Extension of the discrete electron transport capabilities of the Geant4-DNA toolkit to the radiotherapeutic regime

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Background

- Monte Carlo track-structure codes are distinguished from the conventional MC dosimetry codes by their use of discrete physics models that enable detailed simulations w/out using artificial transport steps.
- Track-structure simulations is the preferred theoretical tool for:
  - Mechanistic studies at the (sub) cellular and DNA level.
  - Microdosimetry-based predictions of RBE (and QF).

Motivation

- **There is an increasing need for extending electron track-structure simulations to high-energies (~MeV) for applications such as:**

✓ FLASH radiobiology

✓ Microdosimetry in hadron therapy (δ-ray effects)

✓ Space radiation (electrons in VA belt, δ-rays from GCR)

The challenge

- To develop a discrete physics model suitable for condensed targets (such as liquid water) that is reliable over all energies of interest (eV to MeV).
- For inelastic interactions, commonly used discrete models are limited to:
  - ✓ gaseous targets (e.g. binary-encounter atomic models) or
  - ✓ low-energies (e.g. solid-state dielectric models).

Aim of present work

- Develop a relativistic version of DNA-Option 4 inelastic model that:

✓ Improves the existing models for liquid water (DNA-Option 2 and DNA-Option 4).

✓ Extends up to 10 MeV.

Overview of Geant4-DNA EM models for liquid water medium

- **G4EmDNAPhysics_option2 models**
  - ✓ Default model
  - ✓ Available since Geant4 version 9.1 (released 2007)
  - ✓ Default energy range: 7.4 eV – 1 MeV
- **G4EmDNAPhysics_option4 models**
  - ✓ Recommended low-energy model
  - ✓ Available since Geant4 version 10.2 (released 2016)
  - ✓ Default energy range: 10 eV – 10 keV
- **G4EmDNAPhysics_option6 models**
  - ✓ Adopted from the CPA100 code
  - ✓ Available since Geant4 version 10.4 (released 2017)
  - ✓ Default energy range: 11 eV – 256 keV
  - ✓ Recently extended to include cross section for DNA constituents

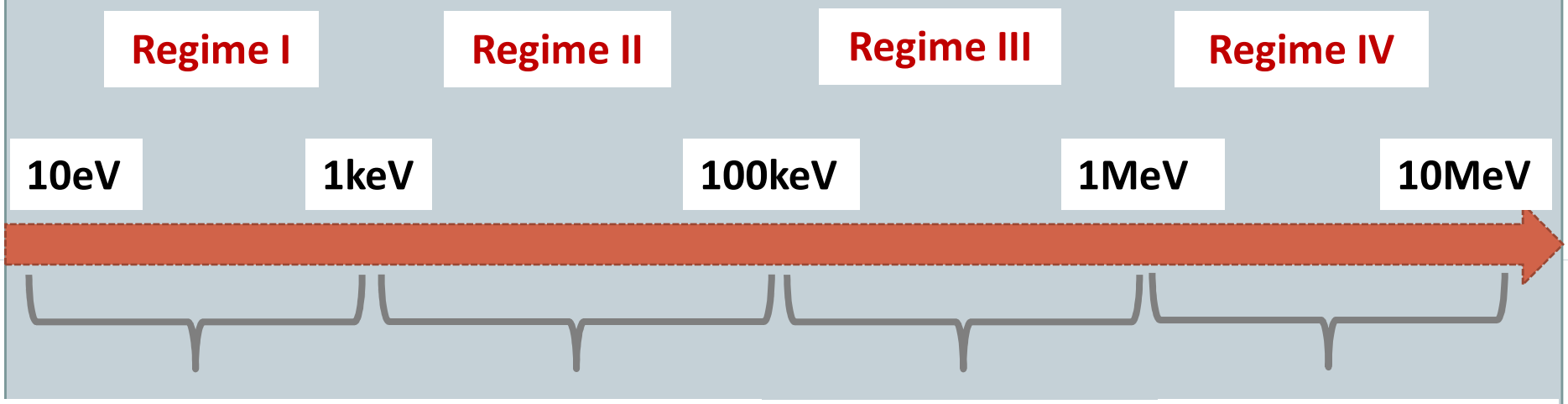
New features in Opt4Rel

i. Implementation of a new Energy-Loss-Function (ELF) using the algorithm developed at the Univ. of Ioannina.
   - ✓ Improved sum-rule consistency tests.
   - ✓ Improved parameterization of experimental data.
   - ✓ Improved high-energy asymptotic trend.

ii. More consistent implementation of low-energy Born corrections.

iii. Implementation of the Fermi density correction to the DCS (differential cross section).

Opt4Rel at a glance



CORRECTIONS:
Low-Energy Born **ON**
Relativistic Longitudinal **OFF**
Relativistic Transverse **OFF**

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Relativistic Transverse **ON**
Asymptotic correction **ON**

CORRECTIONS:
Low-Energy Born **OFF**
Relativistic Longitudinal **ON**
Relativistic Transverse **ON**
Asymptotic correction **ON**
Fermi-density correction **ON**

i. New ELF (algorithm + parameterization)

absorption channels

DNA-Option 2

$$\mathrm{Im}[\varepsilon(E,q=0)] = \sum_{n/k} \mathrm{Im}[\varepsilon_{n/k}(E,q=0)] = \sum_{n/k} \mathrm{Im}[\varepsilon^{(\mathrm{mod})}_{n/k}(E,q=0)]$$

DNA-Option 4

Energy-Loss-Function (ELF)

$$\mathrm{Im}\left[-\frac{1}{\varepsilon(E,q)}\right] = \frac{\mathrm{Im}[\varepsilon(E,q)]}{\mathrm{Re}[\varepsilon(E,q)]^2 + \mathrm{Im}[\varepsilon(E,q)]^2}$$

