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

Electron physics and parameters

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Electrons (positrons) interact via 4 processes

1. **Emission of a bremsstrahlung photon** in the nuclear field or in the field of atomic electrons (electron-electron bremsstrahlung)

2. **Inelastic collision** with atomic electrons (knock-on electron)

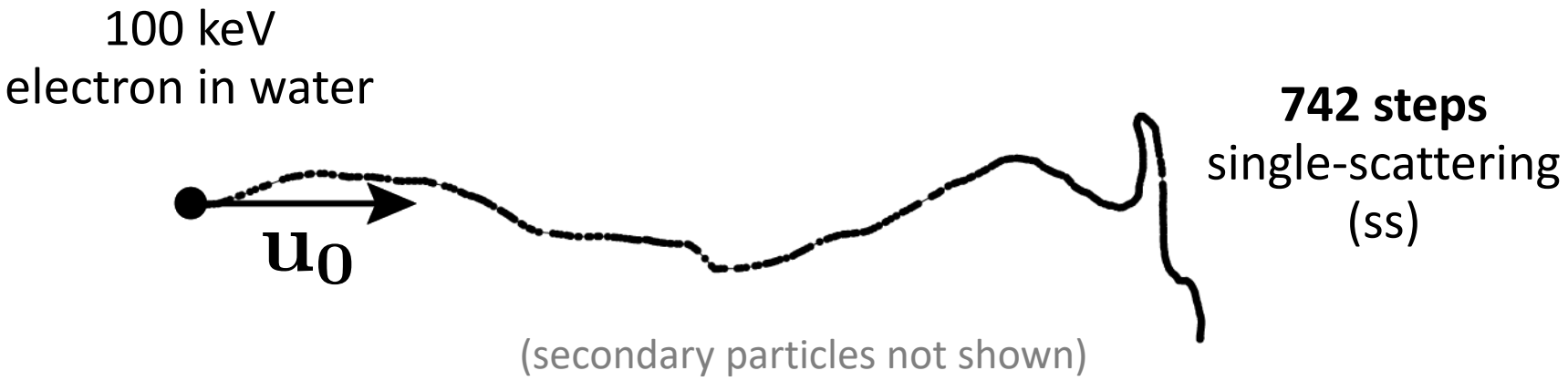
3. **Elastic collision** with nuclei and atomic electrons (deviation)

4. **Positron annihilation** (emission of a photon pair)

The main challenge in modelling the transport of electrons through matter is that the **cross-sections are very large,** because charged particles interact essentially *"all the time"* with the atoms they encounter.

Challenge: electrons interact *"all the time"*

The number of interactions as an electron slows down in a material is very large, for example:

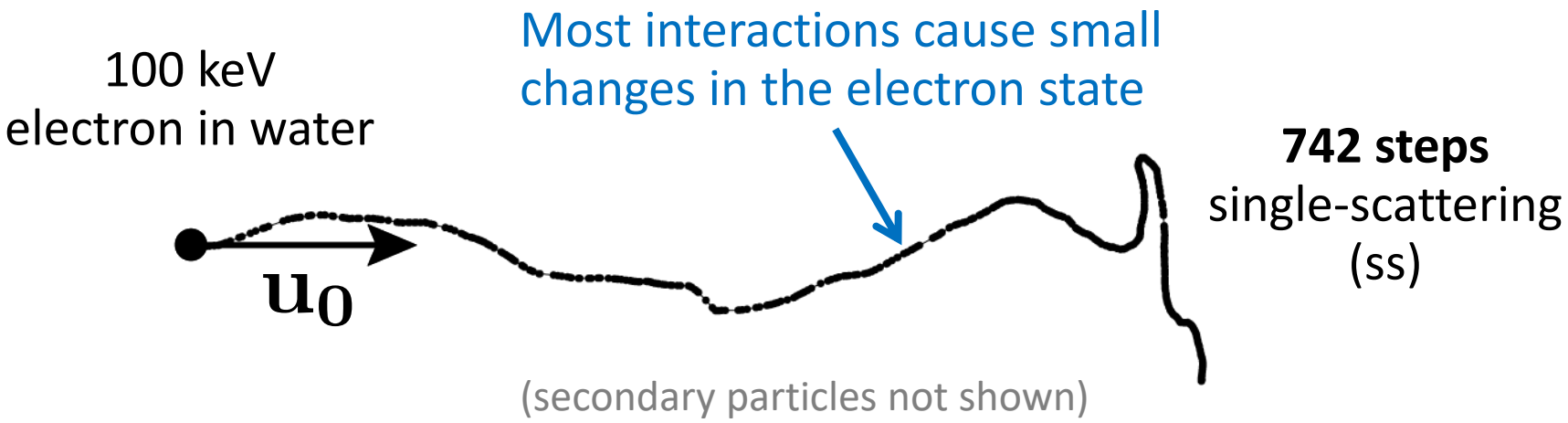


In the radiotherapy (MeV) range, a single incident electron induces ~10^6 interactions before all energy is absorbed: **~1 s of CPU time.**

Simulations typically require ~10^9 histories, which implies more than 10000 days of computation time! **Analog simulation is not practical.**

Solution: condensed history technique (CH)

To curb long simulation times (in 1963!) for electron transport, **Martin Berger** introduced the **condensed history technique.**



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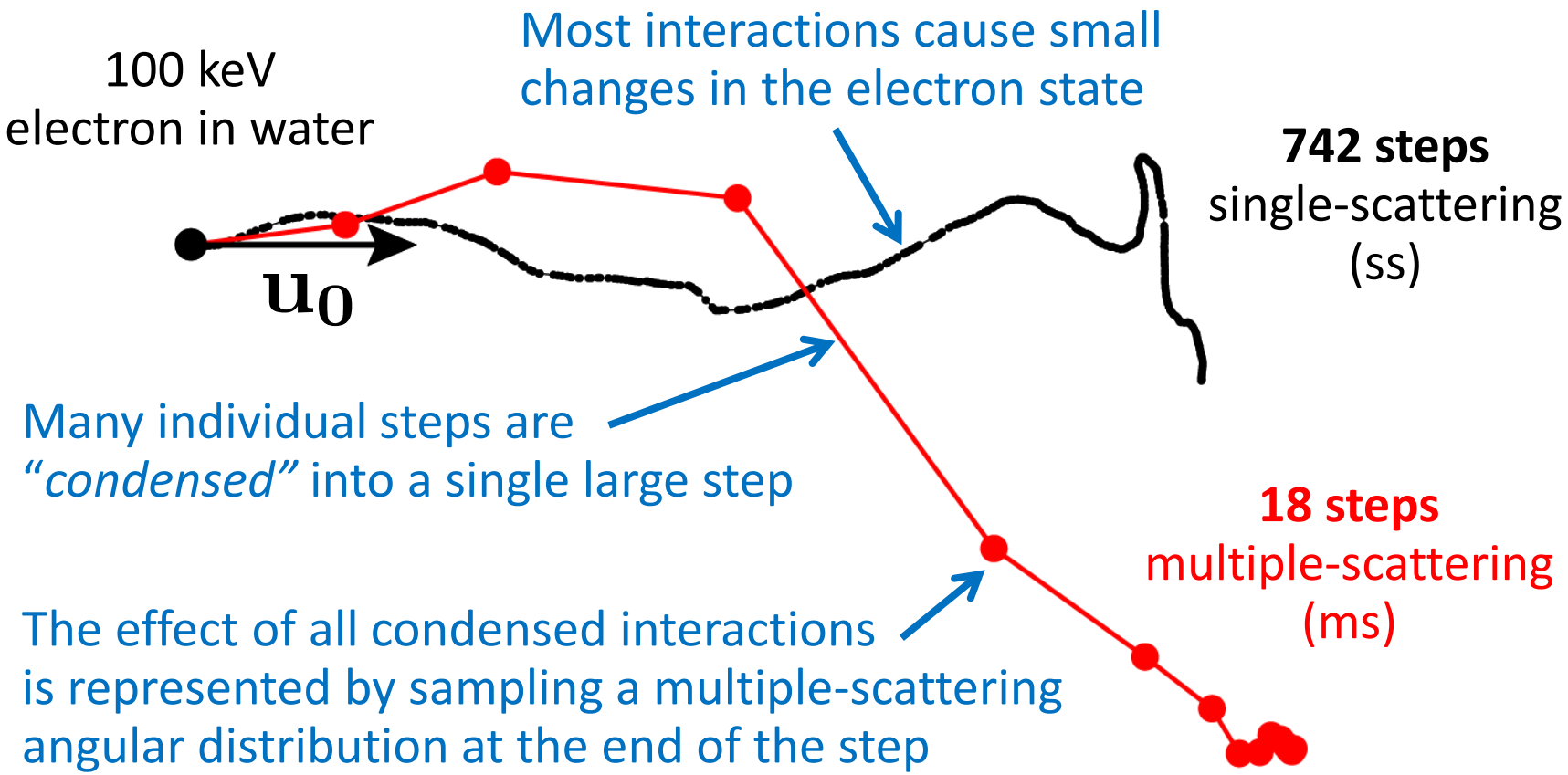

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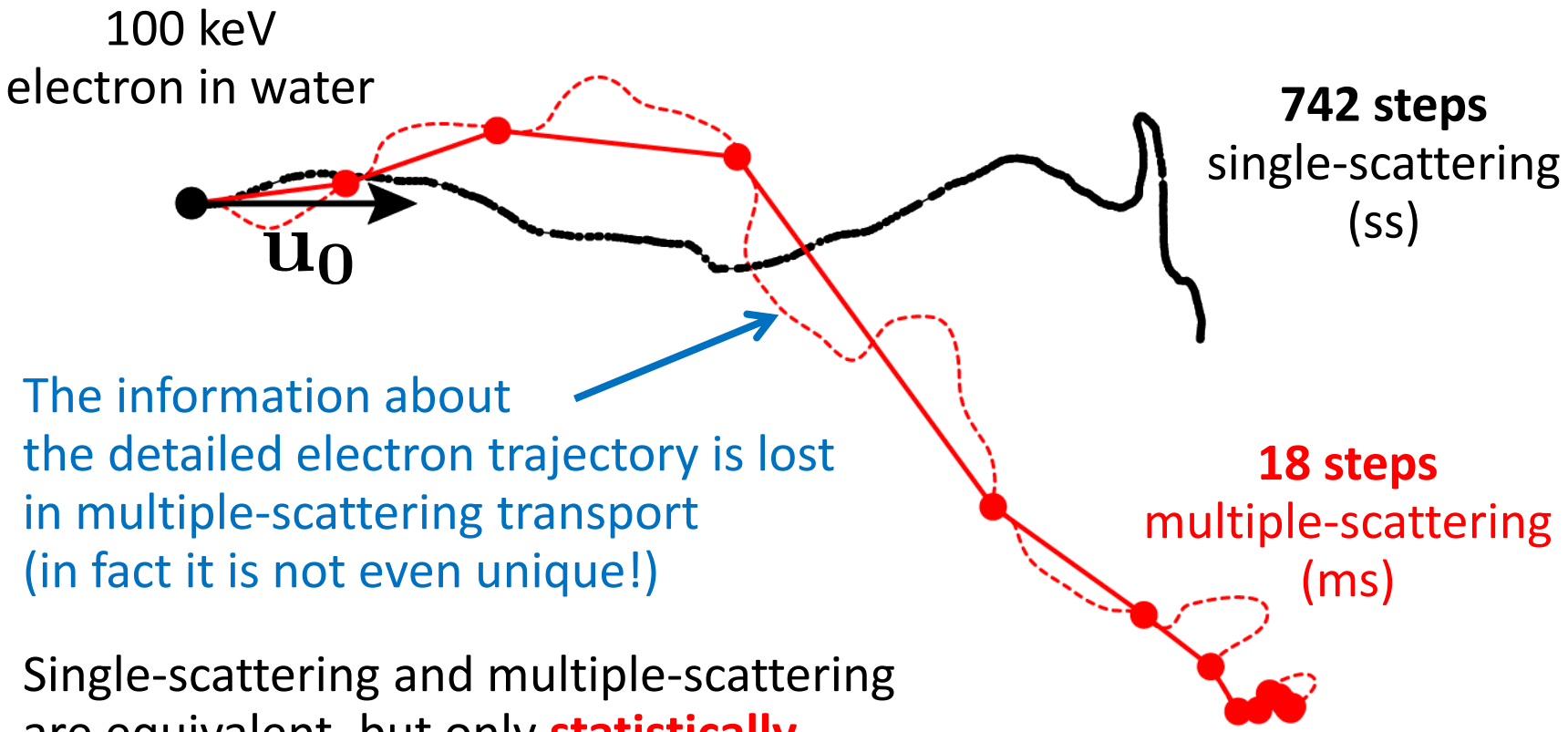


Single-scattering and multiple-scattering are equivalent, but only **statistically**

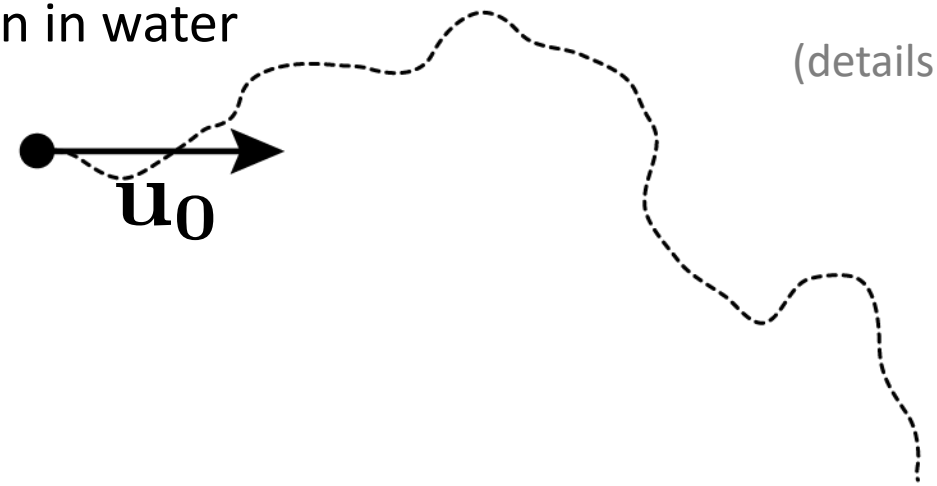
Condensing elastic scattering interactions

EGSnrc uses the screened Rutherford cross section to model elastic single-scattering interactions:

$$\frac{\mathrm{d}\sigma_{\mathrm{el}}}{\mathrm{d}\cos\theta} = C\frac{R(\cos\theta)}{(1-\cos\theta+2\eta)^2}$$

(details in the EGSnrc manual)

100 keV
electron in water



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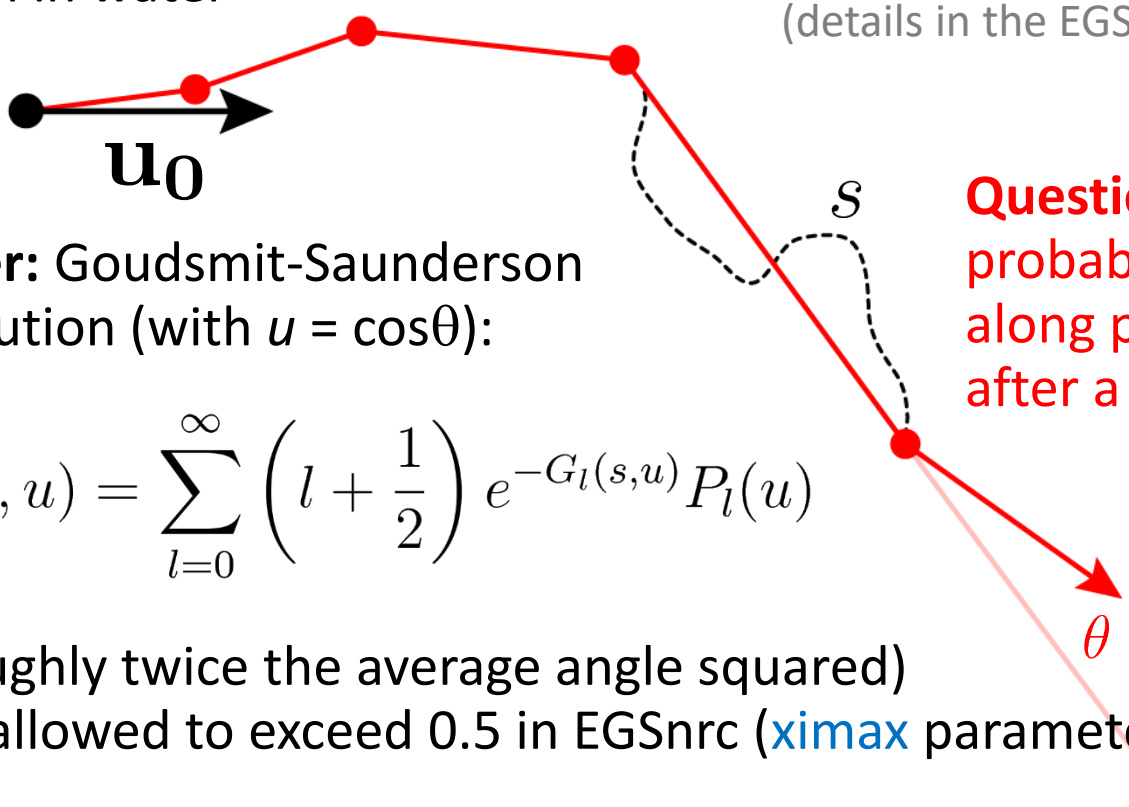


Question: what is the probability to travel along polar angle θ, after a path length s ?

Answer: Goudsmit-Saunderson distribution (with $u = \cos\theta$):

$$F_{\mathrm{MS}}(s,u) = \sum_{l=0}^{\infty}\left(l+\frac{1}{2}\right)e^{-G_l(s,u)}P_l(u)$$

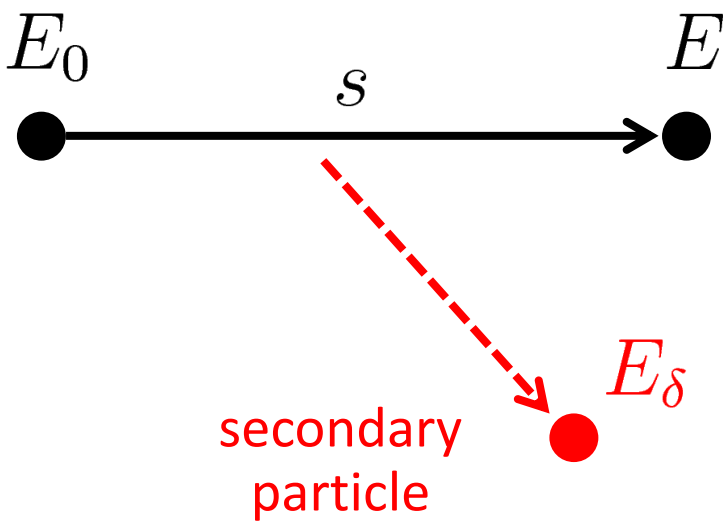
G_1 (roughly twice the average angle squared) is not allowed to exceed 0.5 in EGSnrc (ximax parameter)

Condensing inelastic scattering interactions

Martin Berger defined two condensed history classes:

Class I:

The multiple-scattering step size is sampled from pre-determined distributions of energy loss fractions, and secondary particle emission is sampled independently (ETRAN, ITS, MCNP).



$$E = E_0 - \Delta E(s)$$

Impose energy conservation:

$$E_{\mathrm{dep}} = \Delta E(s) - E_\delta$$

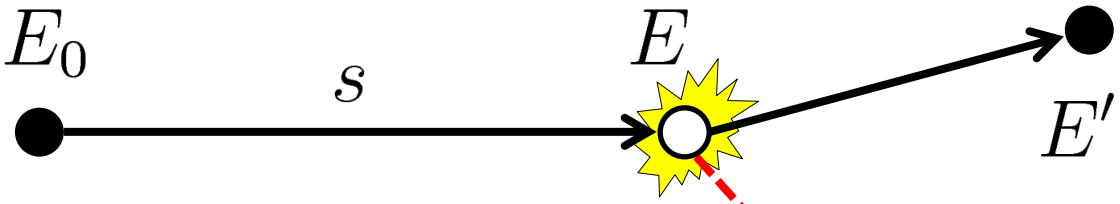
Primary and secondaries are uncorrelated

EGSnrc implements a “class II” CH scheme

Martin Berger defined two condensed history classes:

Class II:

Collisions with energy losses below a certain **threshold** are grouped in the multiple-scattering step, and occasional “catastrophic” collisions with energy losses above the **threshold** are sampled explicitly (EGS4, EGSnrc, Penelope, Geant4, vmc++)



low energy secondaries bundled in continuous energy loss:

$$E = E_0 - E_{\mathrm{dep}}(s)$$

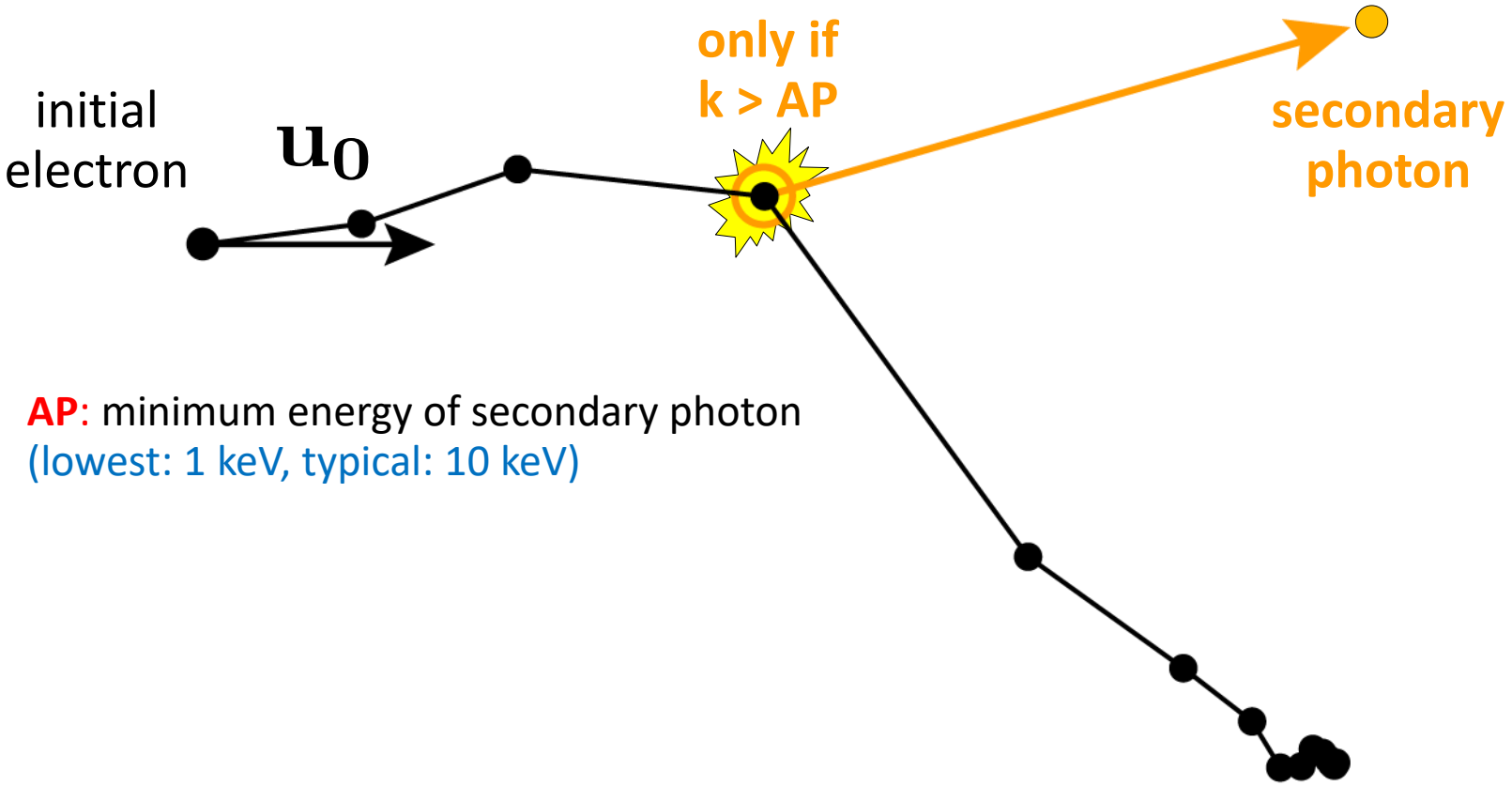
primary and secondaries are correlated

secondary particle

E_δ (above threshold)

The *catastrophic* thresholds are AE and AP

"Hard" events are sampled explicitly if the secondary particle has energy above **AE** (electrons) or **AP** (photons).



