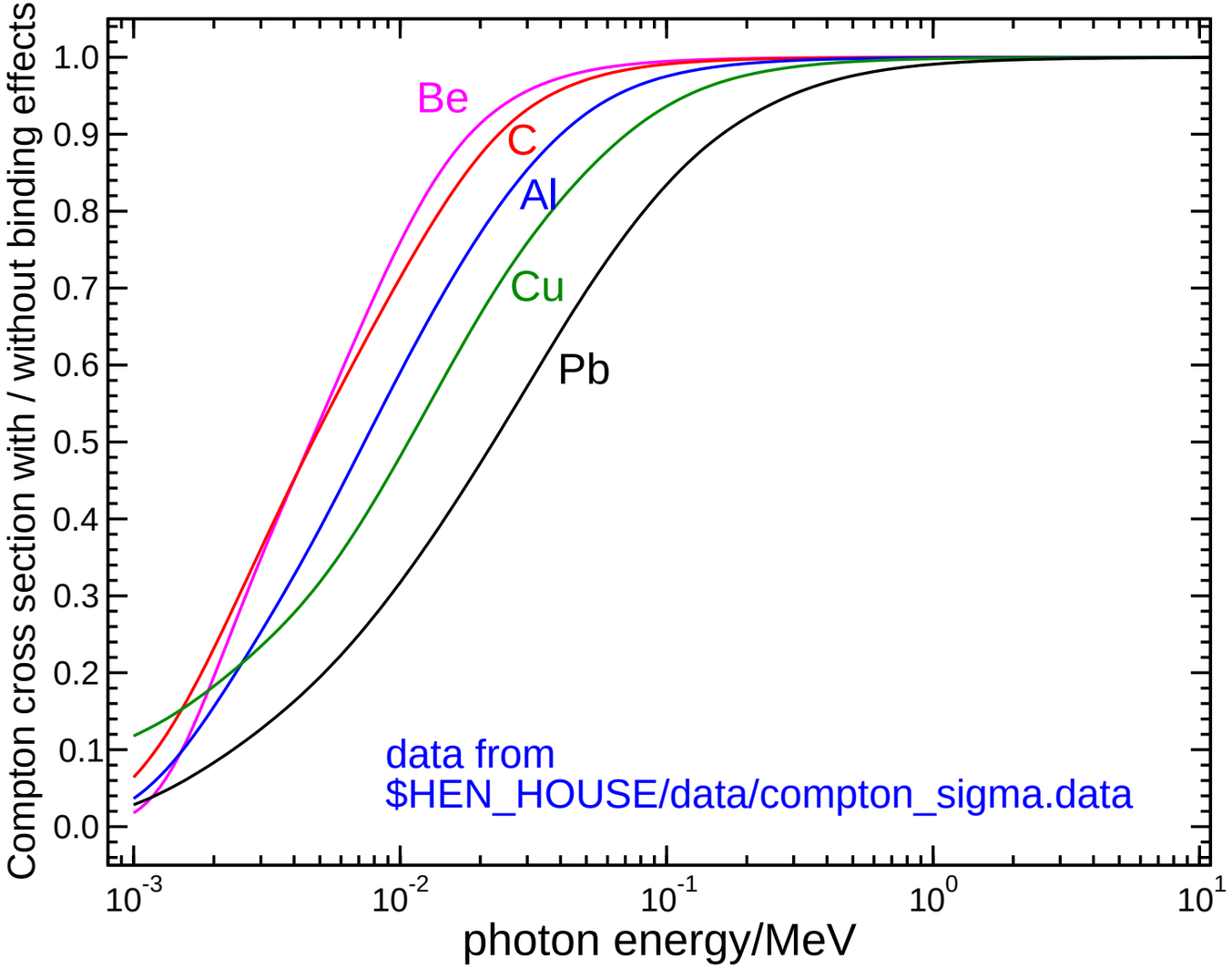
Bound Compton scattering

- Electron binding reduces the total cross section (next slide)
- 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 dominates

$\Rightarrow$ Very small effect for dose calculations.

- Important for detector response function calculations, simulations related to imaging, etc.!

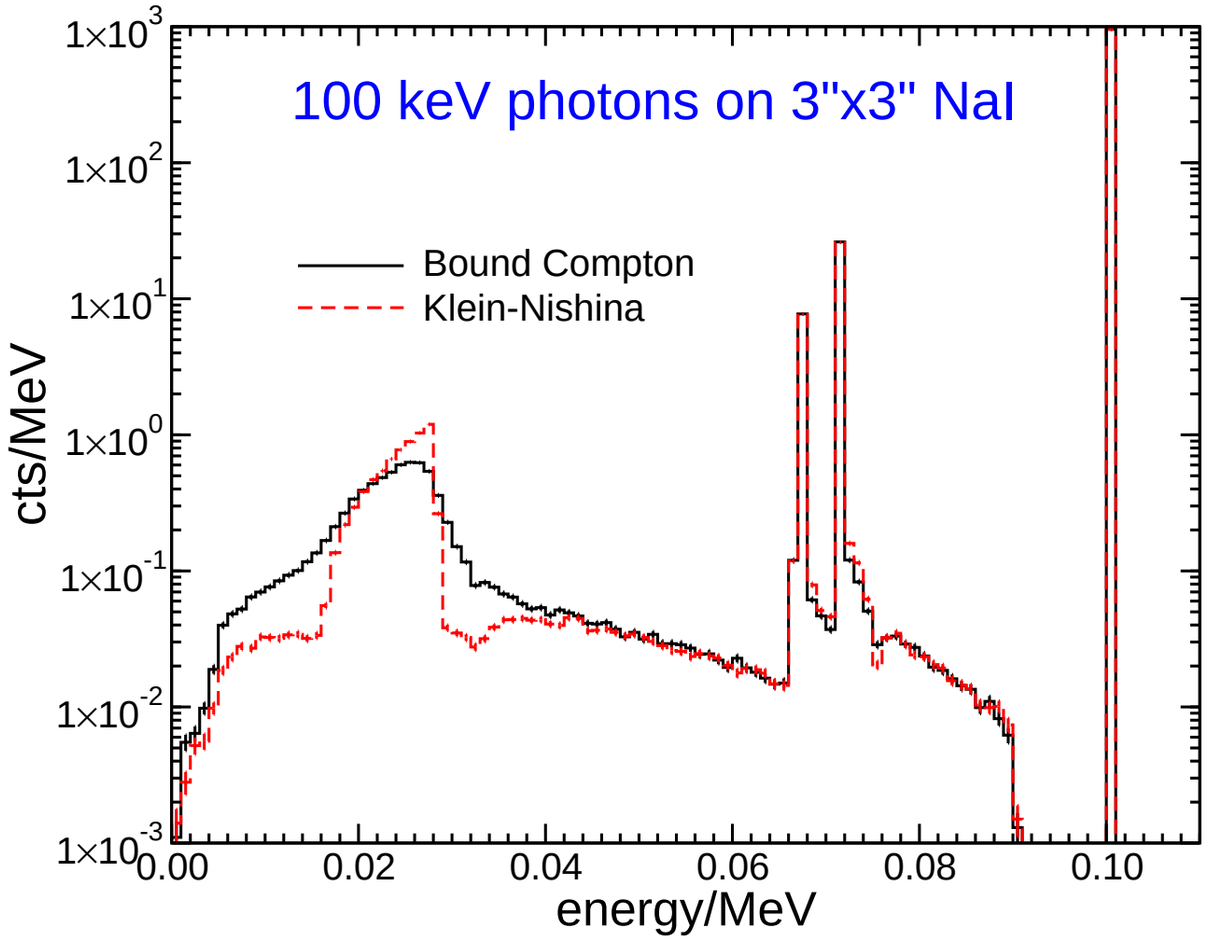
The ratio of bound Compton to Klein-Nishina



Why is this not as important as it appears?

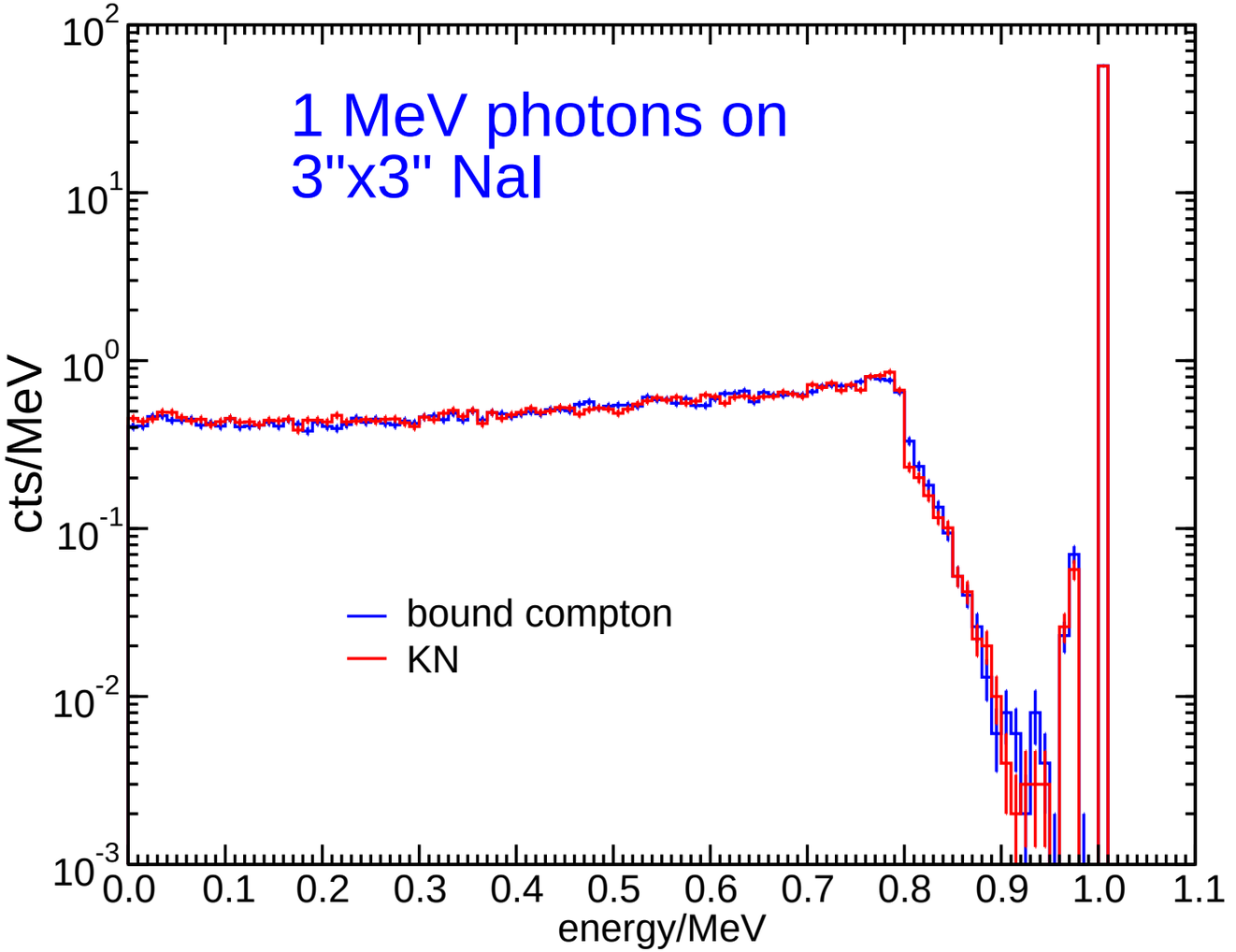
Data provided by Elsayed Ali.

