Towards quantum microdosimetry:
A novel approach for modelling low-energy electron transport in biological tissues

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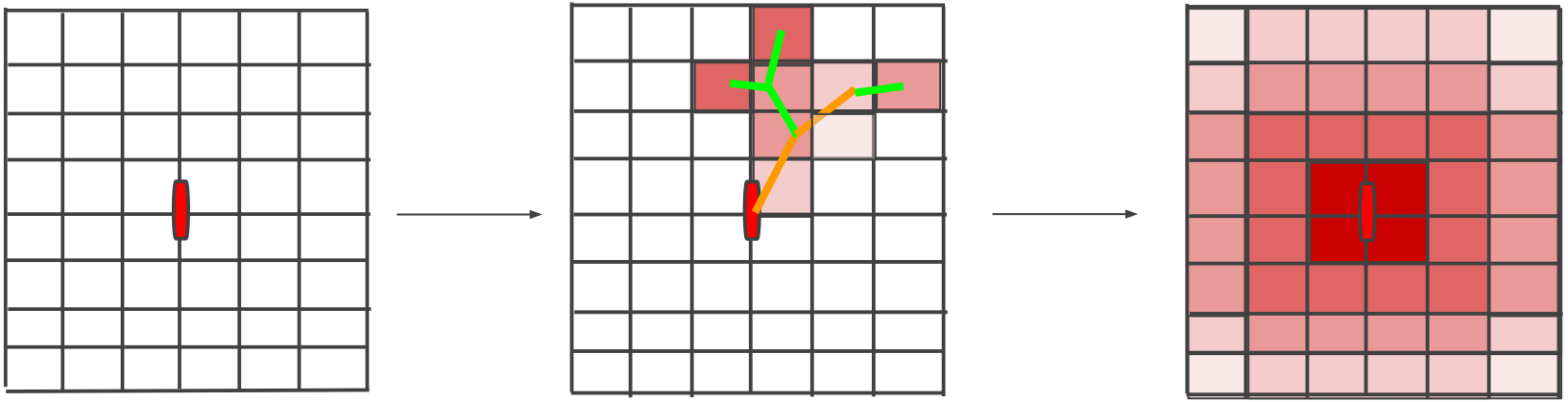
Outline

- Motivation for nanoscale studies
- Current nanoscopic simulations (and problems)
- Previous work that takes QM into account
- Defining a Quantum History
- Measurements that can be made

Motivation for Nanoscale Studies

For treatment planning, one way to predict **dose** is to use Monte Carlo simulations



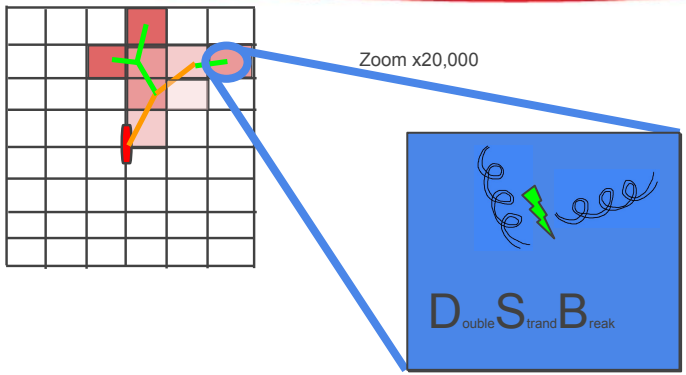
Initial brachytherapy geometry (seed in a phantom)

Simulate a history (Photon source, knock-on electrons)

Average over many many histories

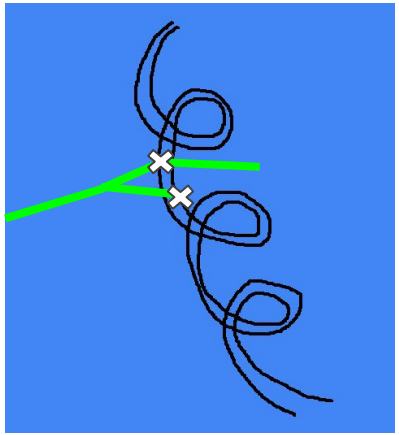
Motivation for Nanoscale (contd.)

But dose is just a **useful heuristic** that correlates well with cell death.