AP: minimum energy of secondary photon
(lowest: 1 keV, typical: 10 keV)

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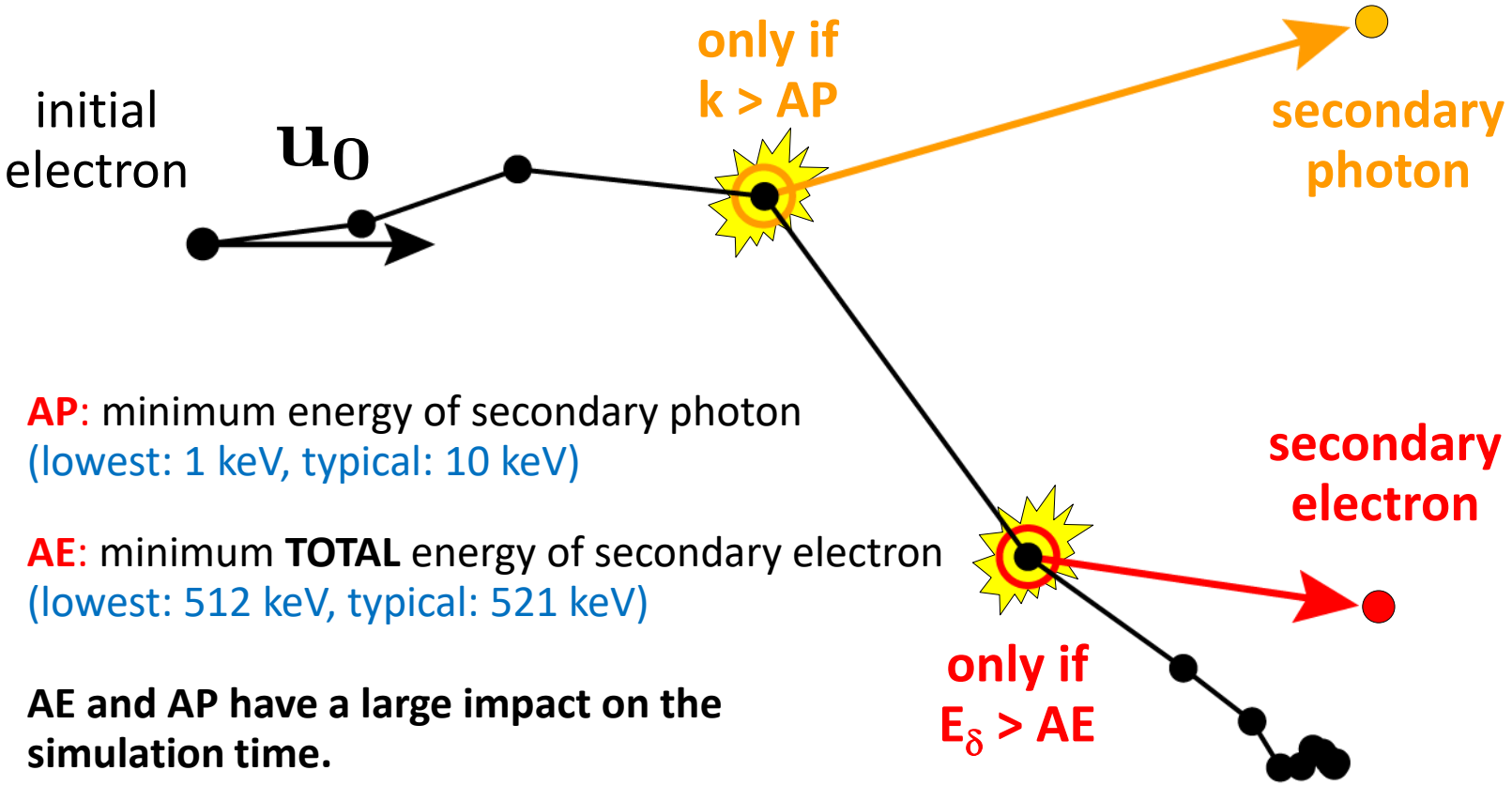


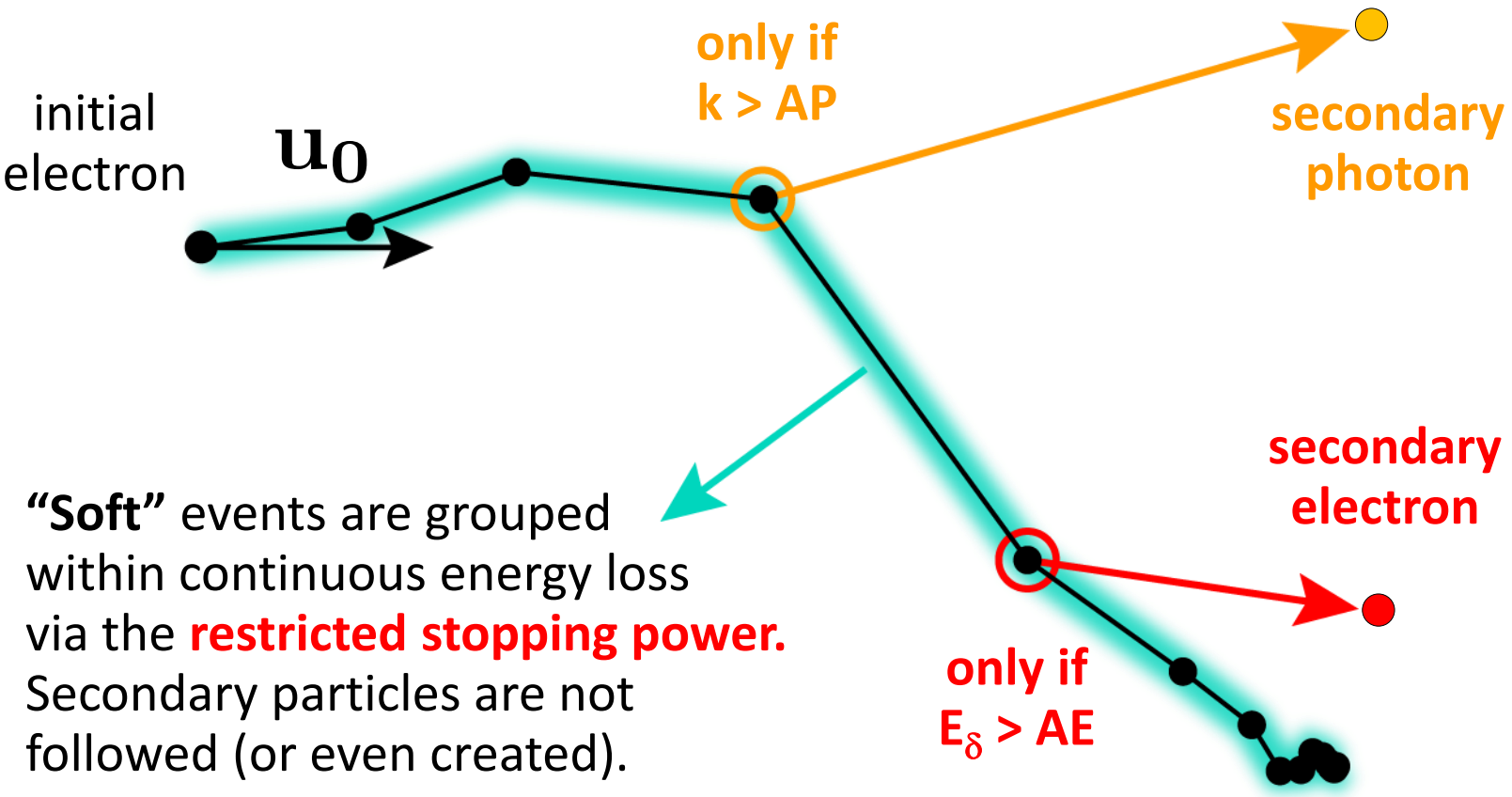
AP: minimum energy of secondary photon (lowest: 1 keV, typical: 10 keV)

AE: minimum **TOTAL** energy of secondary electron (lowest: 512 keV, typical: 521 keV)

AE and AP have a large impact on the simulation time.

The *catastrophic* thresholds are AE and AP

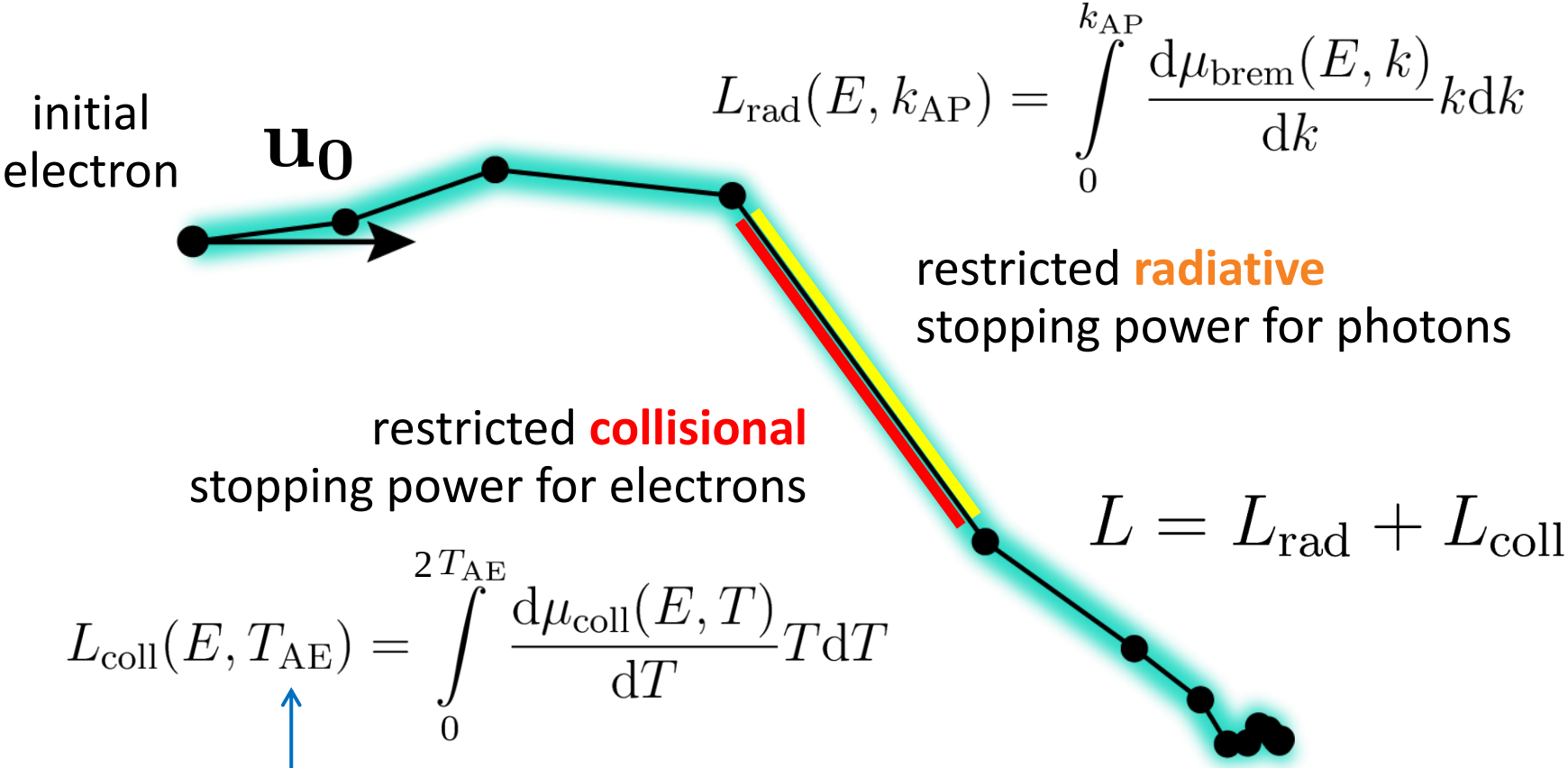
"Hard" events are sampled explicitly if the secondary particle has energy above **AE** (electrons) or **AP** (photons).



"Soft" events are grouped within continuous energy loss via the **restricted stopping power.** Secondary particles are not followed (or even created).

Restricted stopping power below AE and AP

The restricted stopping powers (up to AE and AP) give the average energy lost to sub-threshold events, per unit length.



Can we now transport electrons?

Recall the generic procedure, adjusting for condensed history:

1. sample distance to the next **catastrophic** interaction (using the total cross sections for secondaries above AE and AP).

2. transport electron to interaction site (or to the next boundary), **deposit energy** from sub-threshold events along the way, and sample the **multiple-scattering angle.**

3. sample which interaction occurs, according to the relative cross sections.

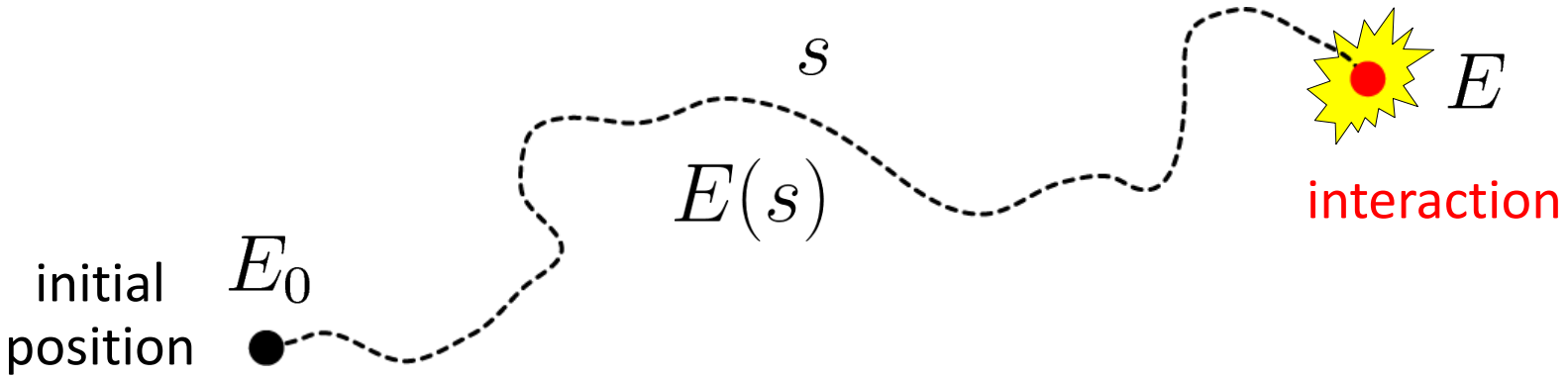
4. sample energies and angles of scattered particles, using the differential cross section.

   (rinse and repeat)

Step 1 issue: continuous energy loss

1. **sample distance to the next catastrophic interaction:**

   electrons are loosing energy continuously to sub-threshold events: **cross sections and stopping powers are not constant!**



Recall: $\mu s = -\ln \eta$

Step 1 issue: continuous energy loss

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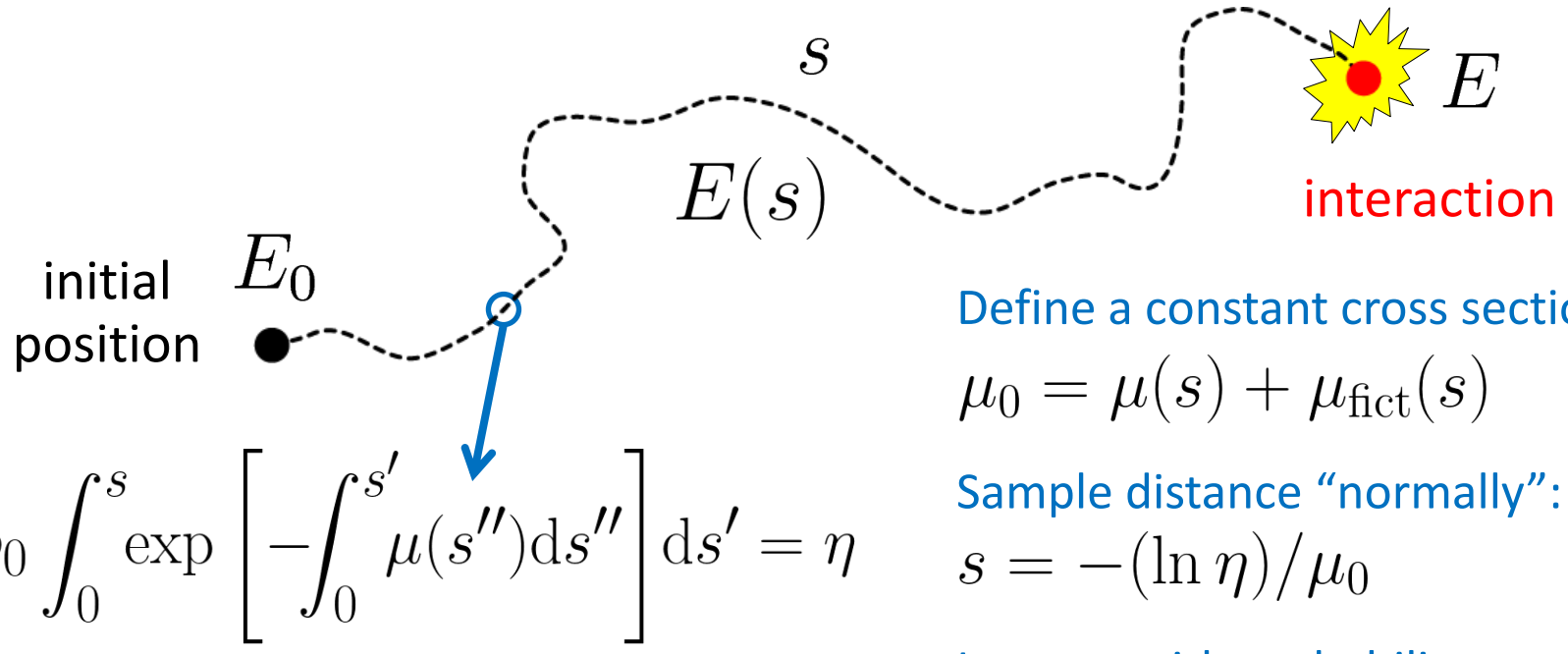

$$\rho_0 \int_0^s \exp\left[-\int_0^{s'} \mu(s'')\mathrm{d}s''\right]\mathrm{d}s' = \eta$$

Use the **fictitious interaction** method to avoid solving explicitly.

Define a constant cross section:

$$\mu_0 = \mu(s) + \mu_{\mathrm{fict}}(s)$$

Sample distance "normally":

$$s = -(\ln \eta)/\mu_0$$

Interact with probability:

$$\mu(s)/\mu_0$$

Step 1 issue: continuous energy loss

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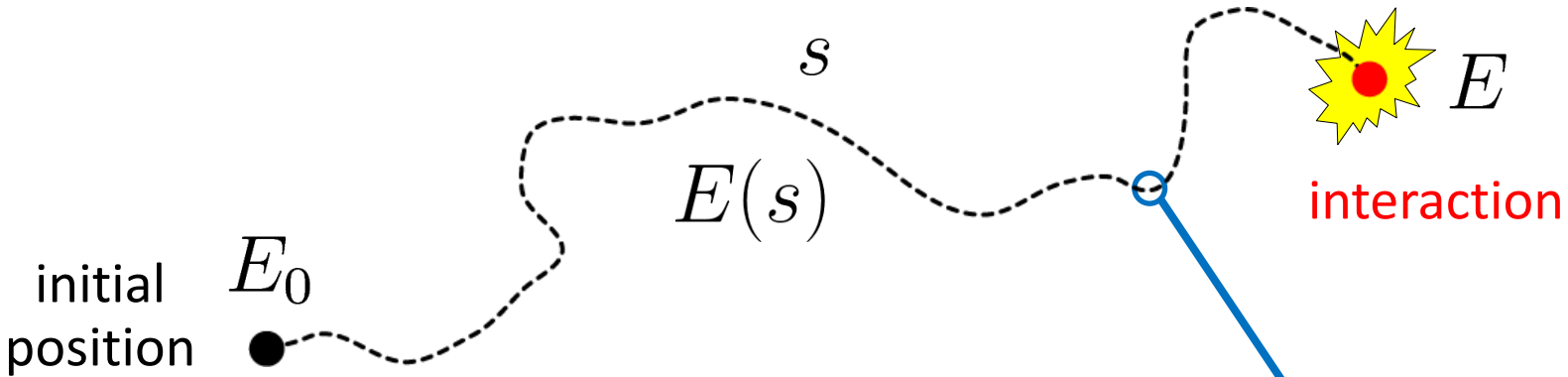


$$\rho_0 \int_0^s \exp\left[-\int_0^{s'} \mu(s'')\mathrm{d}s''\right]\mathrm{d}s' = \eta$$

Use the **fictitious interaction** method to avoid solving explicitly.

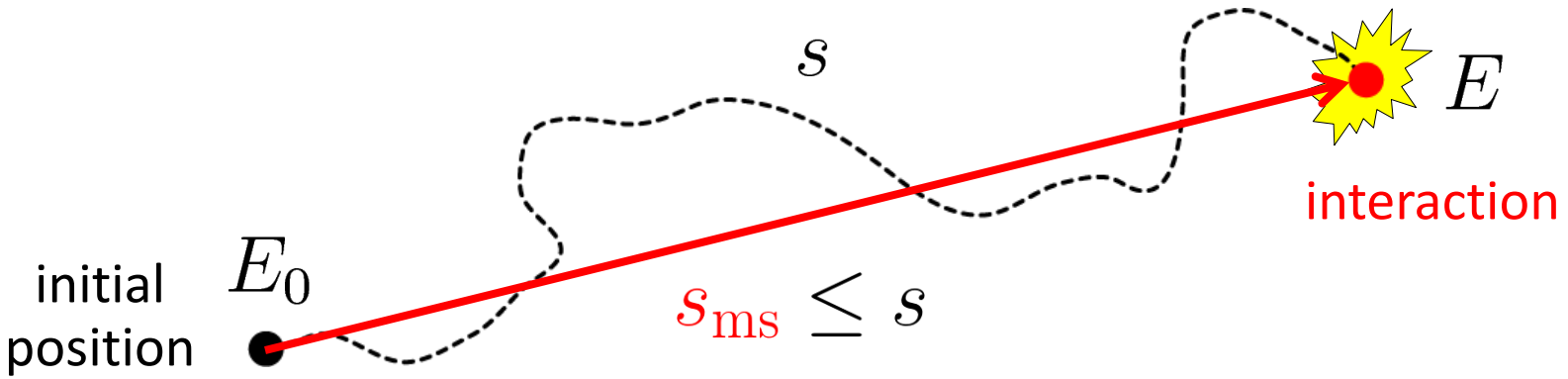
$$\Delta E = \int_0^s L[E(s')]\mathrm{d}s'$$

Use a **series expansion** to express *E* as a function of *s*.

