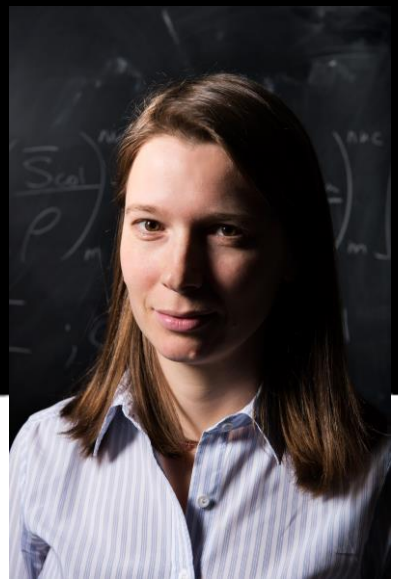
Challenges in Monte Carlo simulations for microdosimetry



Rowan M. Thomson

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Carleton Laboratory for Radiotherapy Physics

Carleton University

Ottawa, Canada

Ottawa Medical Physics Institute

CIRMS Microdosimetry Session, 16 April 2018

Carleton UNIVERSITY

Lifetime probability of developing cancer is considerable.

Lifetime probability of developing cancer is considerable.

Radiation therapy

Alone or with surgery, chemotherapy

- Common - 50% of cancer patients

Advance radiotherapy?

"the majority of our current radiotherapy strategies were derived by empirical optimization of clinical experience performed with inferior technologies."

Chapman & Nahum "Radiotherapy Treatment Planning", 2015

Advance radiotherapy

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Chapman & Nahum "Radiotherapy Treatment Planning", 2015

innovation

research

New technologies

Quantitative evaluations

Advance radiotherapy

"the majority of our current radiotherapy strategies were derived by empirical optimization of clinical experience performed with inferior technologies."

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innovation

research

New technologies

Quantitative evaluations

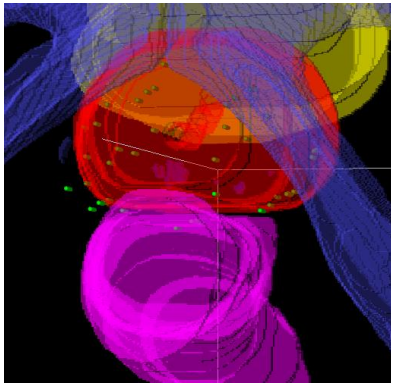
→ Monte Carlo simulations of radiation transport and energy deposition…

Today: Monte Carlo (MC) simulations

Scale

cm

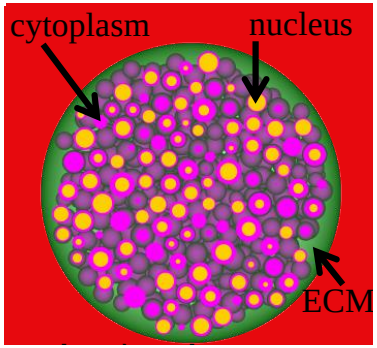
Patient



"Microdosimetry"

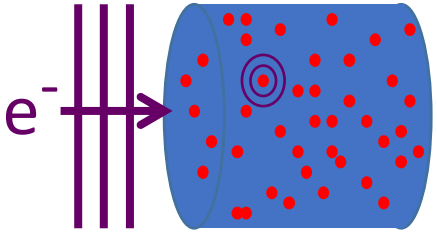
µm

Cells: microscopic tissue models, populations of cells



nm

Subcellular, DNA: low-energy electron transport



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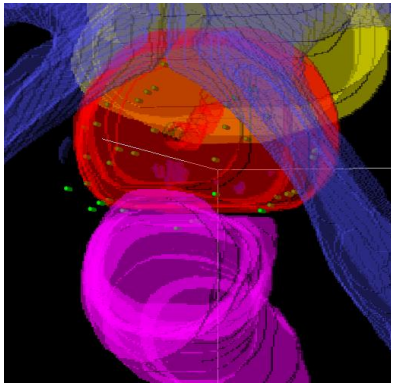

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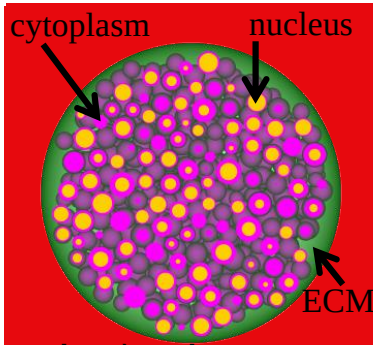

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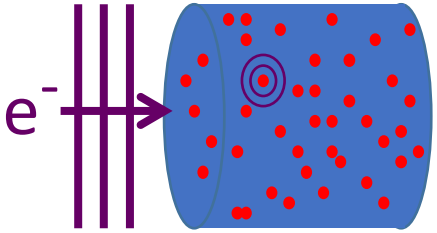


Patient level

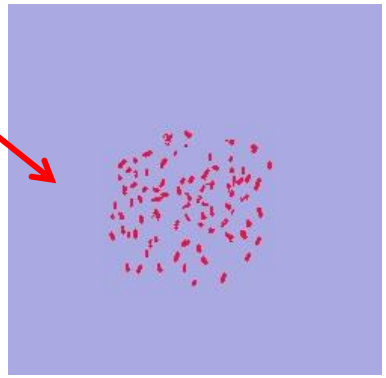
Evolution in dose evaluation…

Image +
treatment data

Patient level

Evolution in dose evaluation…

Image +
treatment data



Traditional approaches
- Water “patient”
- Simplified source(s)