- ***The algorithm permits a <u>sum-rule constrained</u> overlap of ionizations and excitation absorption spectra and it offers <u>greater fitting flexibility</u> near shell binding energies.***

Univ. of Ioannina algorithm

- For ionizations,

$$\mathrm{Im}[\varepsilon_n^{(\mathrm{mod})}(E)] = \{\mathrm{Im}[\varepsilon_n(E)] + S_n + S_{>n} + C_{>n}\}\, C_n, \quad \text{(A1)}$$

where

$$C_n = \mathrm{H}(E - B_n), \quad \text{(A2)}$$

$$C_{>n} = \sum_{j=n+1}^{n_{\max}} \mathrm{Im}[\varepsilon_j(E)]\,\Theta(B_j - E) \times \left(\frac{\mathrm{Im}[\varepsilon_n(E)]}{\sum_{i=1}^{j-1}\mathrm{Im}[\varepsilon_i(E)]\,\mathrm{H}(E - B_i)}\right), \quad \text{(A3)}$$

$$S_{>n} = \sum_{j=n+1}^{n_{\max}} \mathrm{Im}[\varepsilon_j(B_j)]\exp(B_j - E)\,\mathrm{H}(E - B_j) \times \left(\frac{\mathrm{Im}[\varepsilon_n(E)]}{\sum_{i=1}^{j-1}\mathrm{Im}[\varepsilon_i(E)]}\right), \quad \text{(A4)}$$

$$S_n = -\mathrm{Im}[\varepsilon_n(B_n)]\exp(B_n - E). \quad \text{(A5)}$$

- For excitations,

$$\mathrm{Im}[\varepsilon_k^{(\mathrm{mod})}(E)] = \{\mathrm{Im}[\varepsilon_k(E)] + S_{n=1} + C_n\}\, C_k, \quad \text{(A6)}$$

where

$$C_k = \Theta(E - B_{\mathrm{gap}}), \quad \text{(A7)}$$

$$C_n = \sum_{n=1}^{n_{\max}} \mathrm{Im}[\varepsilon_n(E)]\,\Theta(B_1 - E) \times \left(\frac{\mathrm{Im}[\varepsilon_k(E)]\,\Theta(B_1 - E_k)}{\sum_{j=1}^{k_{\max}}\mathrm{Im}[\varepsilon_j(E)]\,\Theta(B_1 - E_j)}\right), \quad \text{(A8)}$$

$$S_{n=1} = \mathrm{Im}[\varepsilon_{n=1}(B_1)]\exp(B_1 - E)\,H(E - B_1) \times \left(\frac{\mathrm{Im}[\varepsilon_k(E)]}{\sum_{j=1}^{k_{\max}}\mathrm{Im}[\varepsilon_j(E)]}\right), \quad \text{(A9)}$$

where $\Theta(\ldots)$ and $H(\ldots)$ are unit step functions with $\Theta(0) = 1$ and $H(0) = 0$.

Sum-rule tests

The sum-rules test the "internal" consistency of the dielectric model

f-sum-rule

$$\frac{2}{\pi E_p^2}\int_0^\infty E\ \mathrm{Im}[\varepsilon(E,0)]\ \mathrm{d}E = 1$$

Tests the absorption spectrum

ELF-sum-rule

$$\frac{2}{\pi E_p^2}\int_0^\infty E\ \mathrm{Im}[-1/\varepsilon(E,0)]\ \mathrm{d}E = 1$$

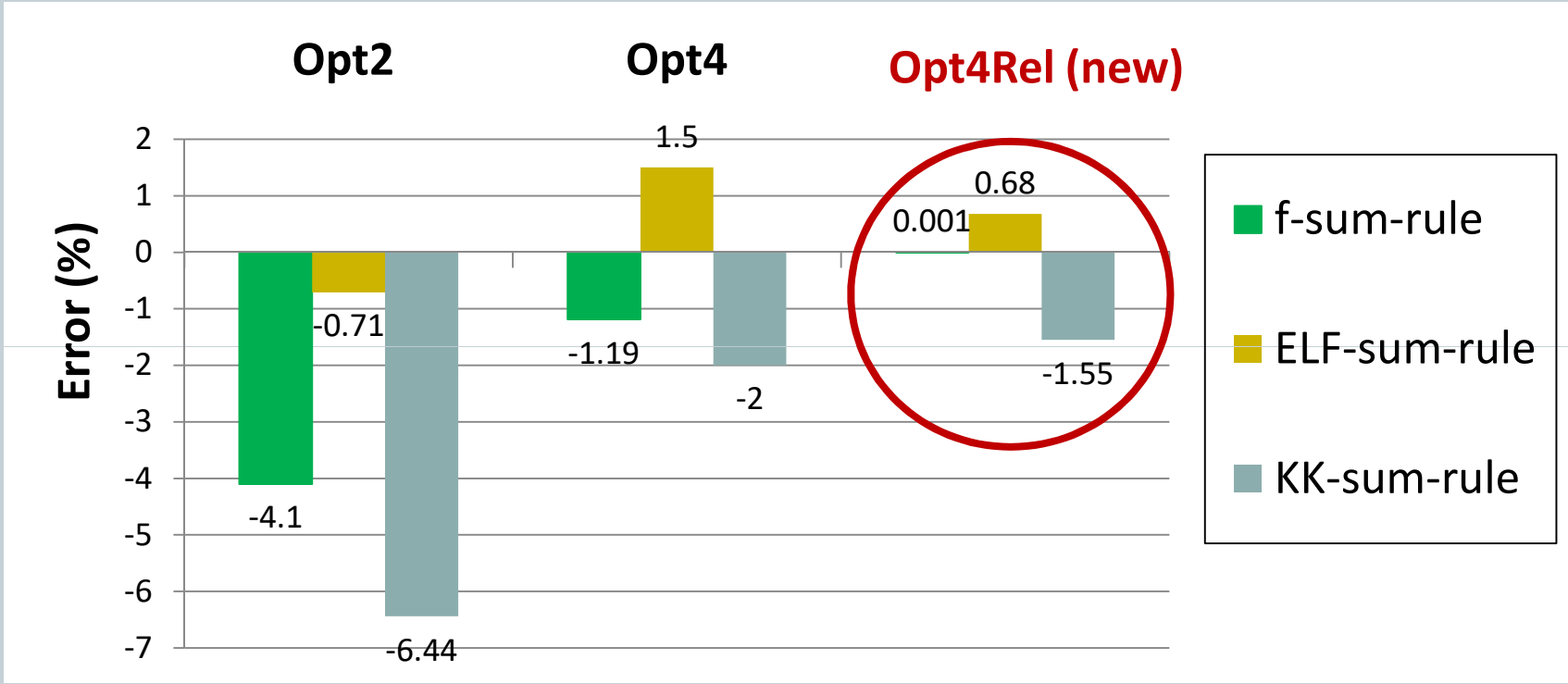
Tests the ELF at intermediate- and high-E