Step 2 issues: curvilinear electron path

2. **transport electron to the interaction site:**

   a) the distance *s* is along the real (curved) electron path: what is the **corresponding straight line step?**



We need an **electron step algorithm**

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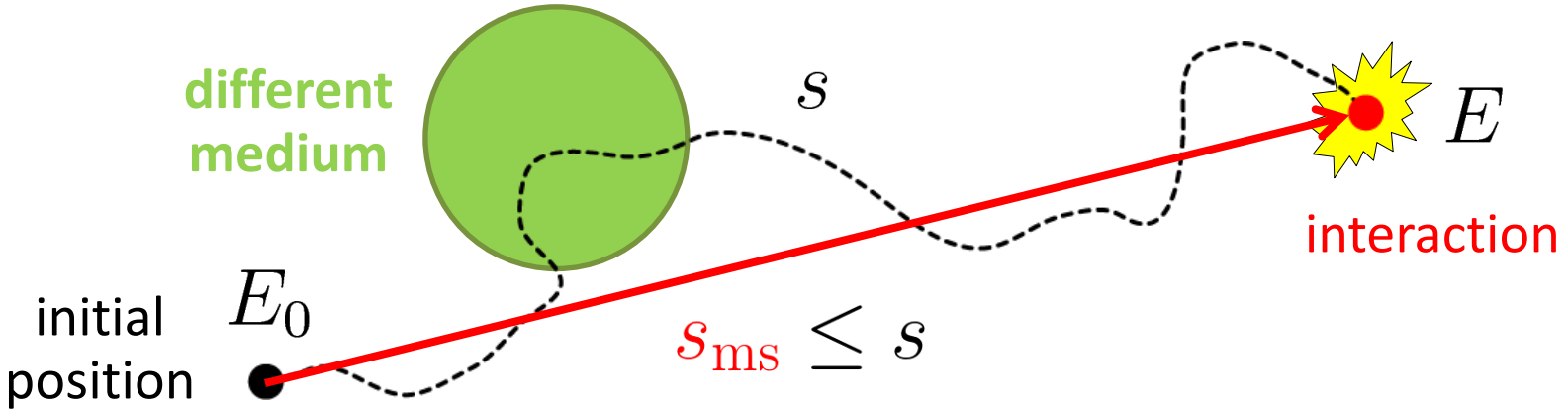
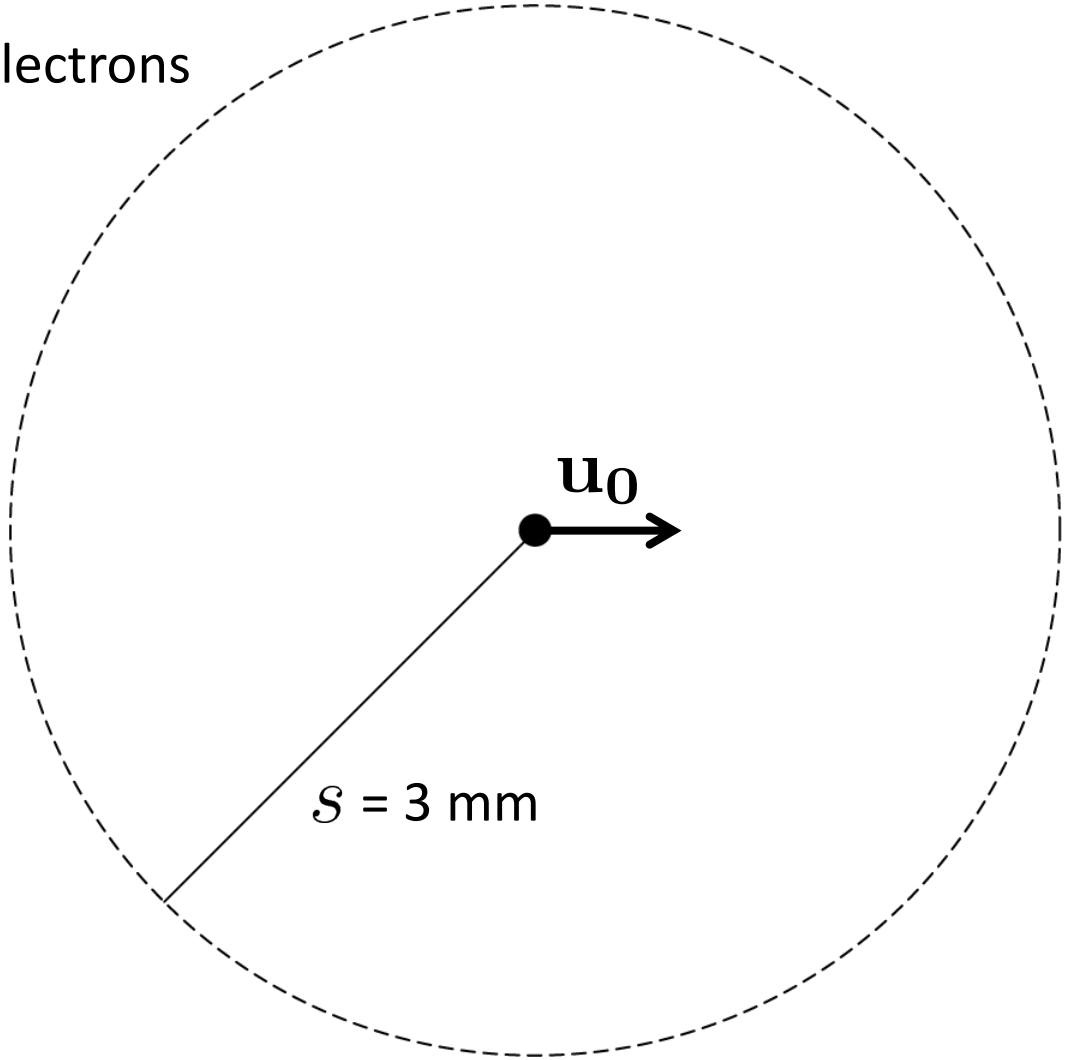


   b) ensure the real (curved) electron path could not have crossed a boundary: **consider distance to boundaries in all directions.**

   c) enforce limits on fractional energy loss (ESTEPE), multiple-scattering angle (ximax), and magnetic deflection (EM ESTEPE).

Electron step should represent “real” paths

1 MeV electrons
in water



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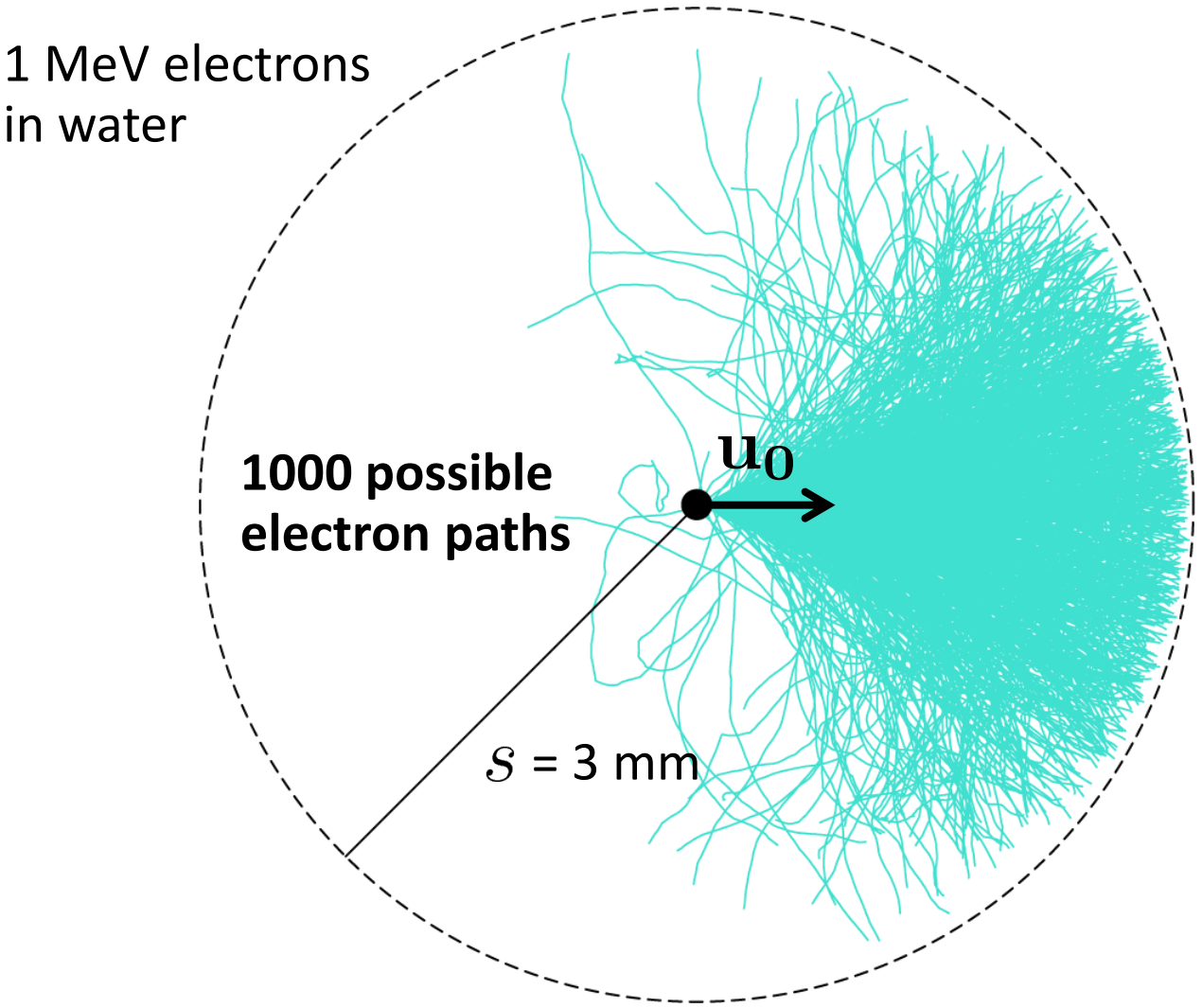

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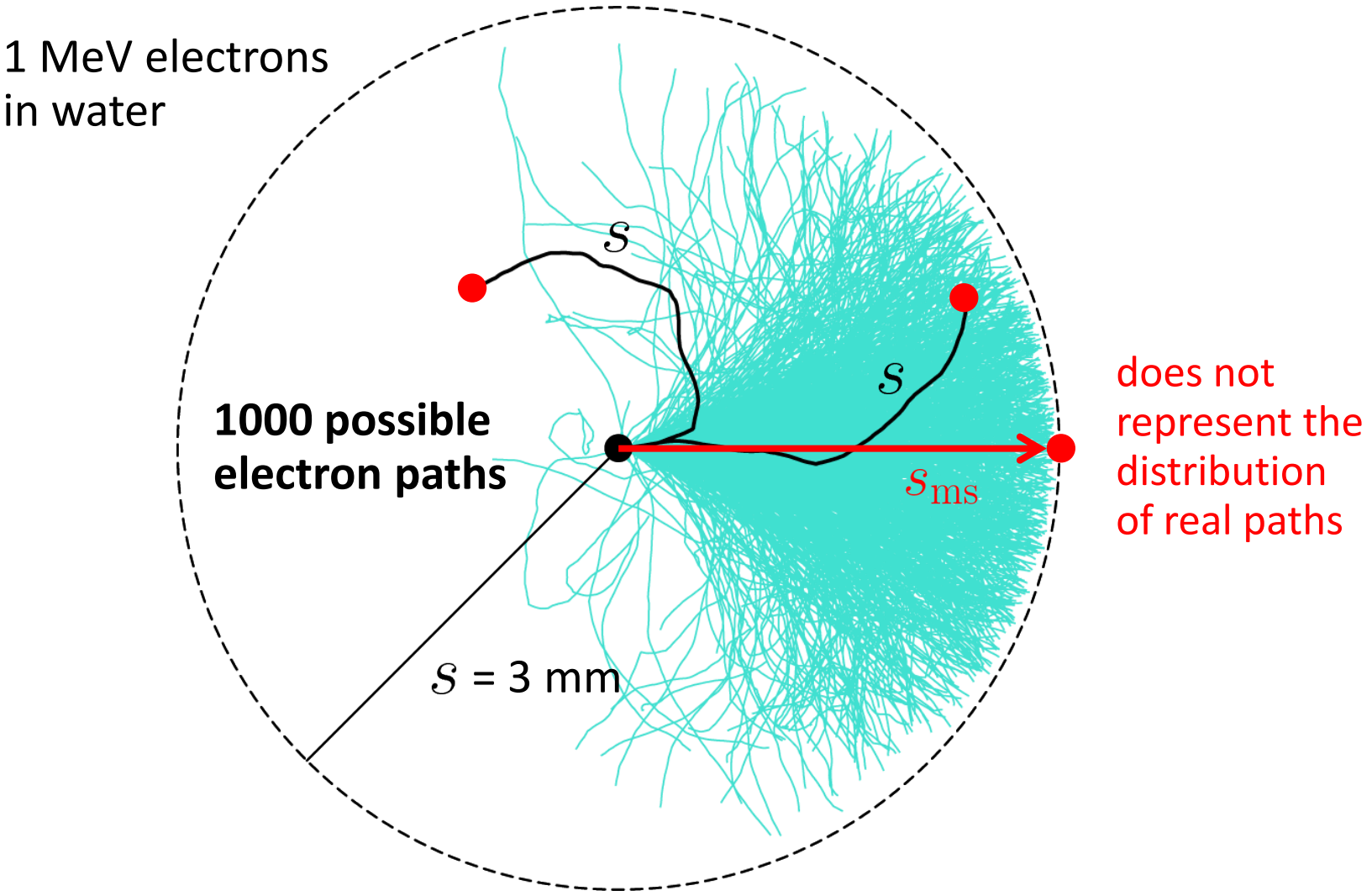

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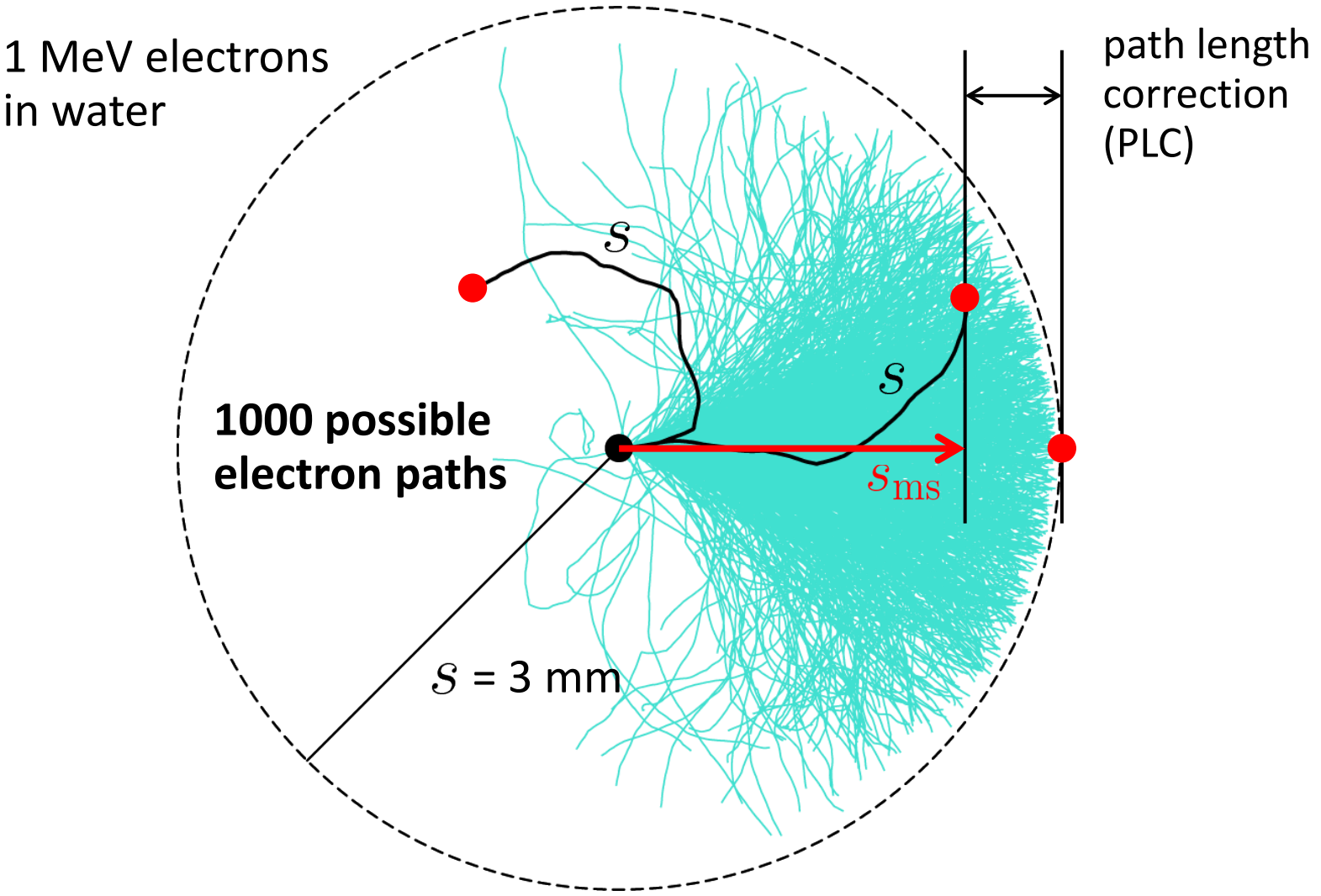

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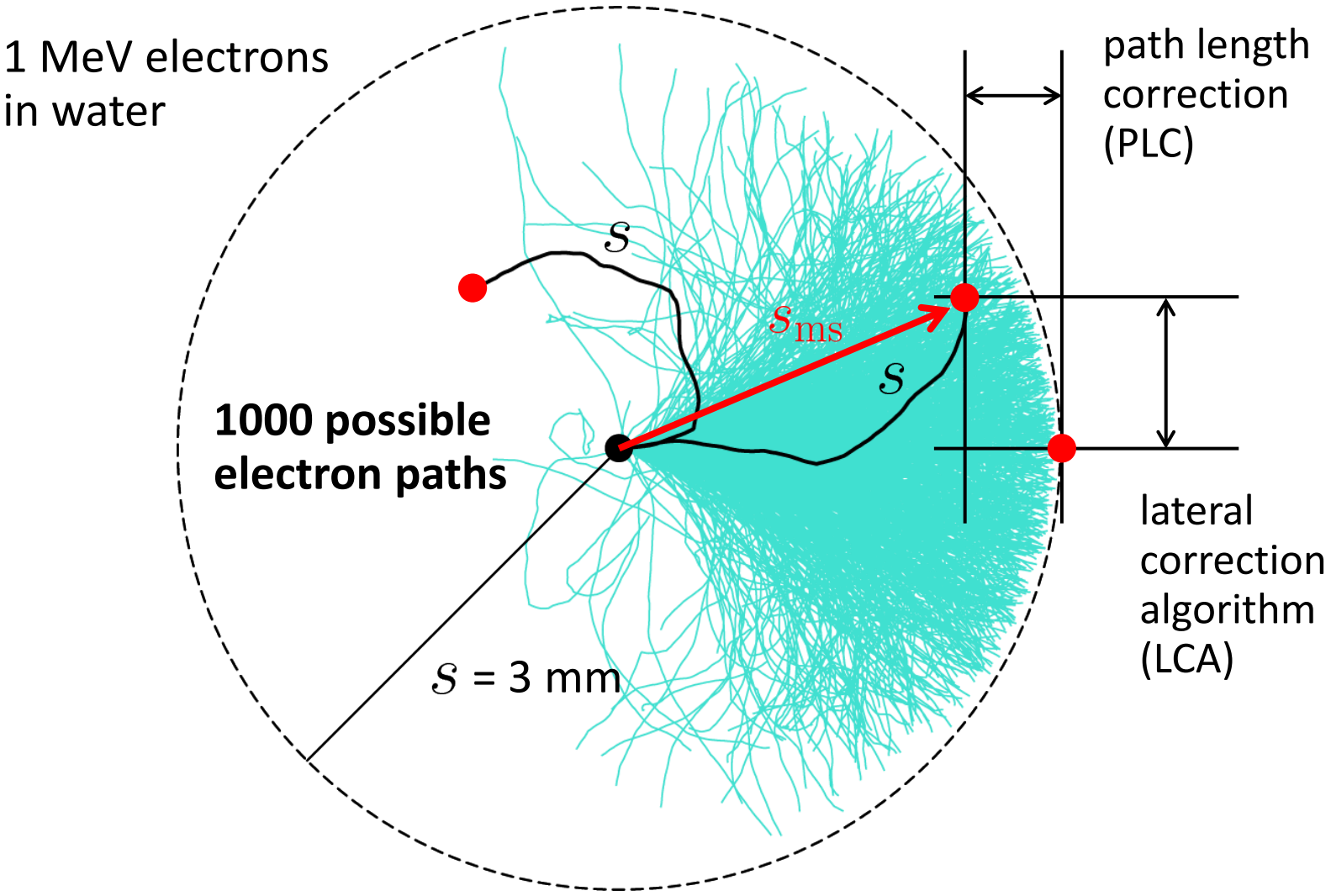
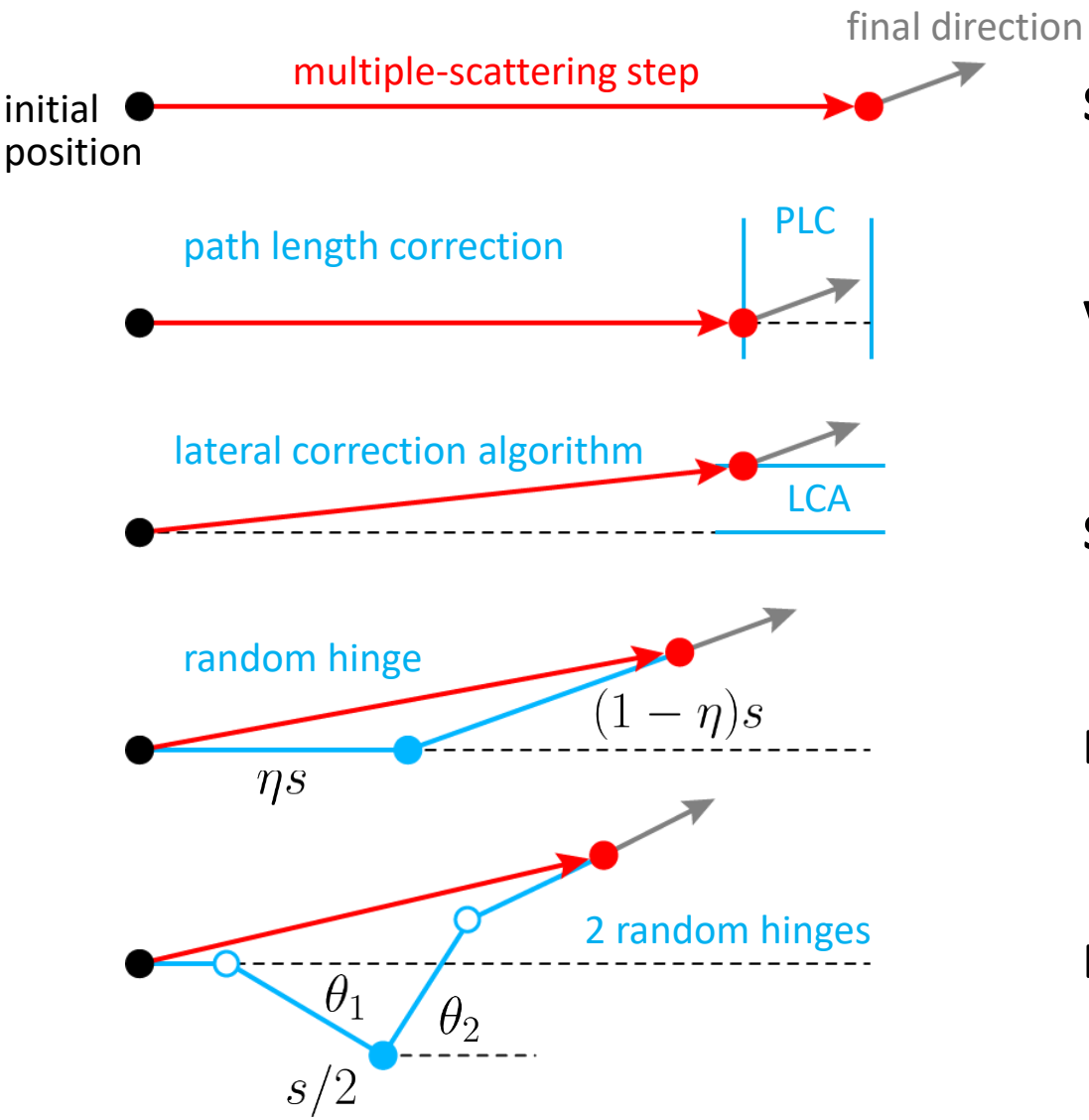


