Geant4-DNA : proximity functions – the new « microprox » extended example

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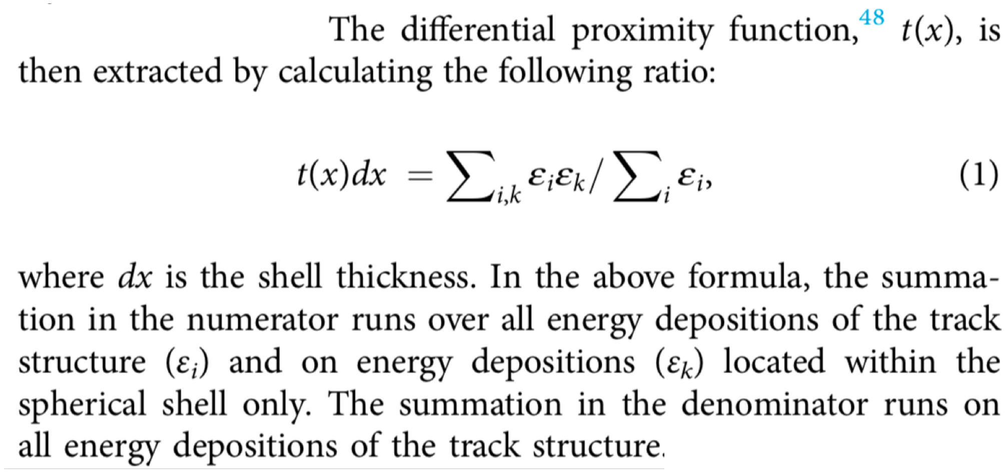
- A way to quickly estimate radiobiological effectiveness of ionising radiation
  - The example calculates proximity functions in liquid water
- Domain of microdosimetry
  - Fundamental description of energy deposition patterns can be obtained through the differential proximity functions of radiation tracks



The differential proximity function,[48] $t(x)$, is then extracted by calculating the following ratio:

$$t(x)dx = \sum\nolimits_{i,k} \varepsilon_i \varepsilon_k \Big/ \sum\nolimits_i \varepsilon_i, \qquad (1)$$

where dx is the shell thickness. In the above formula, the summation in the numerator runs over all energy depositions of the track structure (ε_i) and on energy depositions (ε_k) located within the spherical shell only. The summation in the denominator runs on all energy depositions of the track structure.

- The integral of the differential proximity function is equal to the total energy absorbed in the medium

