Assessing Microdosimetric Uncertainties in Monte Carlo Simulations Due to Quantum Effects in Low-Energy Electron Transport

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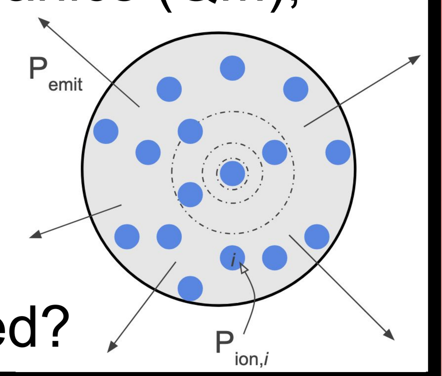
Background

- Monte Carlo (MC) is trustworthy above ~1 keV
- For nanoscale studies of e.g. DNA damage counts, low-energy electrons (~10 eV) are important
- By comparing MC to Quantum Mechanics (QM), studies[1,2,3] have shown bias in the number of scattering events per volume. But only **without** energy loss. Does this trend continue when energy-loss mechanisms are included?



Purpose

To add an energy-loss mechanism to quantum simulations to estimate microdosimetric uncertainties that arise from ignoring quantum effects in Monte Carlo simulations of low-energy electron transport.

Methods

A novel Quantum History approach is compared to classical MC simulations.

Classical Monte Carlo: An electron is emitted isotropically from the centre of a R=2 nm homogeneous sphere. The electron can scatter elastically or can ionize the medium, losing energy and producing a new secondary electron. Every electron is tracked until it leaves the volume, or its energy drops to 10 eV.

Quantum Histories: An isotropic source of probability emanates from the center of a R=2 nm spherical cluster of scatterers. Solving the Schrodinger equation gives the probability of emission from the cluster and the probability of ionization. Ionization reduces the energy of the initial source and produces another source of probability at the ionization location. Iterate until source kinetic energy is less than 10 eV.