Electron step algorithms have evolved



Simplistic (ITS, MCNP)

Very simple (EGS4)

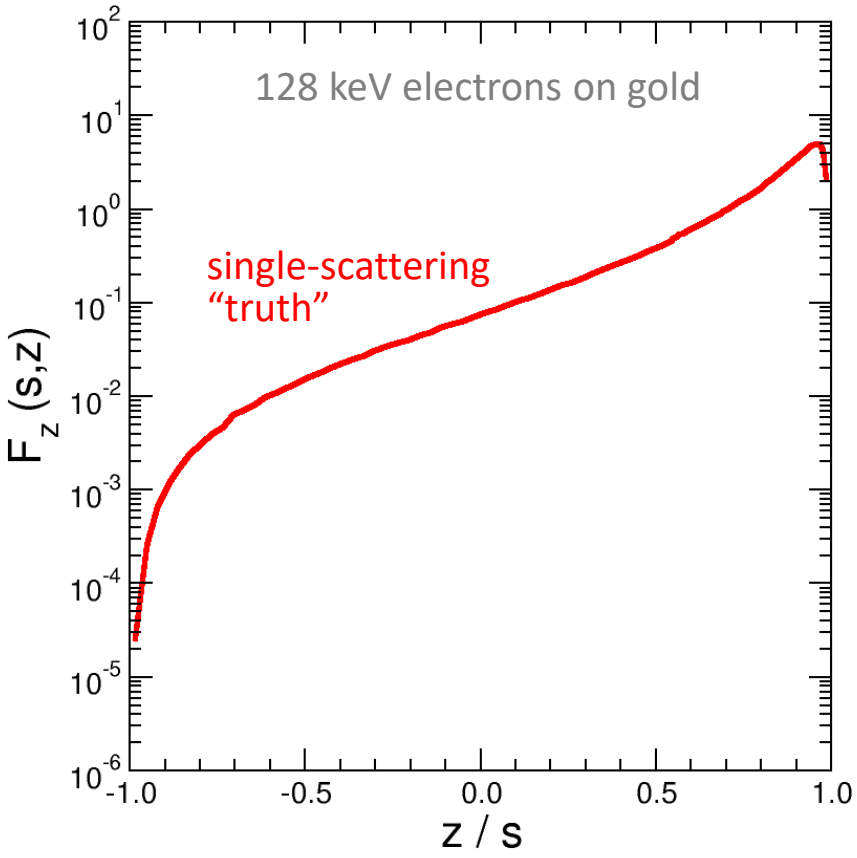
Simple (EGS4/PRESTA)

Better (Penelope)

Best (EGSnrc)

EGSnrc step matches single-scattering

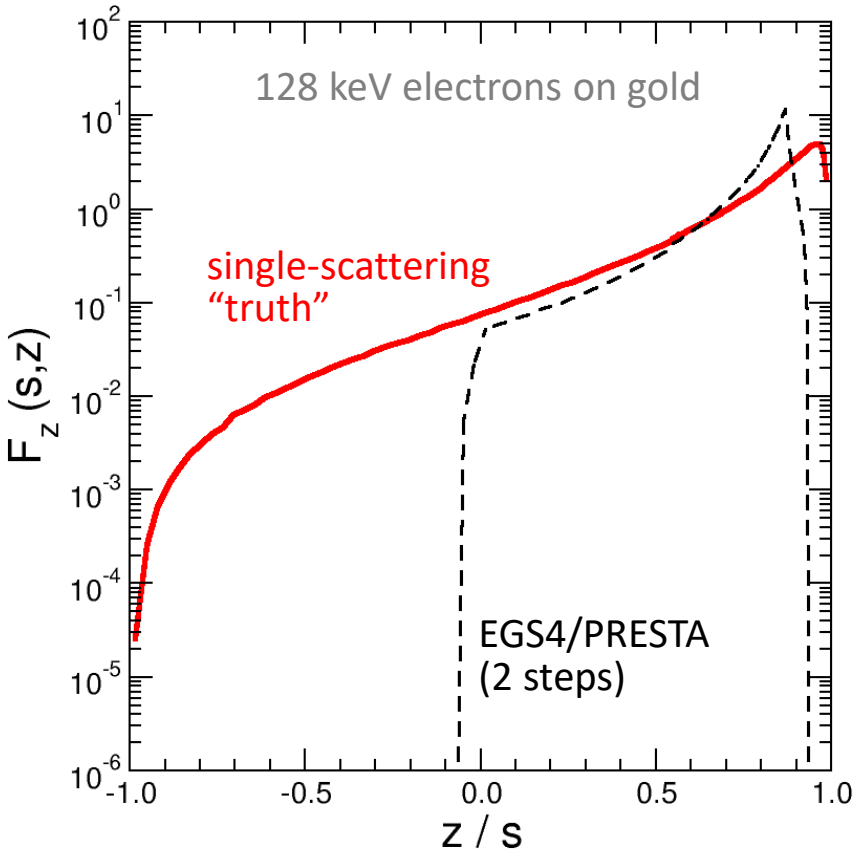
longitudinal distribution



Probability to find the electron at position z after a path length s.

EGSnrc step matches single-scattering

longitudinal distribution



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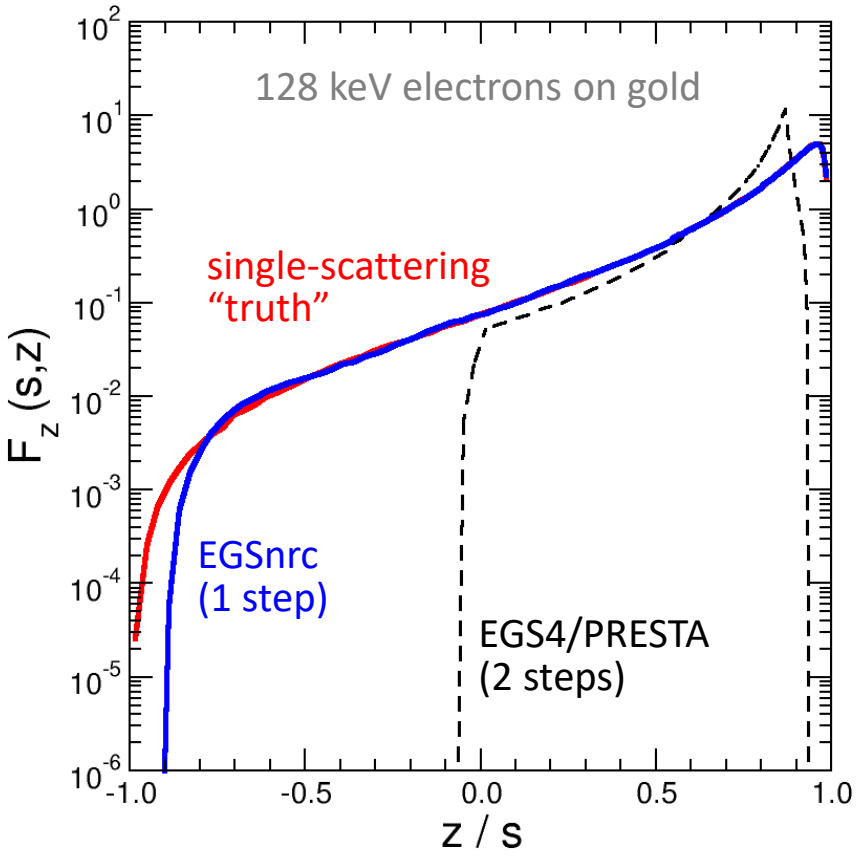

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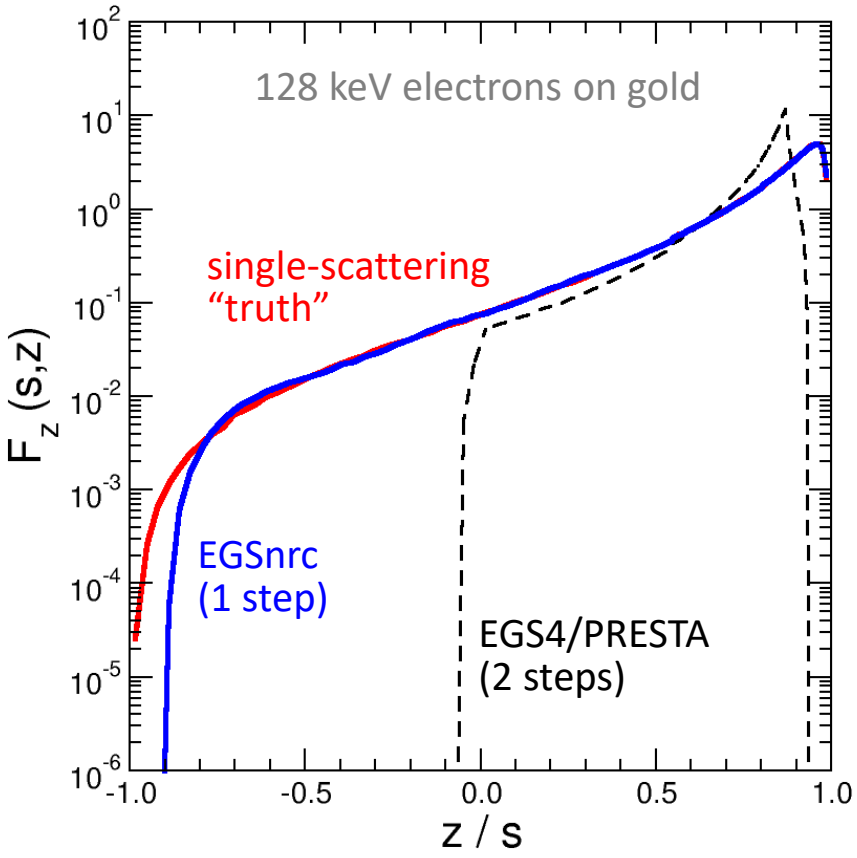
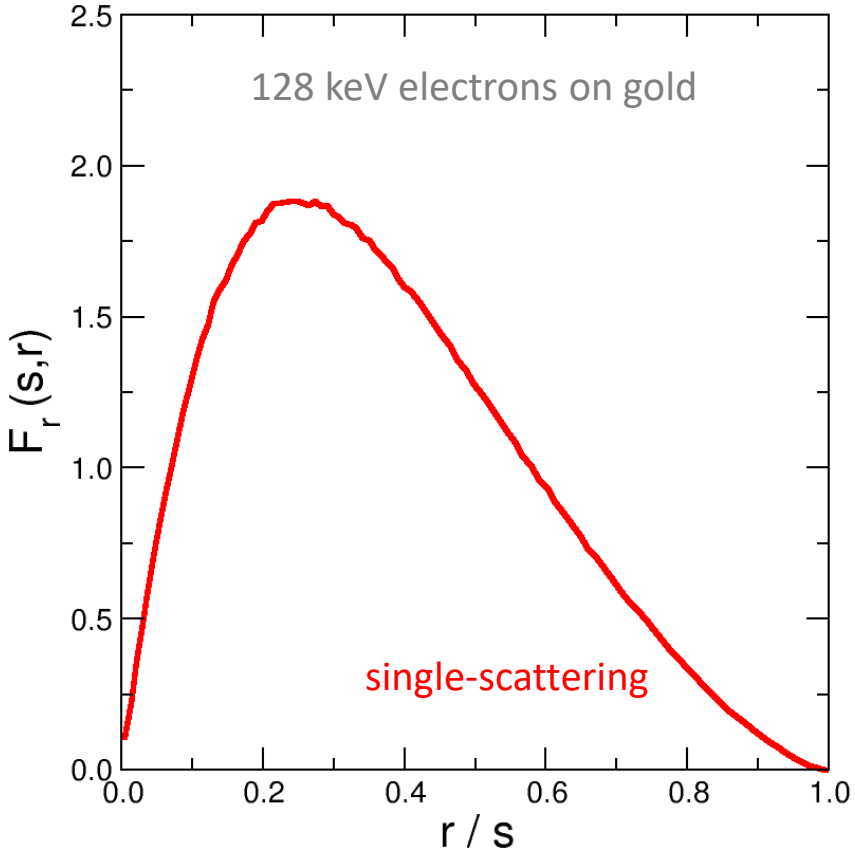


Probability to find the electron at position z after a path length s.

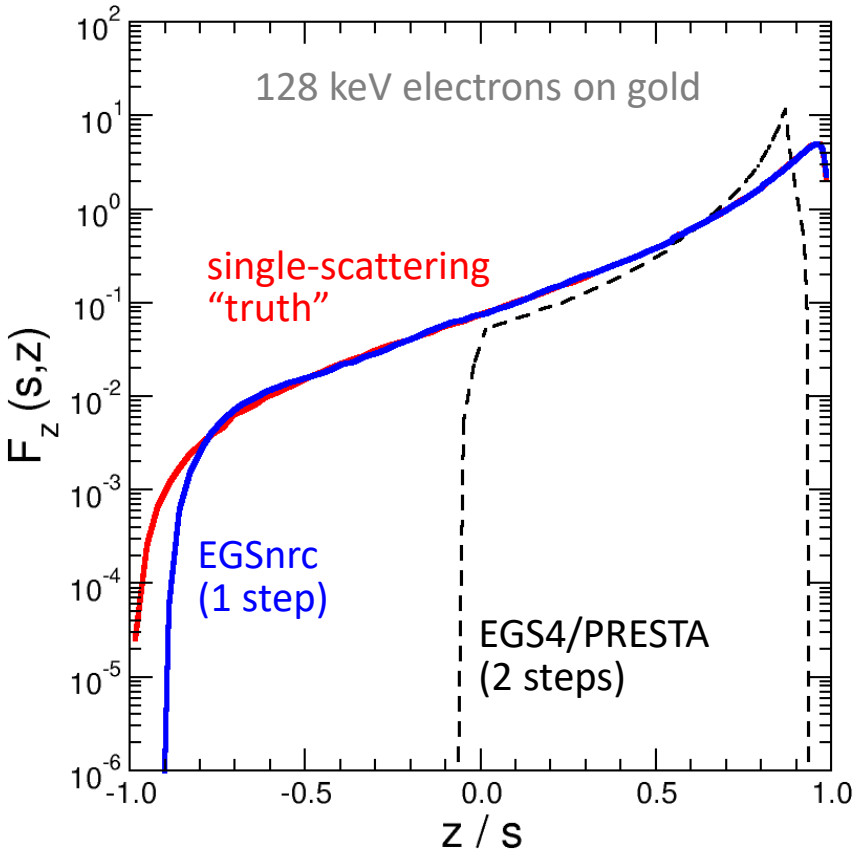
transverse distribution



Probability to find the electron at radial position r after a path length s.

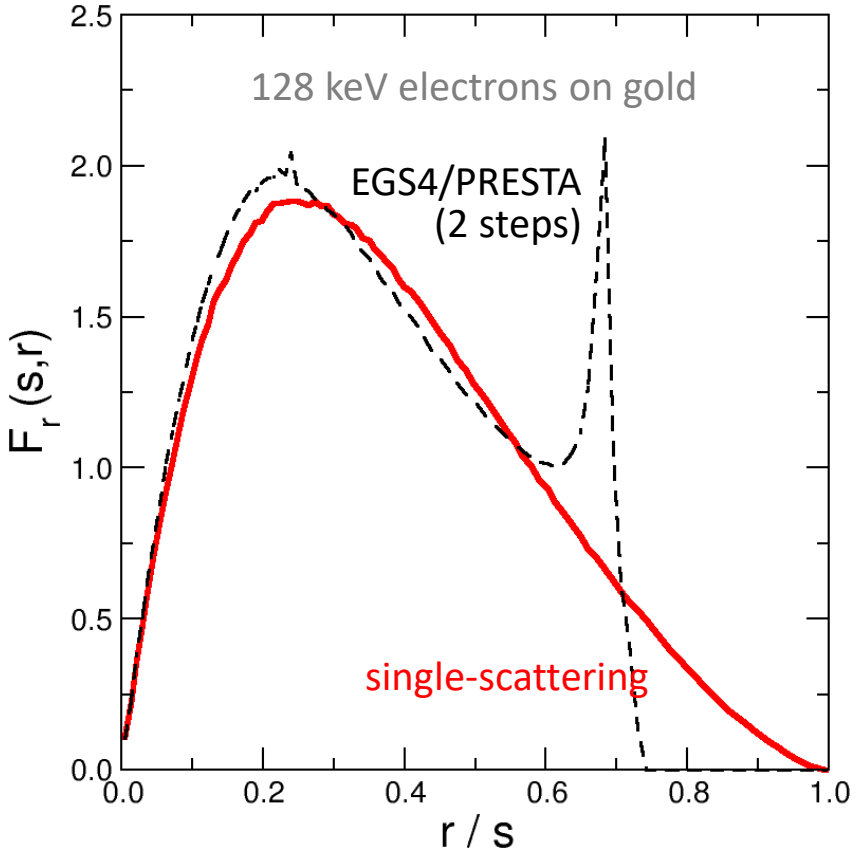
EGSnrc step matches single-scattering

longitudinal distribution



Probability to find the electron at position z after a path length s.

transverse distribution



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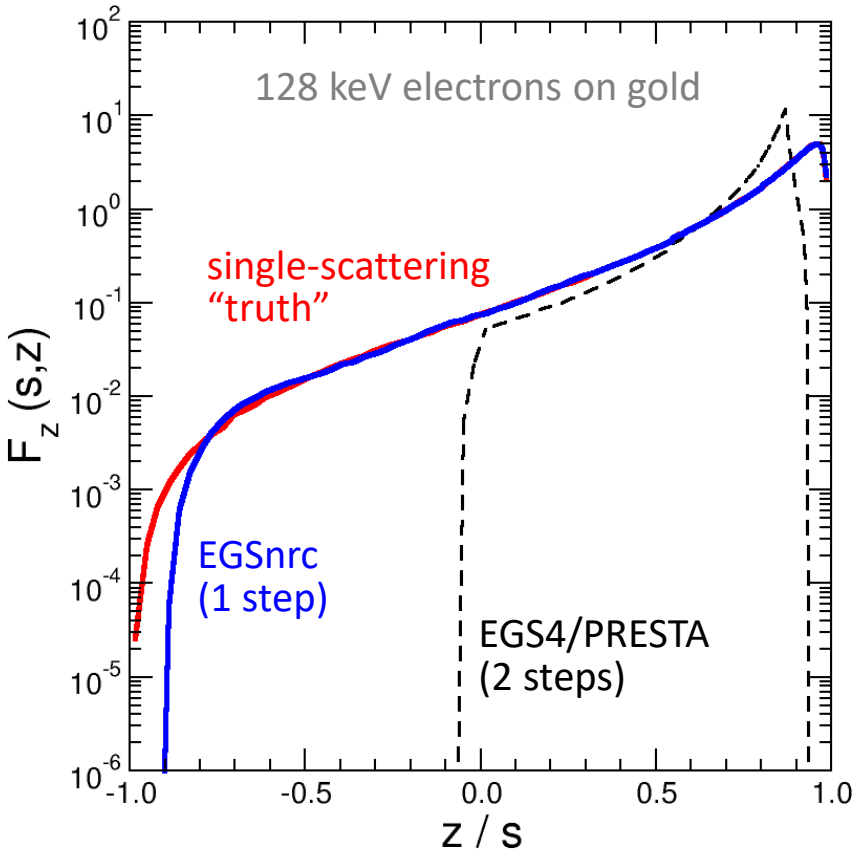
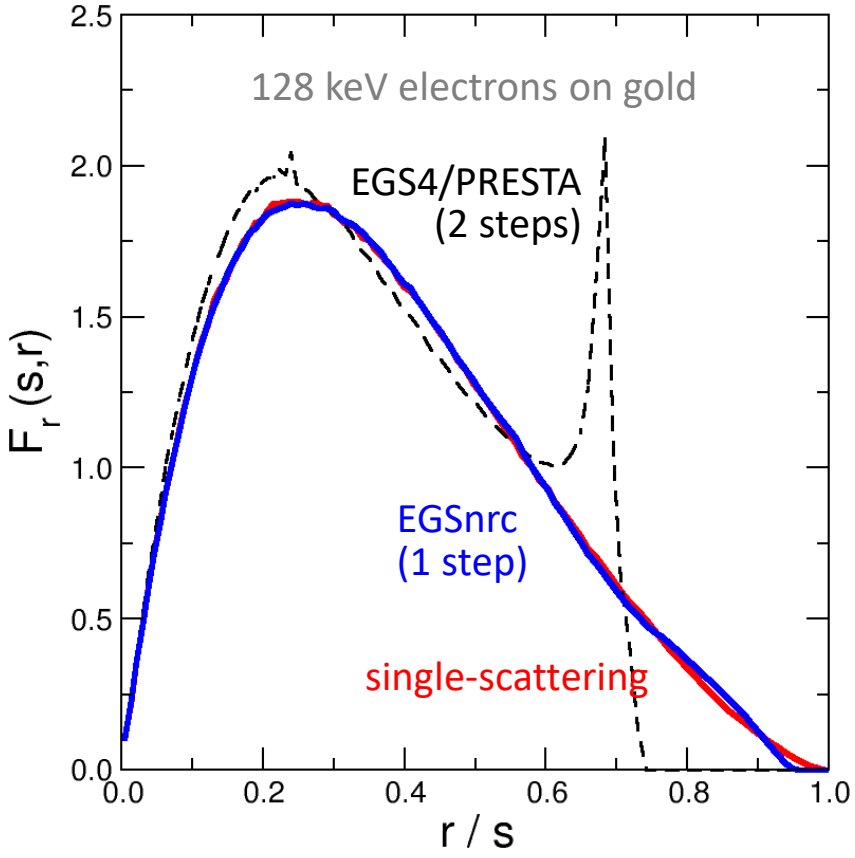


Probability to find the electron at position z after a path length s.

transverse distribution



Probability to find the electron at radial position r after a path length s.