KK-sum-rule

$$\frac{2}{\pi}\int_0^\infty \frac{1}{E}\ \mathrm{Im}[-1/\varepsilon(E,0)]\ \mathrm{d}E + \mathrm{Re}[1/\varepsilon(0,0)] = 1$$

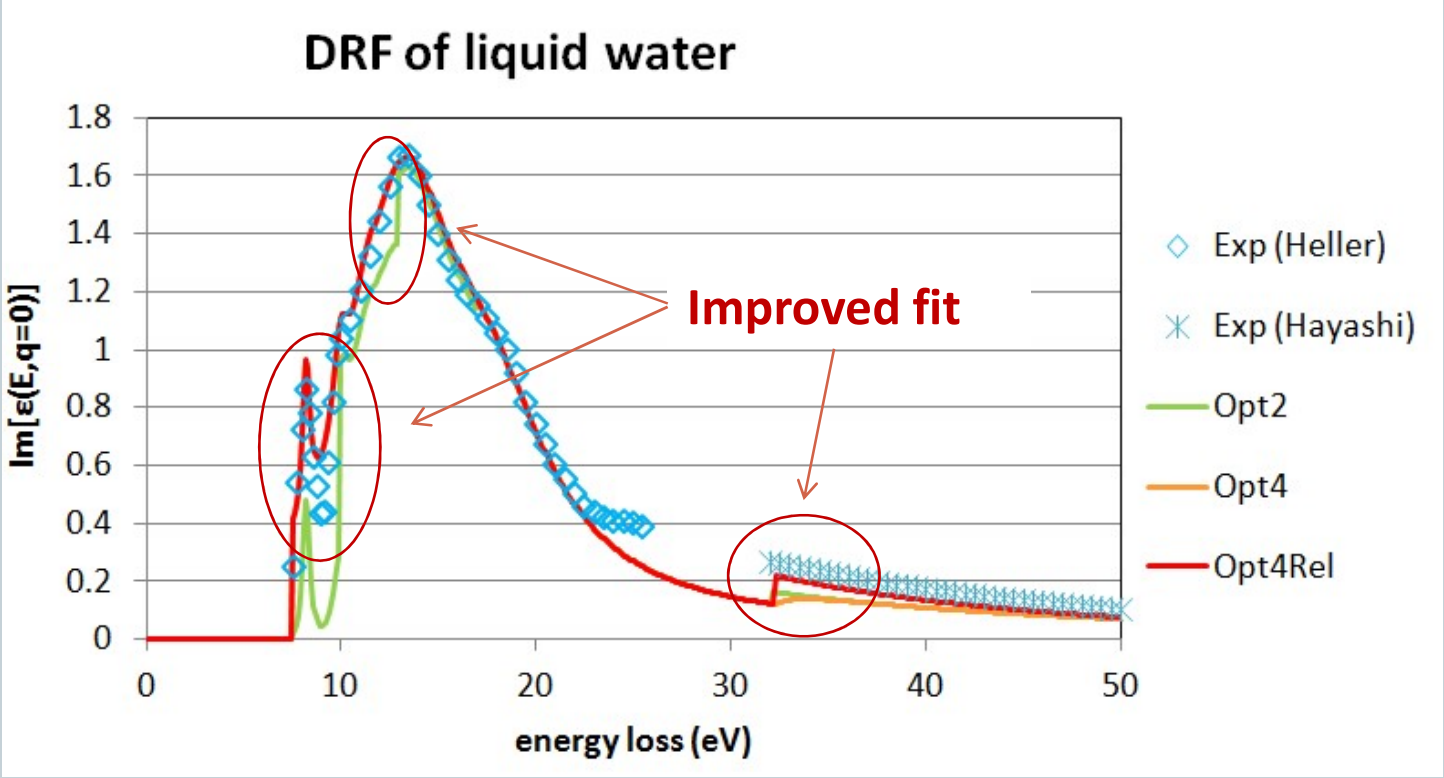
Tests the ELF at low-E (screening)

Improved sum-rule consistency tests



The new model (Opt4Rel) improves <u>all</u> sum rules compared to the existing (Opt2 and Opt4) models.