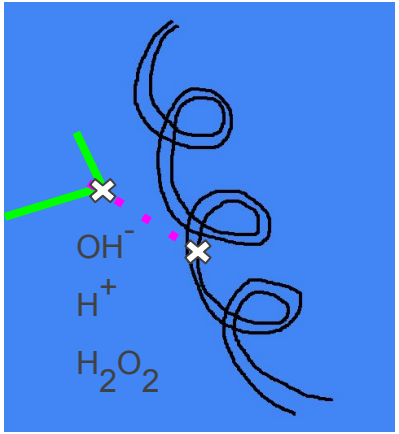


The **physical mechanism** is that ionizing radiation causes damage to DNA (directly or indirectly)

Direct



Indirect



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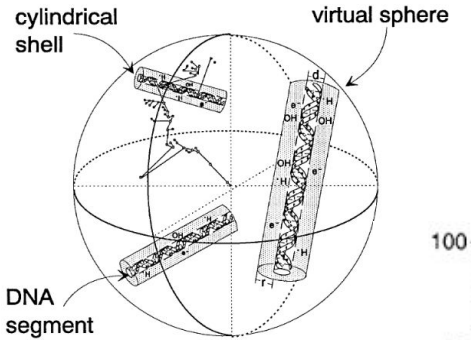
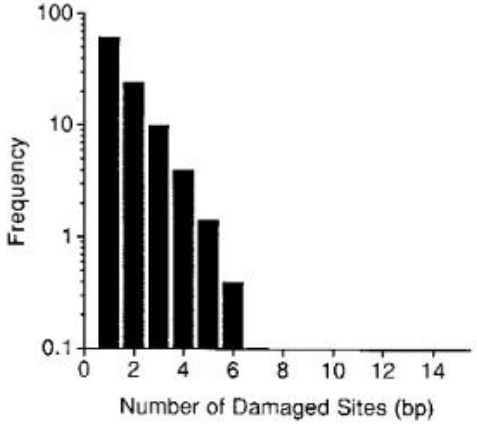
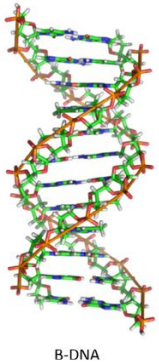
Present Nanoscale Simulations

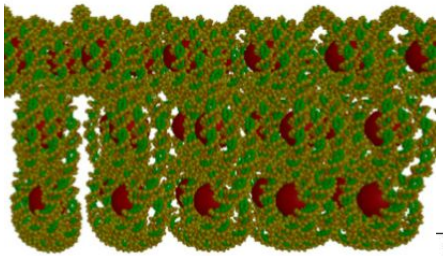
A number of groups simulate electron transport at these nanoscopic length scales



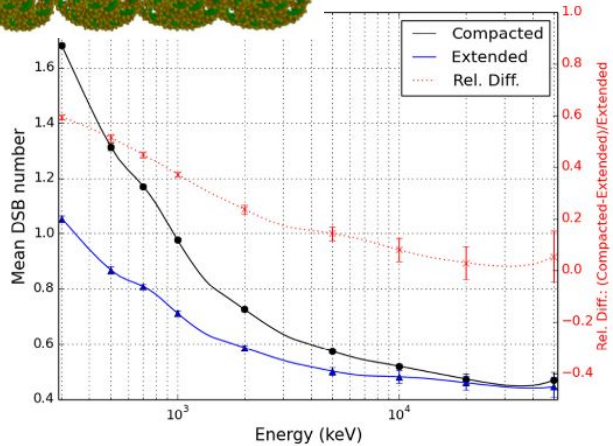
[Nikjoo *et al*, 1997]





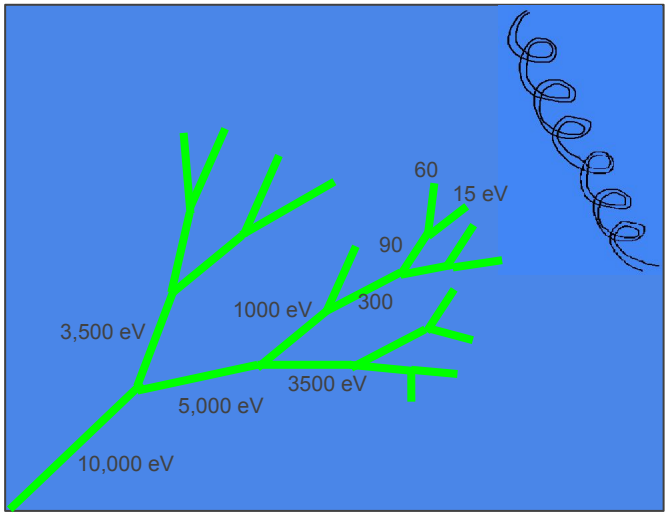


[Meylan *et al*, 2016]



Energy Scales for Nanoscopic Simulations

At these length scales, need to also care about **very low-energy** electrons



High-energy to low-energy cascade to thermalization. High LET at endpoint.