Step 2 issues: curvilinear electron path

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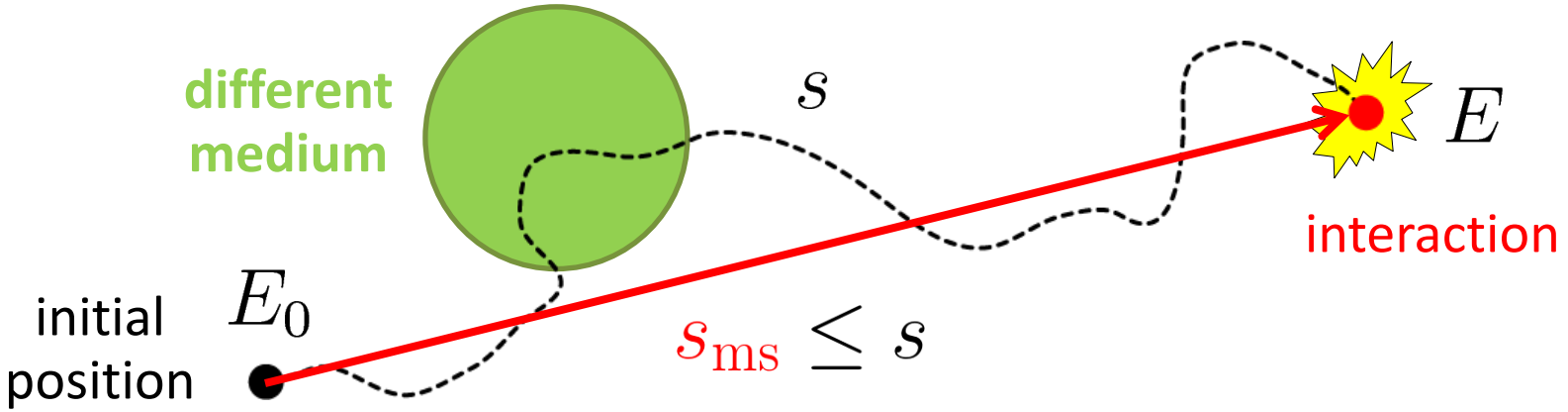
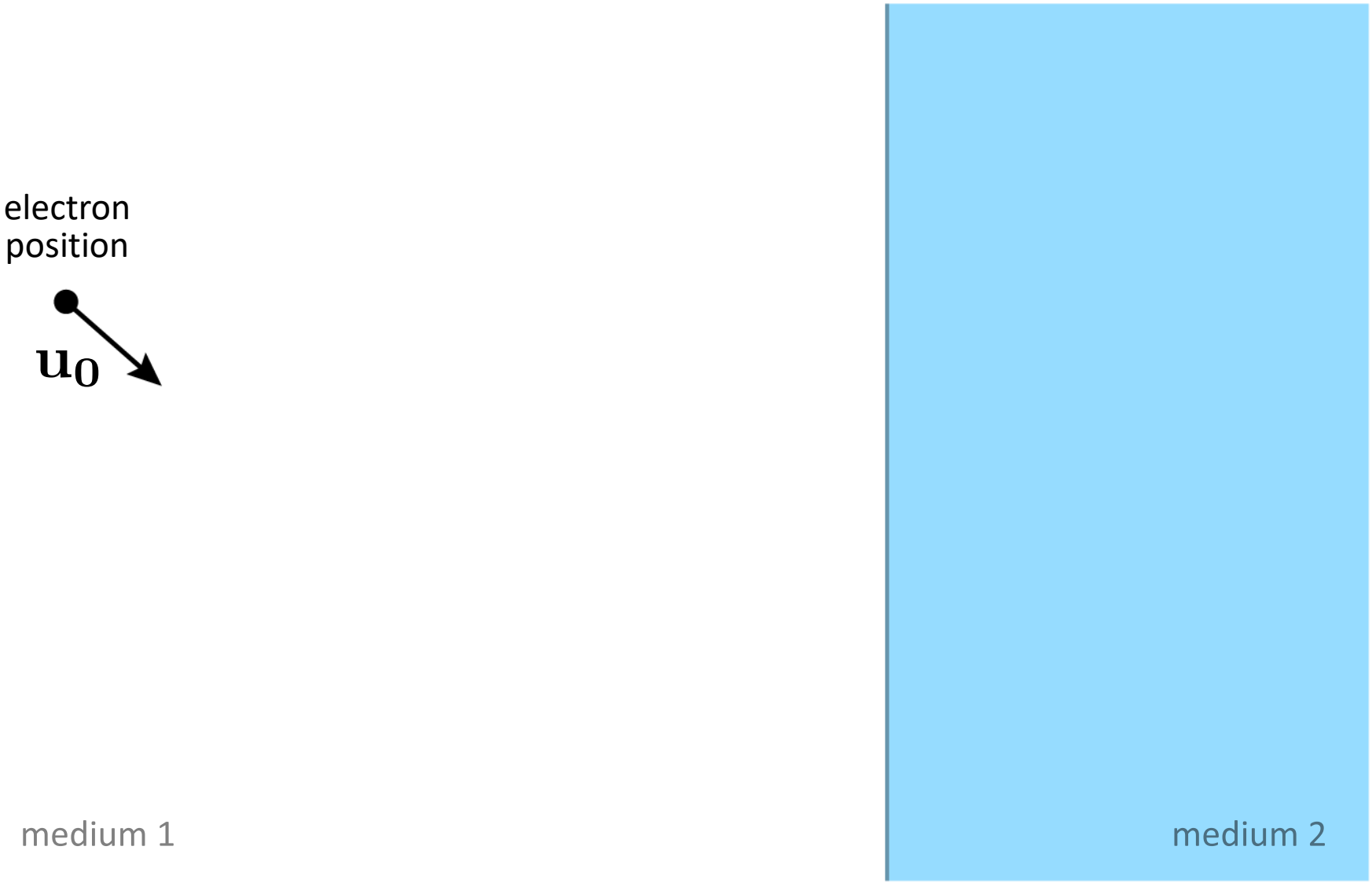


   b) ensure the real (curved) electron path could not have crossed a boundary: **consider distance to boundaries in all directions.**

Limit path length to nearest boundary distance



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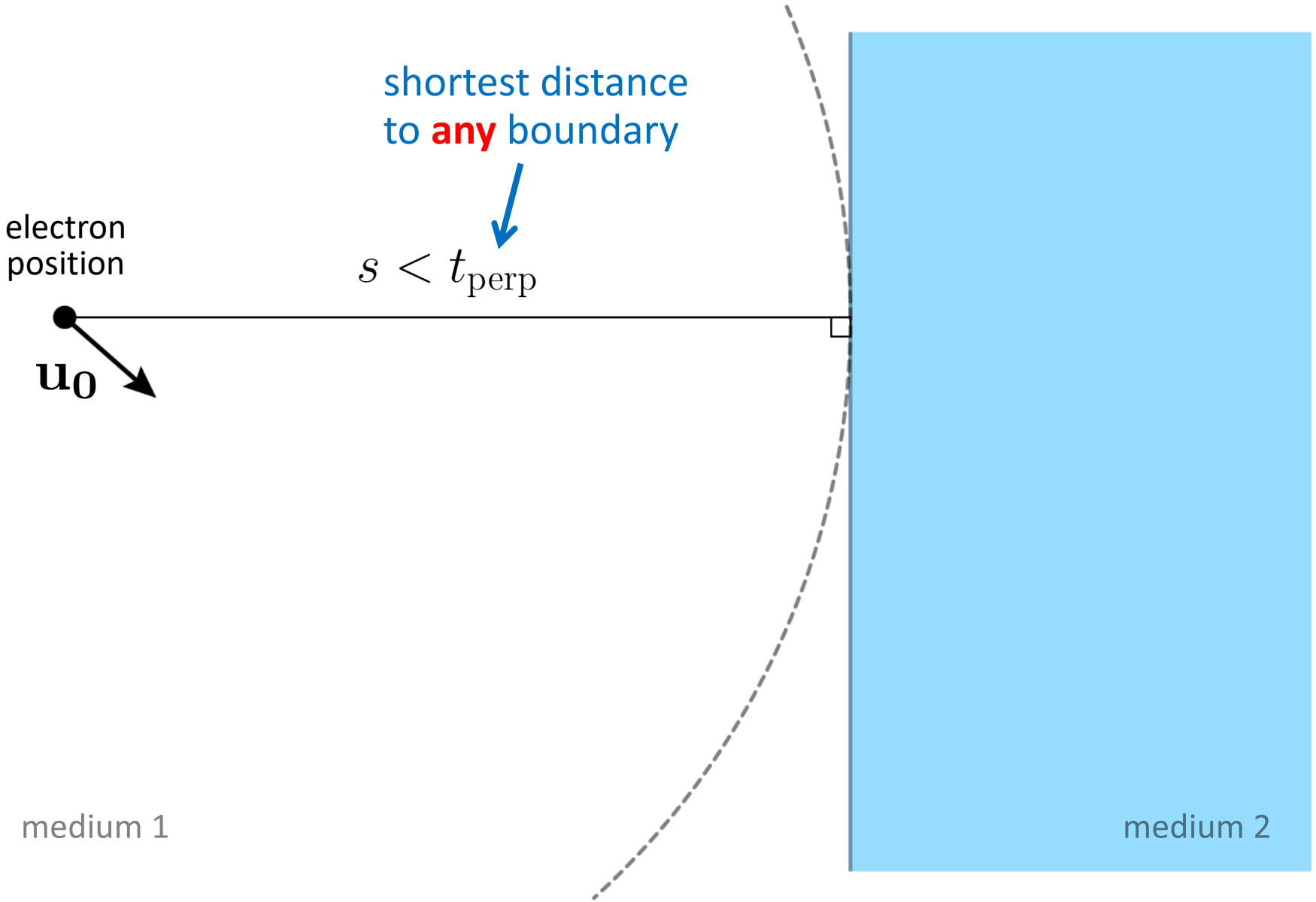

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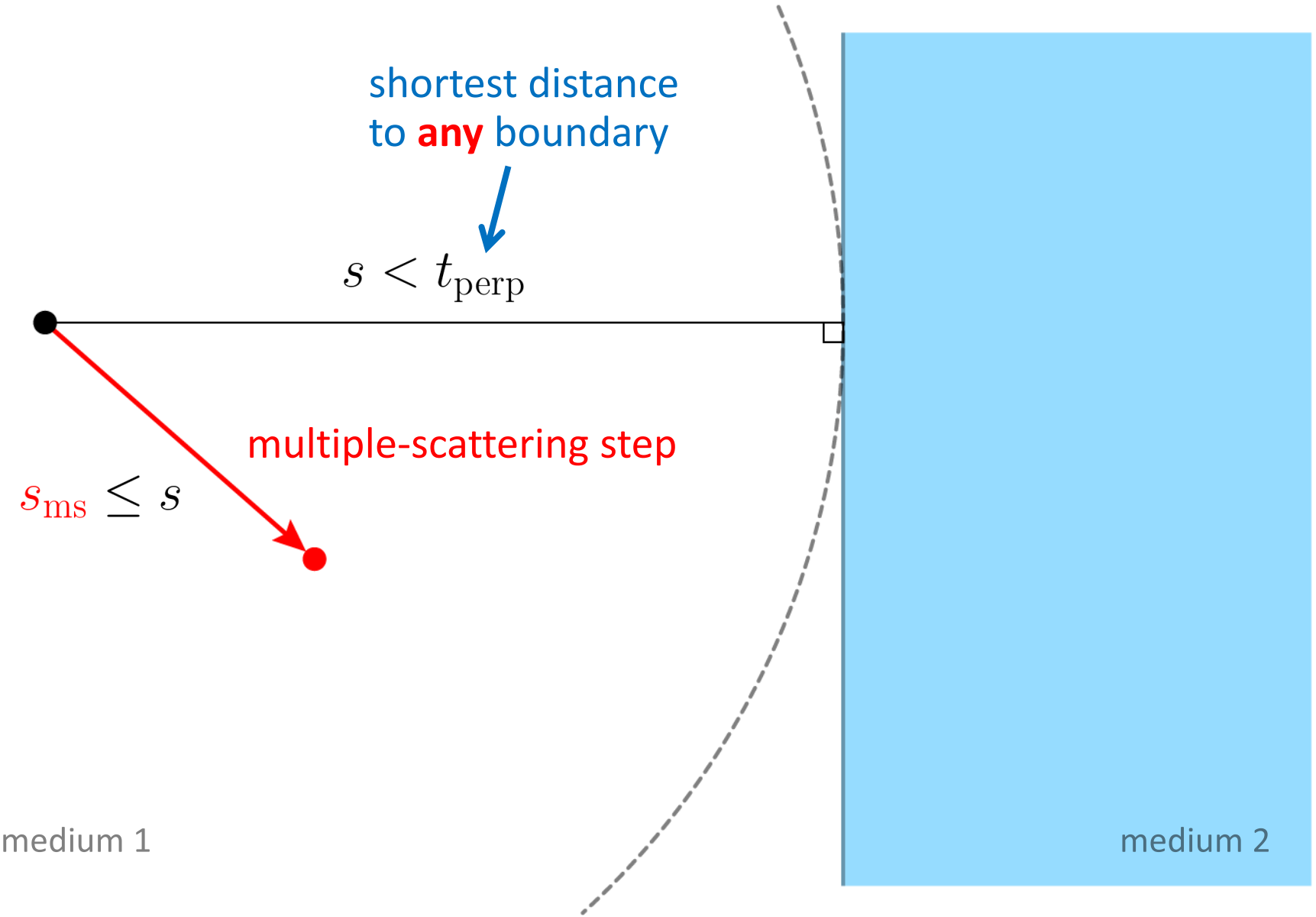

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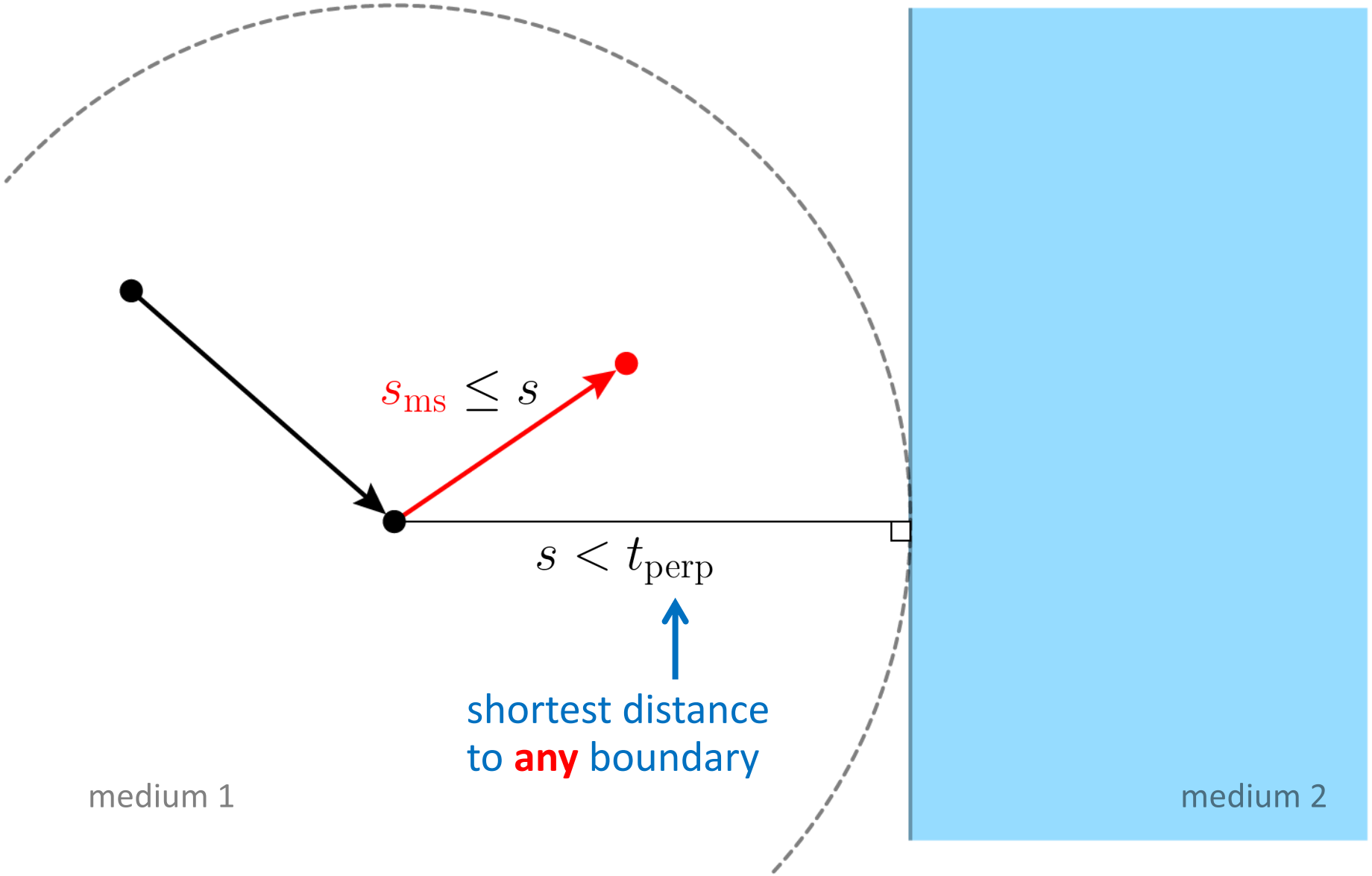

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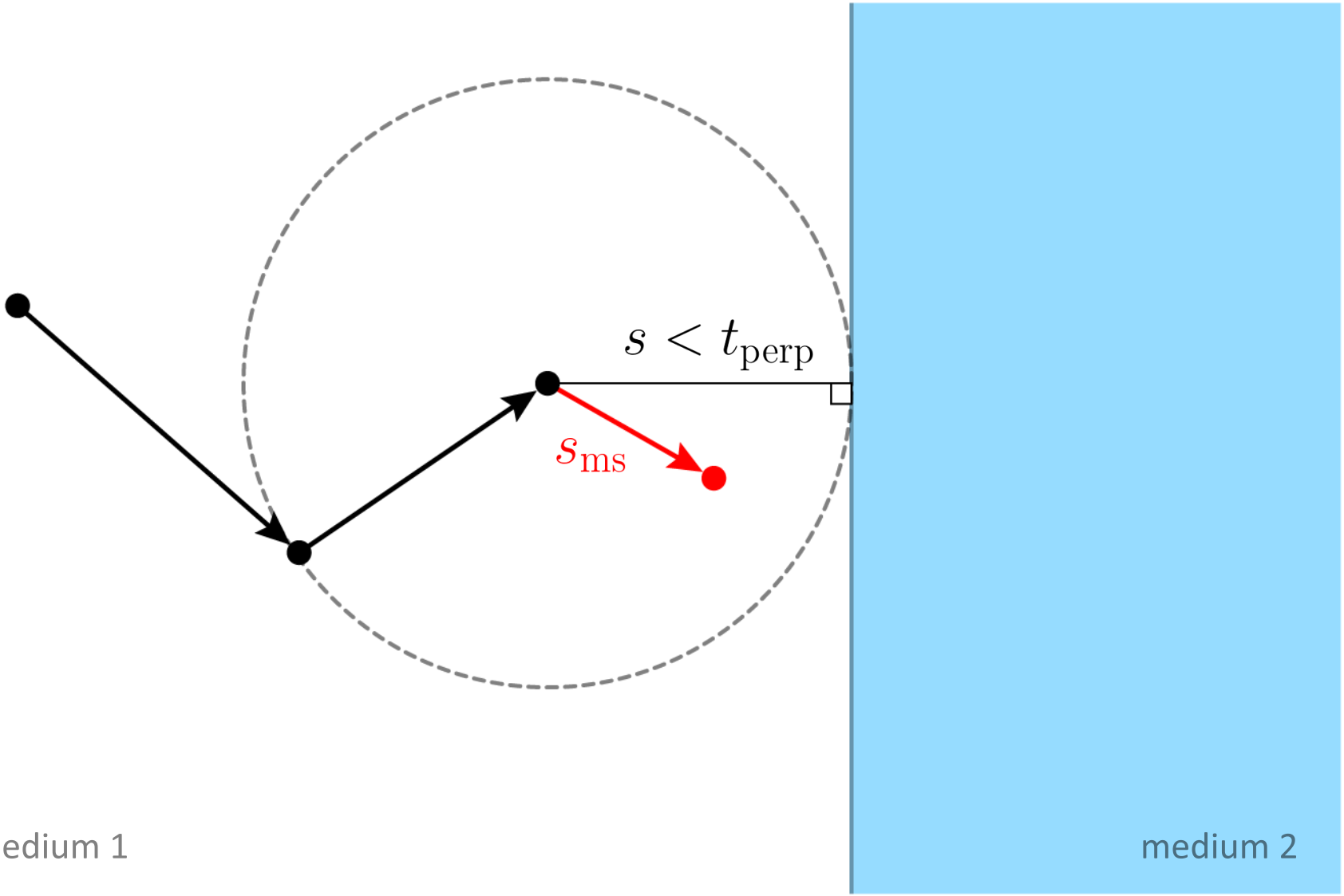

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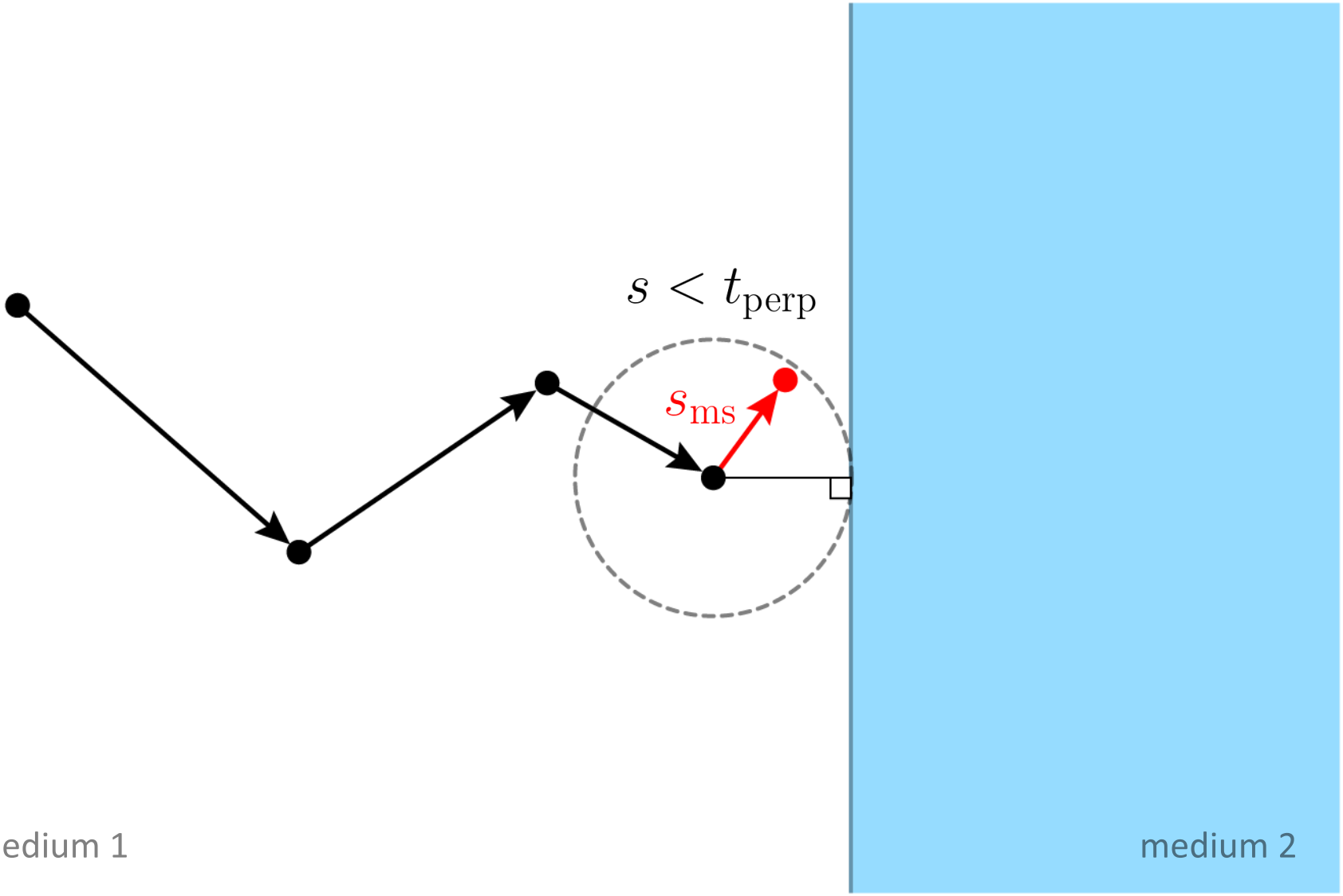
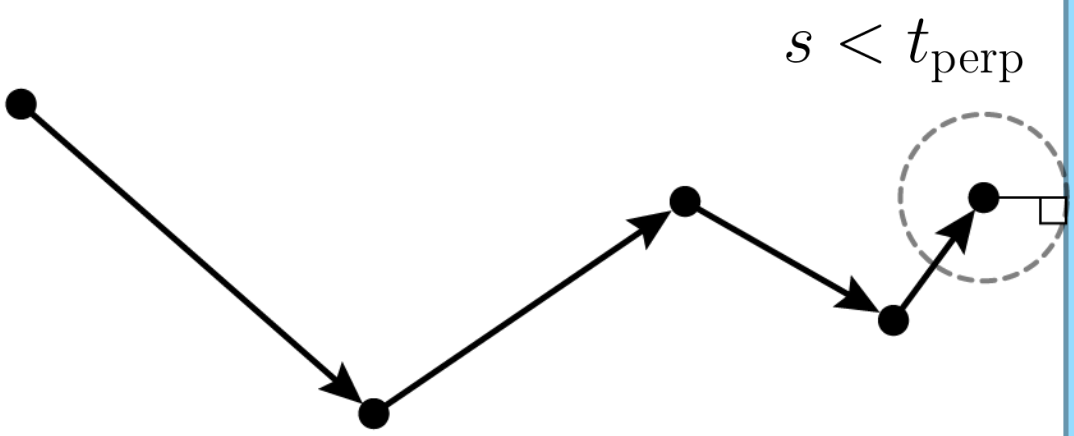


Limit path length to nearest boundary distance

"Zeno's algorithm":
particle never reaches the boundary!