Improved experimental data representation



The new model (Opt4Rel) improves the representation of the experimental data compared to the existing (Opt2, Opt4) models.

Improved high-energy asymptotic trend

- Drude-based ELF models (including DNA-Option 2) overestimate CS and SP at high energies (>>keV) because of the wrong asymptotic trend ($1/E^3$ instead of $1/E^{4.5}$).
- ***An ad hoc high-energy asymptotic correction to the ELF is applied above 100 keV.***

ii. New low-energy Born corrections

The following corrections are applied to the PWBA

Exchange correction

$$\sigma^{(n)}_{\text{Born–EX}}(T) = \sigma^{(n)}_{\text{Born}}(T) + \sigma^{(n)}_{\text{EX}}(T).$$

Mott-exchange

$$\frac{d\sigma^{(n)}_{\text{EX}}(E)}{dE} = \frac{d\sigma^{(n)}_{\text{Born}}(T - E + B_n)}{dE} - \sqrt{\frac{d\sigma^{(n)}_{\text{Born}}(E)}{dE} \times \frac{d\sigma^{(n)}_{\text{Born}}(T - E + B_n)}{dE}}.$$

Exchange-Coulomb correction

$$\sigma^{(n)}_{\text{Born–EX–CO}}(T) = \sigma^{(n)}_{\text{Born–EX}}(T + B_n + U_n) = \sigma^{(n)}_{\text{Born}}(T + B_n + U_n) + \sigma^{(n)}_{\text{EX}}(T + B_n + U_n)$$

U_n: Average KE in the *n*-th shell

New implementation

Proper kinematic arguments (not considered in the default Opt2)

iii. Implementation of the Fermi density effect in the inelastic cross sections

- **Non-negligible contribution to CS and SP above 1 MeV.**
- Affects only transverse interactions.
- We use the optical approximation to calculate the correction to the DCS (Fernandez-Varea et al.):

optical-ELF

$$\frac{d\,\Delta\sigma_T^{(j)}}{dE} \cong -\frac{1}{\pi\alpha_0 N\beta^2 mc^2}\frac{\varepsilon_2^{(j)}(E,0)}{\left|\varepsilon(E,0)\right|^2}\delta_F$$

δ_F is calculated from the Sternheimer model with parameters for liquid water medium.

Medium-specific DCS based on the ELF

$$\frac{d\sigma_{total}^{(j)}(E;T)}{dE} = \left.\frac{d\sigma_{L}^{(j)}(E;T)}{dE}\right|_{RPWBA} + \left.\frac{d\sigma_{T}^{(j)}(E;T)}{dE}\right|_{RPWBA} + \left.\frac{d\sigma_{L}^{(j)}(E;T)}{dE}\right|_{RPWBA\text{-}Ex\text{-}Co}$$

$$\left.\frac{d\sigma_{L}^{(j)}(E;T)}{dE}\right|_{RPWBA} = \frac{1}{\pi\alpha_0 N mc^2\beta^2}\int_{Q_{min}}^{Q_{max}}\left[\frac{\varepsilon_2^{(j)}(E,Q)}{|\varepsilon(E,Q)|^2}\right]\frac{1+Q/mc^2}{Q(1+Q/2mc^2)}dQ$$

New ELF

$$\left.\frac{d\sigma_{T}^{(j)}(E;T)}{dE}\right|_{RPWBA} = \frac{1}{\pi\alpha_0 N mc^2\beta^2}\left[\frac{\varepsilon_2^{(j)}(E,0)}{|\varepsilon(E,0)|^2}\right]\left[\ln\left(\frac{1}{1-\beta^2}\right) - \beta^2 - \delta_F\right]$$