Table 1. ACSs ($\times 10^{-15}$ cm^2) for crosslinks (CLs), DSBs, SSBs, loss of the supercoiled configuration (LS), BD-related crosslinks (BD-CLs), isolated BDs, non-DSB clustered damages (NDCDs), total BDs, and total DNA damages induced by 1–20 eV electrons in 3197 base-pair plasmid DNA. The last two lines are highlighted in color to indicate the ACSs for Arginine-DNA complexes induced by 5 and 10 eV electrons in the same plasmids under identical conditions. * Wang et al. [65].

Energy (eV)	CLs	DSBs	SSBs	LS	BD-CLs	Non-DSB Clustered Damages	Isolated BDs	Total BDs	Total DNA Damages
1	1.7 ± 0.5	n.d.	31.6 ± 4.1	37.1 ± 6.1	1.5 ± 1.0	n.d.	37.1 ± 9.6	39.6 ± 12.4	76.7 ± 13.5
2	n.d.	n.d.	30.2 ± 3.1	34.7 ± 3.0	n.d.	n.d.	46.4 ± 9.2	45.5 ± 7.7	80.2 ± 9.4
3	1.0 ± 0.2	n.d.	23.9 ± 4.0	28.8 ± 3.9	0.5 ± 0.3	n.d.	18.7 ± 8.0	21.1 ± 6.9	49.9 ± 7.8
4	1.4 ± 0.3	1.2 ± 0.3	29.8 ± 3.1	36.2 ± 3.9	0.7 ± 0.6	0.7 ± 0.5	21.1 ± 5.7	25.5 ± 5.1	61.6 ± 6.8
5	2.1 ± 0.3	1.5 ± 0.3	37.5 ± 4.7	44.7 ± 5.8	1.1 ± 0.6	1.3 ± 0.8	22.9 ± 9.8	29.9 ± 13.3	74.6 ± 14.3
6	1.5 ± 0.2	2.3 ± 0.2	18.2 ± 2.2	23.8 ± 3.2	0.9 ± 0.5	1.6 ± 1.0	12.2 ± 3.9	12.7 ± 5.4	36.9 ± 5.5
7	1.5 ± 0.1	1.4 ± 0.5	29.5 ± 3.4	37.6 ± 4.7	0.6 ± 0.4	1.1 ± 0.7	23.4 ± 12.5	25.9 ± 12.5	65.5 ± 13.3
8	1.9 ± 0.3	1.6 ± 0.2	36.6 ± 4.2	42.8 ± 4.7	0.8 ± 0.5	1.2 ± 0.9	24.2 ± 4.2	27.9 ± 10.9	70.7 ± 12.1
9	2.0 ± 0.4	2.7 ± 0.6	39.3 ± 4.2	47.3 ± 6.1	1.5 ± 1.0	1.9 ± 1.2	28.2 ± 11.0	37.4 ± 15.3	84.7 ± 16.5
10	3.7 ± 0.8	3.5 ± 0.6	45.5 ± 4.1	52.0 ± 6.4	2.9 ± 1.1	5.1 ± 1.4	54.0 ± 16.4	51.5 ± 19.7	103.5 ± 21.0

[Dong *et al* 2025]

Complex direct damage observed down to 1 eV

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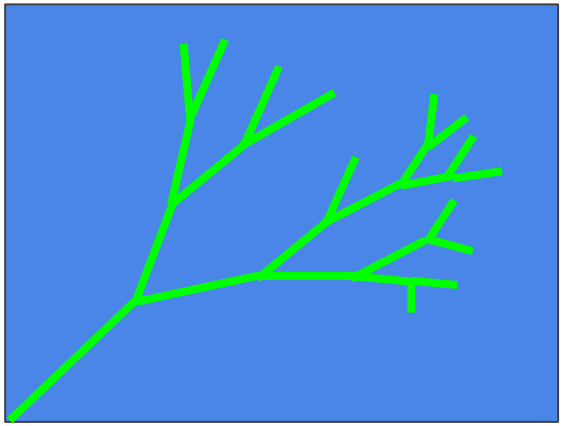
What does Schrödinger Say?

At low energies, electrons **behave like waves**.