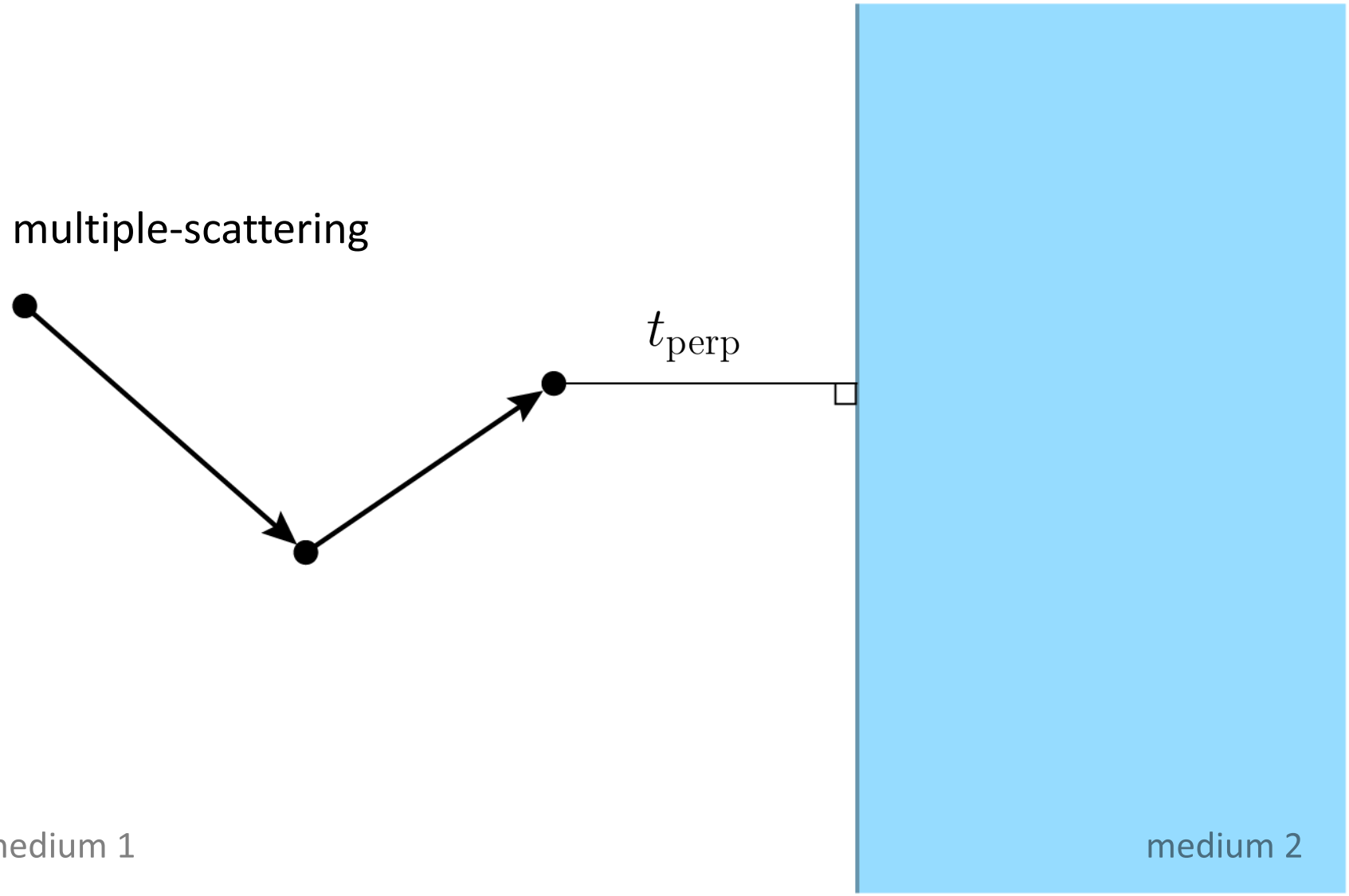


To move across the boundary, we need a
boundary crossing algorithm (BCA)

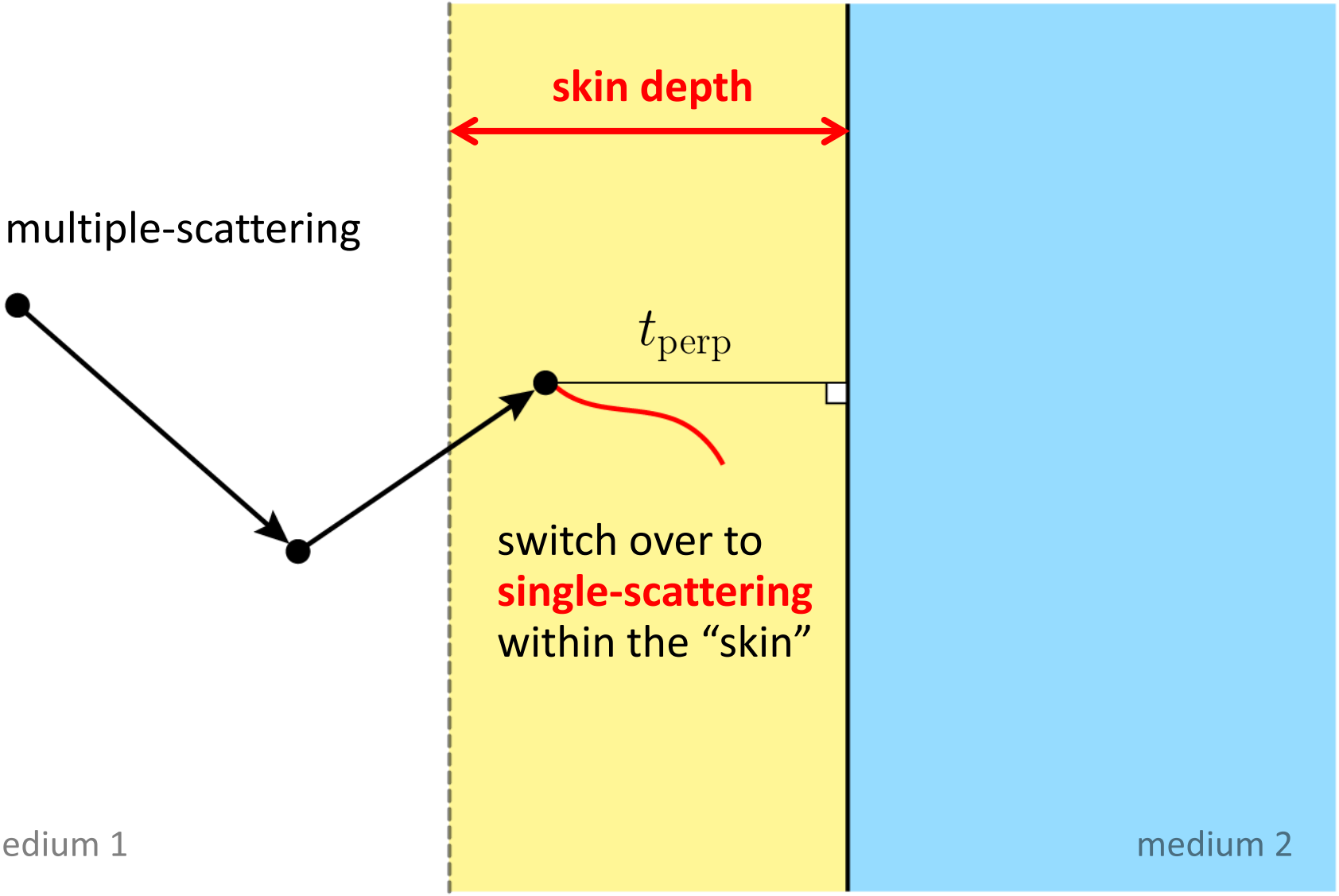
medium 1

medium 2

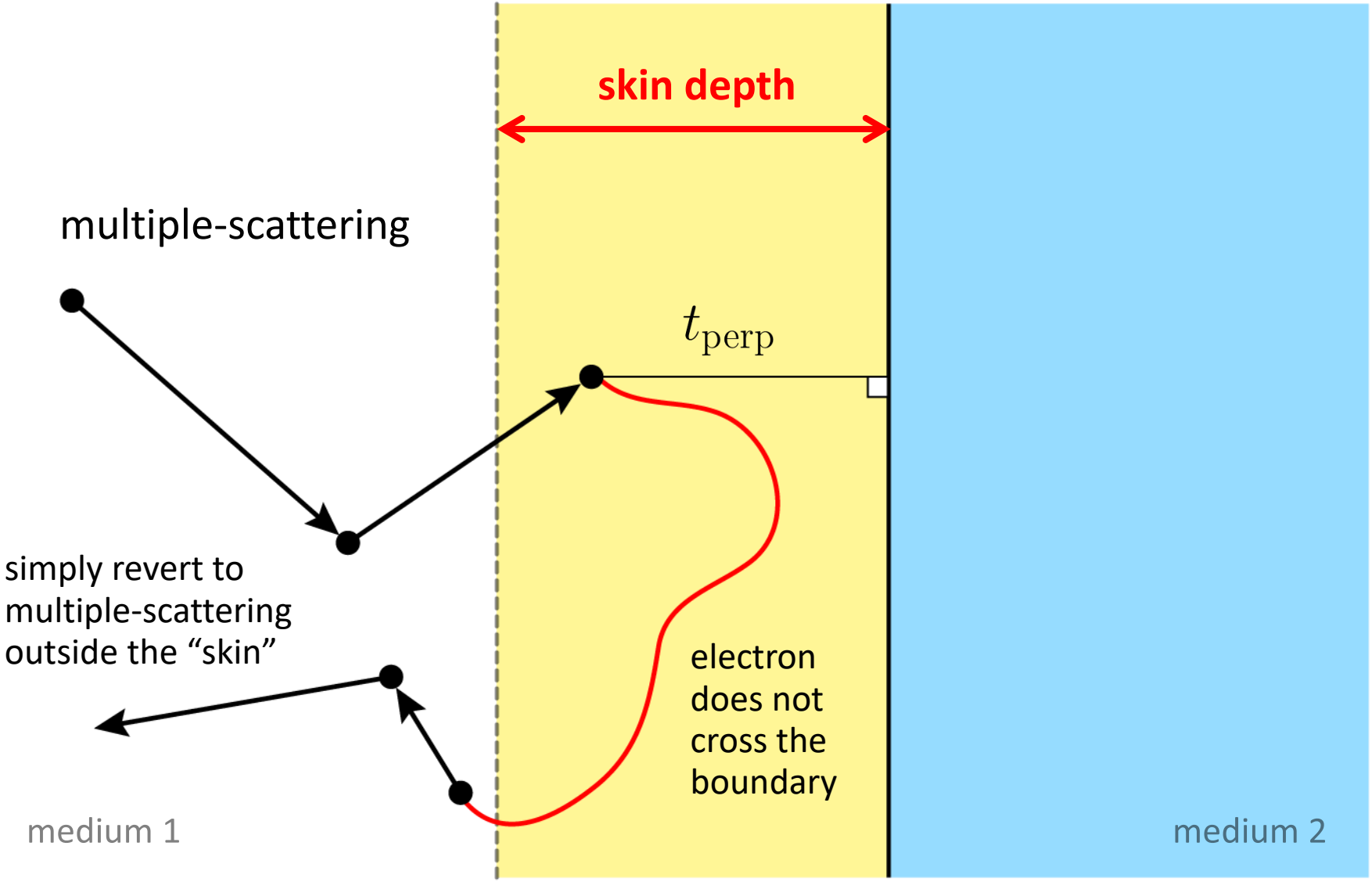
Switch to single-scattering near the boundary



Switch to single-scattering near the boundary



Switch to single-scattering near the boundary



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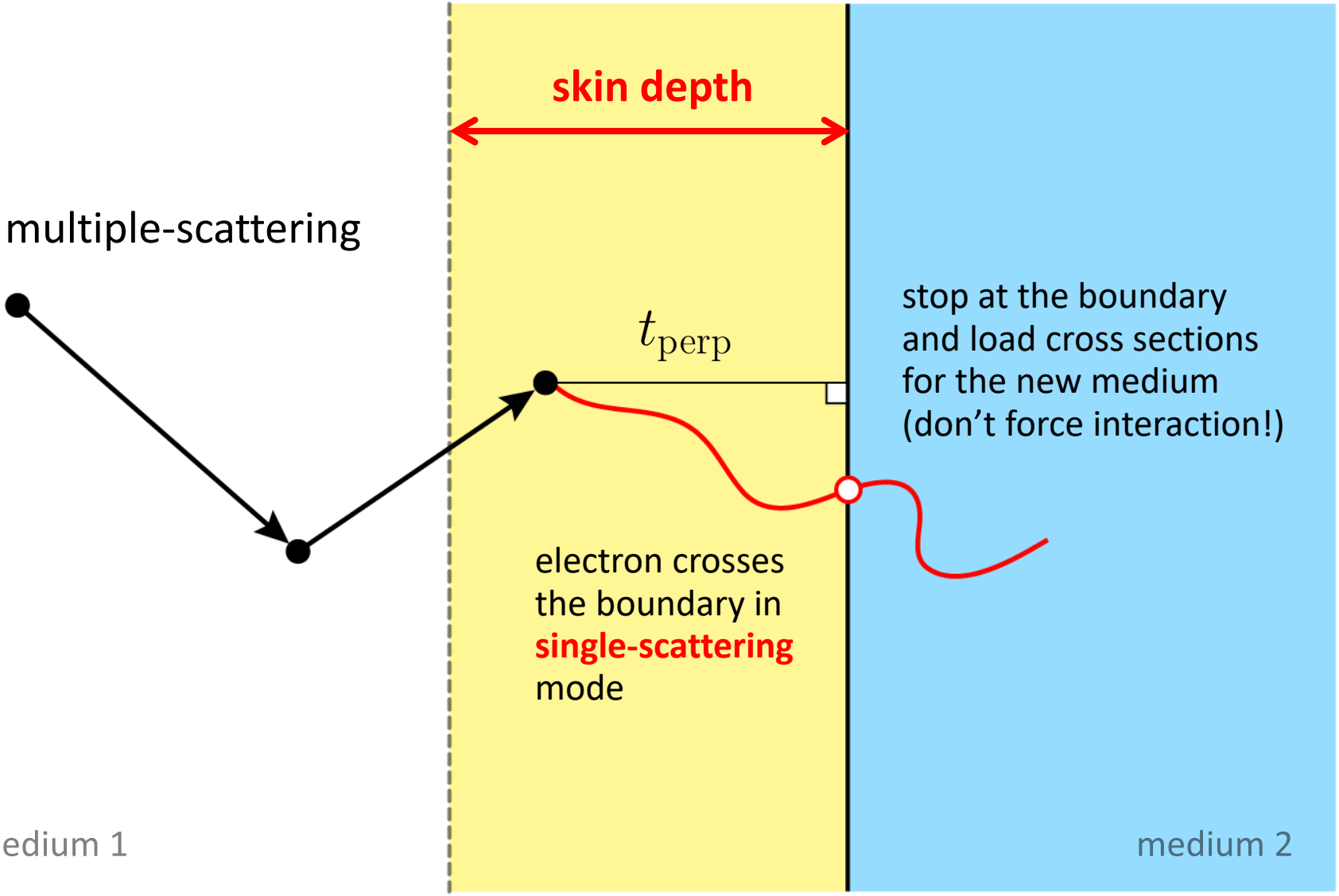
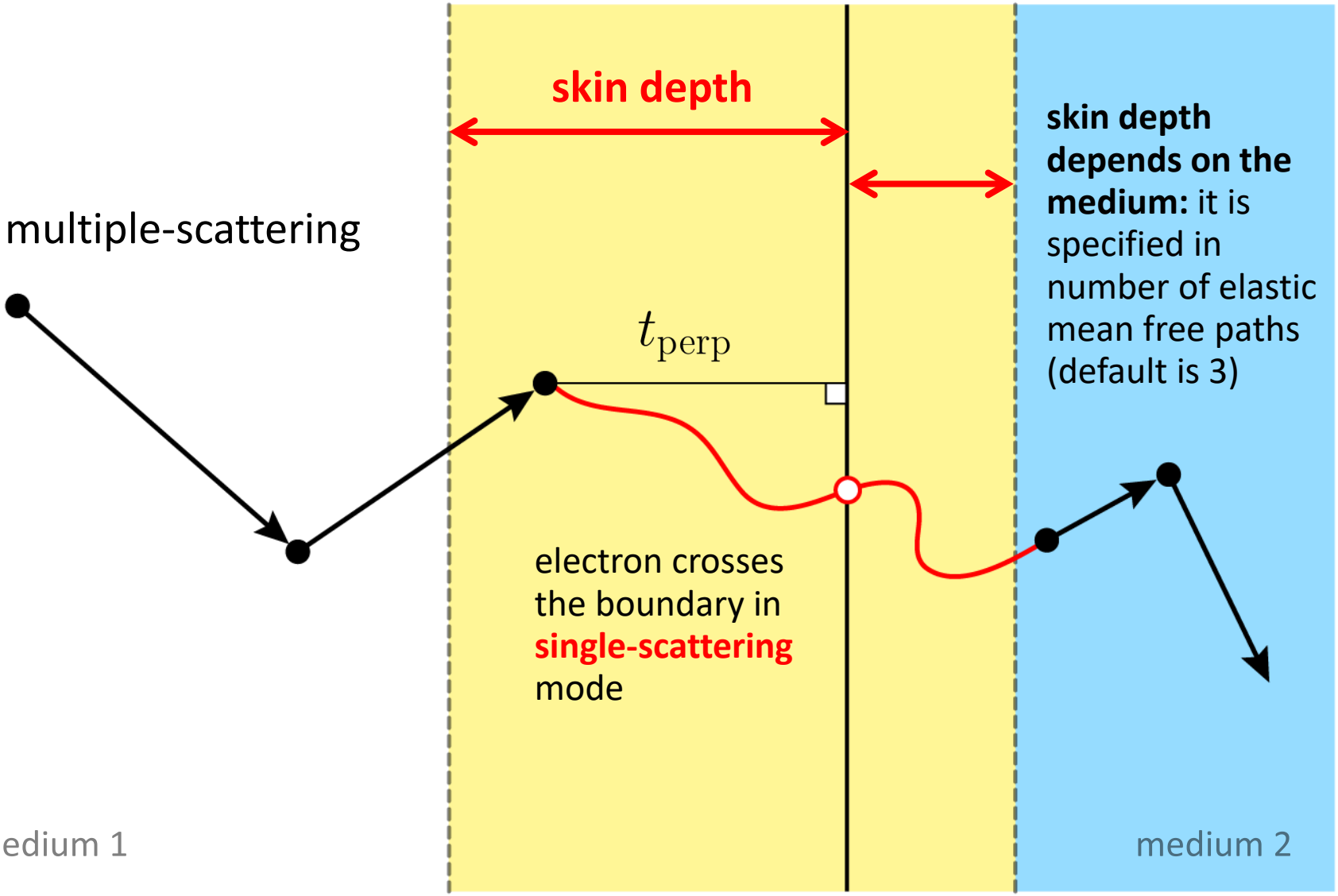
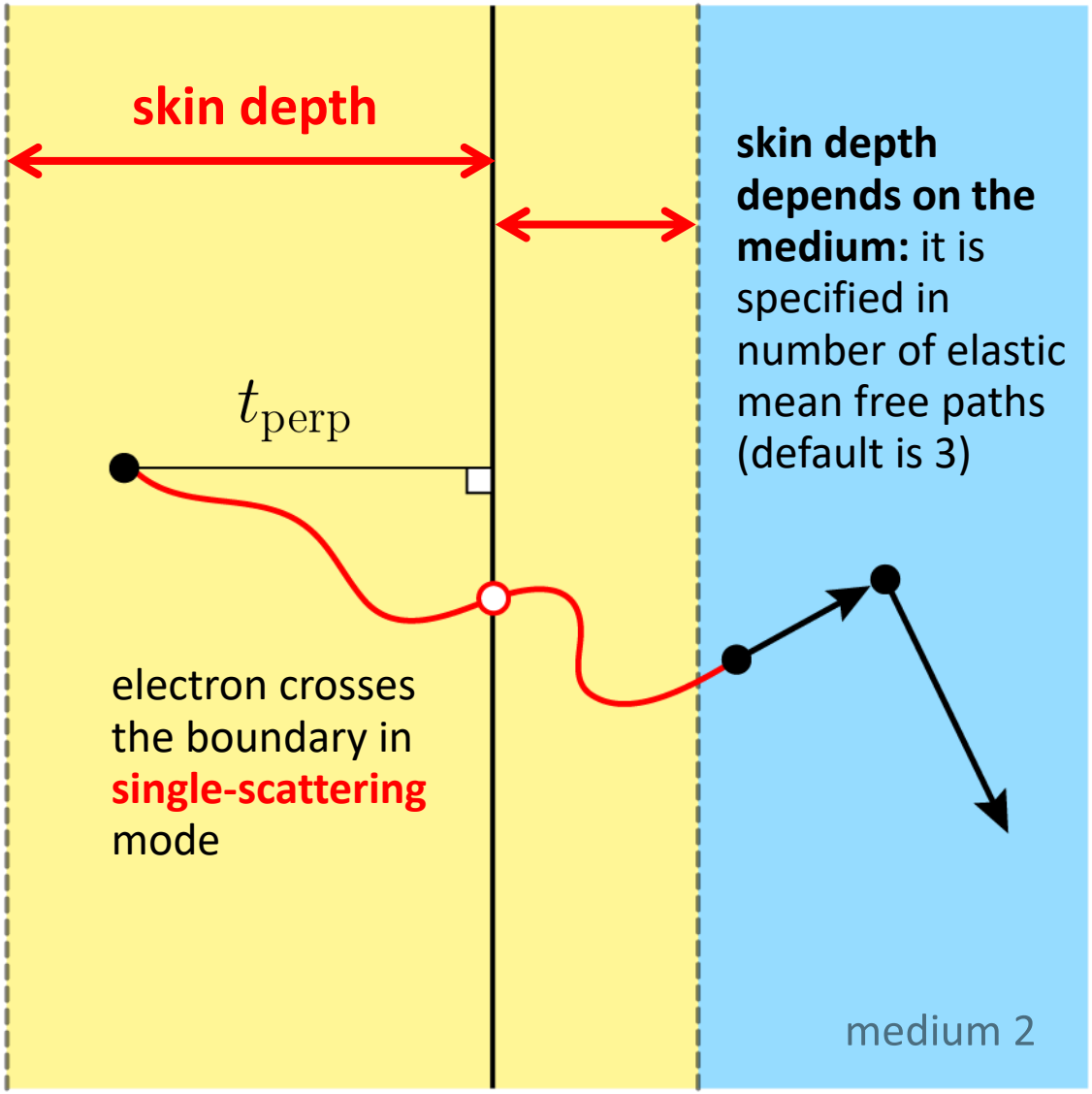


Switch to single-scattering near the boundary



This is called the “Exact BCA” in EGSnrc

- In EGSnrc this is called the **Exact BCA.** There is little reason to use PRESTA-I.
- The default skin depth is **3 elastic mean free paths** because a single step in multiple-scattering “costs” about as much as 3 steps in single-scattering.
- To run an entire simulation in **single-scattering mode,** specify a “huge” skin-depth.
- EGSnrc **converges** to its single-scattering mode with default parameters (large multiple-scattering steps).