$$\int_0^\infty t(x)dx = E_{tot},$$

Geant4-DNA : Principle of calculation of proximity functions

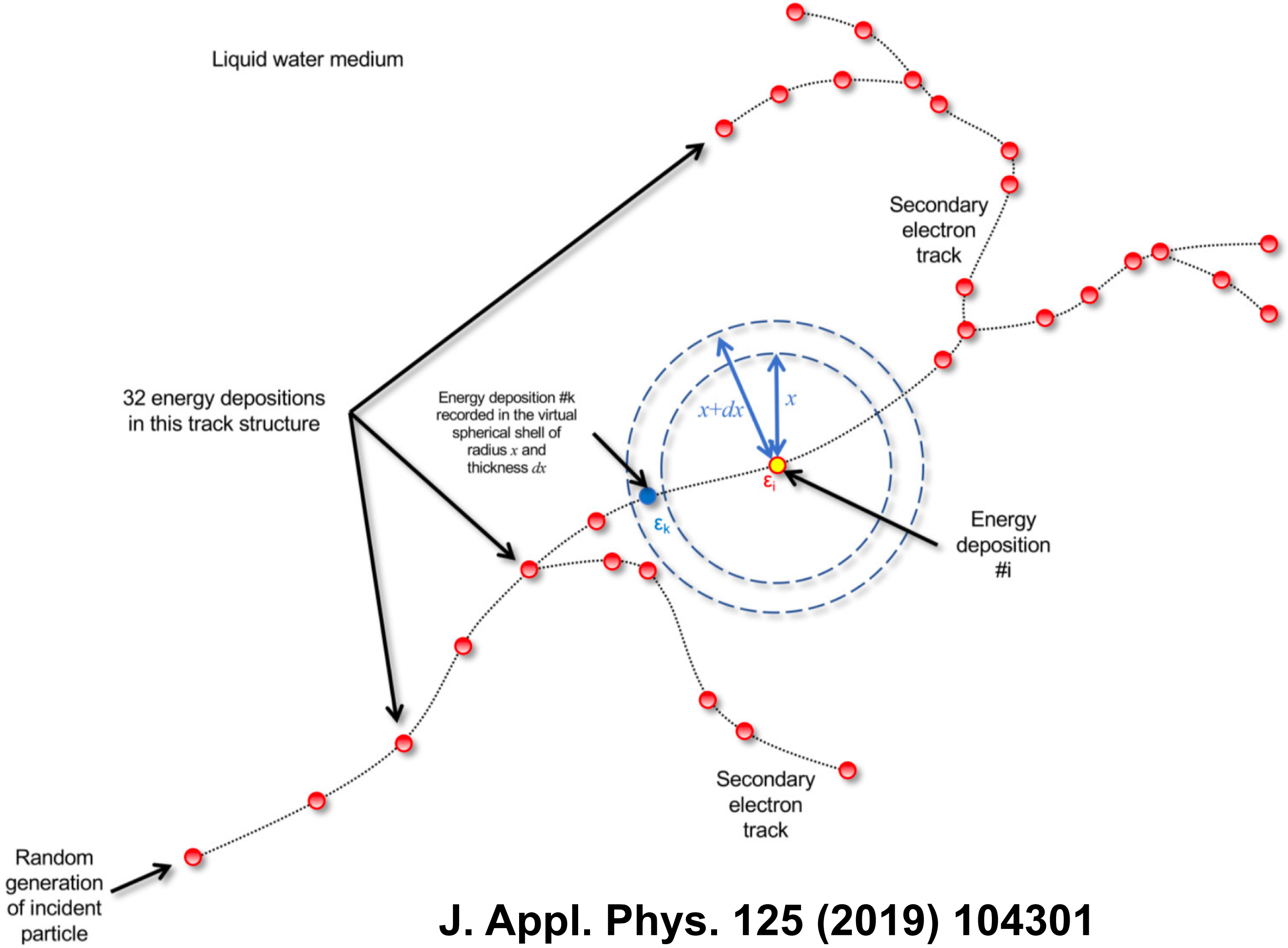


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FIG. 1. Principle of calculation of differential proximity functions $t(x)$ for the track structure of a single incident particle. The track structure illustrated in this figure contains a total of 32 energy depositions (each being represented by a red disk) induced by the incident particle and its secondaries. For each energy deposition (e.g., for energy deposition ε_i marked as a yellow disk) among these 32 depositions, the total energy absorbed in spherical shells of varying radius x and thickness dx (represented by the two blue dashed circles, where the energy deposition ε_k—in blue—is recorded) centered on this energy deposition is recorded. The same procedure is repeated over all remaining 31 energy depositions weighted by their energy value ε_i divided by the total energy deposited in the track, in order to calculate $t(x)dx$ from formula (1). The average value of $t(x)dx$ is obtained by simulating a large number of independent tracks.