The effects on spectrometer response functions



Binding & doppler broadening makes a big difference on the Compton edge. But the effect of relaxation/escape of fluorescent x-rays is more dramatic since detector resolution would already smear the peak out.

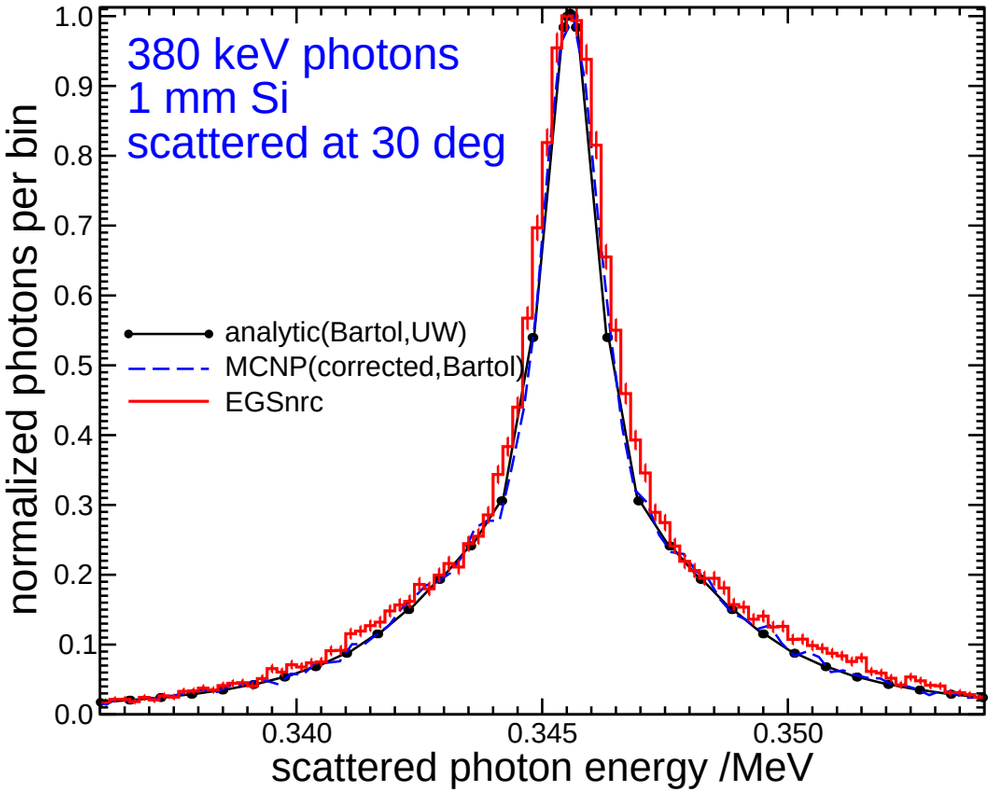
By 1 MeV the effect is negligible



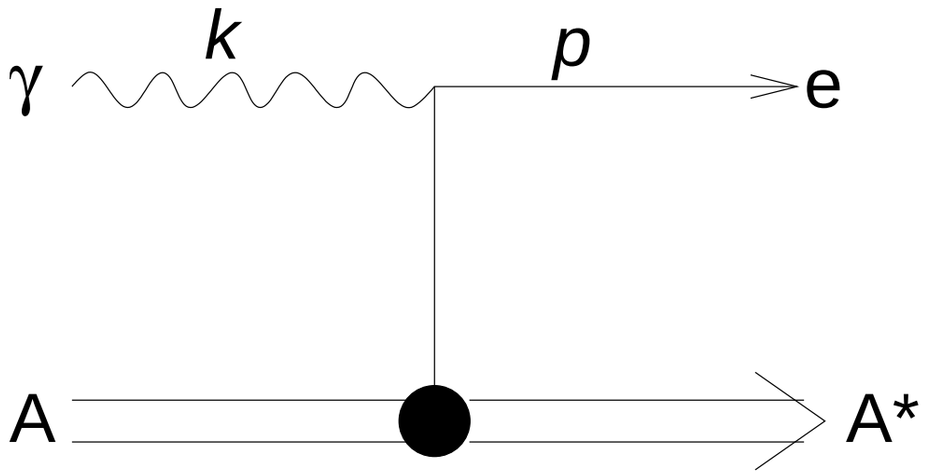
So why waste time including binding/doppler effects?

Verifying the accuracy of the sampling routine

- Bartol and DeWerd (Med Phys 39(2012)5635) corrected the doppler broadening routines in MCNP5
  - verified against an analytic calculation
  - so used it as a check on the EGSnrc implementation



Atomic relaxations



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

Be aware: relaxations in high-Z materials may produce a lot of particles and so a lot of overhead.

Atomic relaxations

Output from watch:

```
Photoelectric about to occur: 1 0.100
   Fluorescent X-ray created: 2 0.073
      Auger electron created: 3 0.009
      Auger electron created: 4 0.002
      Auger electron created: 5 0.002
    Resulting photoelectron: 1 0.012
                                ...
Photoelectric about to occur: 2 0.073
    Coster-Kronig e- created: 3 0.002
      Auger electron created: 4 0.007
      Auger electron created: 5 0.002
      Auger electron created: 6 0.002
```

EII: Electron Impact Ionization

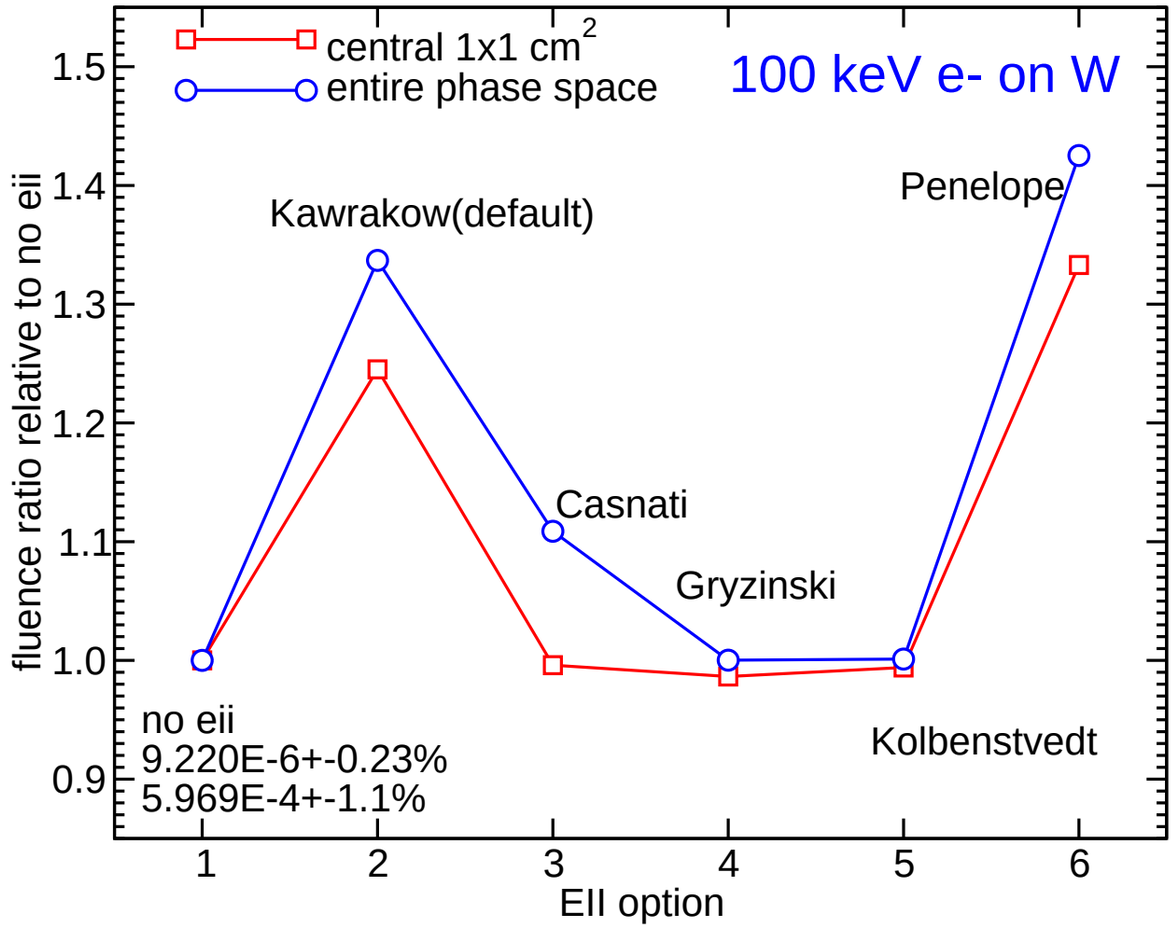
This is creation of electron vacancies directly by electrons (like an internal bremsstrahlung which undergoes a photoelectric event in the same atom).

- EII "on" is essential for calculation of kilo-voltage X-ray spectra (characteristic X-ray lines are underestimated with EII "off")
- Other than for kV spectra, it rarely, if ever, 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

Electron Impact Ionization: options

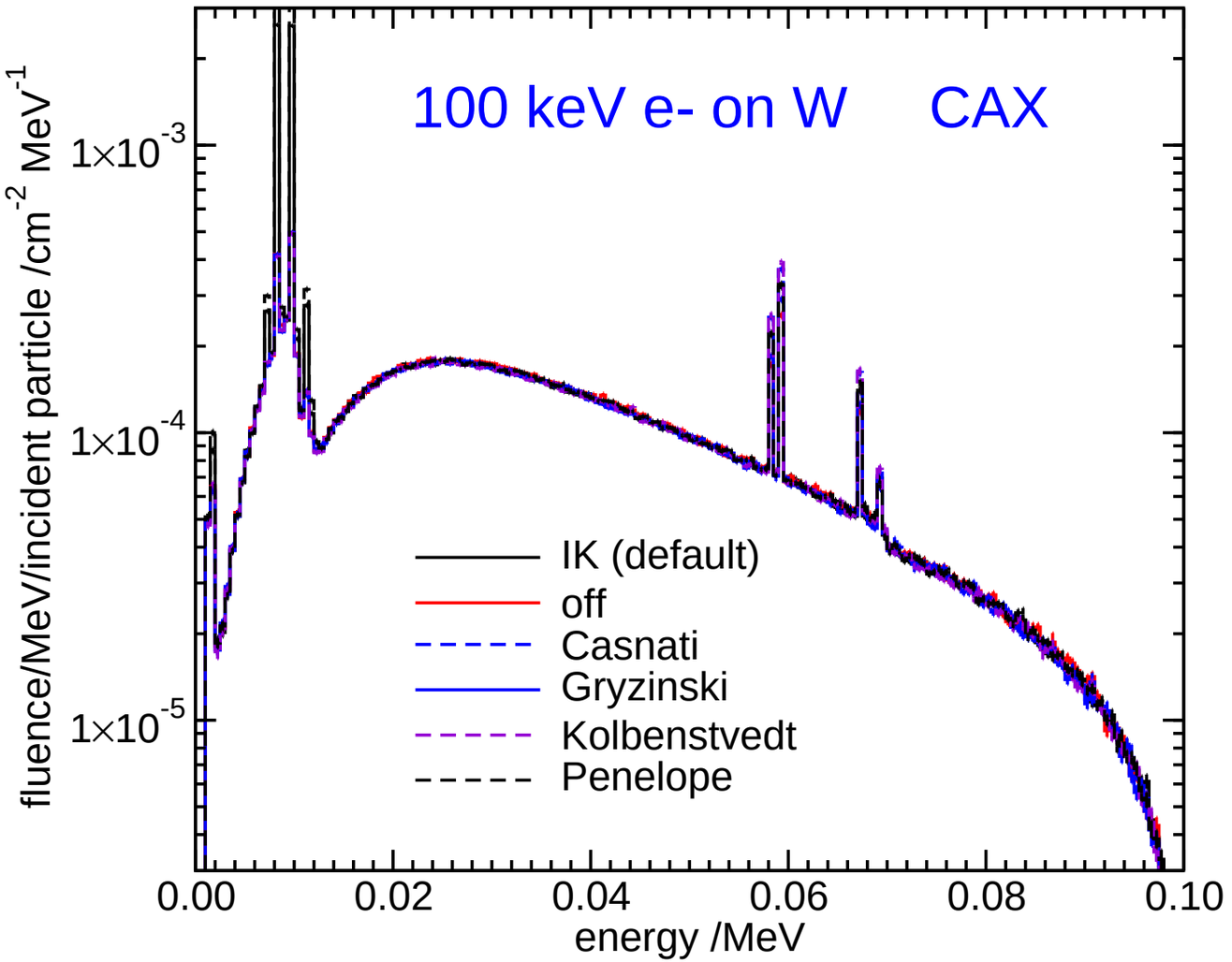
Available options: Off/On/casnati/kolbenstvedt/gryzinski/penelope

Problem: which is right/more accurate?