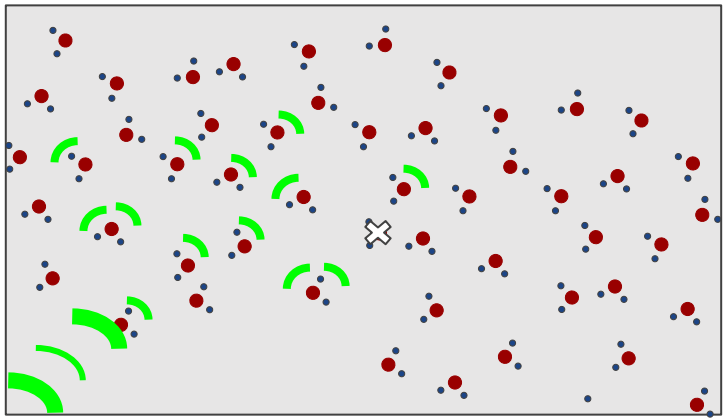
Is this an **issue** for the point-to-point model of current radiation simulations?

T = 100 eV; λ=1.2 Å
H_20 distance = 3.1 Å



Typical Track Structure simulation:

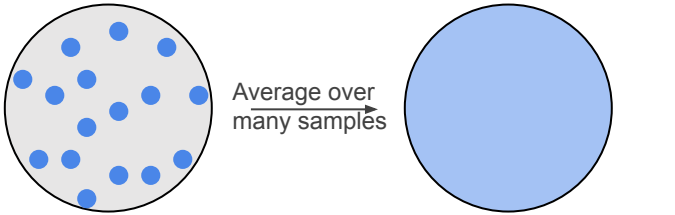
- Each interaction is sampled probabilistically
- 100% momentum and location precision



Reality: wavefield of incident electrons gets reflected and absorbed by molecules

Comparing Monte Carlo to Quantum Mechanics

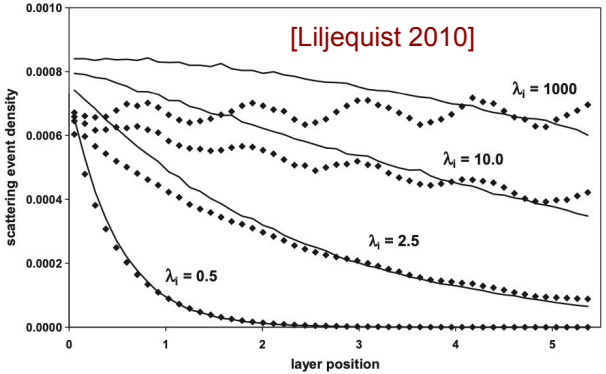
Some groups have already looked into this for cases with **no energy loss**

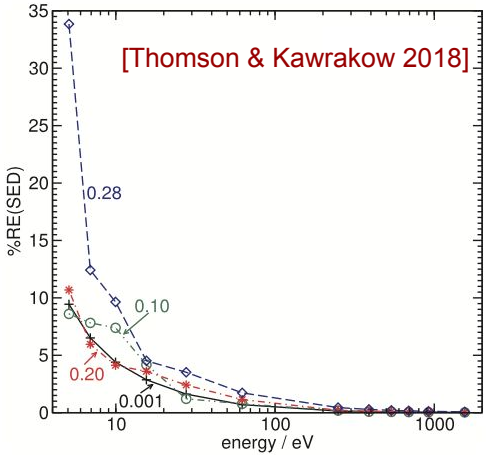


Uniform sample of scatterers in sphere

Homeogeneus sphere with same density

Same density
Same microscopic cross section → Different results
Same incident electron source



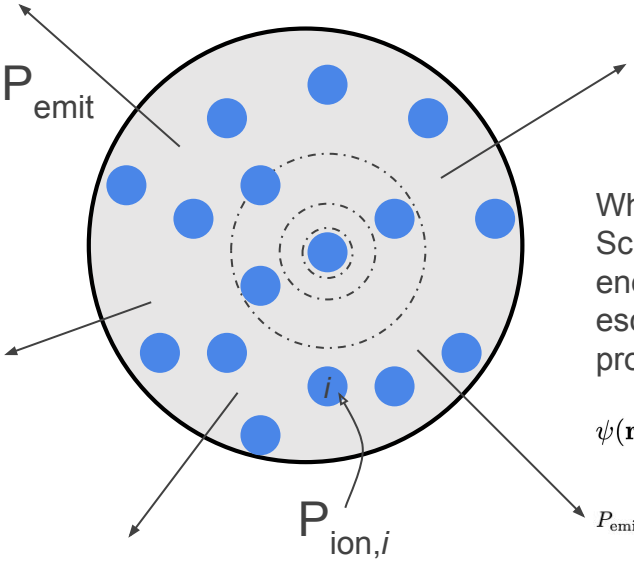


Overarching Goal

How do we **estimate errors** induced from ignoring Quantum Mechanics for typical **microdosimetric** quantities?