Geant4-DNA : Results for the 3 Geant4-DNA Physics constructors (DNA constructors opt2, 4, 6)

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./microprox microprox.in
root plot.C
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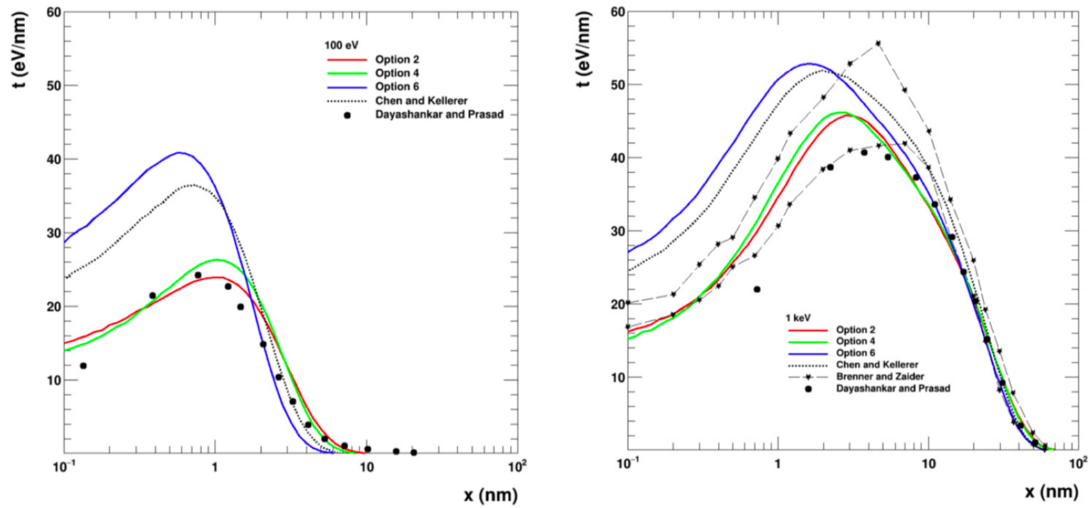