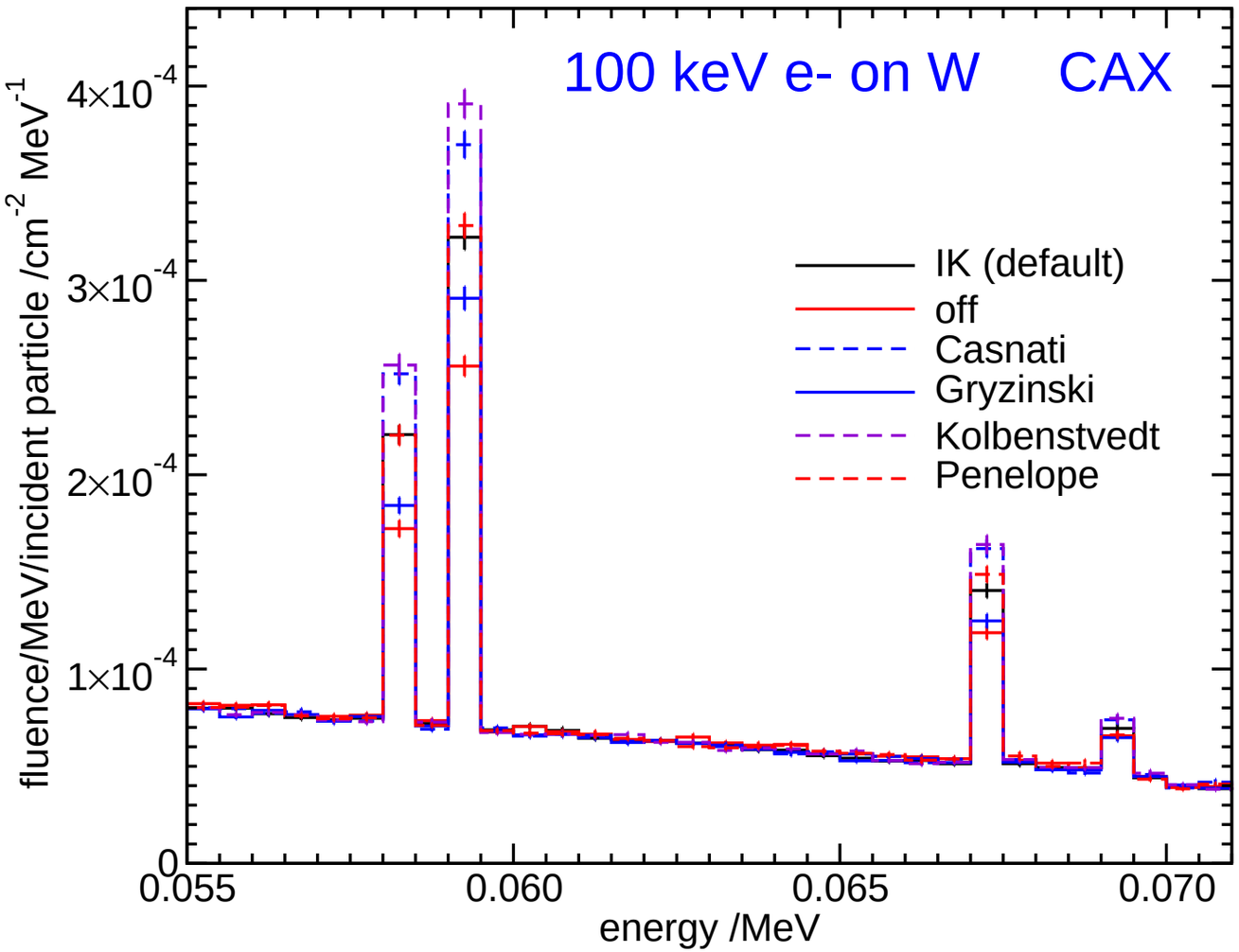
Electron Impact Ionization: options

It doesn't affect the brem component of spectrum



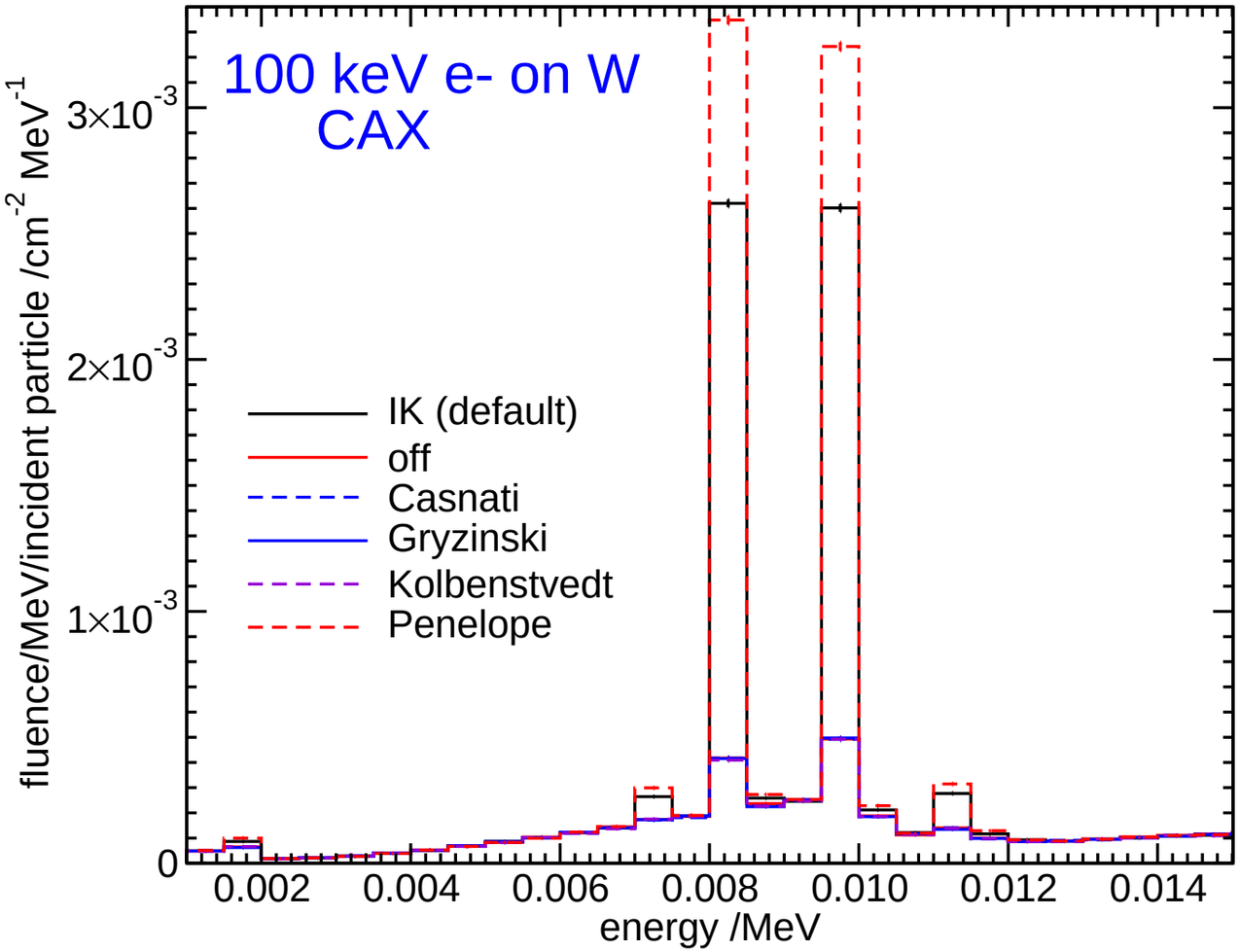
Electron Impact Ionization: options

Problem: which is right/more accurate?



Electron Impact Ionization: options

Problem: which is right/more accurate?



The main difference is decay of the L-shell.

New option re low-energy fluorescence

Previously EGSnrc used K & L shell individual binding energies but averaged values for M & L.