Patient level

Evolution in dose evaluation…

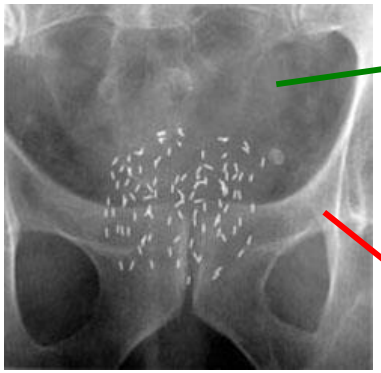
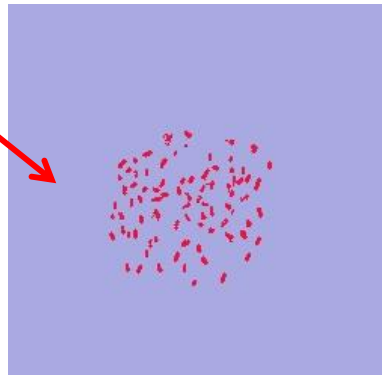


Image +
treatment data



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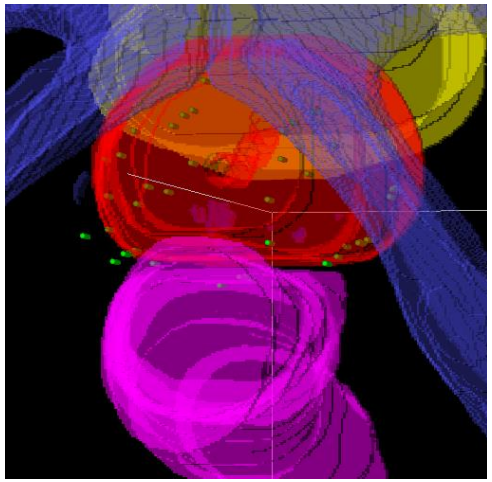

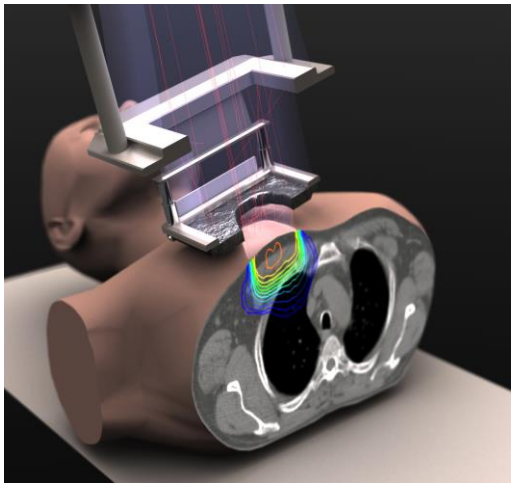

Recently, model-based dose calculations
- Non-water virtual patient models
- Detailed modeling of source(s)

Report of the AAPM Task Group No. 105: Issues associated with clinical implementation of Monte Carlo-based photon and electron external beam treatment planning

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(Received 11 April 2006; revised 11 July 2007; accepted for publication 18 September 2007; published 27 November 2007)

The Monte Carlo (MC) method has been shown through many research studies to calculate accurate dose distributions for clinical radiotherapy, particularly in heterogeneous patient tissues where the effects of electron transport cannot be accurately handled with conventional, deterministic dose algorithms. Despite its proven accuracy and the potential for improved dose distributions to influence treatment outcomes, the long calculation times previously associated with MC simulation rendered this method impractical for routine clinical treatment planning. However, the development of faster codes optimized for radiotherapy calculations and improvements in computer processor technology have substantially reduced calculation times to, in some instances, within minutes on a single processor. These advances have motivated several major treatment planning system vendors to embark upon the path of MC techniques. Several commercial vendors have already released or are currently in the process of releasing MC algorithms for photon and/or electron beam treatment planning. Consequently, the accessibility and use of MC treatment planning algorithms may well become widespread in the radiotherapy community. With MC simulation, dose is computed stochastically using first principles; this method is therefore quite different from conventional dose algorithms. Issues such as statistical uncertainties, the use of variance reduction techniques, the

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From research to clinical practice…

TG-105 for photon and electron external beam treatment planning (2007)

MC for clinical radiotherapy dose evaluation:
→ "emerging technology"
→ "preliminary report"

Report of the Task Group 186 on model-based dose calculation methods in brachytherapy beyond the TG-43 formalism: Current status and recommendations for clinical implementation

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(Received 7 May 2012; revised 26 July 2012; accepted for publication 2 August 2012; published 25 September 2012)

The charge of Task Group 186 (TG-186) is to provide guidance for early adopters of model-based dose calculation algorithms (MBDCAs) for brachytherapy (BT) dose calculations to ensure practice uniformity. Contrary to external beam radiotherapy, heterogeneity correction algorithms have only recently been made available to the BT community. Yet, BT dose calculation accuracy is highly dependent on scatter conditions and photoelectric effect cross-sections relative to water. In specific situations, differences between the current water-based BT dose calculation formalism (TG-43) and MBDCAs can lead to differences in calculated doses exceeding a factor of 10. MBDCAs raise three major issues that are not addressed by current guidance documents: (1) MBDCA calculated doses are sensitive to the dose specification medium, resulting in energy-dependent differences between dose calculated to water in a homogeneous water geometry (TG-43), dose calculated to the local medium in the heterogeneous medium, and the intermediate scenario of dose calculated to a small volume of water in the heterogeneous medium. (2) MBDCA doses are sensitive to voxel-by-voxel interaction cross sections. Neither conventional single-energy CT nor ICRU/ICRP tissue composition compilations provide useful guidance for the task of assigning interaction cross sections to each voxel. (3) Since each patient-source-applicator combination is unique, having reference data for each possible combination to benchmark MBDCAs is an impractical strategy. Hence, a new commissioning process is required. TG-186 addresses in detail the above issues through the literature review

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From research to clinical practice…

TG-186 for brachytherapy dose calculation methods beyond TG-43 formalism (2012)

"Model-based" dose calculations → MC simulations

Develop patient & treatment model

"Raw" patient treatment and image data
CT, MRI

Develop patient & treatment model

"Raw" patient treatment and image data
CT, MRI

Develop patient model

- Map CT number (HU) to mass density (g cm^{-3})
- Voxel = volumetric pixel
- In each voxel: assign tissue elemental compositions