New ELF

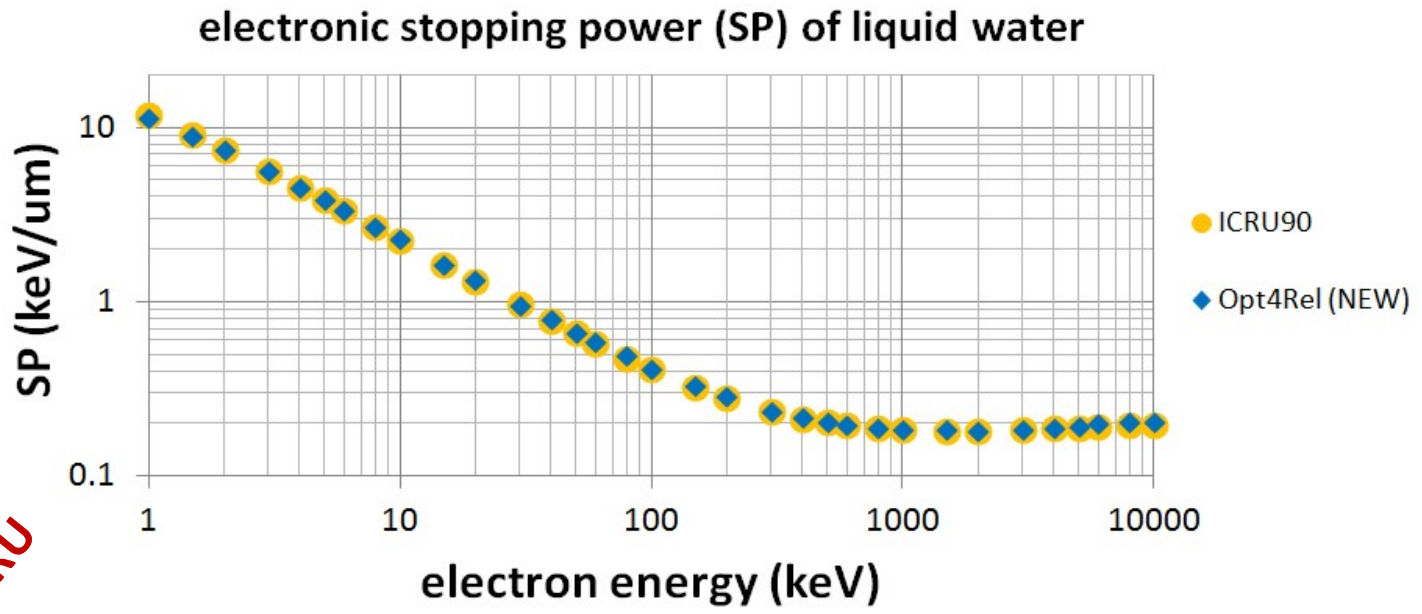
Fermi density effect

$$\left.\frac{d\sigma_{L}^{(j)}(E;T)}{dE}\right|_{RPWBA\text{-}Ex\text{-}Co} = \frac{d\sigma_{L}^{(j)}(T-E+B_n;T+B_n+U_n)}{dE} - \sqrt{\frac{d\sigma_{L}^{(j)}(T;T+B_n+U_n)}{dE}\times\frac{d\sigma_{L}^{(j)}(T-E+B_n;T+B_n+U_n)}{dE}}$$