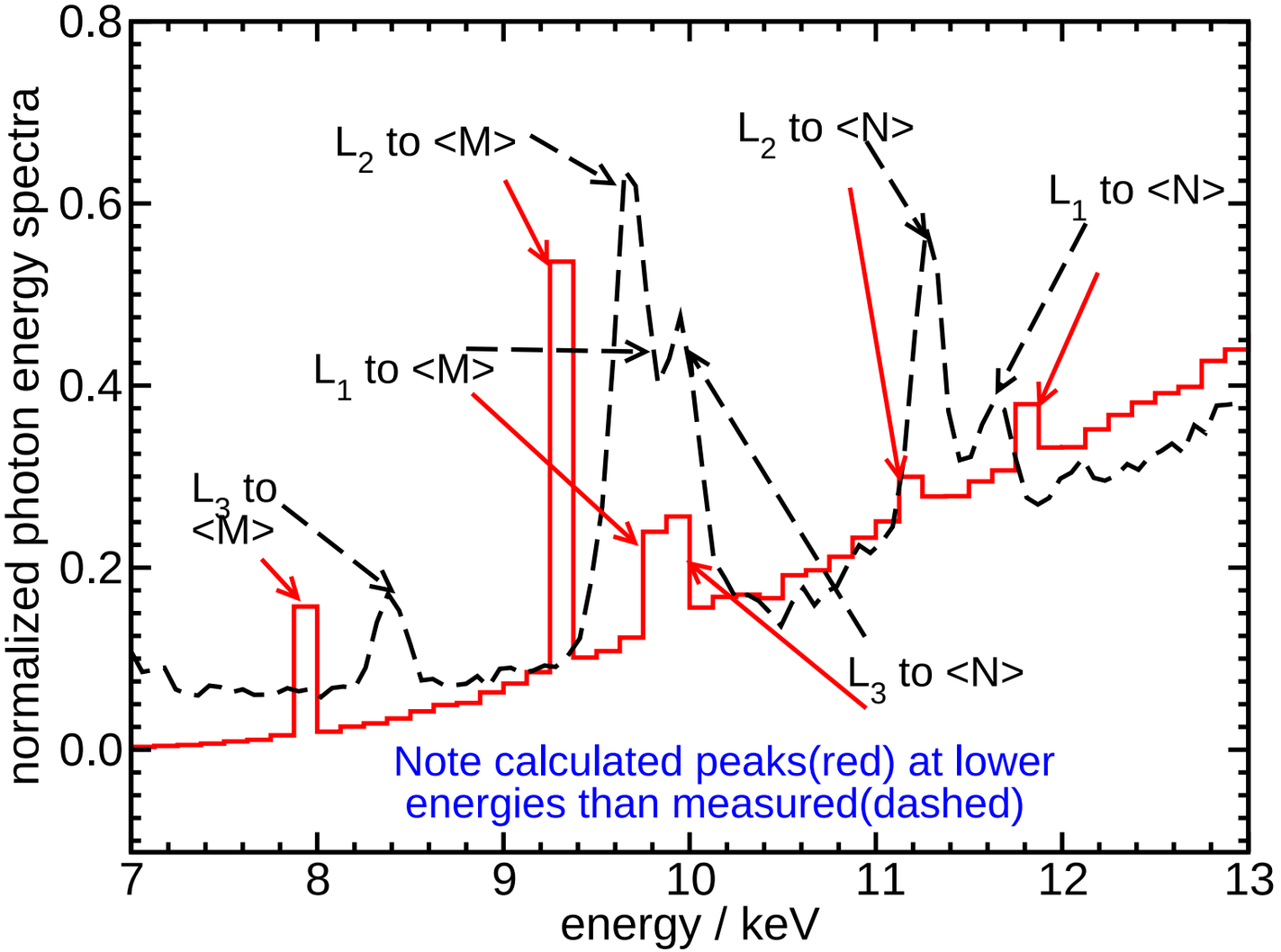
Shell energies (in keV) used previously in EGSnrc for Tungsten

K	L1	L2	L3	$< M >$	$< N >$
69.5	12.1	11.5	10.2	2.27	0.301

$$< M_k >= \frac{\sum \nu_{KM_j} E_{M_j}}{\sum \nu_j}$$ where ν_{KM_j} is probability of an M_j to K transition

But: If used $L - M_j$ probabilities, then $< M >= 1.88$ keV not 2.27 keV.

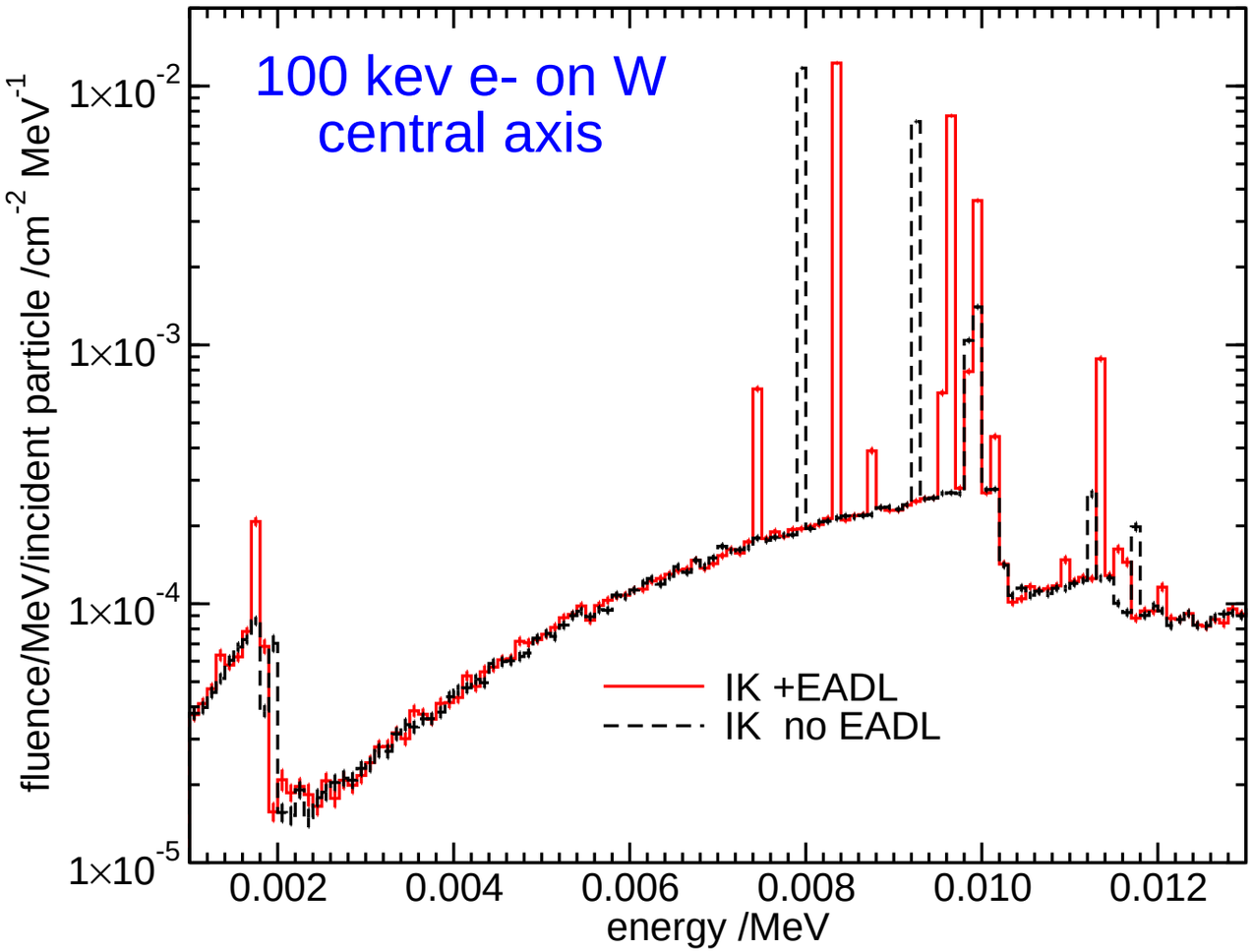
Effects of using shell averages



50 kV XOFT source. From Randy Taylor's MSc thesis (2008)

New option: use of the EADL relaxation dataset

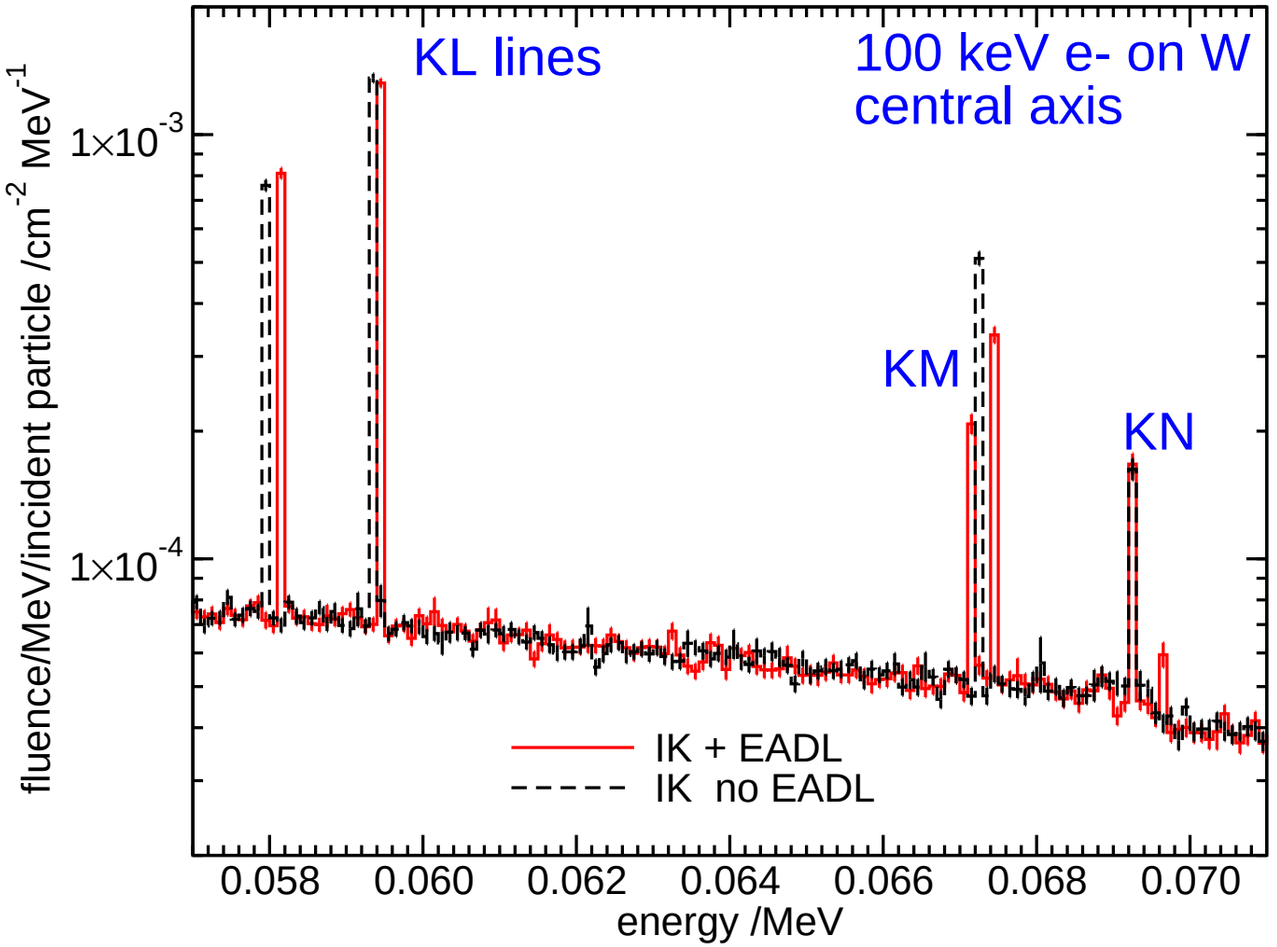
Uses LLNL Evaluated Atomic Data Library (1991)



Extra lines when M and N shells not averaged. Main peaks shifted up.

EADL option: (now default)

REPLACE {$EADL_RELAX} WITH {.true.} in egsnrc.macros



Extra lines when M and N shells not averaged.