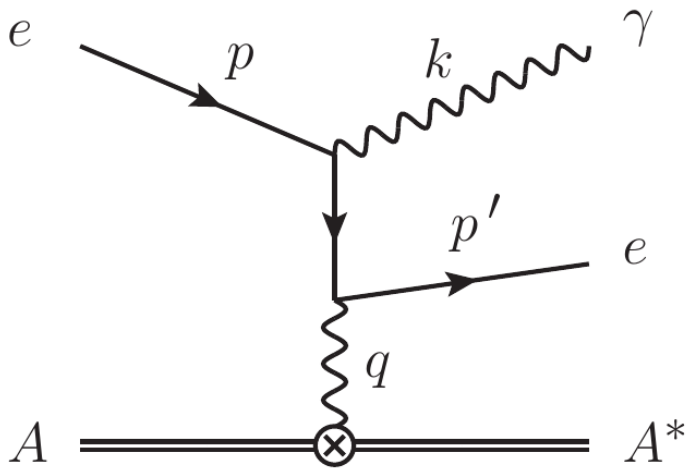
Electrons (positrons) interact via 4 processes

1. **Emission of a bremsstrahlung photon** in the nuclear field or in the field of atomic electrons (electron-electron bremsstrahlung)
2. **Inelastic collision** with atomic electrons (knock-on electron)
3. **Elastic collision** with nuclei and atomic electrons (deviation)
4. **Positron annihilation** (emission of a photon pair)

The main challenge in modelling the transport of electrons through matter is that the **cross-sections are very large,** because charged particles interact essentially *"all the time"* with the atoms they encounter.

Bremsstrahlung emission

- Simulated only for $T > AP$ ($k > AP$)
- Restricted stopping powers for sub-threshold, "soft" bremsstrahlung
- Dominates at high energies
- Scales as Z^2



Options:

Bethe-Heitler (default) | ICRU37 | better electron-electron bremsstrahlung

```
Brems cross sections = BH | NIST | NRC
```

```
Brems angular sampling = Simple | KM
```

← modified Koch-Motz (default)

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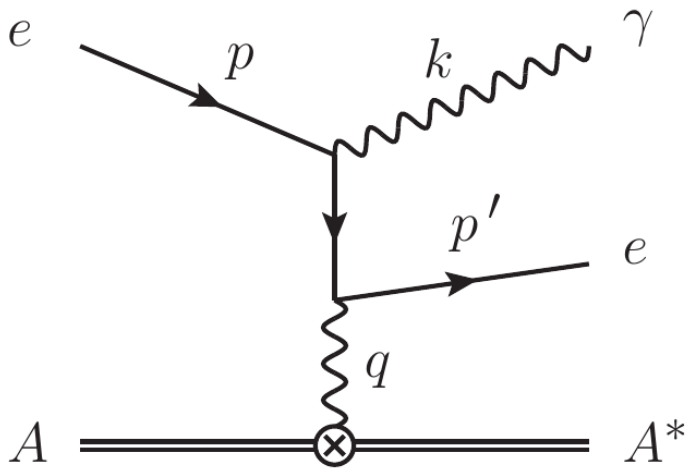

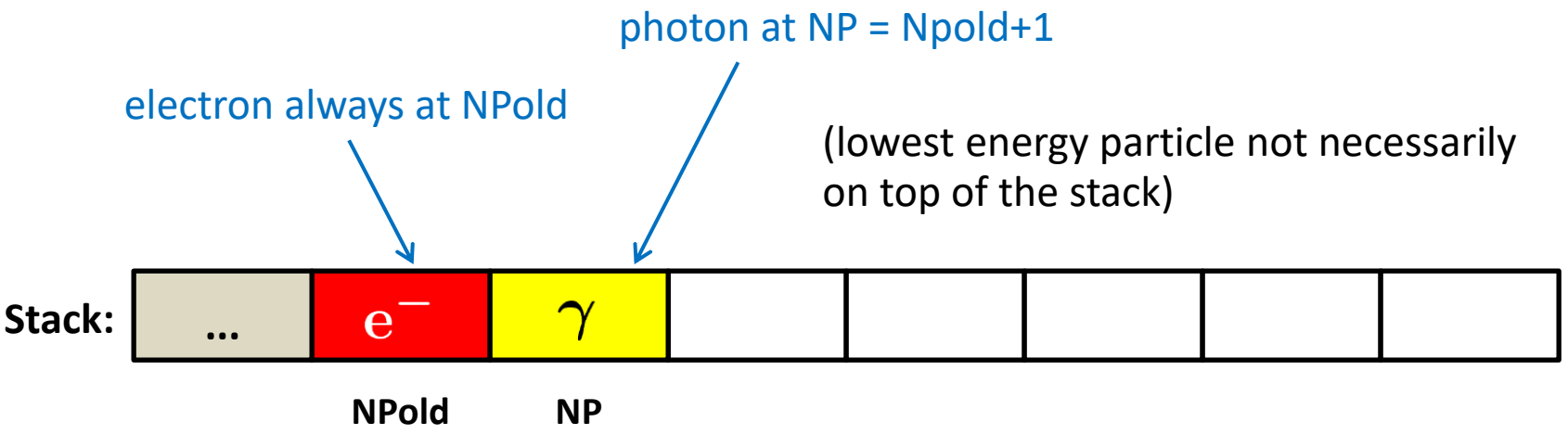

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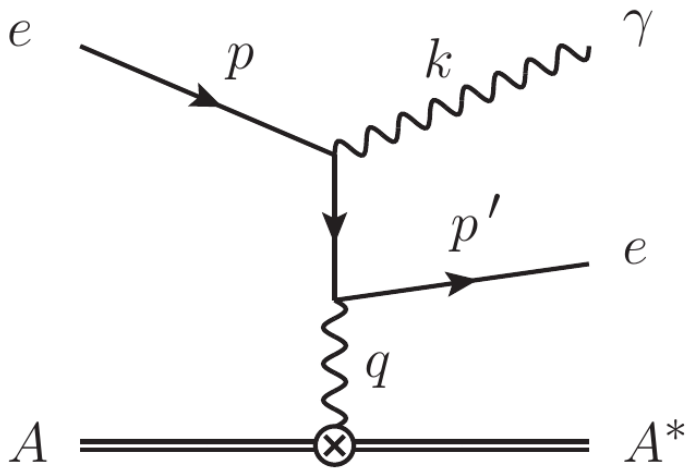
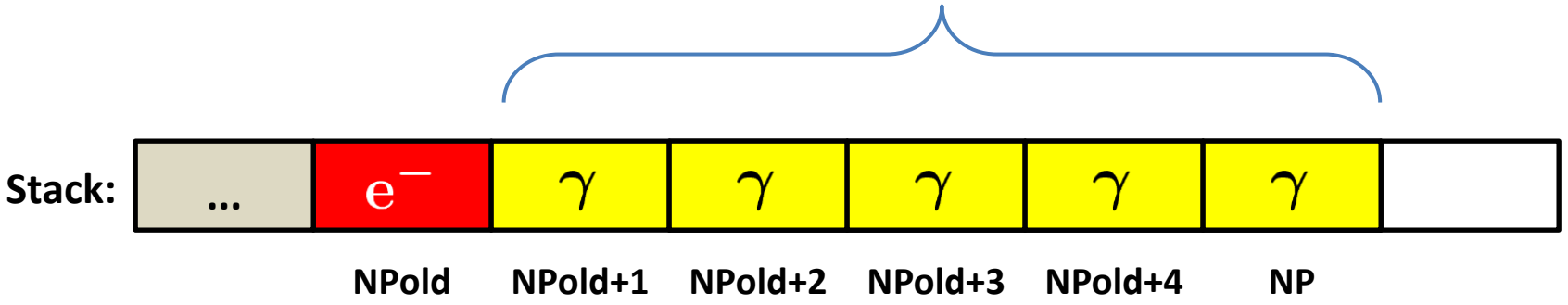
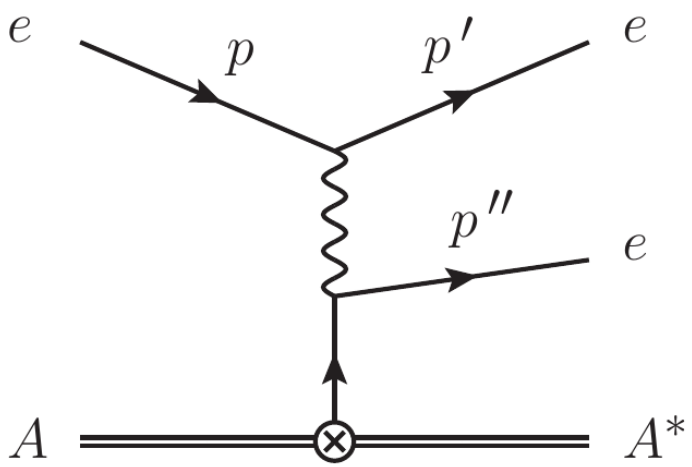


when **splitting** is used, photons are between NPold+1 and NP (not ordered by energy)

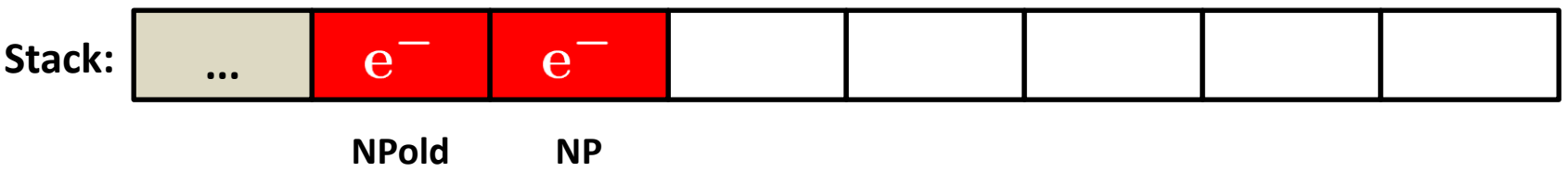


Electron inelastic collision (Møller scattering)

- Simulated only for $T > 2T_{AE}$ because electrons are indistinguishable.
- Restricted stopping powers for sub-threshold, “soft” collisions
- Generally, dominates at low and intermediate energies
- Scales as Z
- **Ignores binding**



secondary, **lower energy** electron is at NP = NPold+1



Electron impact ionization (Eii)

Incident electron knocks out a **bound electron,** and **atom relaxes** emitting fluorescent photons, Auger and Coster-Kronig electrons. Essential for accurate kilovoltage X-ray spectra.

- Treated within the Møller routine, as a type of inelastic collision.
- Simulated for K and L shells with binding energies $E_b > T_{AE}$.
- When Eii is turned on, Eii interactions are based on the bound electron cross section. All other interactions are treated as Møller.

Options:

```
Electron Impact Ionization =
Off | On | casnati | kolbensvedt | gryzinski | penelope
```

default

EGSnrc's own Eii cross section derived by Iwan Kawrakow

Electron impact ionization (Eii)

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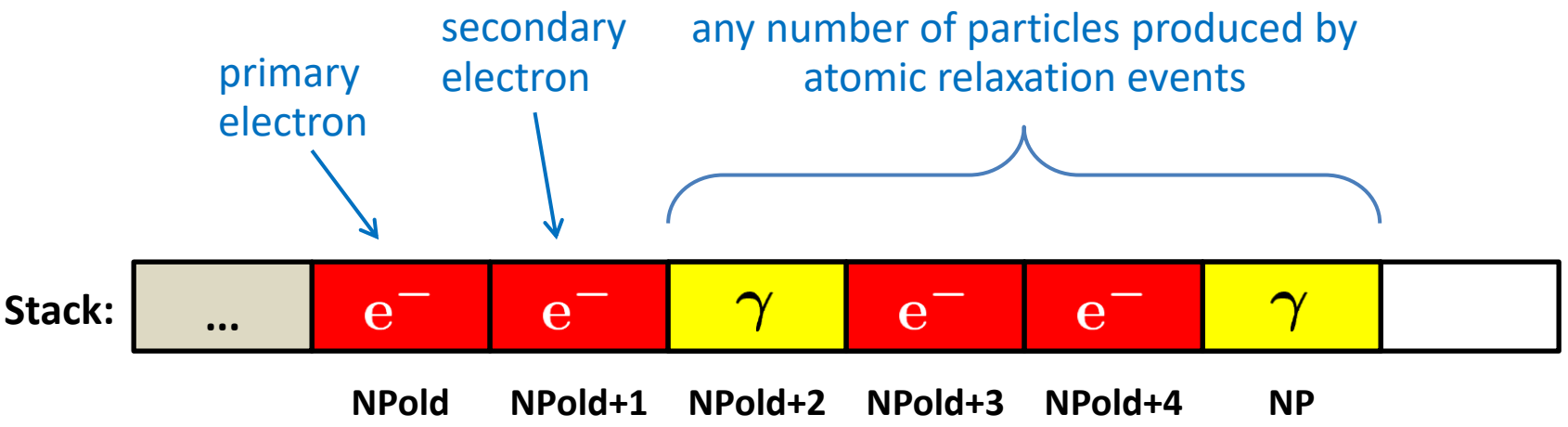
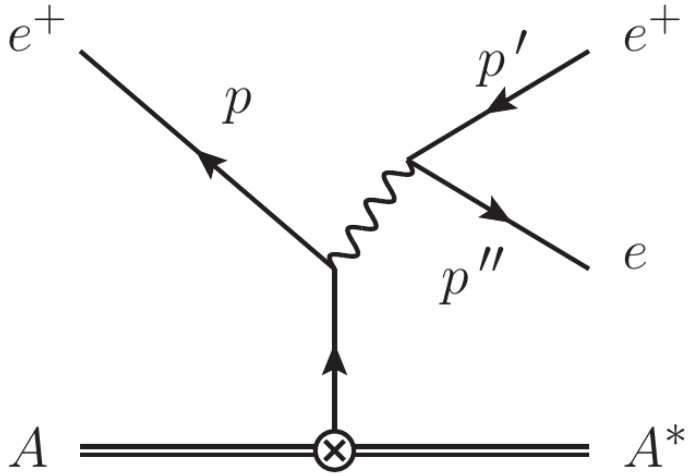
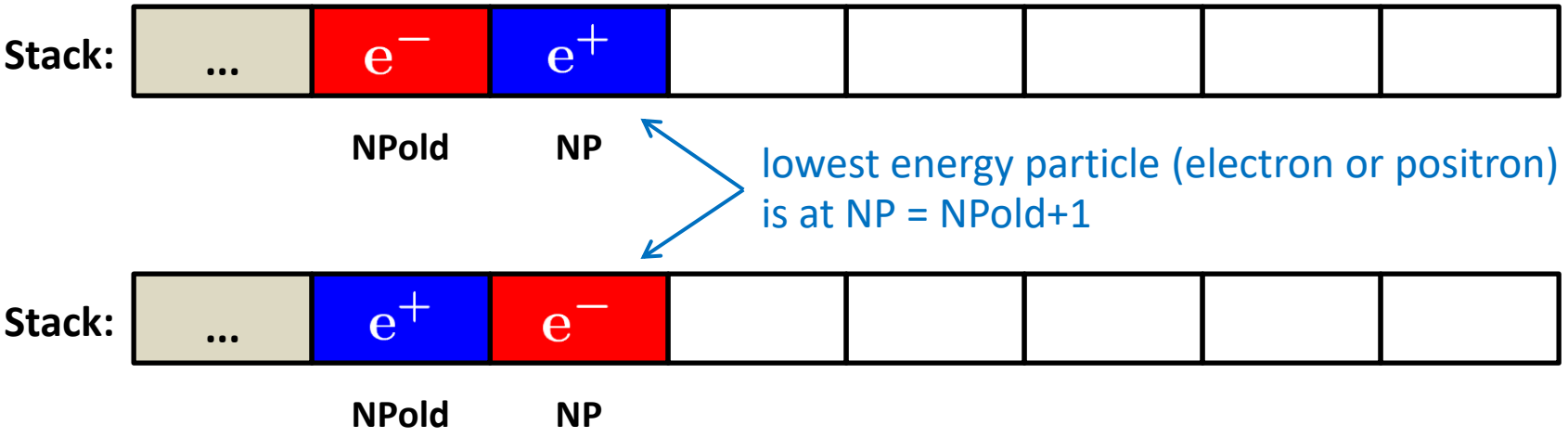


Positron inelastic collision (Bhabha scattering)

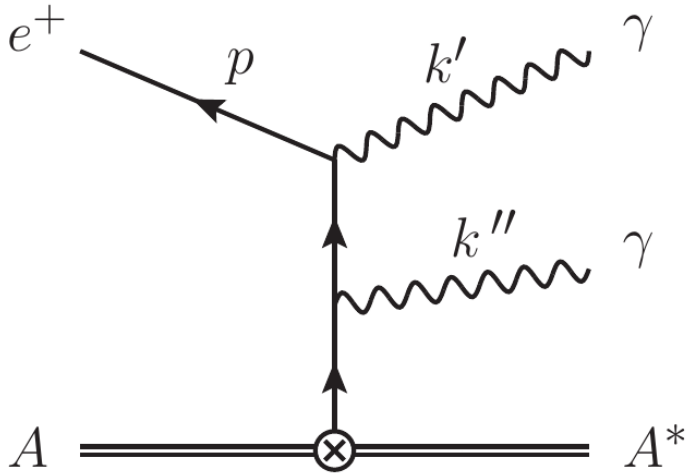
- Simulated only for $T > T_{AE}$ because particles are distinguishable.
- Generally, dominates at low and intermediate energies
- Scales as Z
- **Ignores binding**

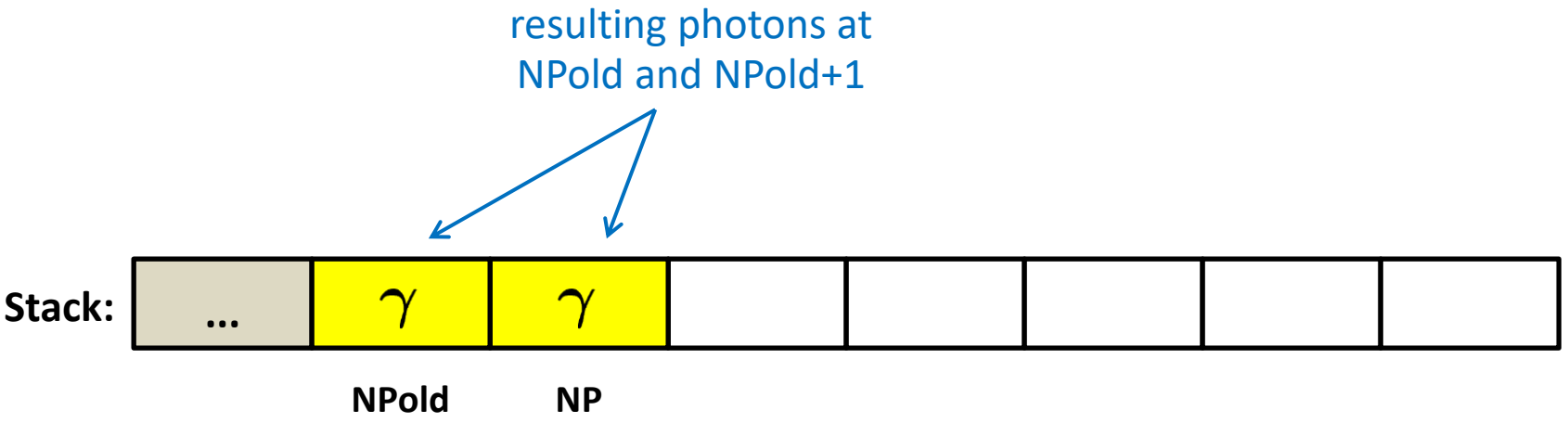




Positron annihilation

- Only two-photon annihilation is simulated, in first Born approximation.
- Two-photon annihilation is by far the dominant process.
- Important only at low energies: positrons always annihilate at rest, if not before!
- Scales as Z