Building a Quantum History

To connect with the microdosimetry literature, need to include an **energy loss mechanism**



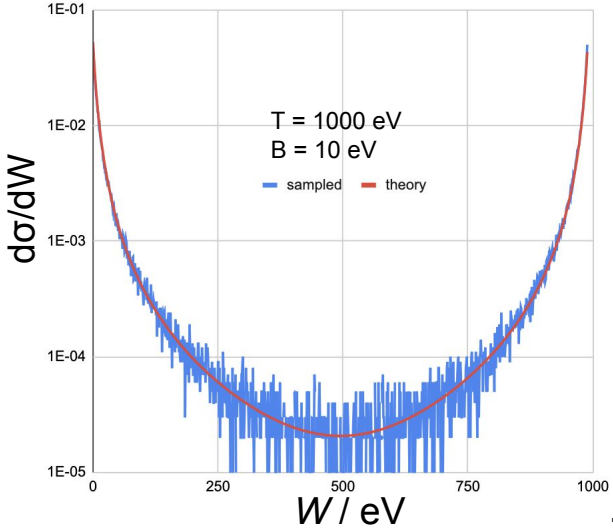
When you solve the Schrodinger equation for one energy, you get a probability to escape the system, or a probability to ionize

$$\psi(\mathbf{r}) = \phi(\mathbf{r}) + f_0 \sum_j K(\mathbf{r}, \mathbf{r}_j)\psi(\mathbf{r}_j)$$

$$P_{\text{emit}} = \frac{J_{\text{emit}}}{J_{\text{emit}} + J_{\text{abs}}}, \quad P_{\text{abs}} = \frac{J_{\text{abs}}}{J_{\text{emit}} + J_{\text{abs}}}$$

The ionization energy-loss spectrum (W) depends on a chosen binding energy B

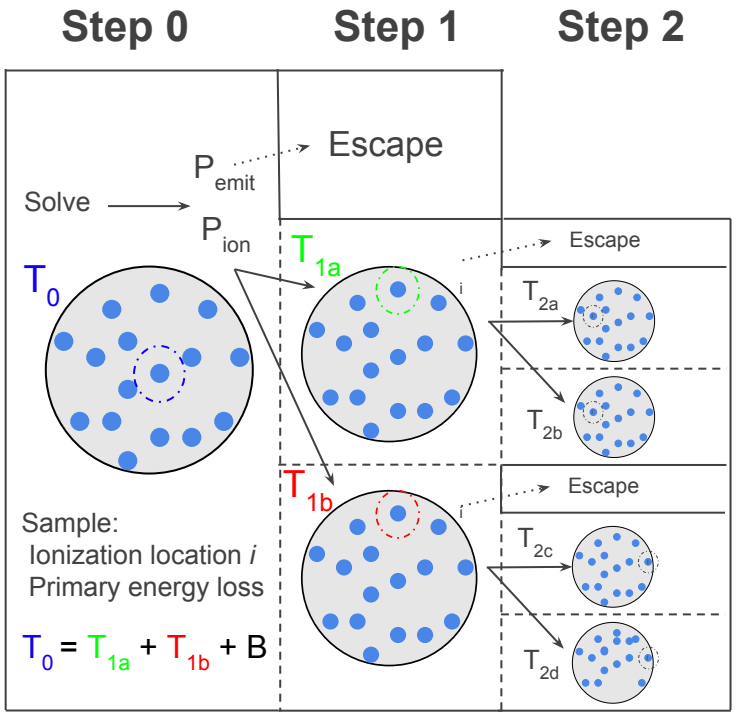
$$\frac{d\sigma_{\text{ion}}}{dW} \propto \frac{1}{W^2} + \frac{1}{(T+B-W)^2} - \frac{1}{W(T+B-W)}$$