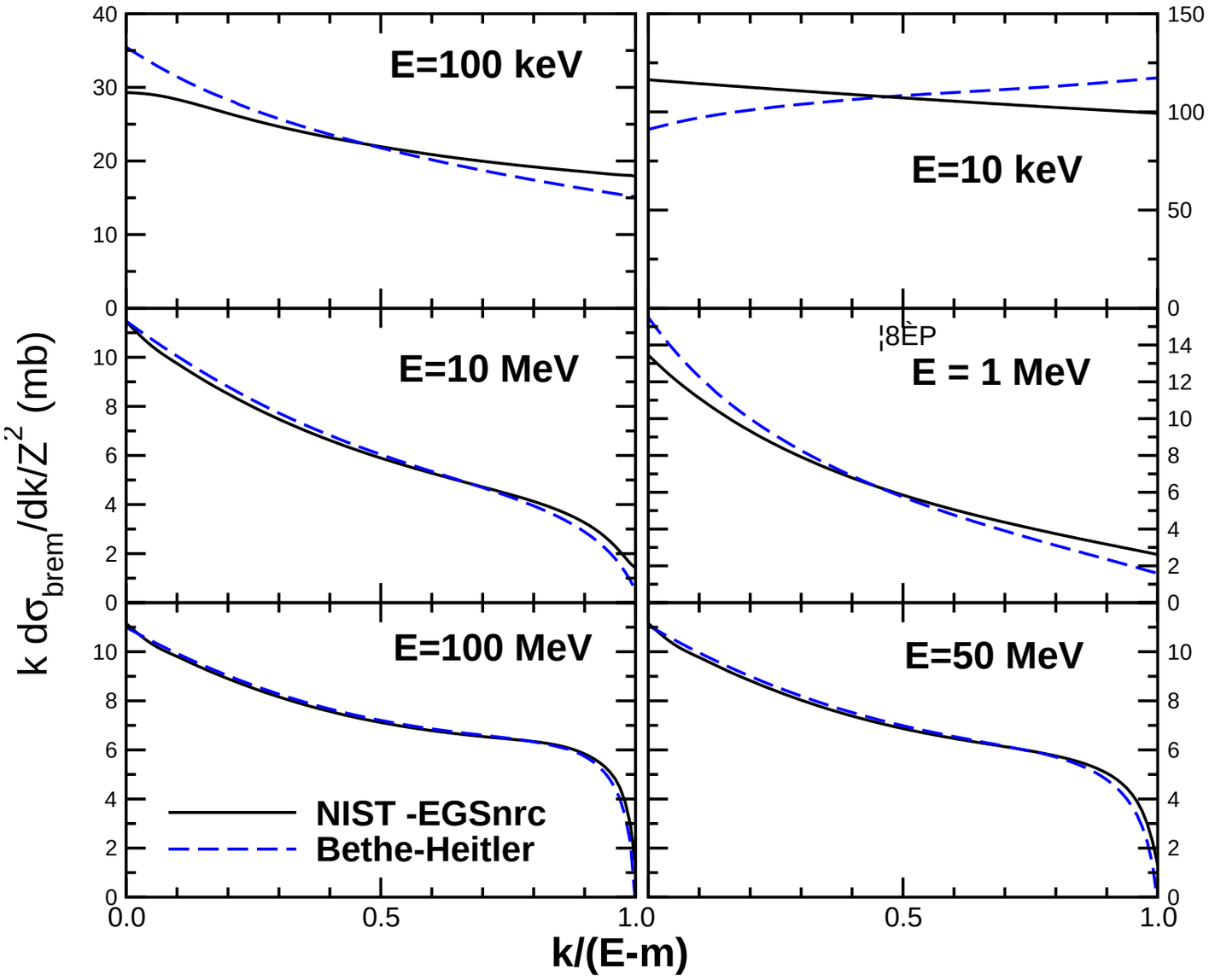
Bremsstrahlung cross sections

- there are three differential cross section options
  - Bethe-Heitler cross section as used in EGS4
  - NIST database = Coulomb corrected Bethe-Heitler $>\sim$50 MeV.
  - NIST database for nuclear brem but with new electron brem modelled using Tessier and Kawrakow, Nucl. Instr. Meth. B **266** (2008)625-634.
- There are significant differences at low energies between NIST and Bethe-Heitler (although 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.

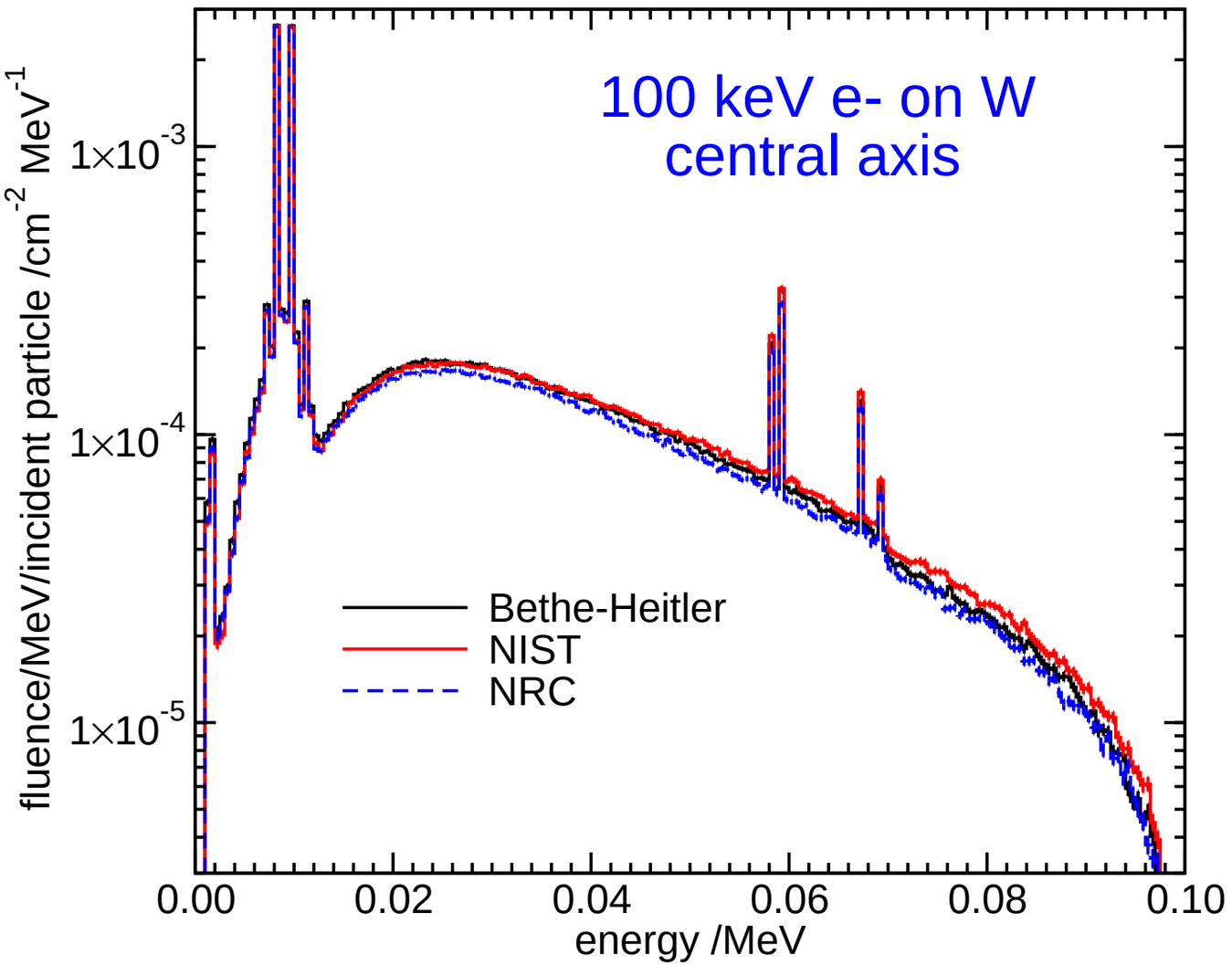
$\Rightarrow$ Don't use the NIST or NRC option for energies above 100 MeV

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

Brem cross sections: NIST vs Bethe-Heitler



Brem cross sections: NIST vs Bethe-Heitler vs NRC



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 BEAMnrc. Ali's work demonstrated several cases where it appears to be important/more accurate.
- Note: when using DBS this translates into a factor of up to $\sim$6 penalty in CPU time!

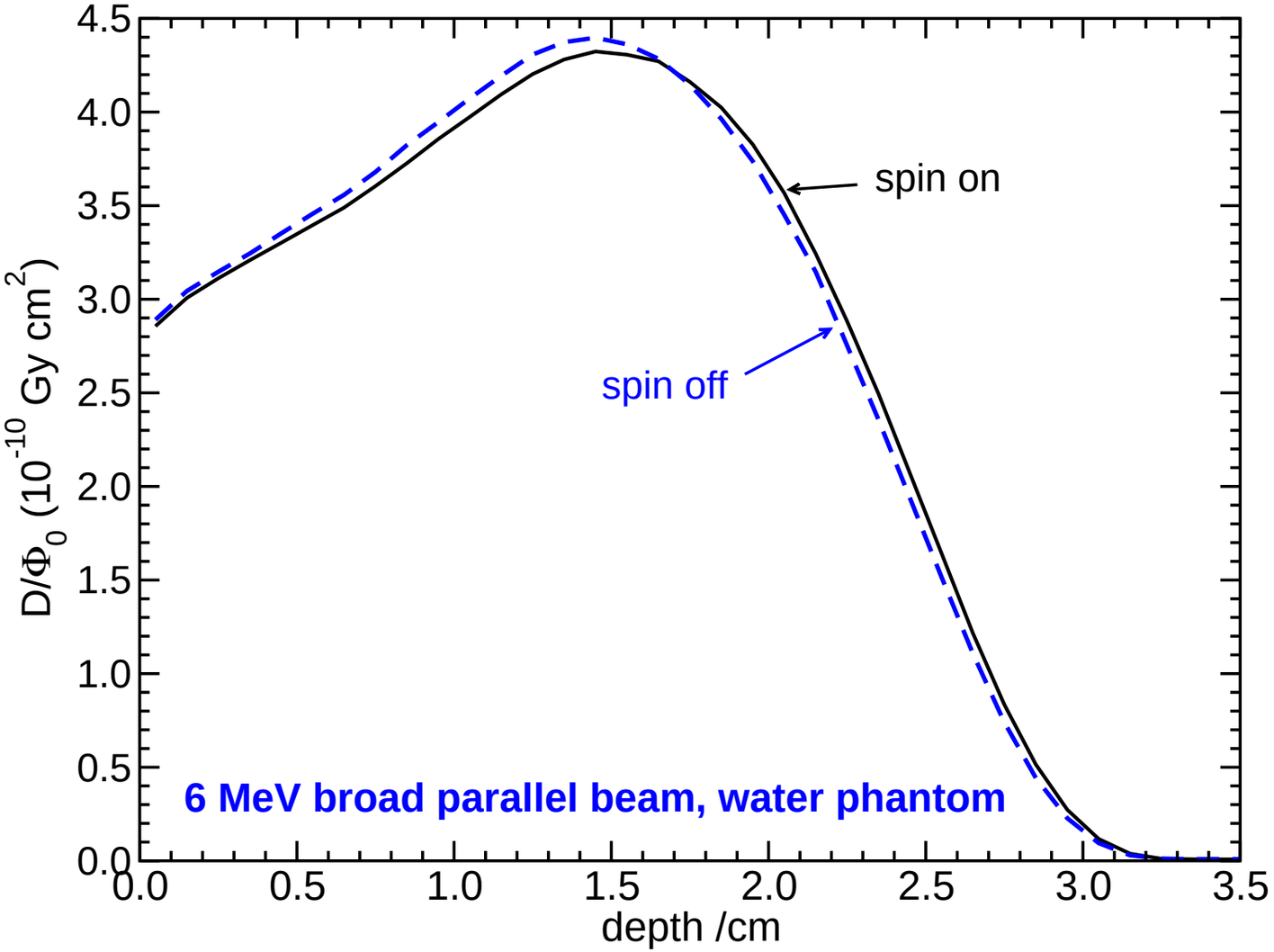
Spin effects

- 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)