Fig 1: One Quantum History

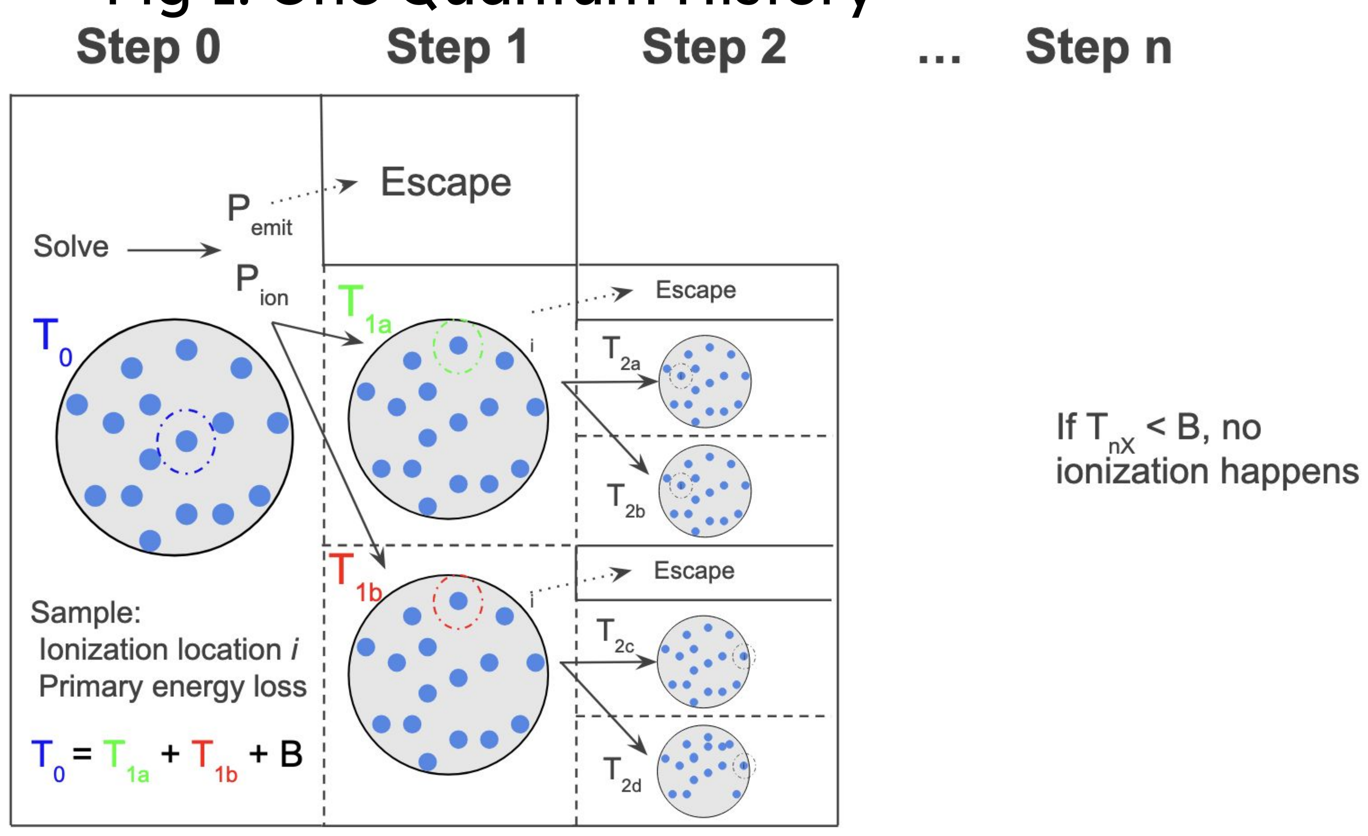