Quantum History's Treelike Structure

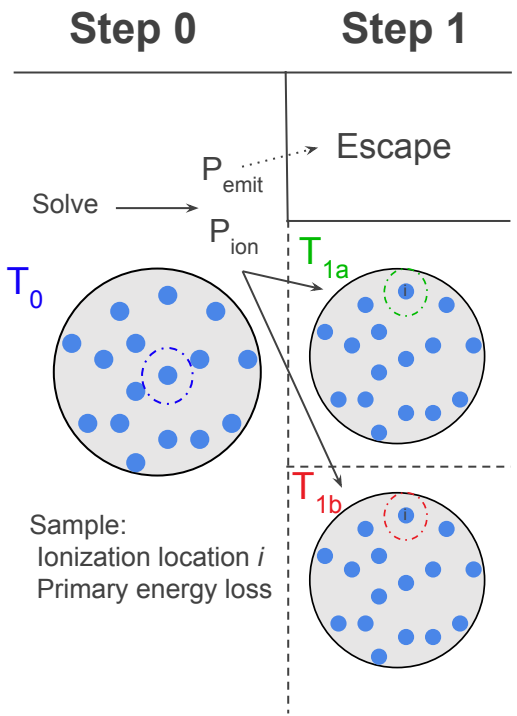
Initialization:

Set MFPs $\ell_{elastic}$ $\ell_{inelastic}$
Set density
Set initial kinetic energy
Set binding energy
Set ionization spectrum
Sample scatterer positions



If $T_{nX} < B$, no ionization happens

Extracting Observables

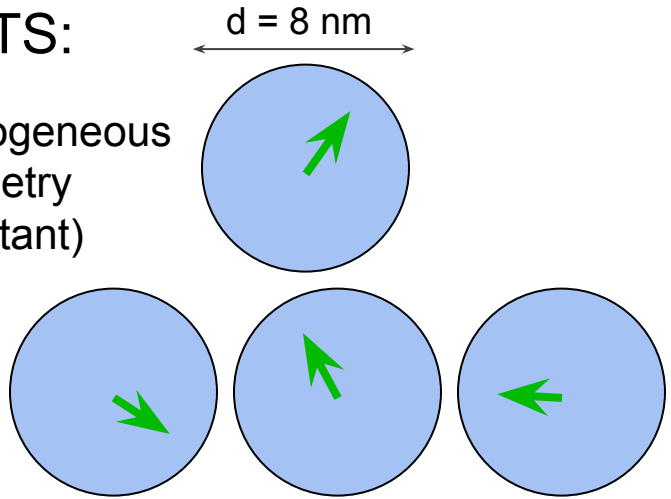


Look at step *0*. How to extract e.g. ionization count ν ?

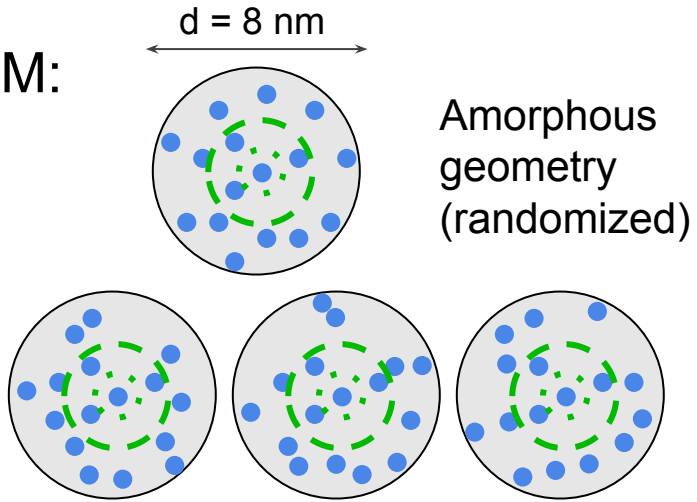
$$\nu^{(0)} = P_{\text{emit}}\{0\} + P_{\text{ion}}\{1\} \oplus \nu^{(1a)} \oplus \nu^{(1b)}$$

Comparing Monte Carlo (TS) to Quantum Histories (QM)

TS:



QM:



~10^7 histories

~10^3 quantum histories

Density, cross sections, initial energy, are all equal

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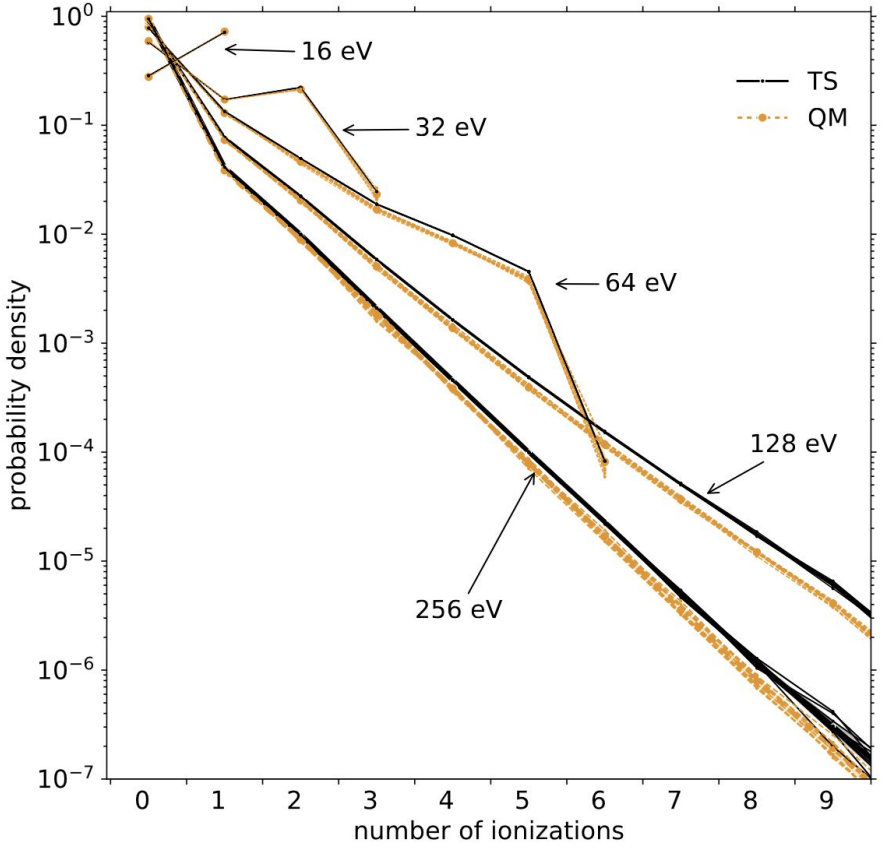
(Number of Ionizations)

Results from Microdosimetry



Summary statistics:

T_0 / eV	$\langle \nu_{QM} \rangle$	$\langle \nu_{TS} \rangle$	ε=(TS-QM)/QM
16	0.722	0.716	(-0.9 ± 0.1)%
32	0.668	0.691	(3.4 ± 1.1)%
64	0.326	0.352	(8.0 ± 1.5)%
128	0.138	0.150	(8.9 ± 1.5)%
256	0.064	0.070	(9.2 ± 1.4)%

- Relative uncertainty ε<10% across all energies

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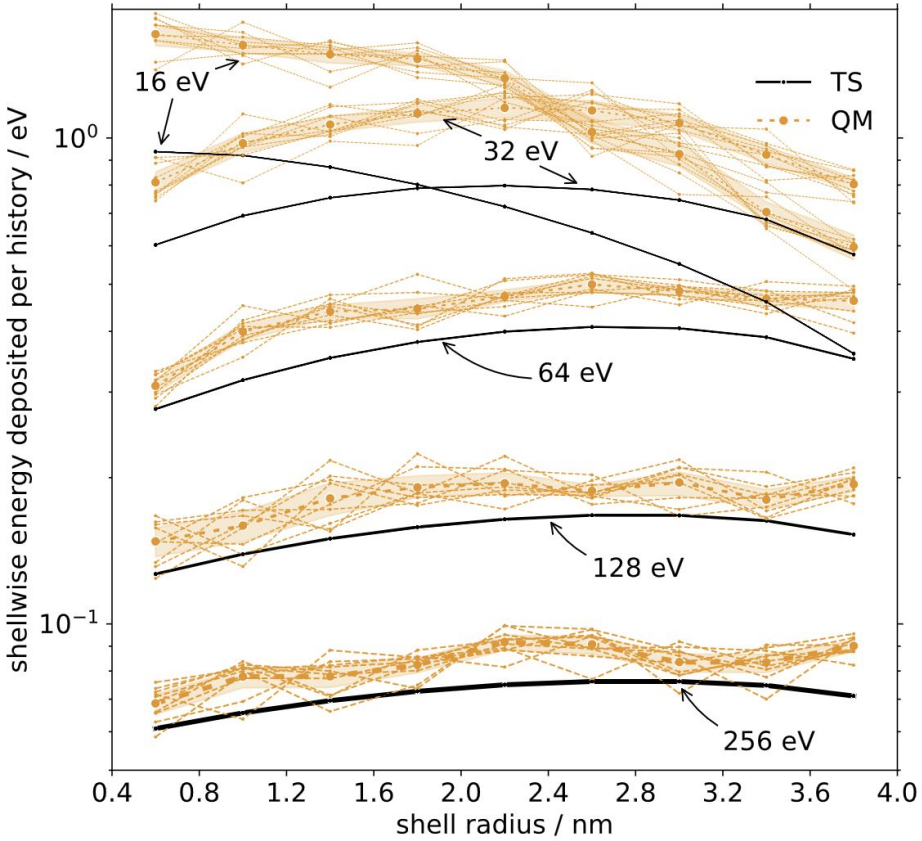
Results from Microdosimetry