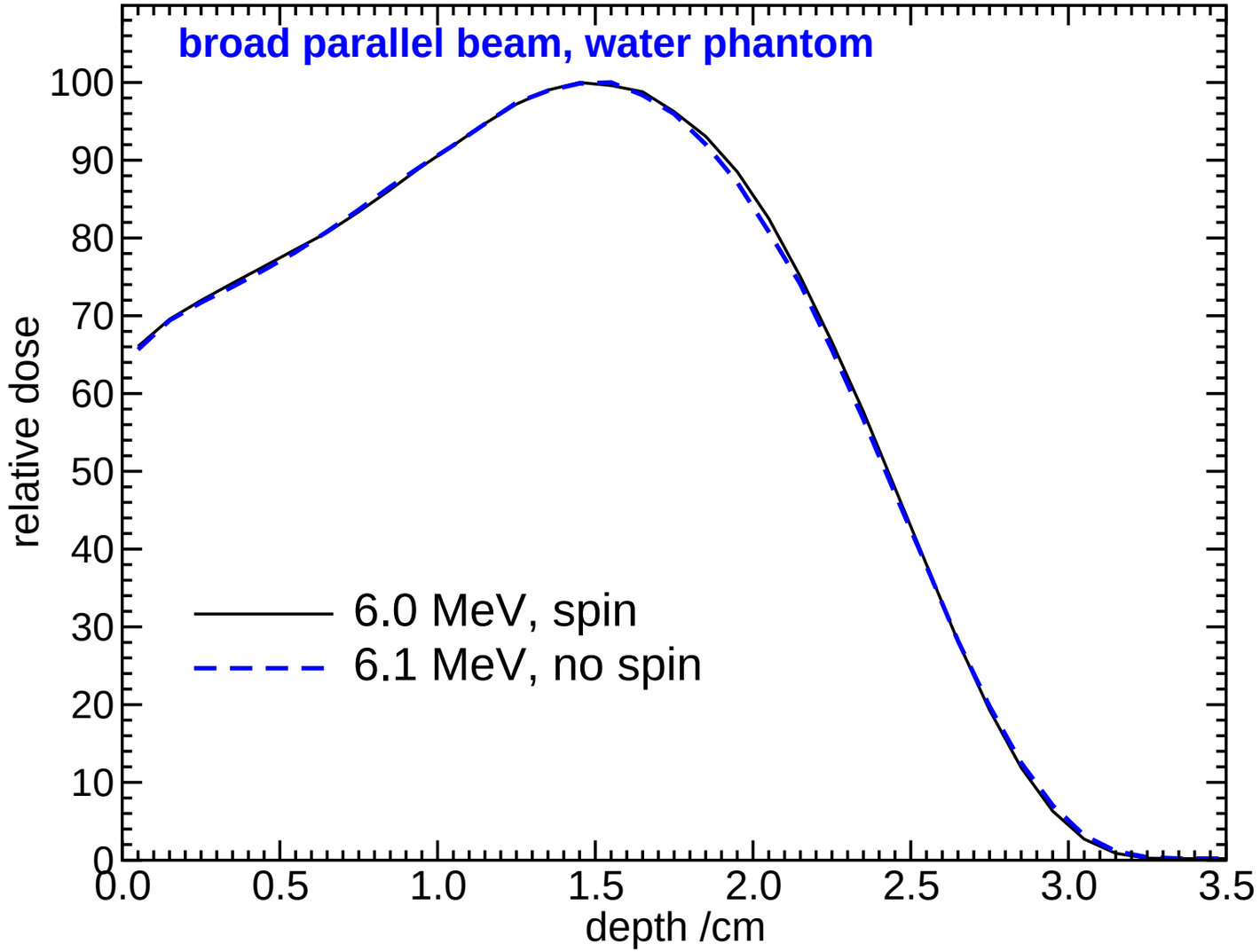
$\Rightarrow$ You must have some very strong arguments to turn the spin off.

Spin effects: example



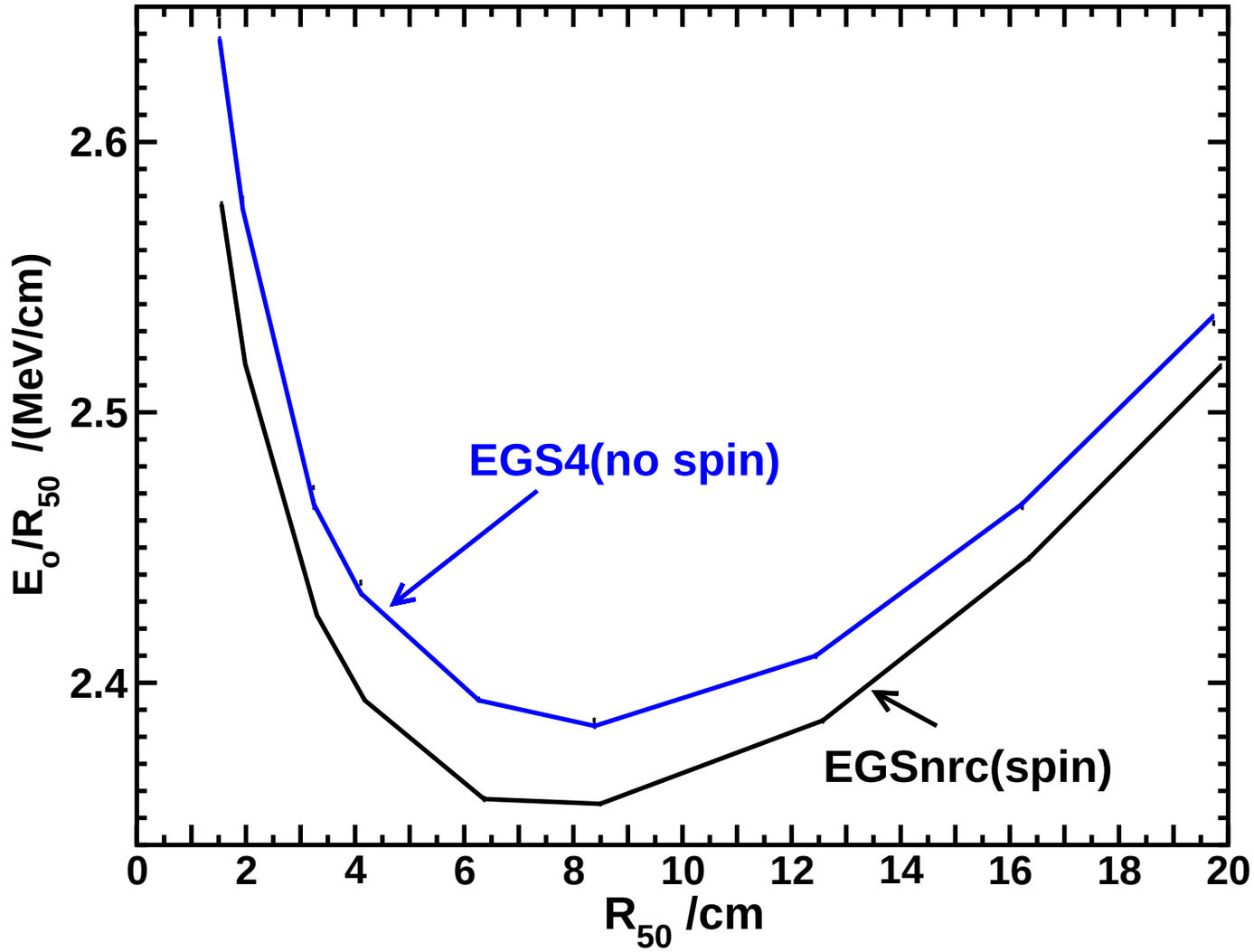
Spin has increased R_{50} for low Z but it is the reverse for high Z.

Spin effects: example



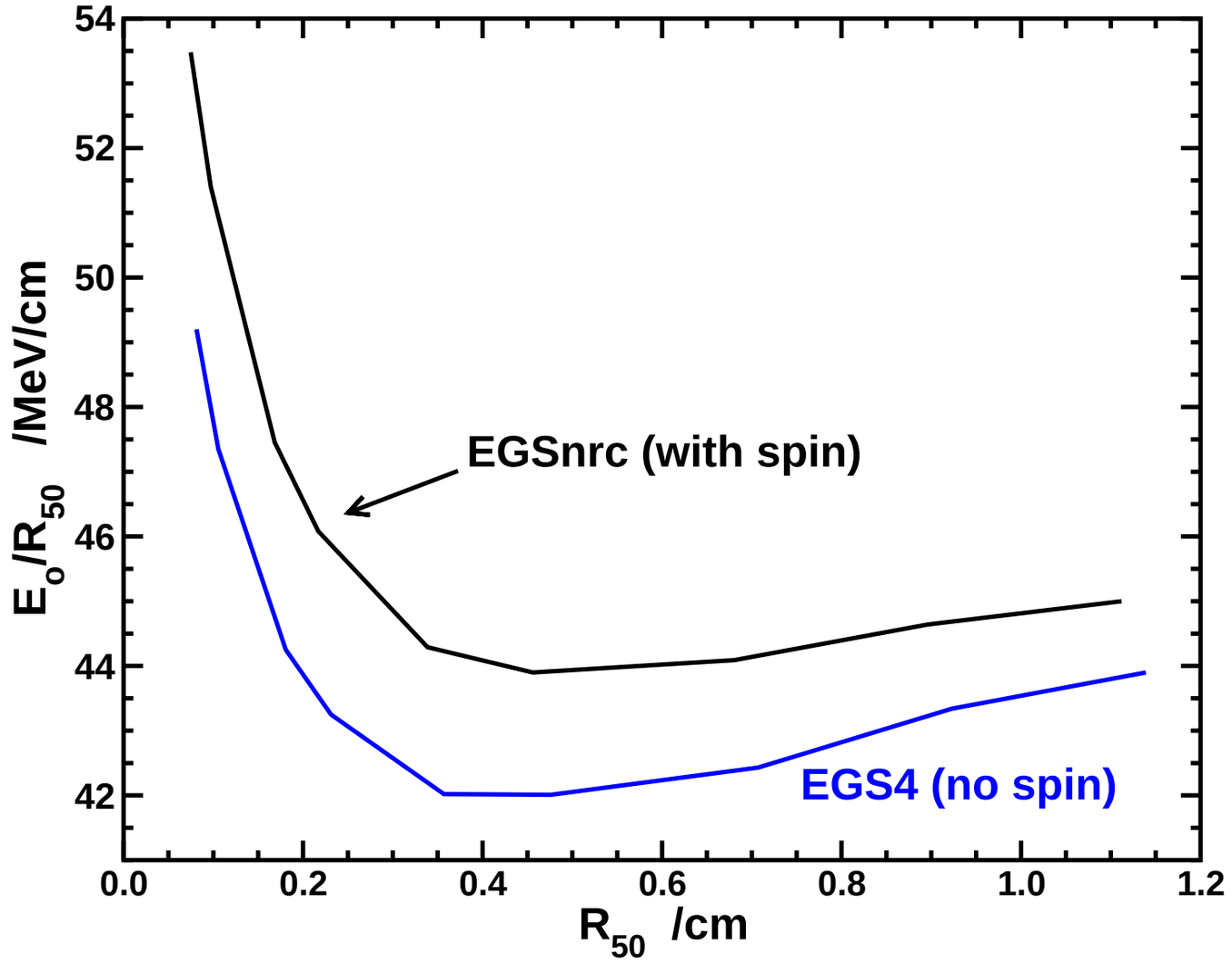
When modelling electron beams, one matches $R_{50} \Rightarrow$ hard to see a problem.