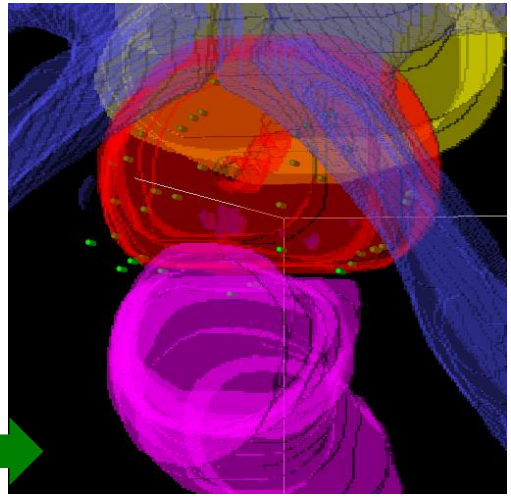
Develop patient & treatment model

"Raw" patient treatment and image data
CT, MRI

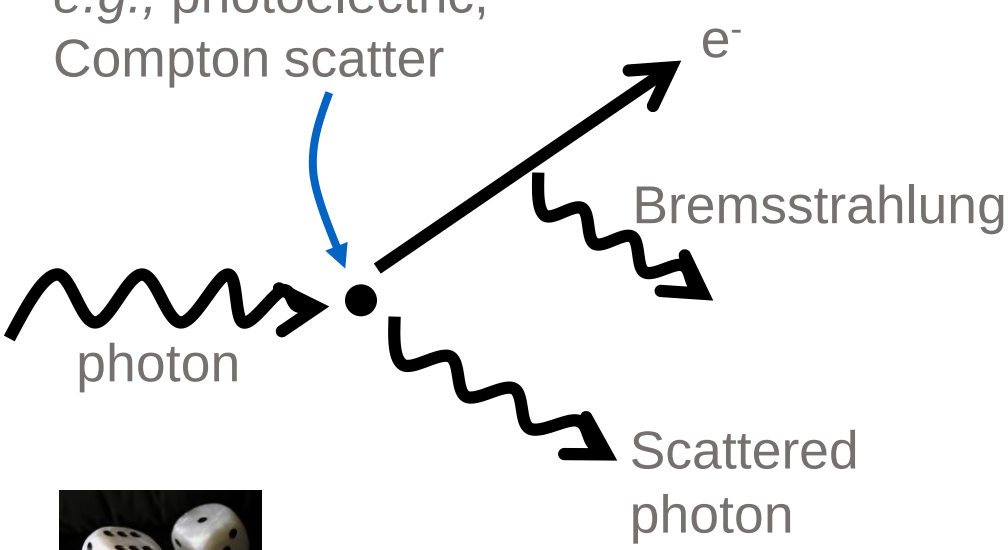
Develop patient model

- Map CT number (HU) to mass density (g cm^{-3})
- Voxel = volumetric pixel
- In each voxel: assign tissue elemental compositions

- 3D voxelized patient model with non-water tissues
- Detailed source model



MC simulation



Particles (radiation quanta):

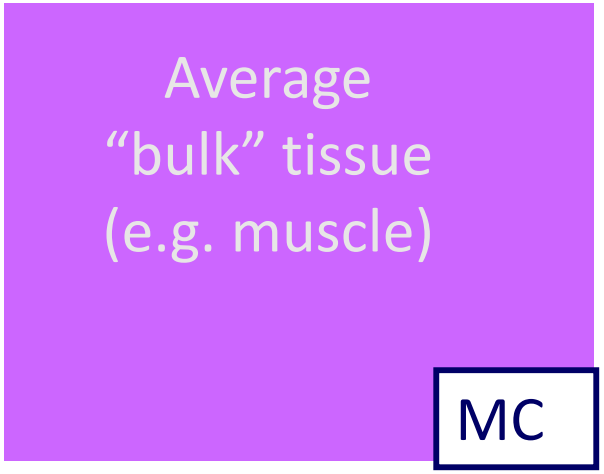
- "Born" according to distributions describing source
- Travel distances determined by probability distributions (interaction cross sections for media simulated) to site of collision/scatter
- Continue/repeat until particle is absorbed or leaves the geometry

Calculate dose: up energy deposited in tissue (divide by mass).

Patient voxels

- MC simulations: radiation transport, dose in ~mm voxels

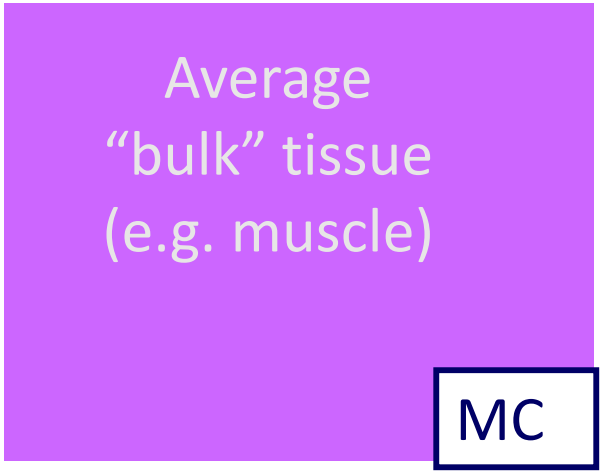
mm-sized voxel



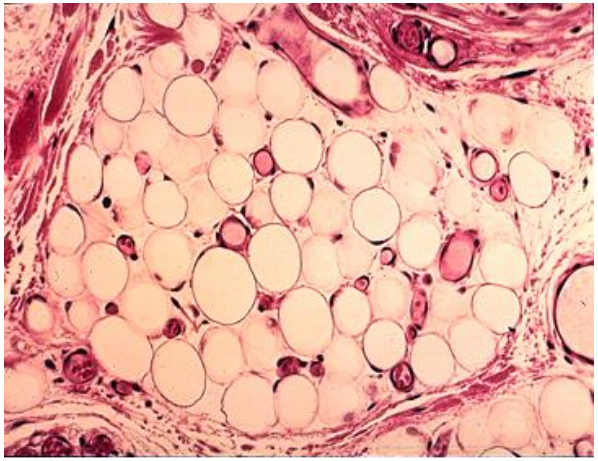
Cells

- MC simulations: radiation transport, dose in ~mm voxels
- Cellular structures underlie tissues modeled in MC simulations → Neglected for radiotherapy dose calculations

mm-sized voxel



Underlying cells



Voxel bulk tissue ←→ cells?