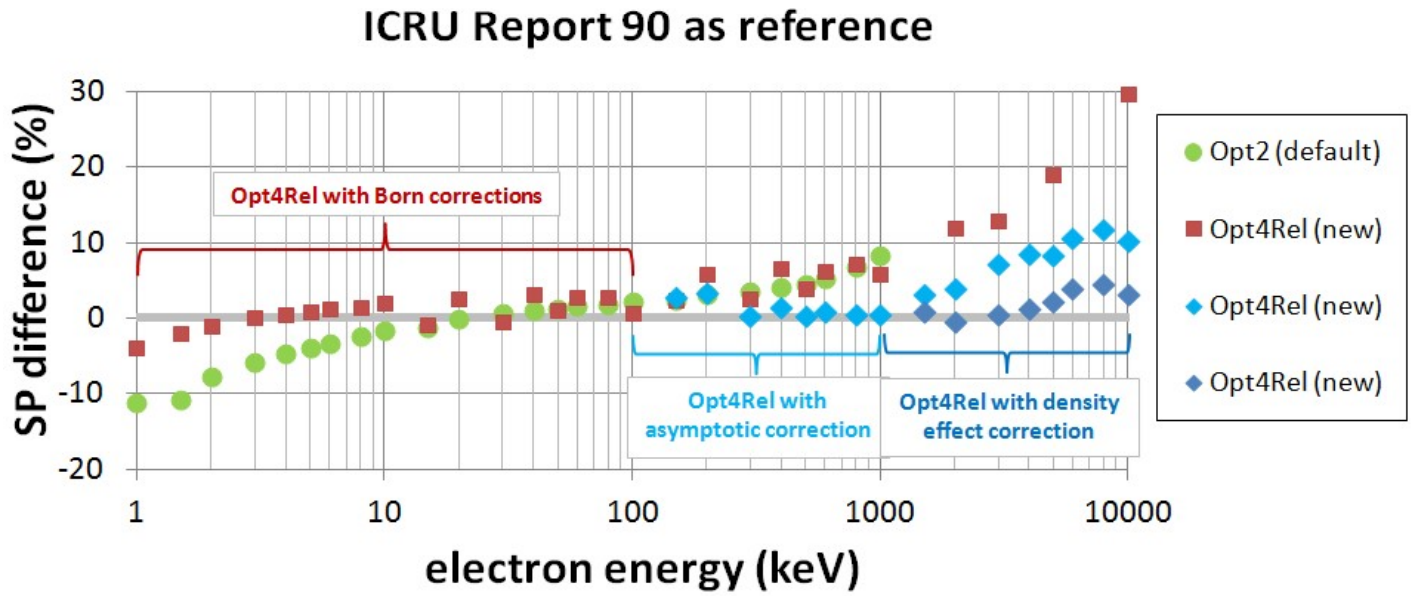
New formulation

Benchmarking Simulations

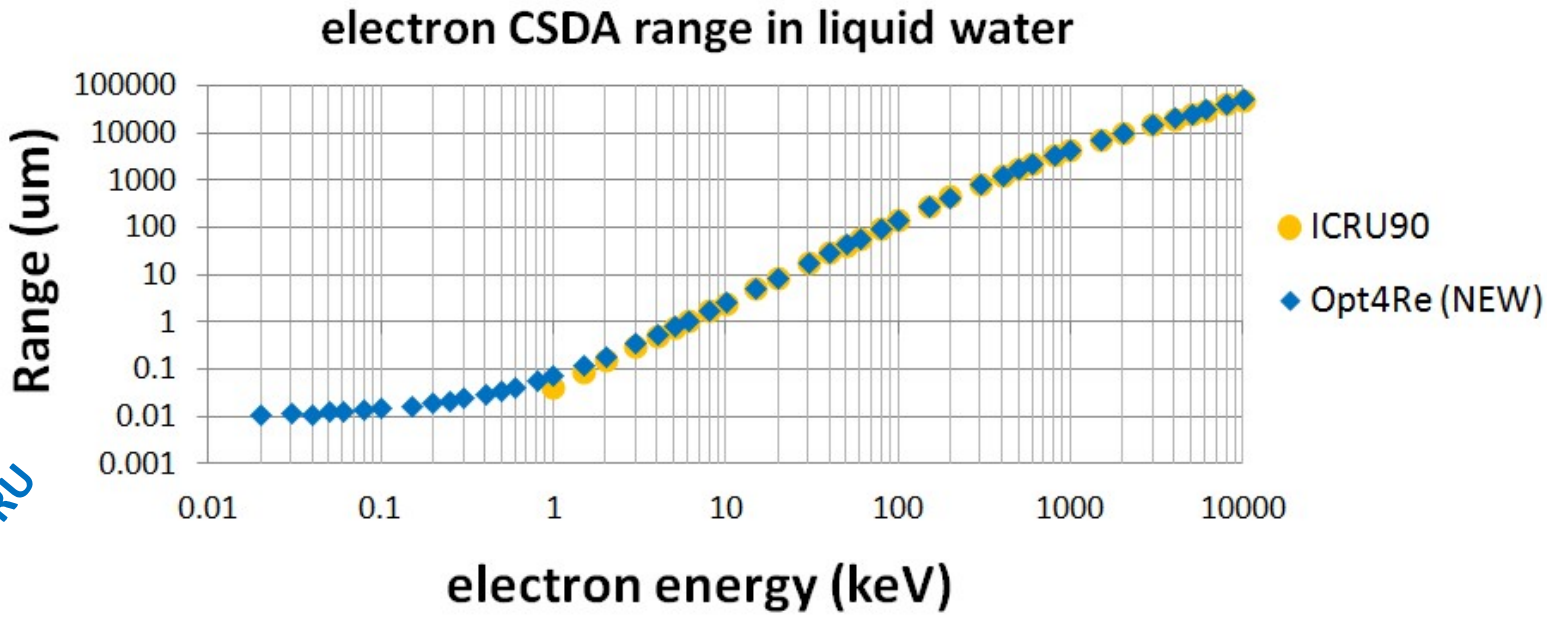
- ✓ Stopping power (spower)
- ✓ Range (range)
- ✓ DPK (TestEm12)
- ✓ Lineal Energy (microyz)