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



This implies that R_{50} increases for a given E_0.

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



This implies that R_{50} decreases for a given E_0.

Electron-step (transport) algorithm

- The default EGSnrc algorithm needs ~ 1.7 times longer per step compared to PRESTA (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

  - ~ 1.5 times slower than using PRESTA with the same step size
  - BUT: much faster to achieve the same accuracy since it can use much larger step sizes (no need for 1% ESTEPE).

- In a geometry with many boundaries, CPU time is more strongly influenced by boundary crossing algorithm than by 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)
- It is perhaps not necessary for high-energy calculations (say, $>$ 100 MeV)
- In the intermediate and low-energy range the error introduced due to PRESTA-I's BCA is strongly dependent on the situation
- For a typical RTP type calculation 3 times more CPU time is needed compared to transport setting corresponding to EGS4/PRESTA.

Boundary Crossing Algorithm

-electron may not take any step $> t_{\perp}$, the perpendicular distance to the closest boundary

-to prevent transport in another medium

PRESTA-I

Within 'skindepth_for_bca'(in mfp) of a boundary (t_{min}), turn off lateral correlation algorithm and transport to boundary

$=>$ multiple scatter event at boundary

'skindepth_for_bca' value is large.

EXACT

-EGSnrc default is to switch to single scattering at 'skindepth_for_bca $= 3$'

-there is no scatter at boundary

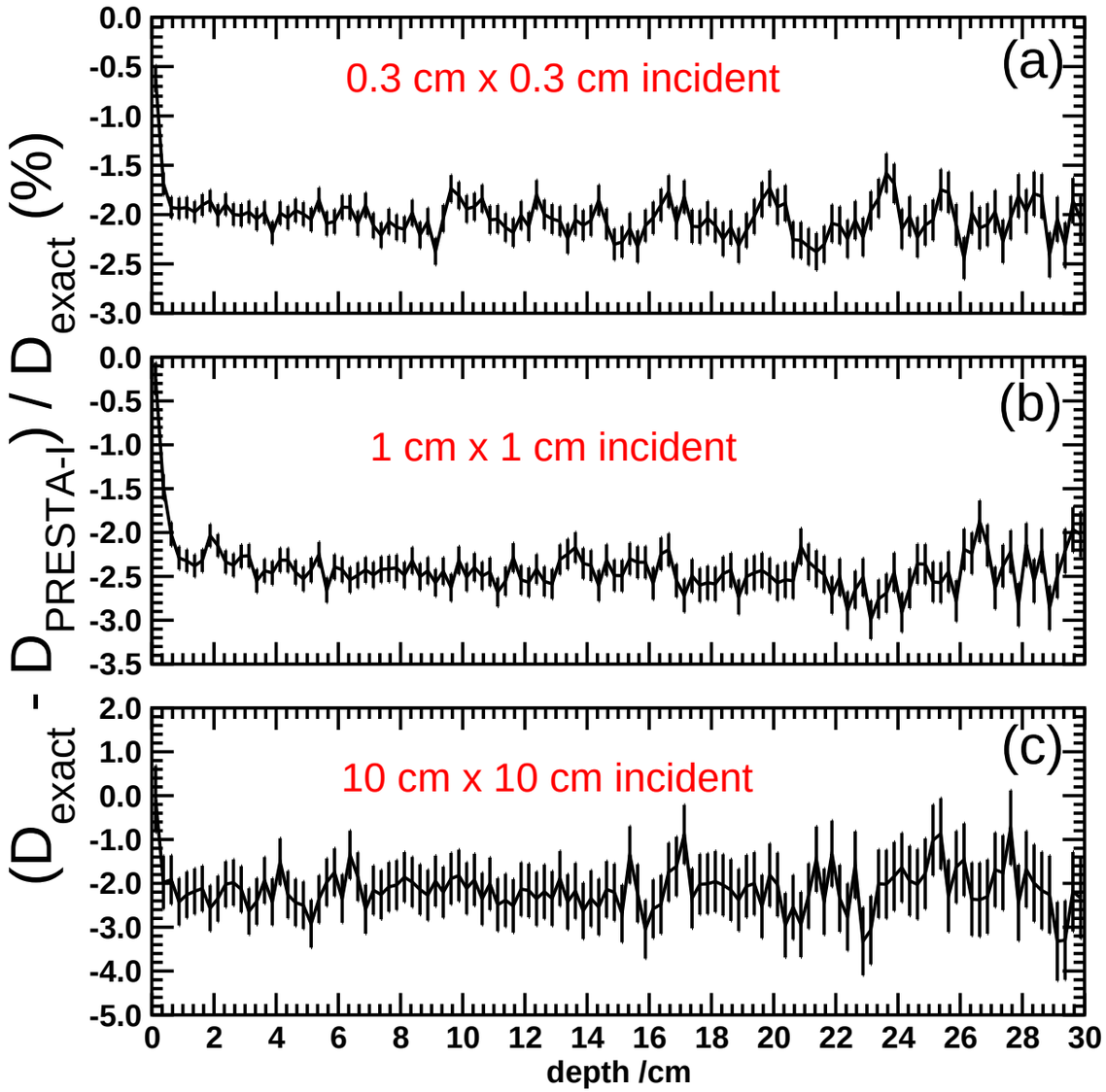
PRESTA-I BCA vs EXACT BCA

EXACT BCA is much slower for DOSXYZnrc (factor of 3) and somewhat slower for a photon accelerator (30%) and much slower for an electron accelerator (factor of 2).

Give same answers in most cases, but not all.

Problems occur for small scoring regions laterally or when using CHAMBER for central axis depth-doses.

6 MV photons: CHAMBER phantom: CAX r=0.14 cm



From Walters and Kawrakow, Med Phys 34 (2007) 847–850

BCA Defaults in BEAMnrc code system

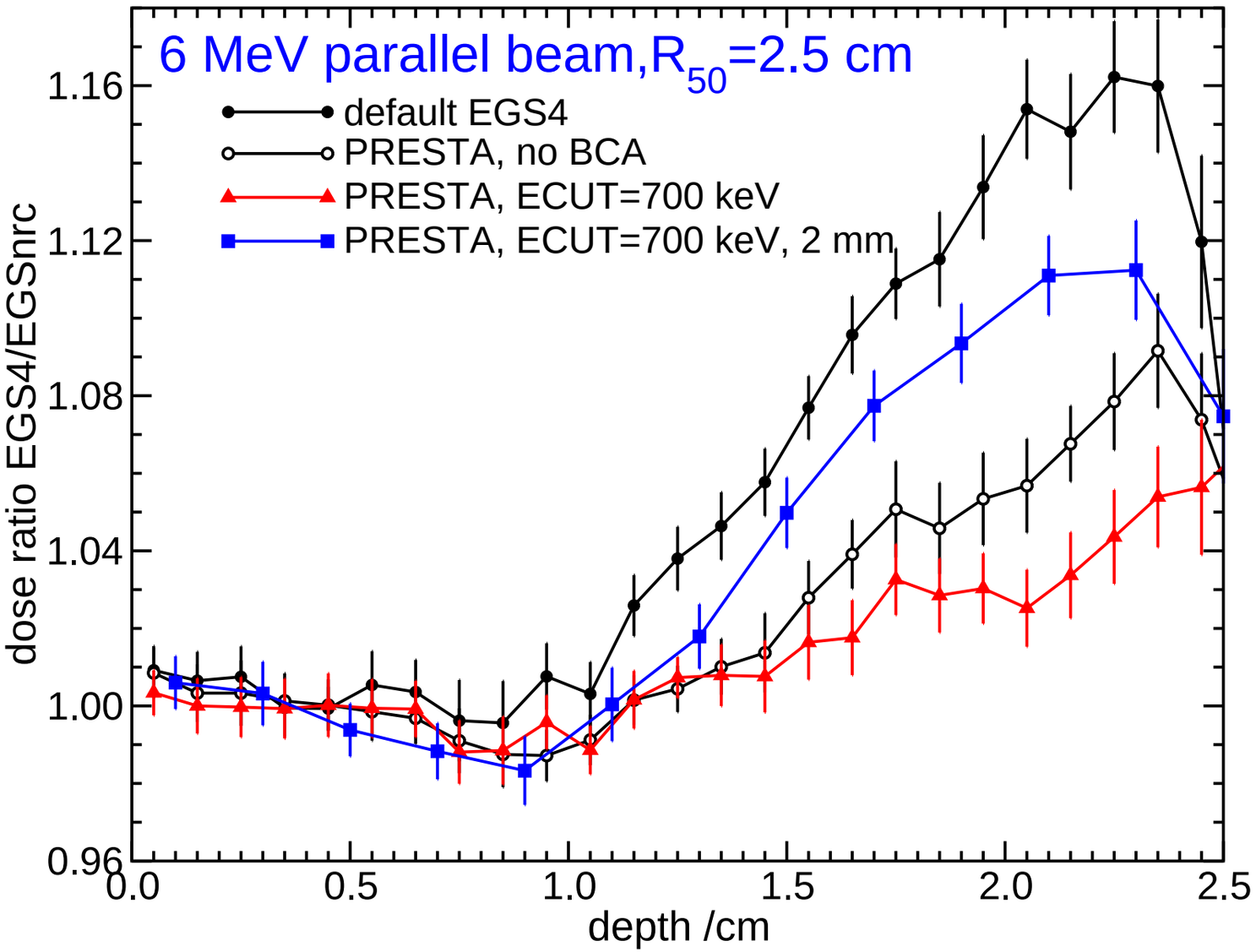
Default until 2007: PRESTA-I BCA for BEAMnrc and DOSXYZnrc

Now **BEAMnrc default** is EXACT
–30% slow down for photon accelerators
–factor of 2 slow down for electron accelerators
Reset to PRESTA-I unless you are scoring small region depth-dose with CHAMBER CM