- MC simulations: radiation transport, dose in ~mm voxels
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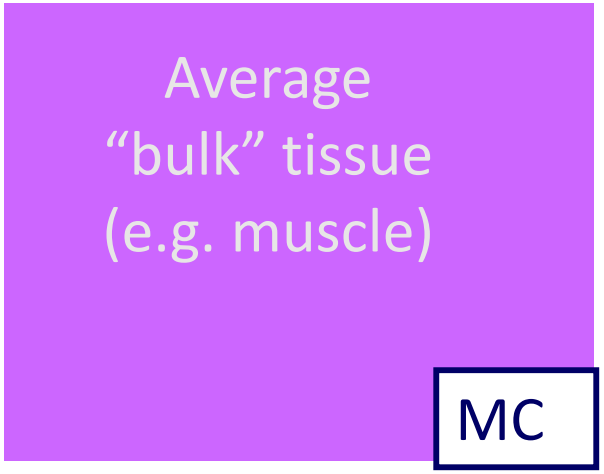
mm-sized voxel



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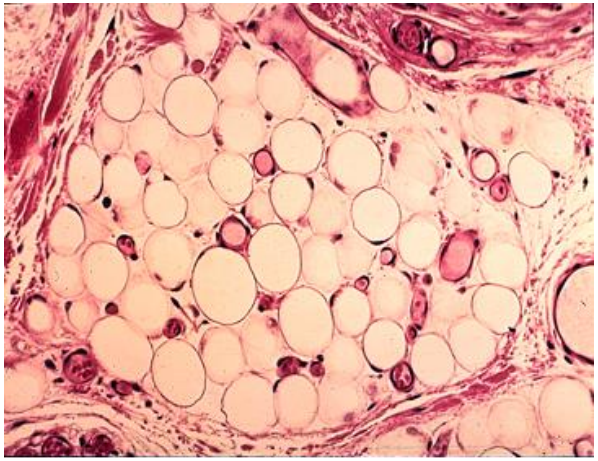


Voxel bulk tissue ←→ cells?

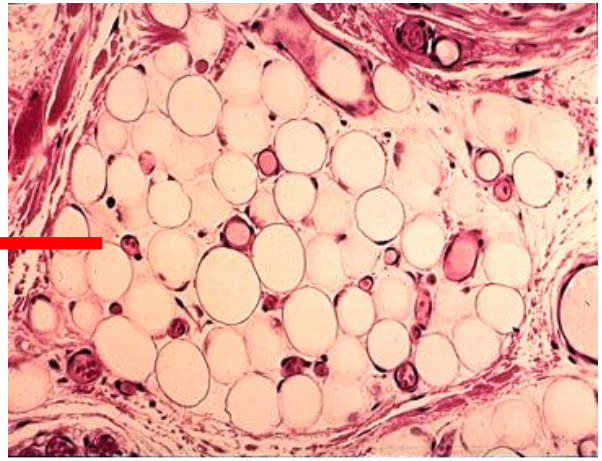
- MC simulations: radiation transport, dose in ~mm voxels
- Cellular structures underlie tissues modeled in MC simulations → Neglected for radiotherapy dose calculations

mm-sized voxel

Average
"bulk" tissue
(e.g. muscle)