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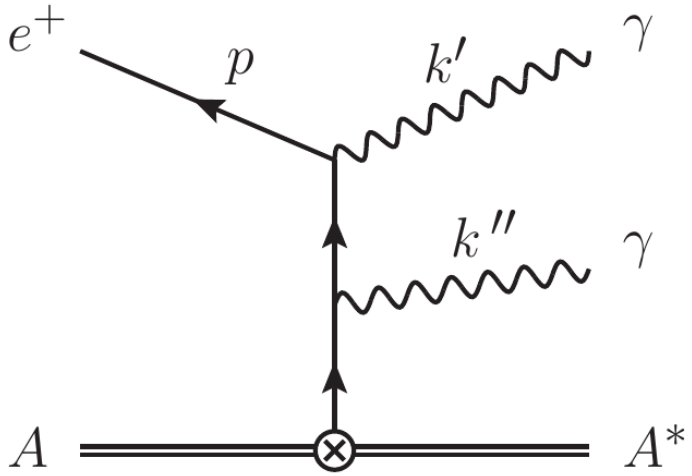
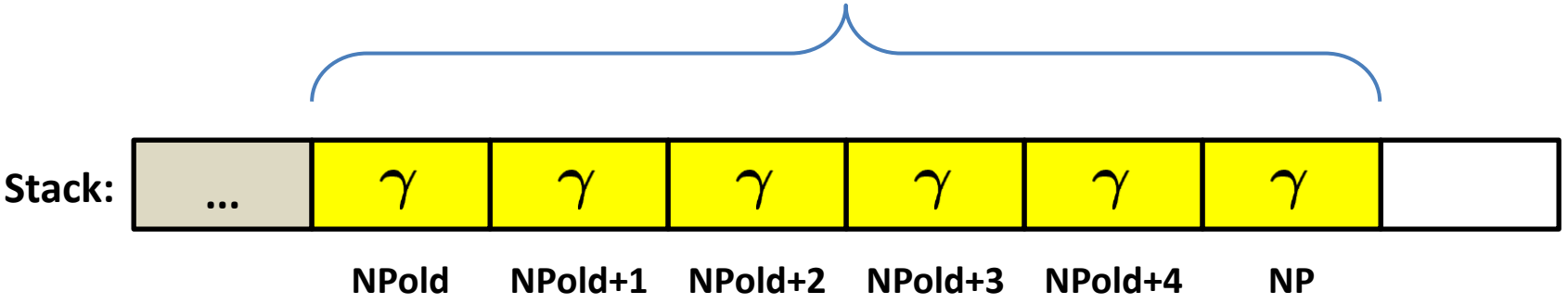
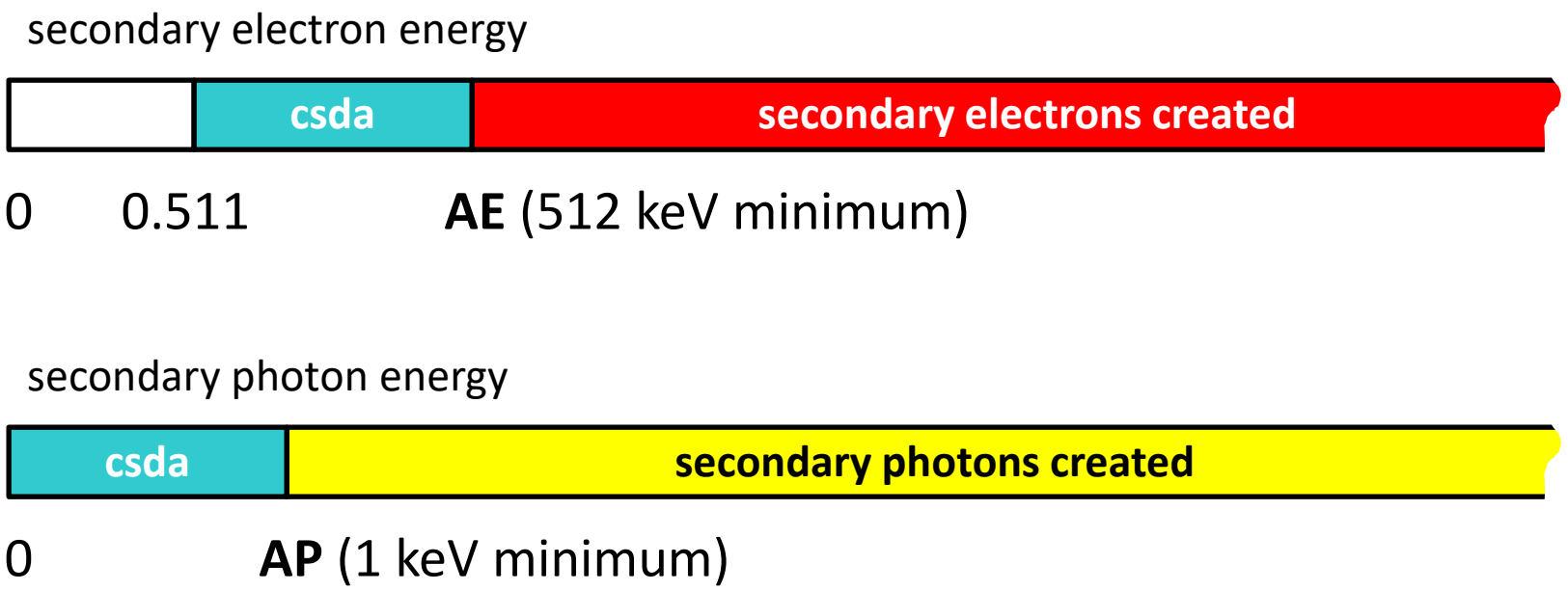


when **splitting** is used, there are `nbr_split` photon pairs on the stack



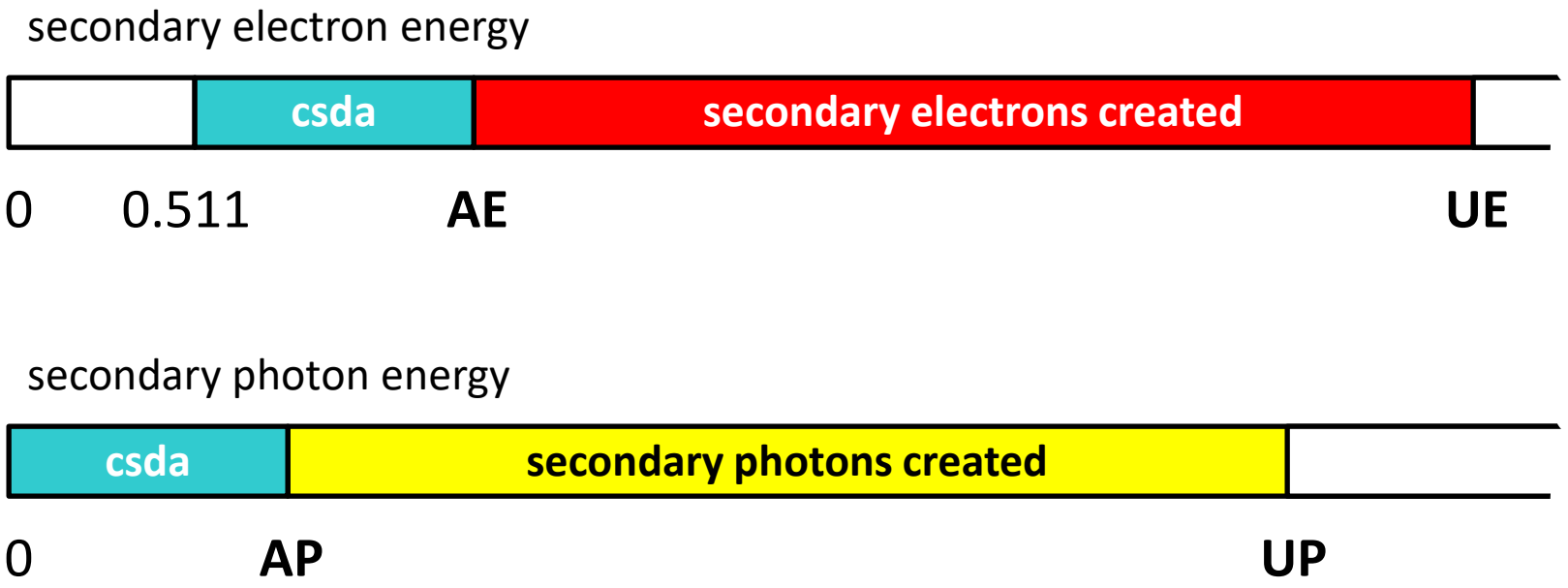
There are 3 sets of energy thresholds

1. **Lower thresholds AE and AP:** lowest energies of secondary electrons and photons. Below these energies, interactions are grouped as part of the continuous slowing down approximation.



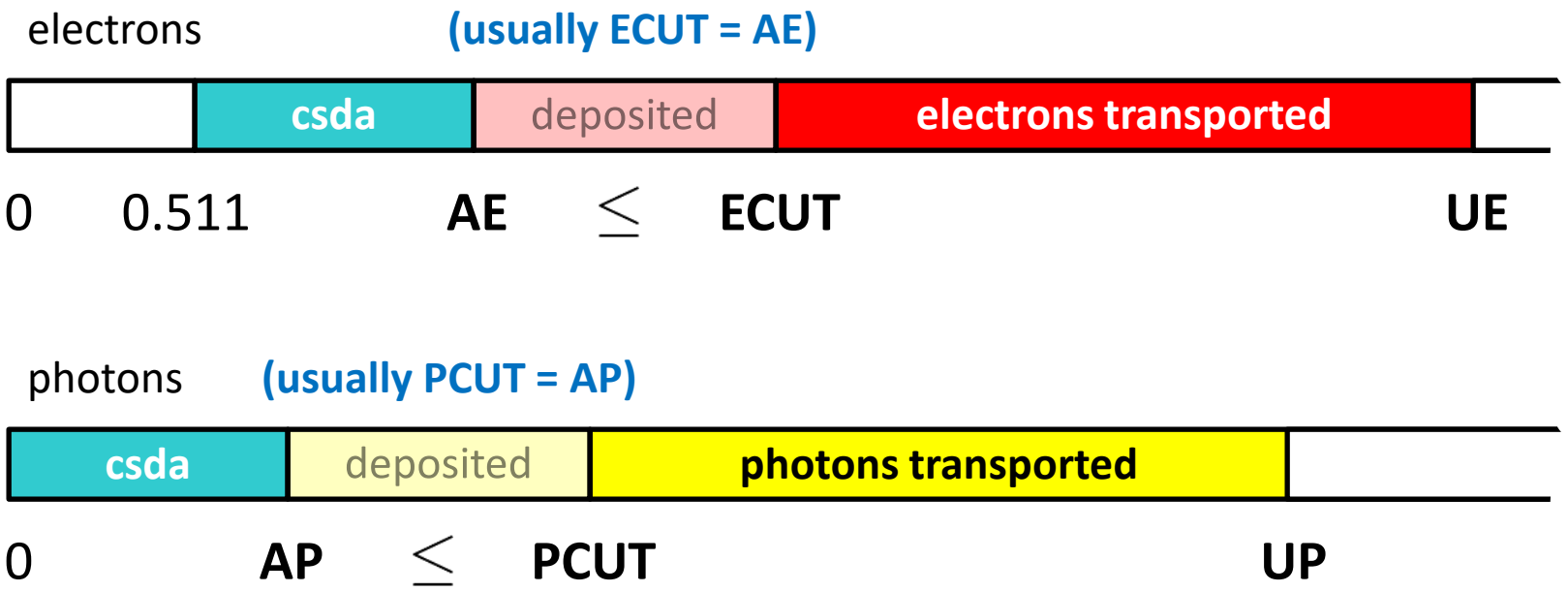
There are 3 sets of energy thresholds

2. **Upper thresholds UE and UP:** upper limit on the energy of electrons and photons (simply set those above the maximum energy of source particles).



There are 3 sets of energy thresholds

3. **Transport cutoffs ECUT and PCUT:** energy threshold below which electron and photon transport is stopped, and remaining energy is deposited locally (approximation).



Select electron transport parameters

```
:start media definition:    # or in PEGS file!

    AE = 0.521     # (MeV), minimum is 0.512
    AP = 0.010     # (MeV), minimum is 0.001
    UE = 50.511    # (MeV)
    UP = 50        # (MeV)

    # ...

:stop media definition:
```

have a large impact on simulation time

Select electron transport parameters

```
:start MC transport parameter:

    Global ECUT                    = 0.521    # AE by default (MeV)
    Global PCUT                    = 0.010    # AP by default (MeV)
```

Select electron transport parameters

```
:start MC transport parameter:

    Global ECUT                    = 0.521    # AE by default (MeV)
    Global PCUT                    = 0.010    # AP by default (MeV)

    Spin effects                   = On       # [On], Off
```

Spin effects incur a 30–100% penalty in simulation time. But it always has an impact on results (when electrons transport matters). **You must have some very strong argument to turn this off!**

Select electron transport parameters

```
:start MC transport parameter:

    Global ECUT                    = 0.521    # AE by default (MeV)
    Global PCUT                    = 0.010    # AP by default (MeV)

    Spin effects                   = On       # [On], Off
    Brems angular sampling         = KM       # [KM], Simple
    Brems cross sections           = NRC      # [BH], NIST, NRC
```

Not the default option

BH only accurate for energies above ~ 50 MeV

Select electron transport parameters

```
:start MC transport parameter:

    Global ECUT                     = 0.521    # AE by default (MeV)
    Global PCUT                     = 0.010    # AP by default (MeV)

    Spin effects                    = On       # [On], Off
    Brems angular sampling          = KM       # [KM], Simple
    Brems cross sections            = NRC      # [BH], NIST, NRC
    Electron Impact Ionization      = On       # [Off], On ...
```

Not the default option

Required for accurate characteristic X-rays

Select electron transport parameters

```
:start MC transport parameter:

    Global ECUT                     = 0.521    # AE by default (MeV)
    Global PCUT                     = 0.010    # AP by default (MeV)

    Spin effects                    = On       # [On], Off
    Brems angular sampling          = KM       # [KM], Simple
    Brems cross sections            = NRC      # [BH], NIST, NRC
    Electron Impact Ionization      = On       # [Off], On ...

    Electron-step algorithm         = EGSnrc   # [EGSnrc], PRESTA-I
    Boundary crossing algorithm     = Exact    # [Exact], PRESTA-I
    Skin depth for BCA              = 3        # [3]
    ESTEPE                          = 0.25     # [0.25]
    ximax                           = 0.5      # [0.5]

:stop MC transport parameter:
```

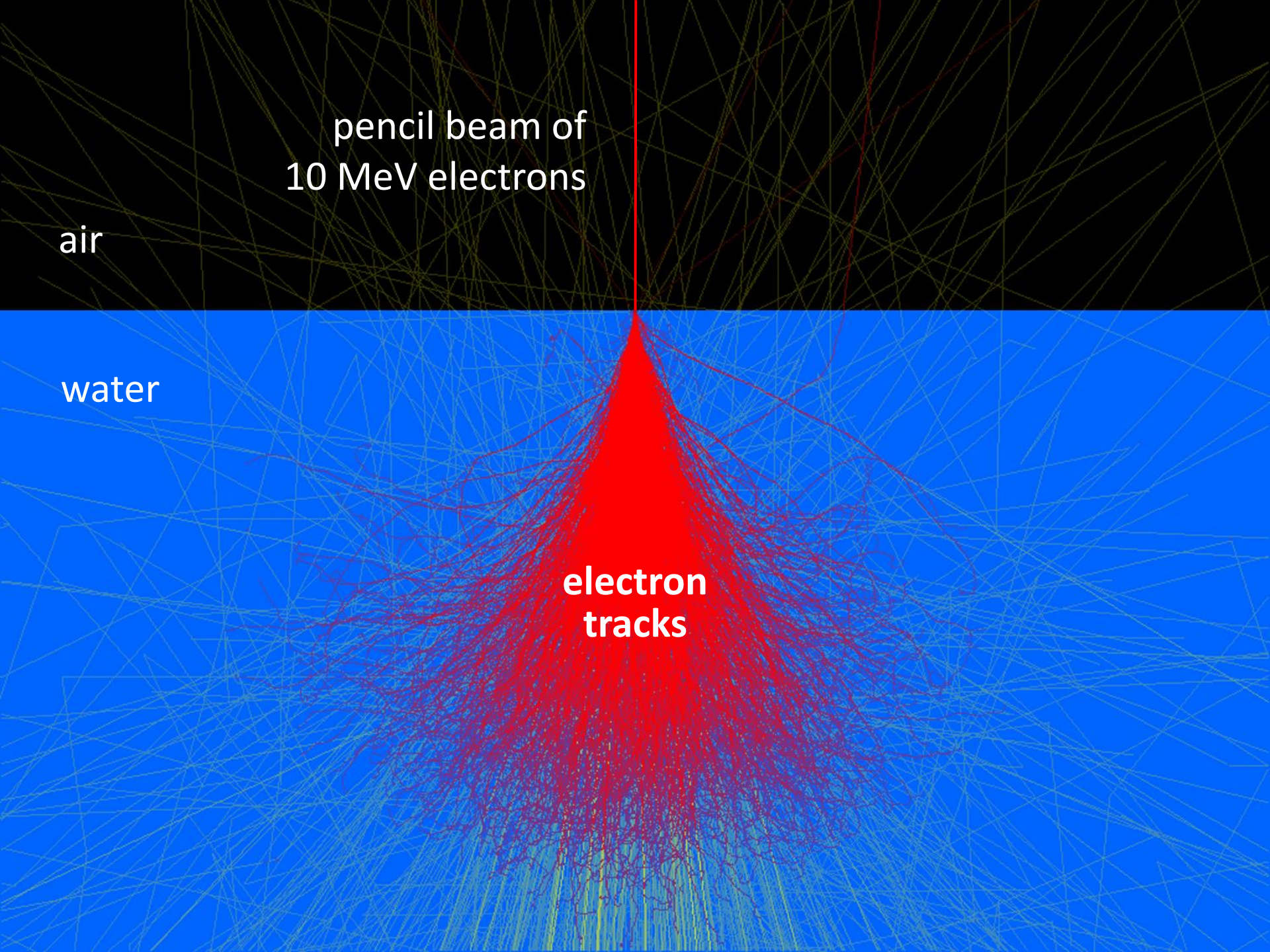
EGSnrc can model electromagnetic fields

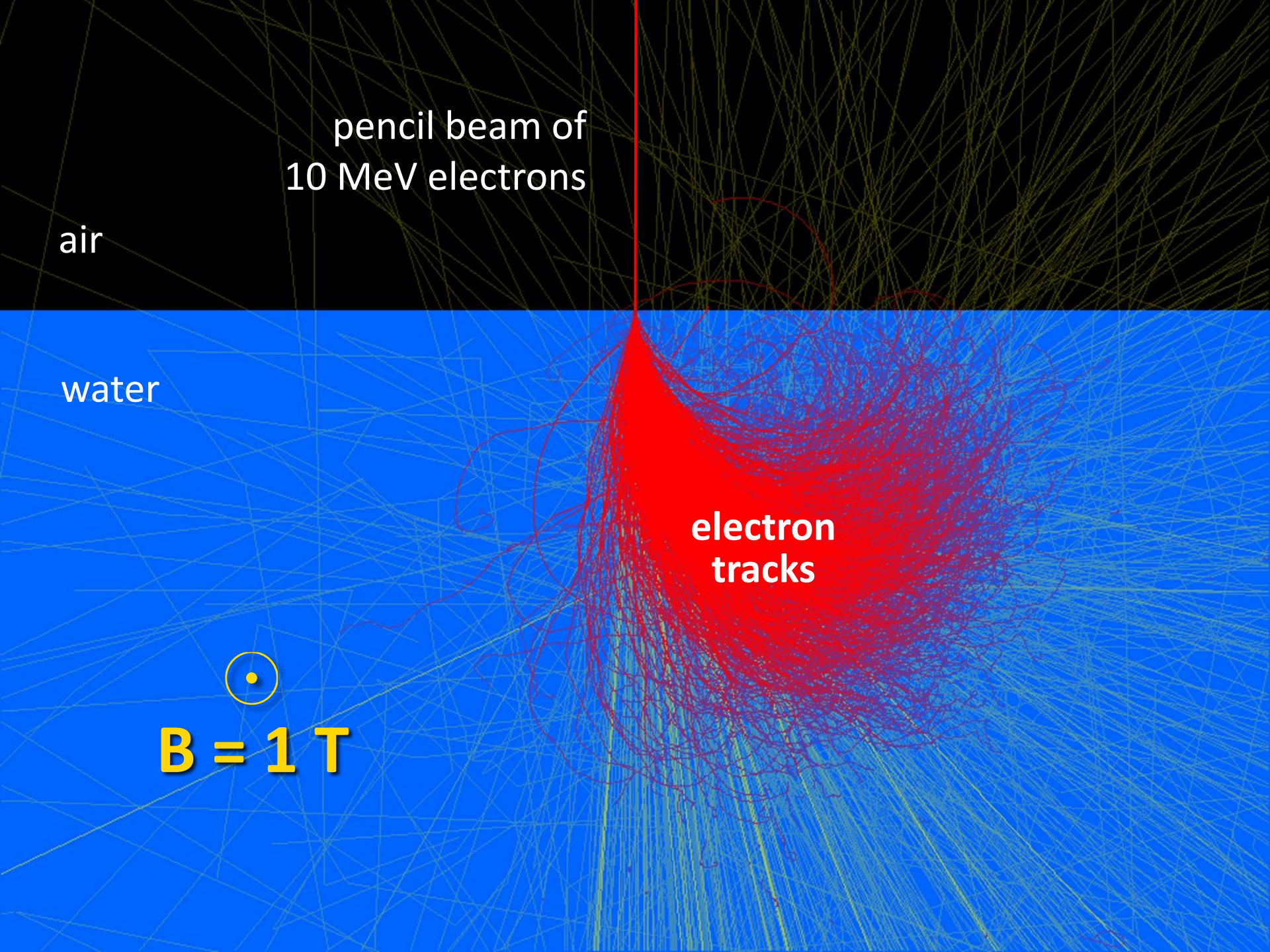
- Static magnetic and electric field components can be set by input
- Electric fields are not fully consistent (electron is discarded if its energy drops below AE upon changing direction!)
- A refined implementation has been developed by Malkov and Rogers, and will be added to EGSnrc: *Med. Phys.* **43**(7), 4447.

```
:start MC transport parameter:

    Magnetic field      = 0, 0, 0.5    # (x, y, z) components in Tesla
    Electric field      = 0, 0.1, 0    # (x, y, z) components in V/cm
    EM ESTEPE           = 0.02         # [0.02]

:stop MC transport parameter:
```


pencil beam of
10 MeV electrons
air
water
electron
tracks


pencil beam of
10 MeV electrons
air
water
electron
tracks
B = 1 T

Suggested parameter selection strategy

1. Start with the **most accurate** electron transport parameters available (defaults, except NRC brems cross section, and Eii turned on if relevant).

2. Consider **faster options** if simulation is too long; but don't turn off spin effects!

3. In most situations, proper selection of **AE**, **AP**, **ECUT** and **PCUT** proves the most critical parameters affecting simulation time.

4. **Rule of thumb:** set ECUT so that the electron range at ECUT is less than 1/3 the dimension of interest (e.g., voxel size).

5. Remember that higher thresholds imply an **approximation**, so convince yourself that your results are valid by running a representative simulation with lower thresholds. (Better yet: use range rejection and variance reduction!)

Conclusion

- Analog simulation (every single interaction) of charged particle interaction is **costly** because cross-sections are very large.
- The **condensed history technique** solves the efficiency problem, by grouping particle steps into large, statistically equivalent steps.
- EGSnrc implements a **class II scheme:** "soft" events are grouped within the restricted stopping power, while "catastrophic" events above energy thresholds AE and AP are handled explicitly.
- **Multiple-scattering** introduces new complexities due to the unknown "real" particle path: continuous energy loss, electron step algorithm, and boundary crossing algorithm.
- The thresholds **AE** and **AP**, and transport cutoffs **ECUT** and **PCUT**, have the most impact on simulation efficiency (and accuracy!)