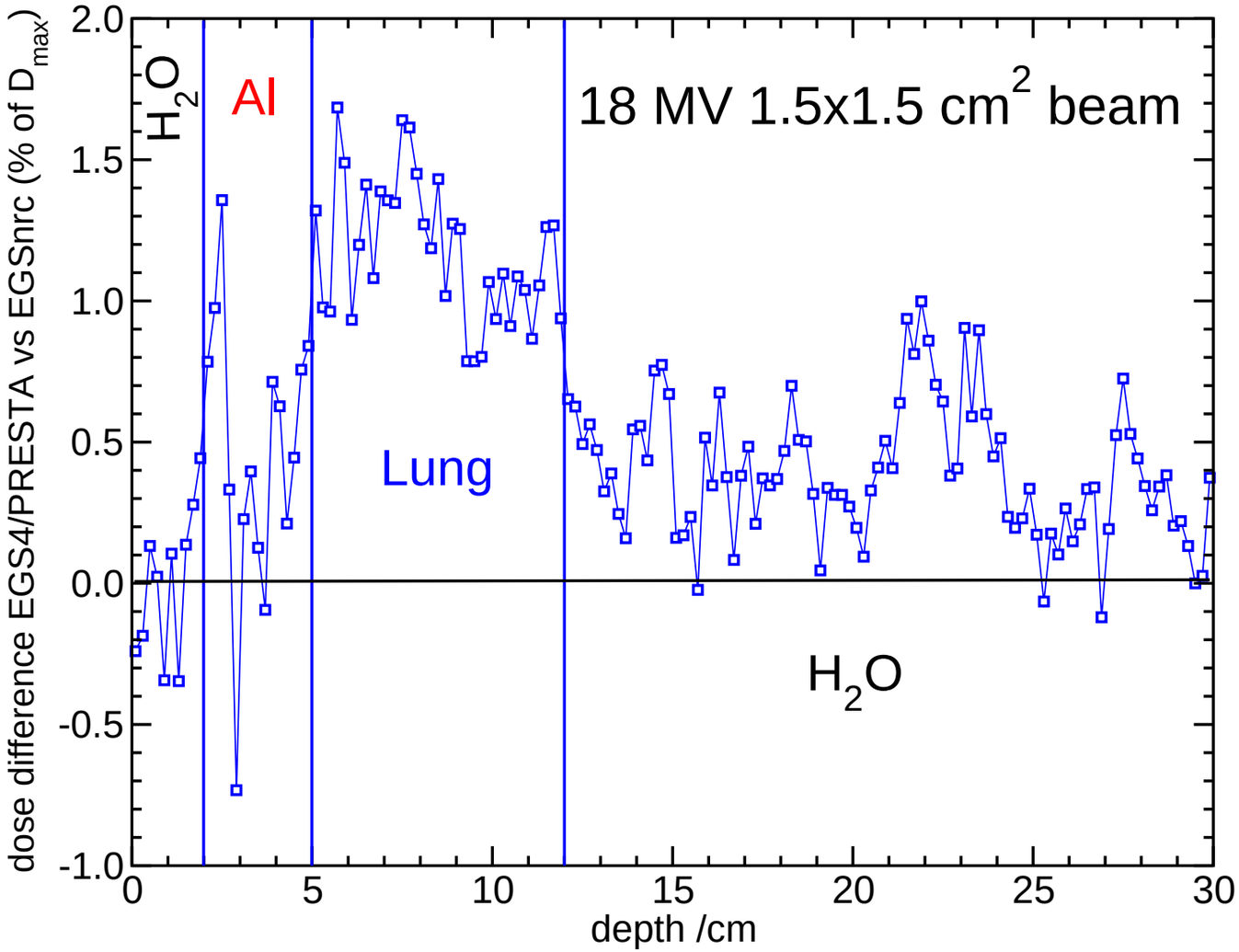
DOSXYZnrc default is PRESTA-I since factor of 3 slow down unacceptable

Must use EXACT for small voxels without lateral CPE.

Narrow electron beam



Narrow photon beam



$\Rightarrow$ Don't make compromises if you want to use EGSnrc as a benchmark against (allegedly) less accurate algorithms!

Step sizes

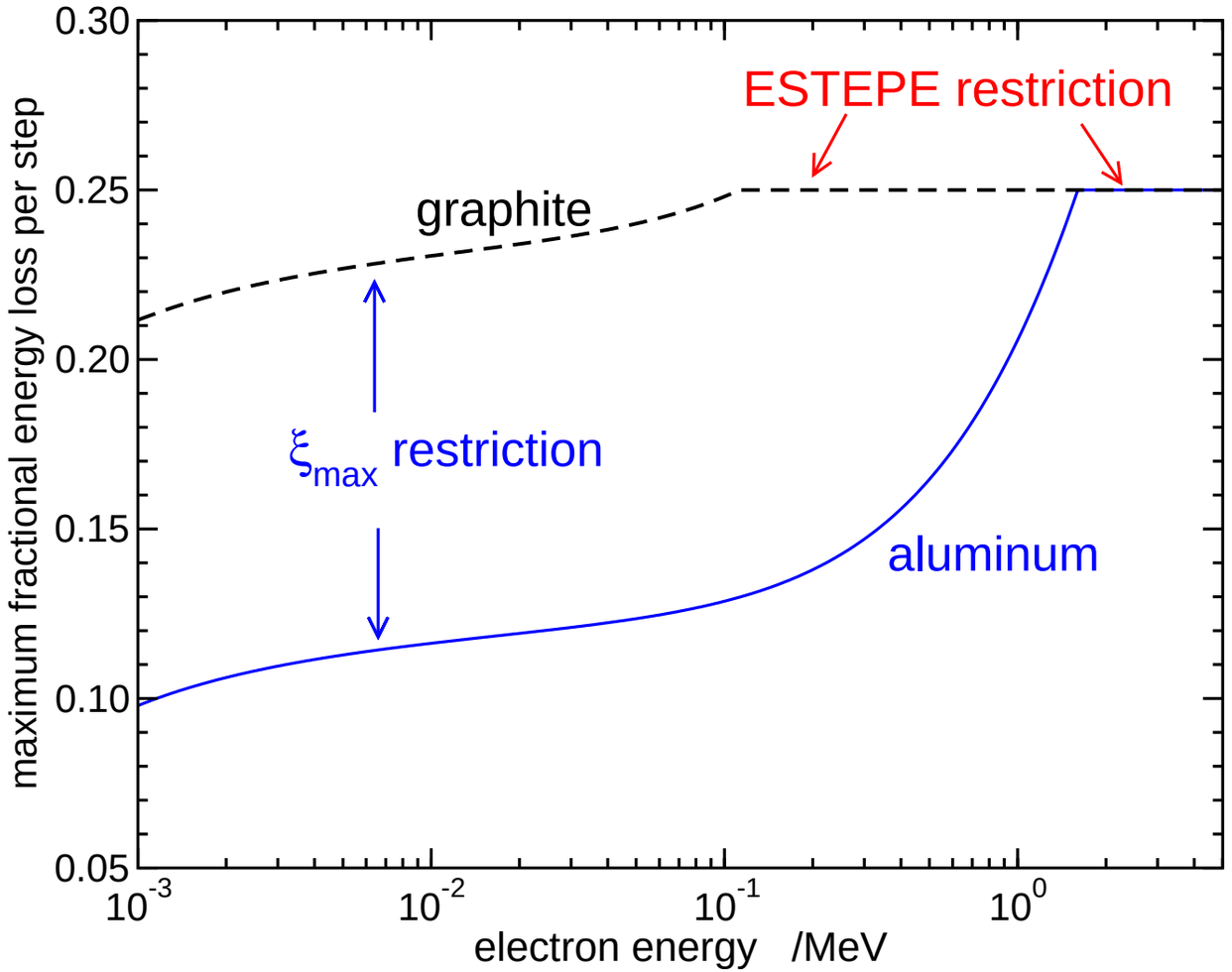
Using EGSnrc default electron-step algorithm (PRESTA-II) and BCA (EXACT)

- estepe, ximax and skin_depth_for_bca controls on step size are NOT needed
- by default they are set automatically for maximum accuracy.
- If you find step size dependencies, please let us know!

For default EGSnrc (see next slide)

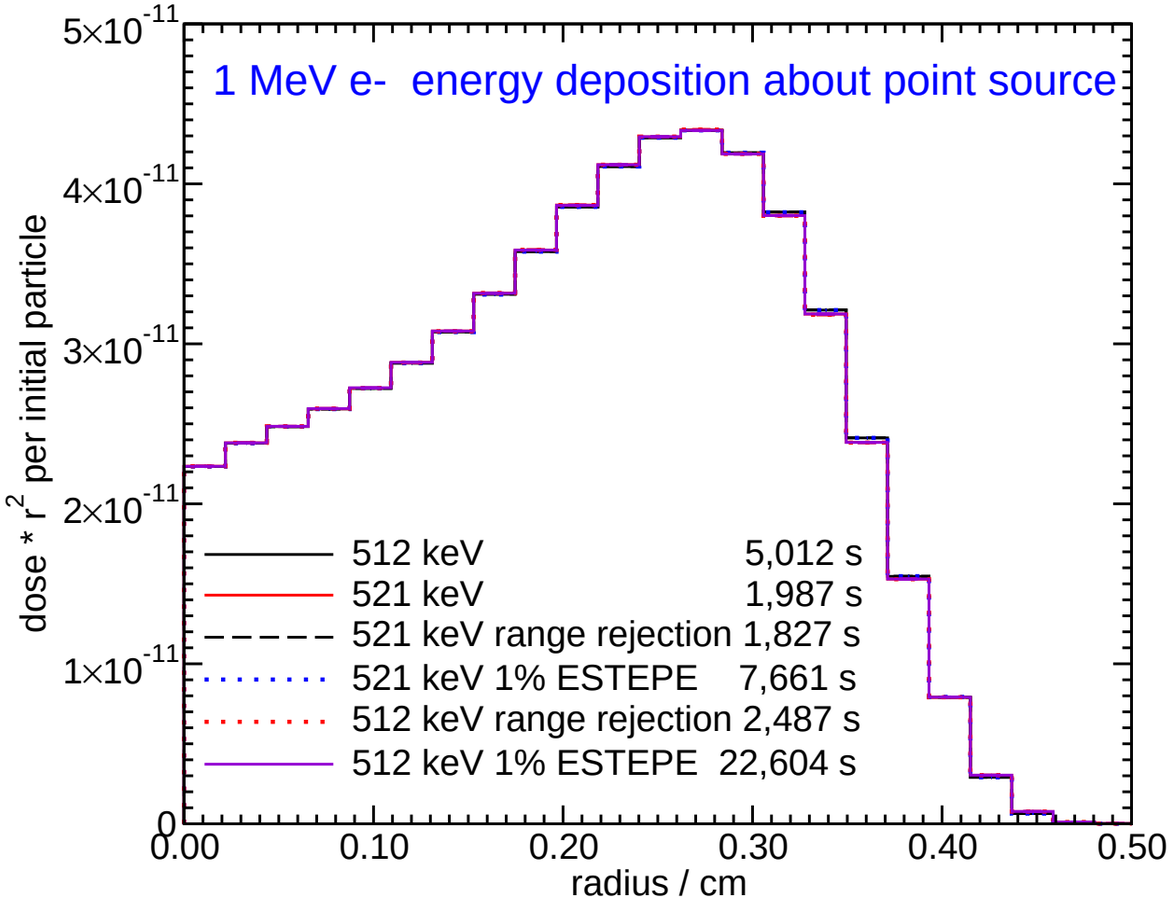
- At low energies the ximax restriction dominates
  - restricts the maximum scattering in a step so theory accurate
- At high energies the estepe restriction (=0.25) is more important
  - restricting maximum energy loss per step so certain approximations hold

Step sizes



Actual step size used is affected by AE, AP (distance to next discrete interactions) and by geometry.

Step size effects on energy deposition kernels



Timing EGSnrc vs Geant4, authors used 1% ESTEPE for EGSnrc and AE=ECUT=512 keV for a 'fair comparison' (needed to get right answer with Geant4). EGSnrc gets right answer with longer steps and higher AE.

NRC pair cross sections and triplet production

- Relatively new option, not much experience
- CPU time penalty is negligible (pair_nrc is even more efficient than BH for energies below $\sim$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.

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 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 investigations of imaging devices
  - there is an option to read in molecular form factors if you want.
- CPU cost negligible (unless running calculation without e- 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

Conclusions

- parameter selection is important for efficiency considerations with EGSnrc
- the default settings in most cases give accurate results
- still some research needed on electron impact ionization options

Acknowledgments

Iwan Kawrakow, then at NRC, now at ViewRay, was the main developer of EGSnrc. We all owe him a debt of gratitude for making the code what it is today.

Ernesto Mainegra-Hing, Blake Walters and Frederic Tessier of NRC play major roles in maintaining the system today.

Parts of this talk have been used at EGSnrc/BEAMnrc courses and all of the above have contributed in one way or another.

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