MC

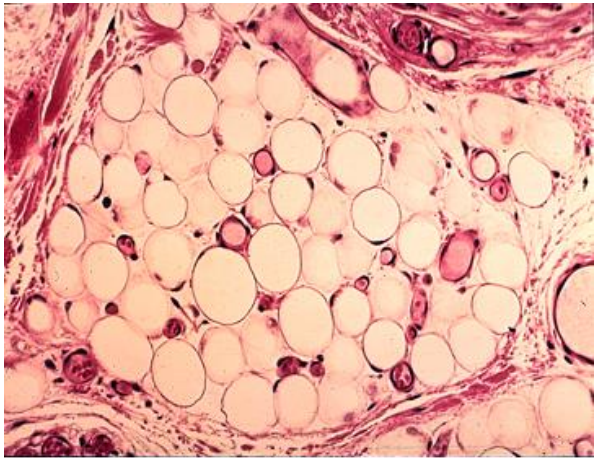
Underlying cells

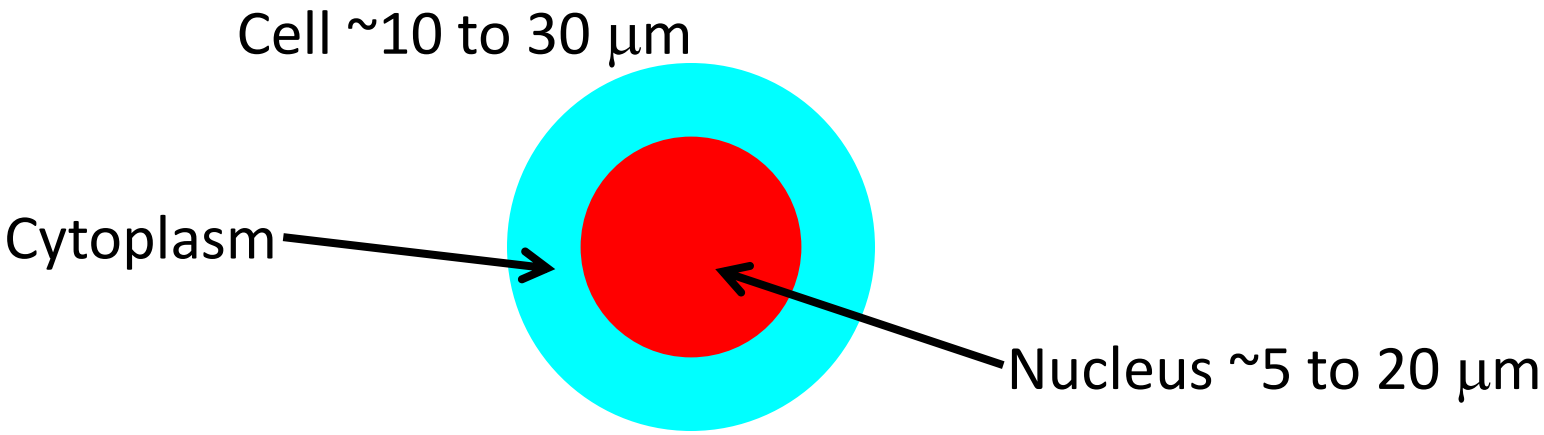


Radiation targets

Primary targets for radiation: cell and cell components (~microns)

- DNA – important target; nucleus
- Whole cell – receptors on cell membrane and mitochondria play roles relating to apoptosis, DNA repair





How are macroscopic dose descriptors related to doses to cellular targets?

mm-sized voxel

Underlying cells

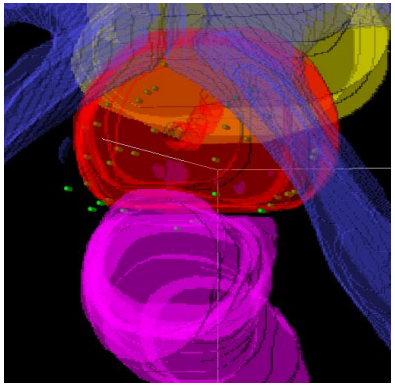
Thomson et al, Phys. Med. Biol. **58** (2013)
Oliver & Thomson, Phys. Med. Biol. **62** (2017) X 2

Today: Monte Carlo simulations

Scale

cm

Patient



"Microdosimetry"

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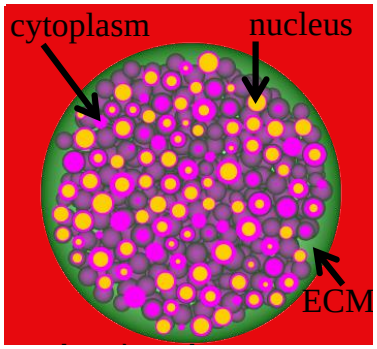
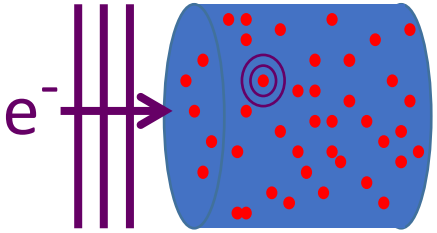


nm

Subcellular, DNA: low-energy electron transport



How to model cells?

- Many MC simulations assume cells are water equivalent
- Cell morphology literature (50 years)
- Size, composition, shape of cell constituents (nucleus, cytoplasm)

Thomson et al, Phys. Med. Biol. **58** (2013)
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How to model cells?

- Many MC simulations assume cells are water equivalent
- Cell morphology literature (50 years)
- Size, composition, shape of cell constituents (nucleus, cytoplasm)

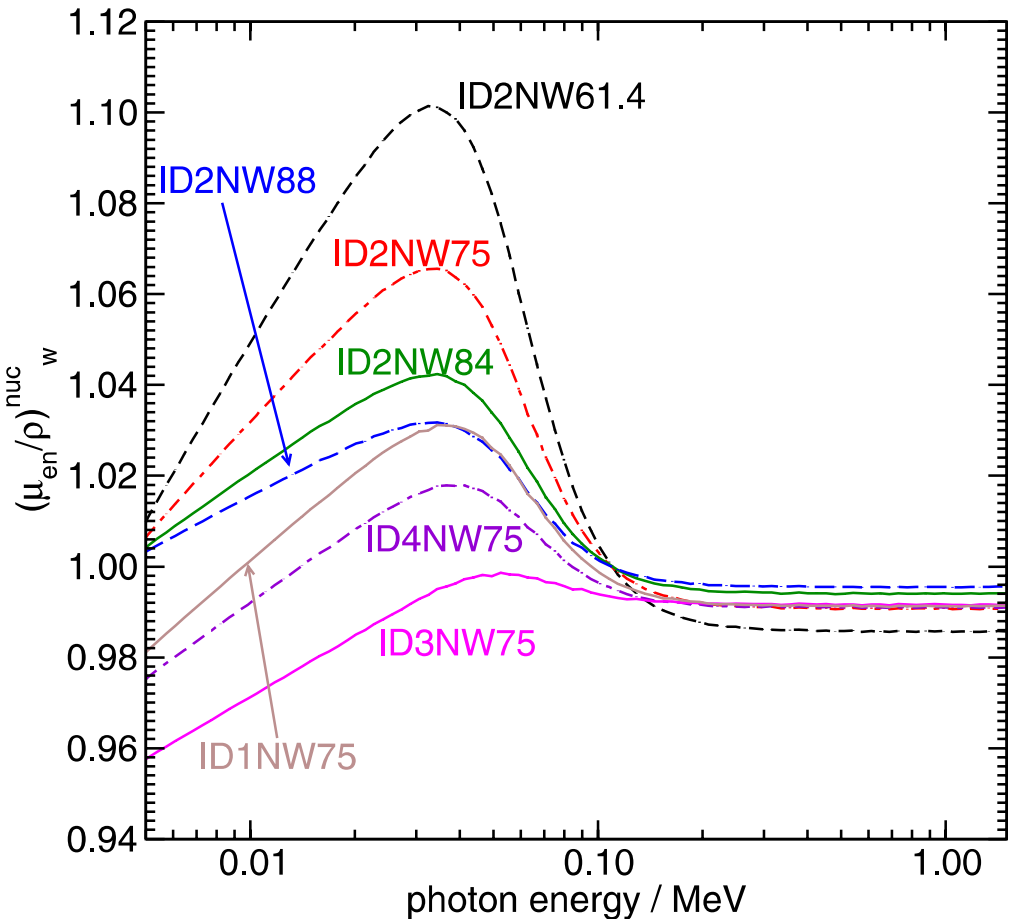
→Significant mass fractions of proteins, inorganic elements (sodium, calcium), and lipids (adipocytes only); water content varies