Summary statistics:

T_0 / eV	ΣE_{QM} / eV	ΣE_{TS} / eV	ε=(TS-QM)/QM
16	10.71	6.26	-(41.5 ± 1.5)%
32	9.06	6.42	-(29.2 ± 1.7)%
64	3.98	3.28	-(17.5 ± 1.6)%
128	1.63	1.39	-(14.9 ± 2.5)%
256	0.75	0.64	-(14.0 ± 2.0)%

- Relative uncertainty **grows** at small energies

Conclusions

- We have provided a model that can calculate microdosimetric quantities in nanovolumes
- Quantum mechanics is important at low energies
- Uncertainty is observable-dependent, so can’t just quote a flat error rate for all classical simulations

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Next steps

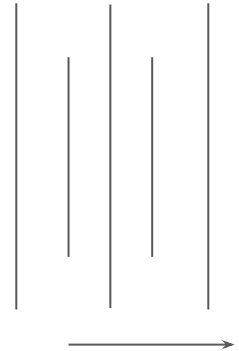
- Need more interactions beyond ionization (elastic beyond s-wave, electronic excitation)
- Model is useful even beyond microdosimetry
- Need to connect with measured data for cross sections (water, DNA)

Thanks for listening!

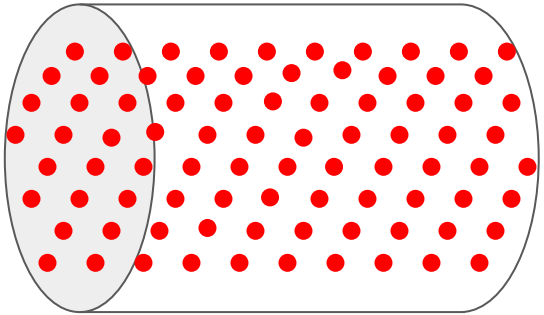
Questions?

Backup Slides

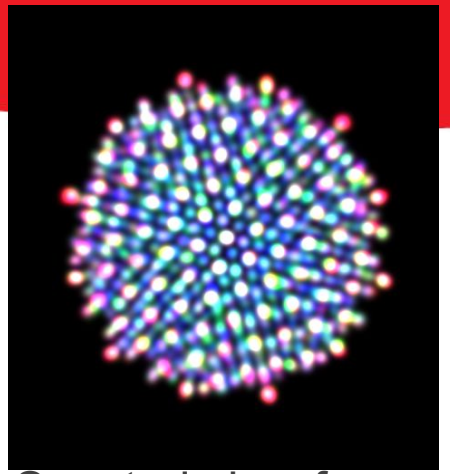
Not just microdosimetry!



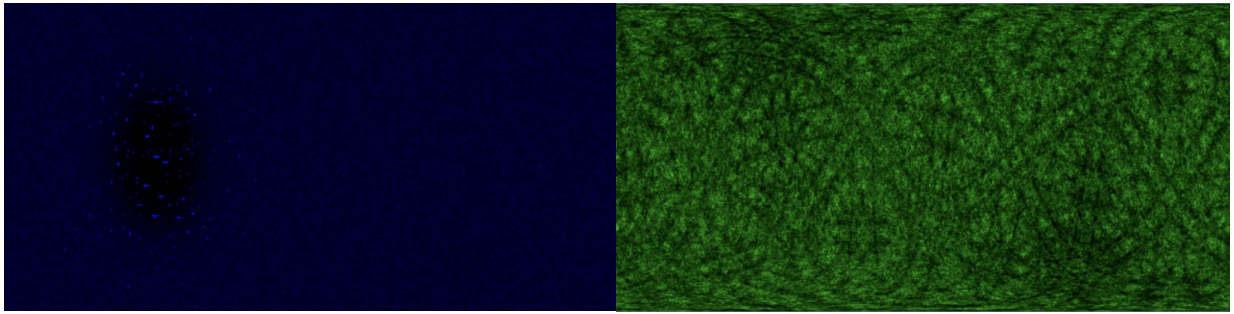
Plane wave



Silicon lattice at nonzero temperature



Spectral view from viewpoint of beam



Far field pattern, important for crystallography (Mercator projection)

Templates