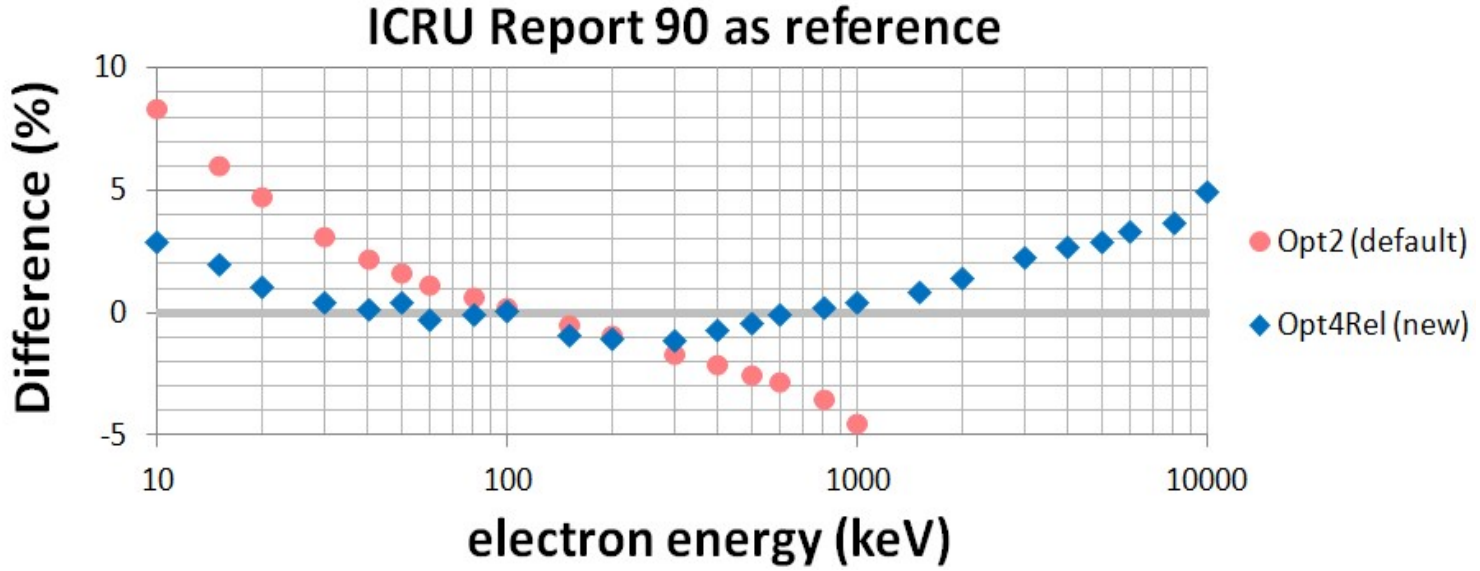
New model within 5% from ICRU



Default model within 10% from ICRU

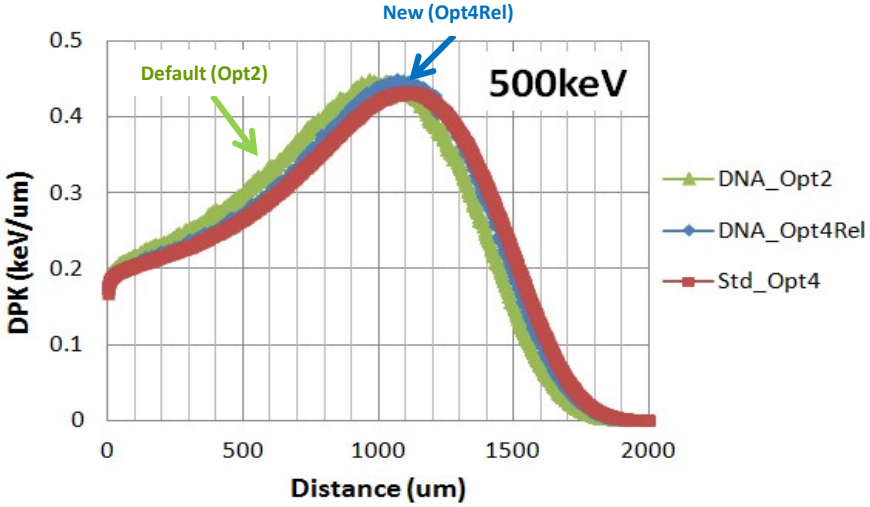


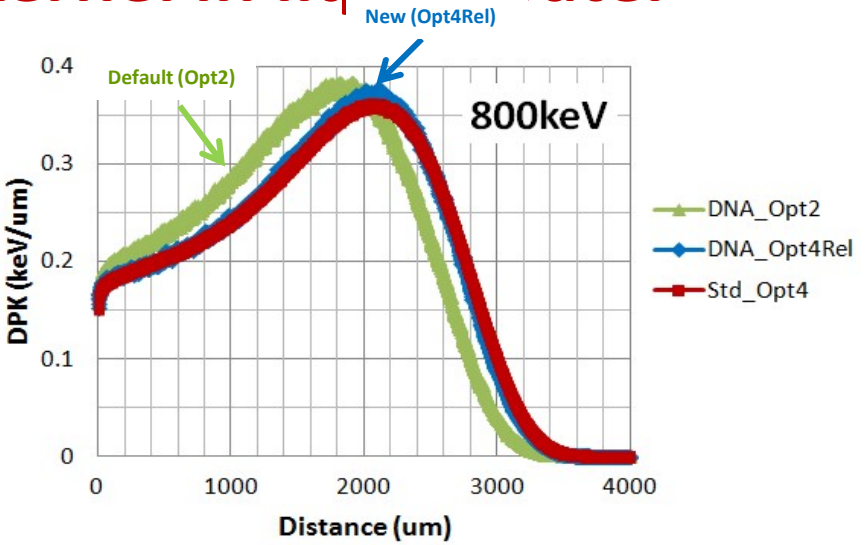
New model within 5% from ICRU

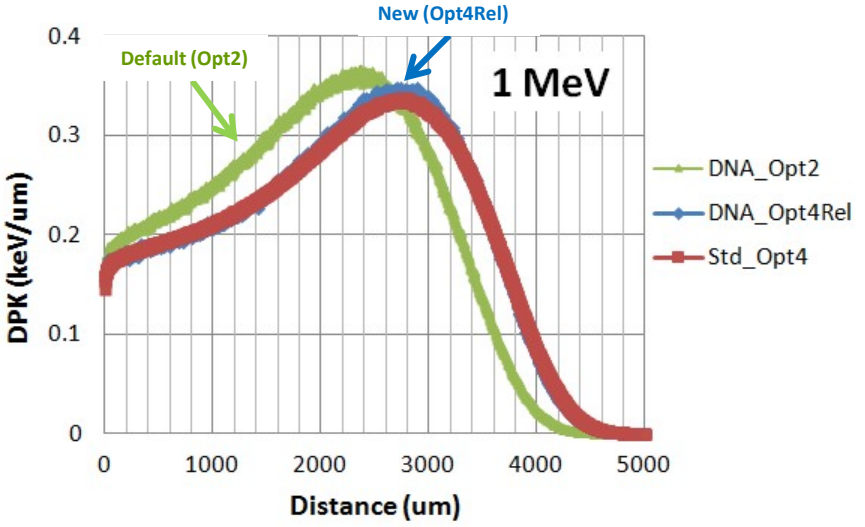


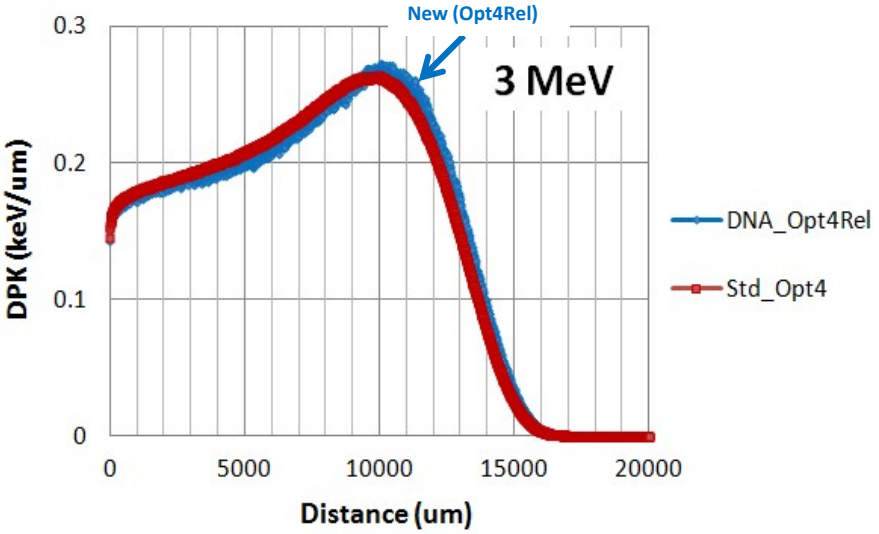
Default model within 8% from ICRU

Electron dose point kernel in liquid water



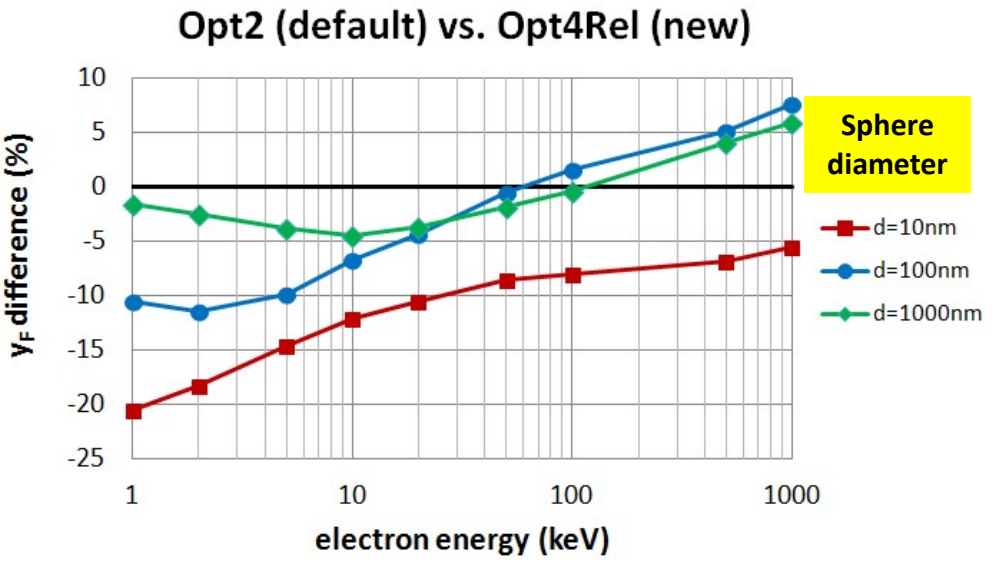


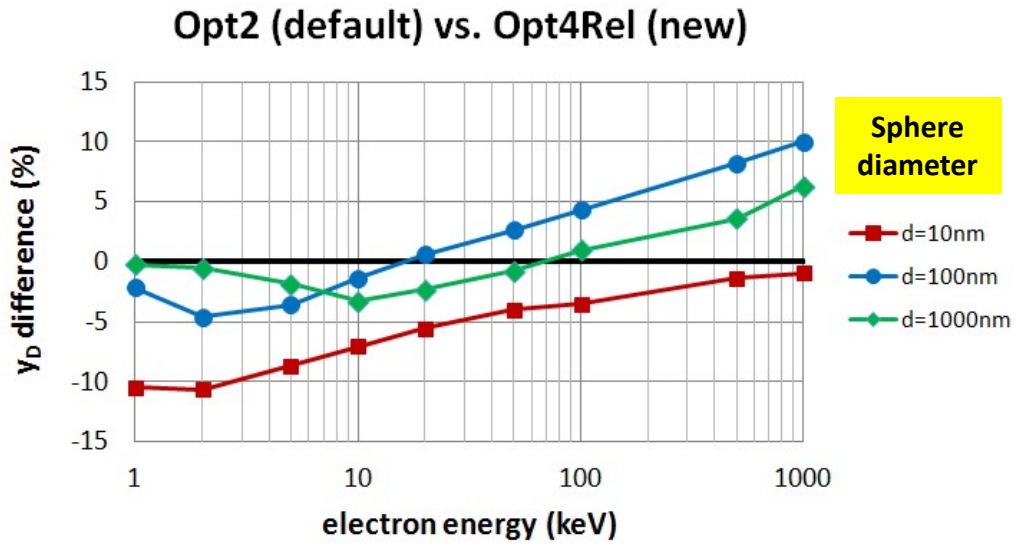




✓ **The new model (DNA-Opt4Rel) is in good agreement with StdOpt4 at high energies (>500 keV) contrary to the default DNA-Opt2.**

Electron lineal energy in liquid water





- Maximum differences between the default (Opt2) and the new model (Opt4Rel) depend on sphere size:

✓ 5% for the 1µm sphere

✓ 10% for the 100nm sphere

✓ 20% for the 10nm sphere

Summary of Results

- The new model:
  - ✓ Reduces sum-rule errors below 1.5% (default model 6.5%).
  - ✓ Improves the fit to the experimental dielectric data.
  - ✓ Reduces the differences from ICRU SP and Range data below ~5% (default model ~10%).
  - ✓ Calculates DPK in good agreement with StdOpt4 at high-energies (contrary to the default model).
  - ✓ Differs from the default model for mean values of microdosimetry quantities by 5-20% (or more).

Conclusion

- The DNA-Opt4 model has been improved and extended up to 10 MeV.
- This development extends Geant4-DNA electron track-structure capabilities from its current 1 MeV upper limit to 10 MeV.
- The new model (DNA-Opt4Rel) uses the same methodology as the existing Geant4-DNA dielectric models (Opt2, Opt4) but employs (i) an improved ELF for liquid water, (ii) a more consistent implementation of low-energy Born corrections, and (iii) various relativistic corrections.

Future

- Perform a systematic comparisons with StdOpt4 up to 10 MeV (now up to 3 MeV).
  - To validate the ELF asymptotic correction and the density effect implementation.
- Revise the ELF parameterization according to more recent experimental dielectric data for liquid water.
  - e.g. adopt the ECN model (used by KURBUC code) ?
- Correct the ELF for exchange-correlation effects.
  - e.g. implement many-body local-field-corrections (LFC) ?

☆ *The last two are expected to have a strong influence on very-low-energy (sub-100eV) electron transport.*

Acknowledgement

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  - European Space Agency (ESA)
  - Institut de radiophysique, CHUV, Lausanne

Thank you!