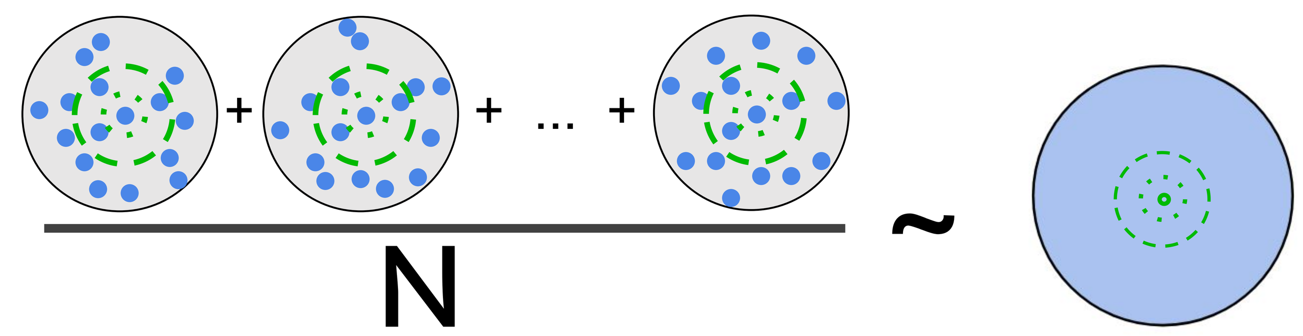
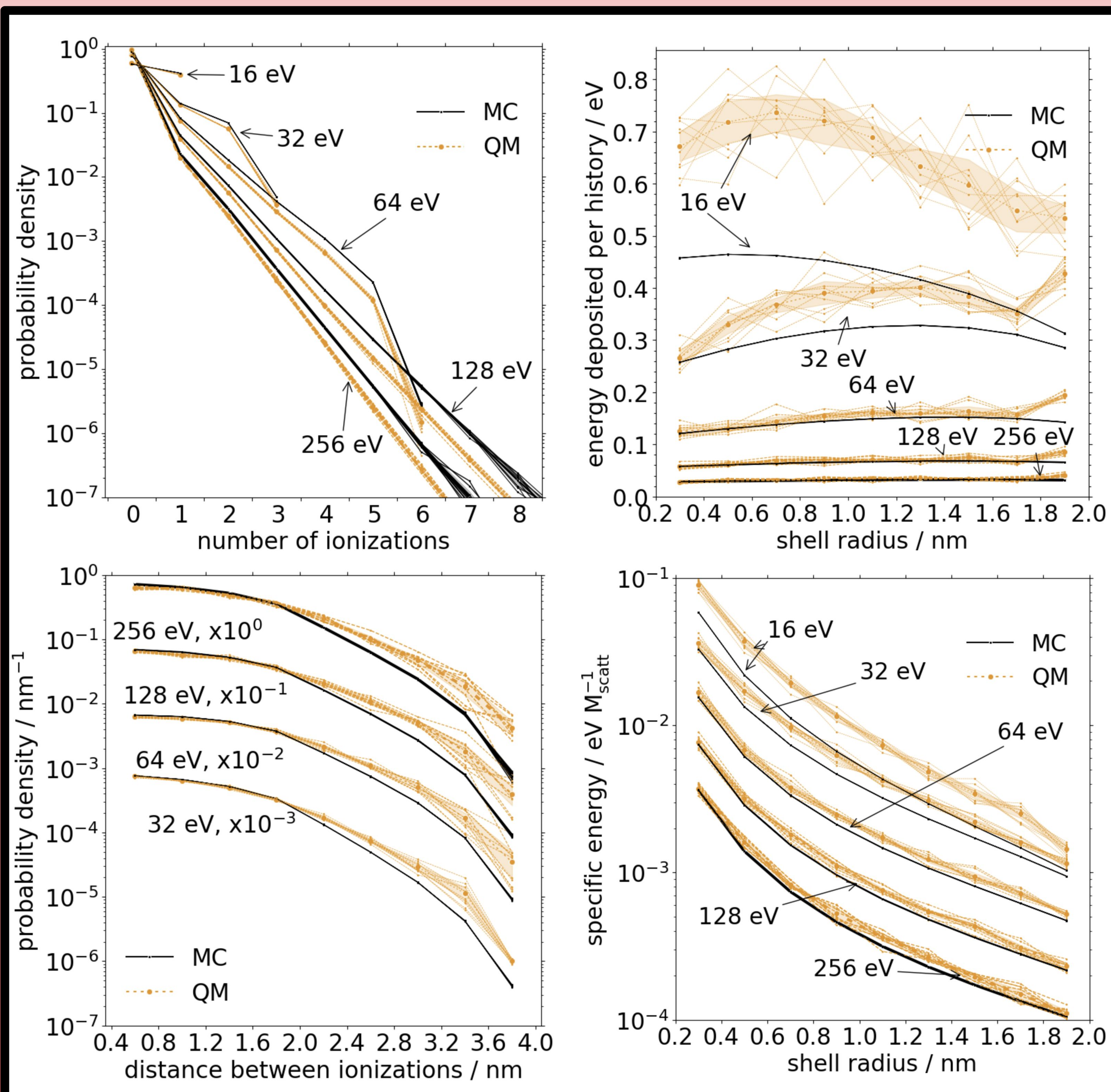