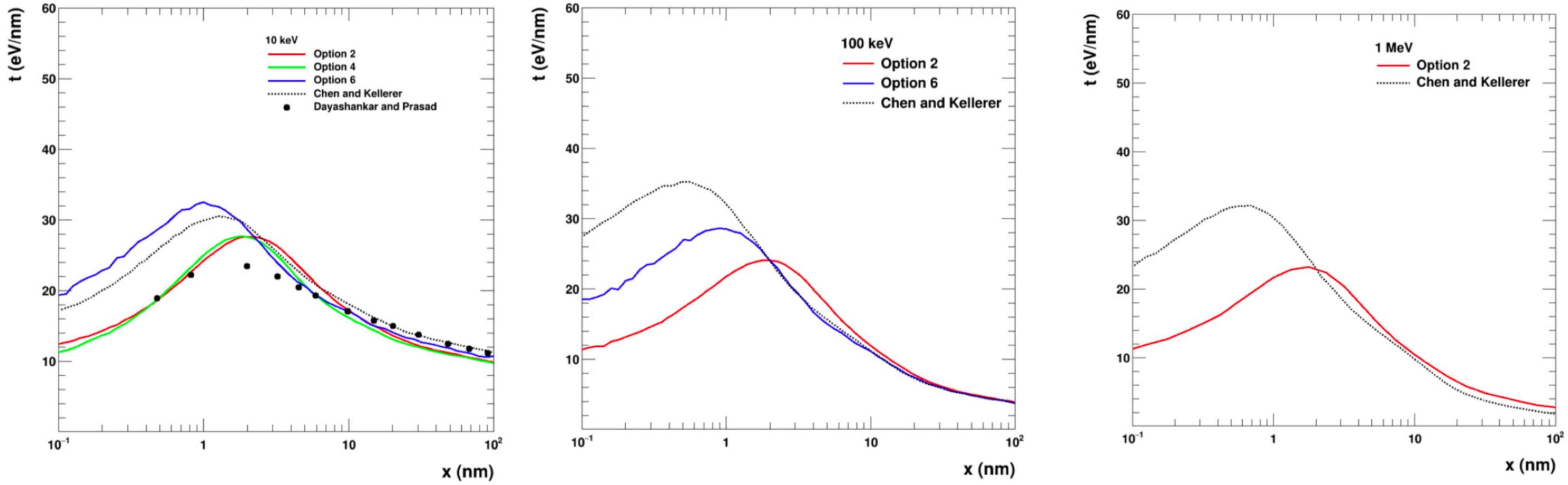

FIG. 4. (Differential) proximity functions $t(x)$ as a function of radius x for monoenergetic electrons with incident energies of 100 eV, 1 keV, 10 keV, 100 keV, and 1 MeV. For the comparison with the simulations of Chen and Kellerer[48] (black dotted line), a 12.6 eV tracking cut has been applied to all Geant4-DNA simulations. These simulations were performed using the three physics constructors "option 2" (red line), "option 4" (green line), and "option 6" (blue line). In the case of 1 keV electrons, upper and lower limits of proximity functions calculated by Brenner and Zaider[44] for the vapor phase are qualitatively shown by the black stars and the dashed lines. Finally, and for completeness, we also added the data of Dayashankar and Prasad[46] for vapor and for a 4.5 eV tracking cut (black disks).

Users can now simulate such functions with the « microprox » extended/medcal/dna example

Geant4-DNA : Biophysical implications

$$\mathrm{RBE} = \frac{\zeta_{\mathrm{test}}}{\zeta_{\mathrm{ref}}}, \qquad \zeta = \int_0^{\infty} t(x)\gamma(x)dx,$$

- γ(x) is a biological function related to the interaction probability of sublesions (separated by a distance x) to form a lesion.

- the form of γ(x) depends on both the geometrical and biological properties of the system. A commonly used form for γ(x) is that derived for V79 cells, which exhibits a rather constant value (±10%) up to about 10 nm, sharply falling (but not vanishing) at larger distances. Thus, as an application example of the present results, we can approximate γ(x) by a step function, i.e., γ(x)=1 for x≤10nm and γ(x)=0 for x>10nm.

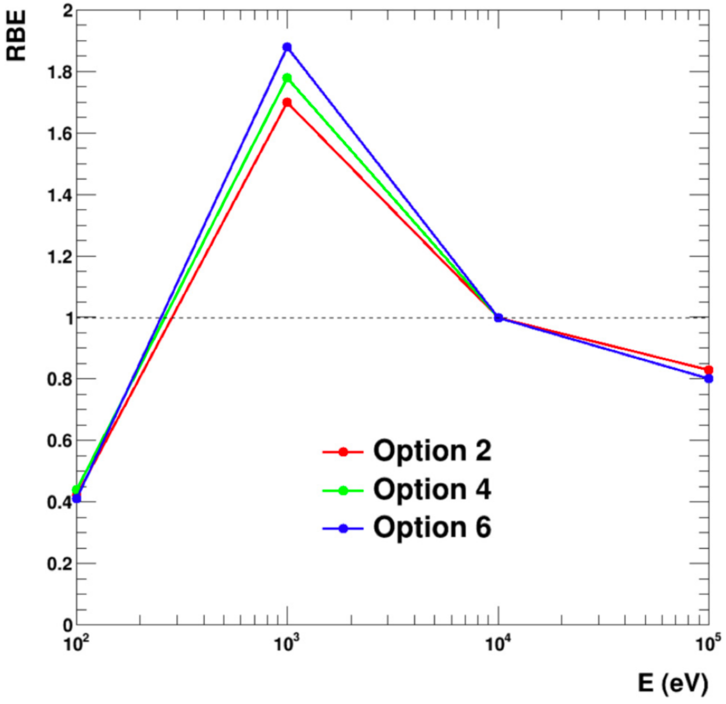

FIG. 9. RBE calculations as a function of incident kinetic energy for monoenergetic electrons with incident energies of 100 eV, 1 keV, 10 keV, and 100 keV. The "option 2" physics constructor has been used with its default tracking cut of 7.4 eV (red curves). The red, green, and blue curves show results obtained with the "option 2," "option 4," and "option 6" physics constructors, respectively. 10 keV is used as the "reference" radiation energy for the calculation of RBE (see Sec. III D for details).