→Cell morphology (composition, size, shape) varies considerably with cell type and normal/cancerous tissue

Thomson et al, Phys. Med. Biol. **58** (2013)
Oliver & Thomson, Phys. Med. Biol. **62** (2017)

Cells ≠ water

Mass energy absorption coefficients for cell nucleus relative to water; different cell models.

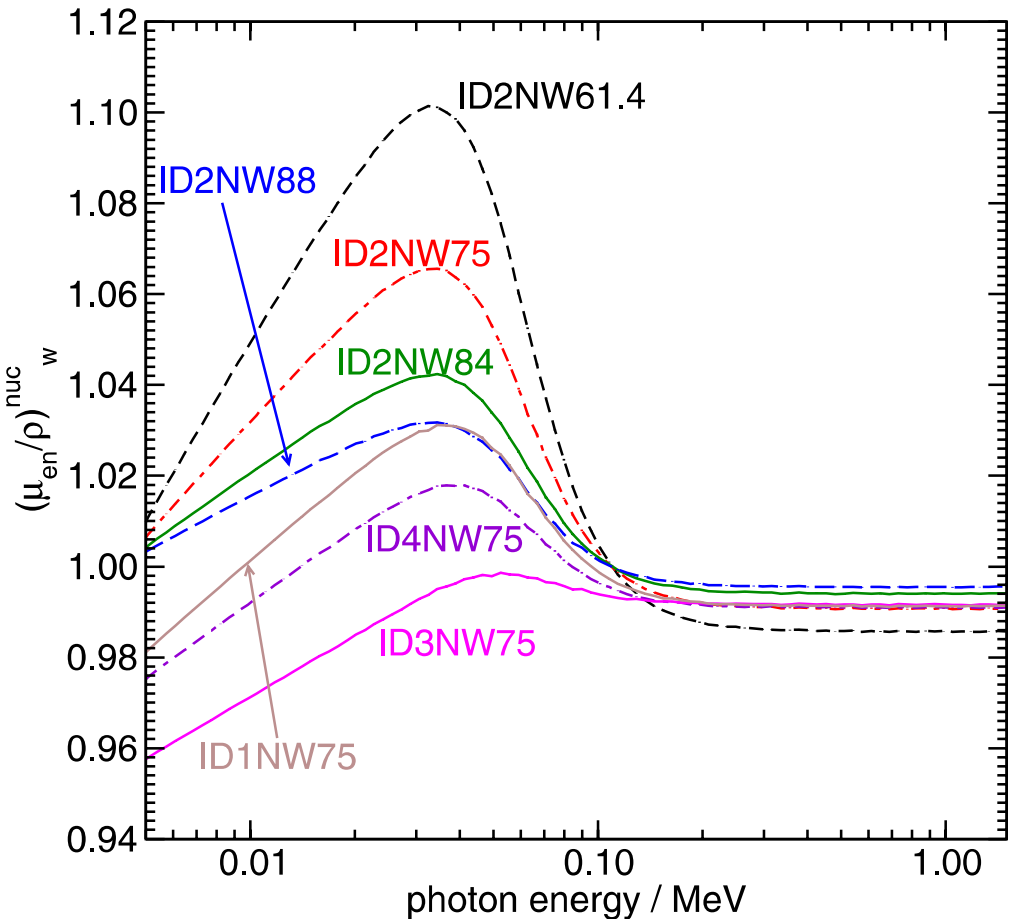


Thomson et al, Phys. Med. Biol. **58** (2013)

Cells ≠ water

Mass energy absorption coefficients for cell nucleus relative to water; different cell models.

- Below 100 keV:
  - Up to 10% deviations from unity
  - Energy absorption coefficients vary by 10% with cell model
- Differences smaller with increasing energy
- Similar for cytoplasm



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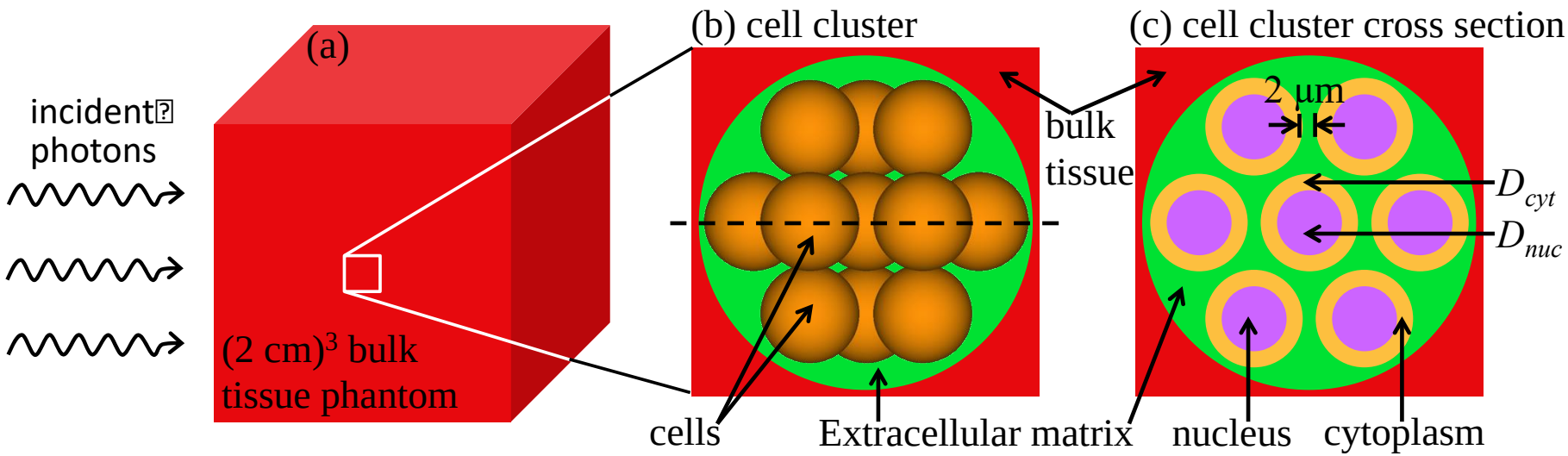
Multicellular models