Fig 2: Averaging Multiple Quantum Histories

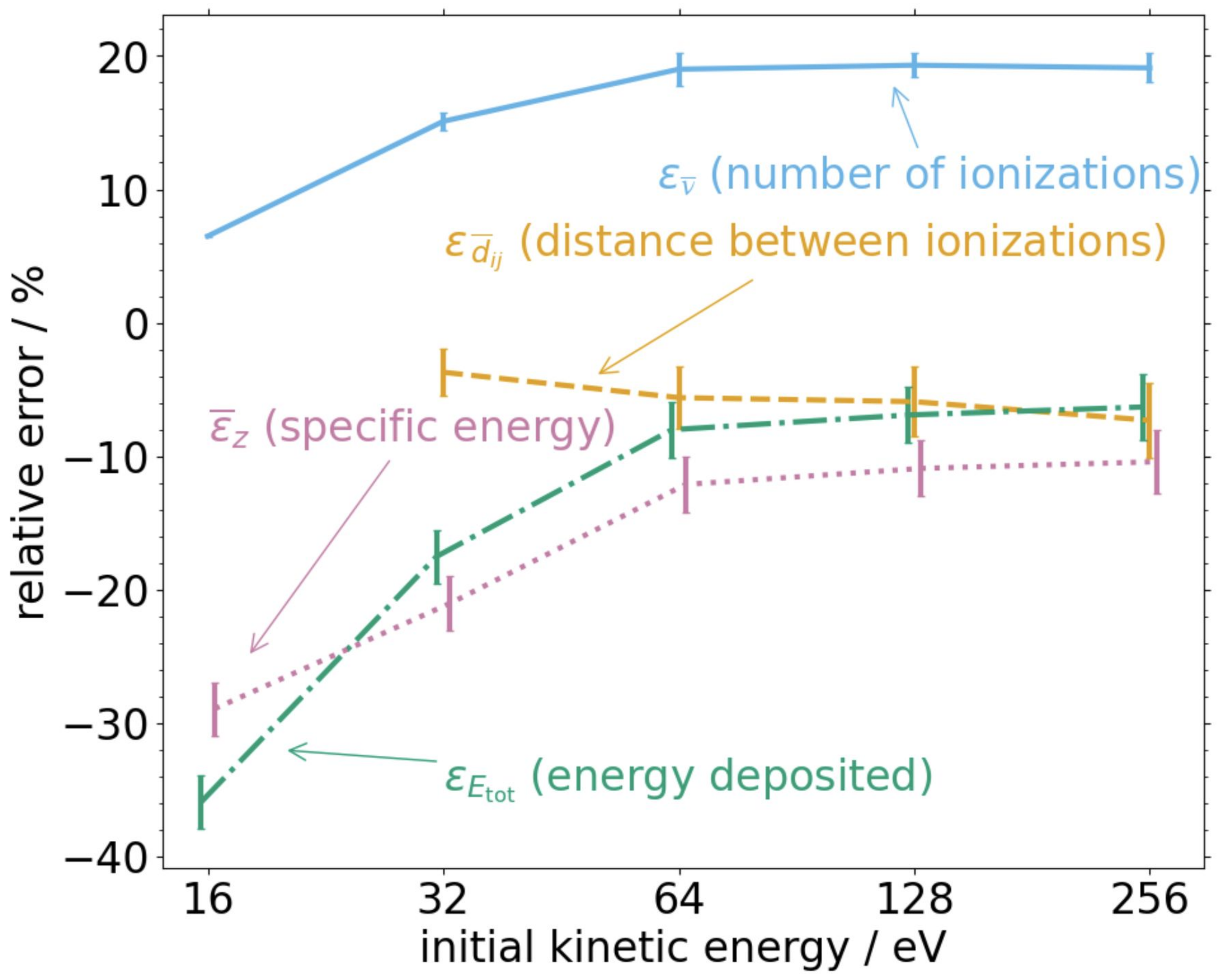


Key point: Averaging across sampled microstates of scatterer positions with the same macrostate (density, cross sections) captures uncertainty from unknowable scatterer positions.



Results

- Classical MC overestimates number of ionizations
- MC underestimates energy deposited, specific energy, and probability of large-distance ionization pairs
- Some observables have larger relative error at small energies, some do not ⇒ Observable-specific!



Conclusions

- Our model can calculate microdosimetric observables in a water-like medium
- We can estimate uncertainty due to ignoring quantum effects for microdosimetric quantities
- Uncertainty is observable-specific (no universal bias)

Next Steps

- More thorough set of physical processes (electronic excitation, non-isotropic scattering)
- True binding energies and cross sections
- Multiple scatterer types (think DNA in water)

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Joint COMP | AAPM Annual Meeting 2026

References:

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[2] D Liljequist and H Nikjoo, Rad. Phys. and Chem. **99** (2014) 45–52
[3] RM Thomson and I Kawrakow, Phys. Med. **54** (2018) 179–188