Develop microscopic tissue models (13 cells)…



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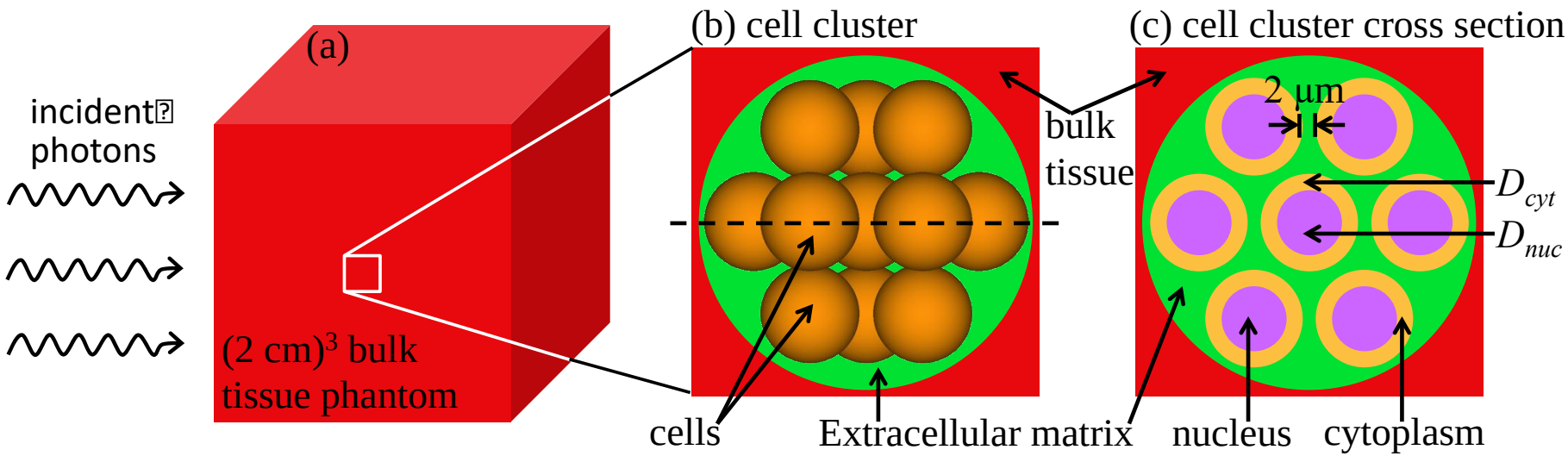
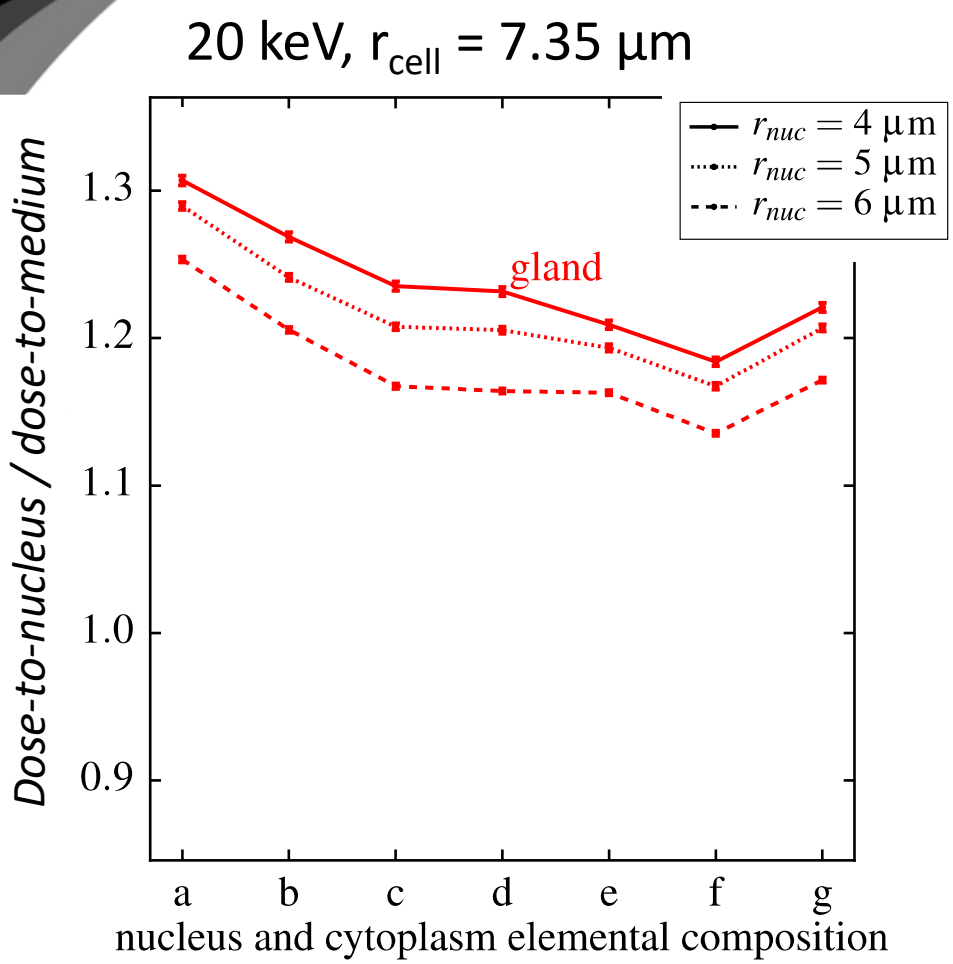
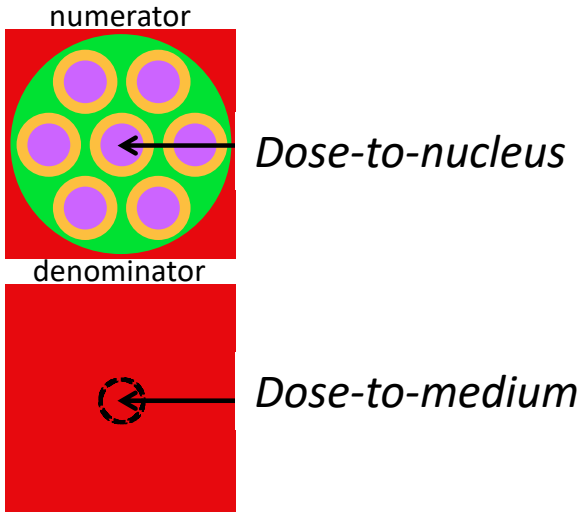


- Various cell/nucleus radii, cytoplasm/nucleus elemental compositions, bulk tissues, and photon energies
- MC simulations with egs_chamber (EGSnrc); radiation transport modeled to 1 keV (e- range <40 nm).

Thomson et al, Phys. Med. Biol. **58** (2013)
Oliver & Thomson, Phys. Med. Biol. **62** (2017) X 2

Nucleus dose varies with cell type, size





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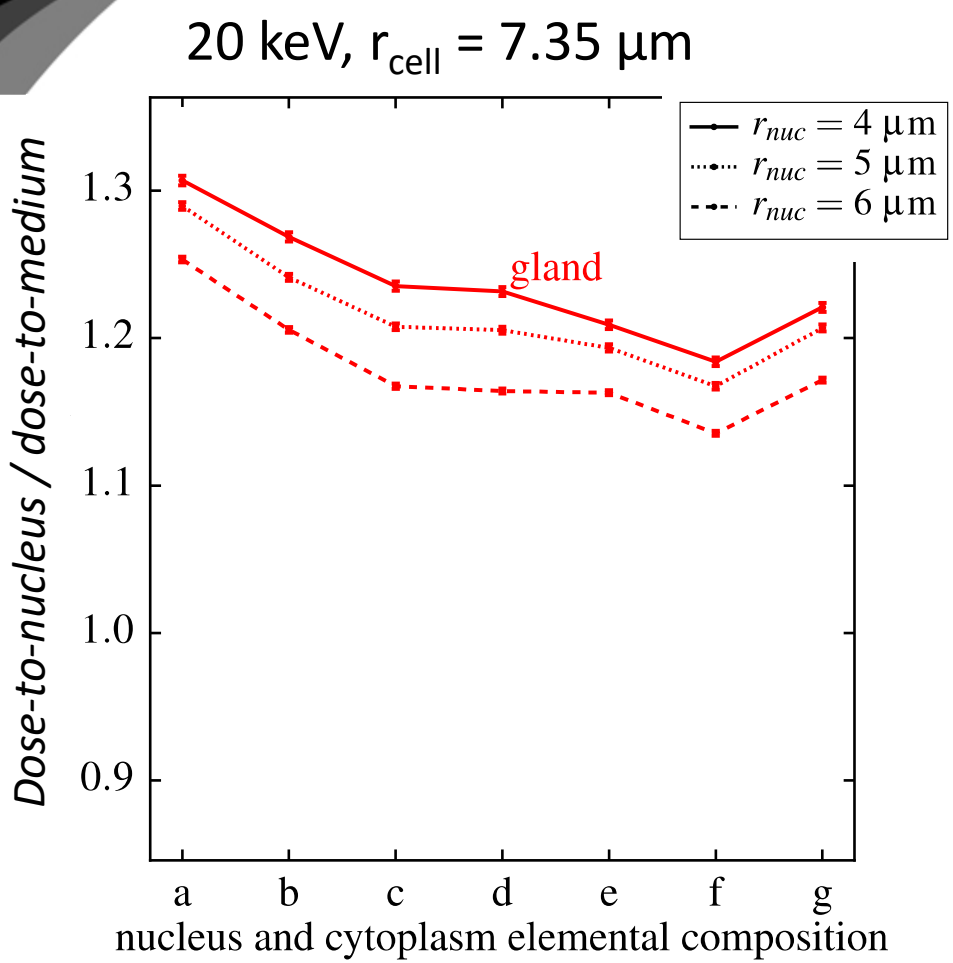
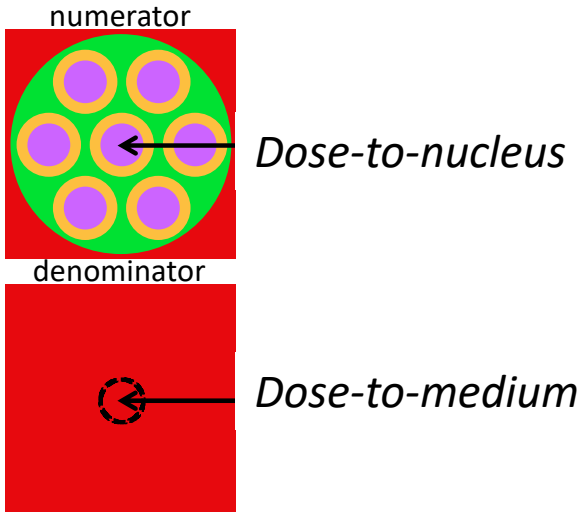
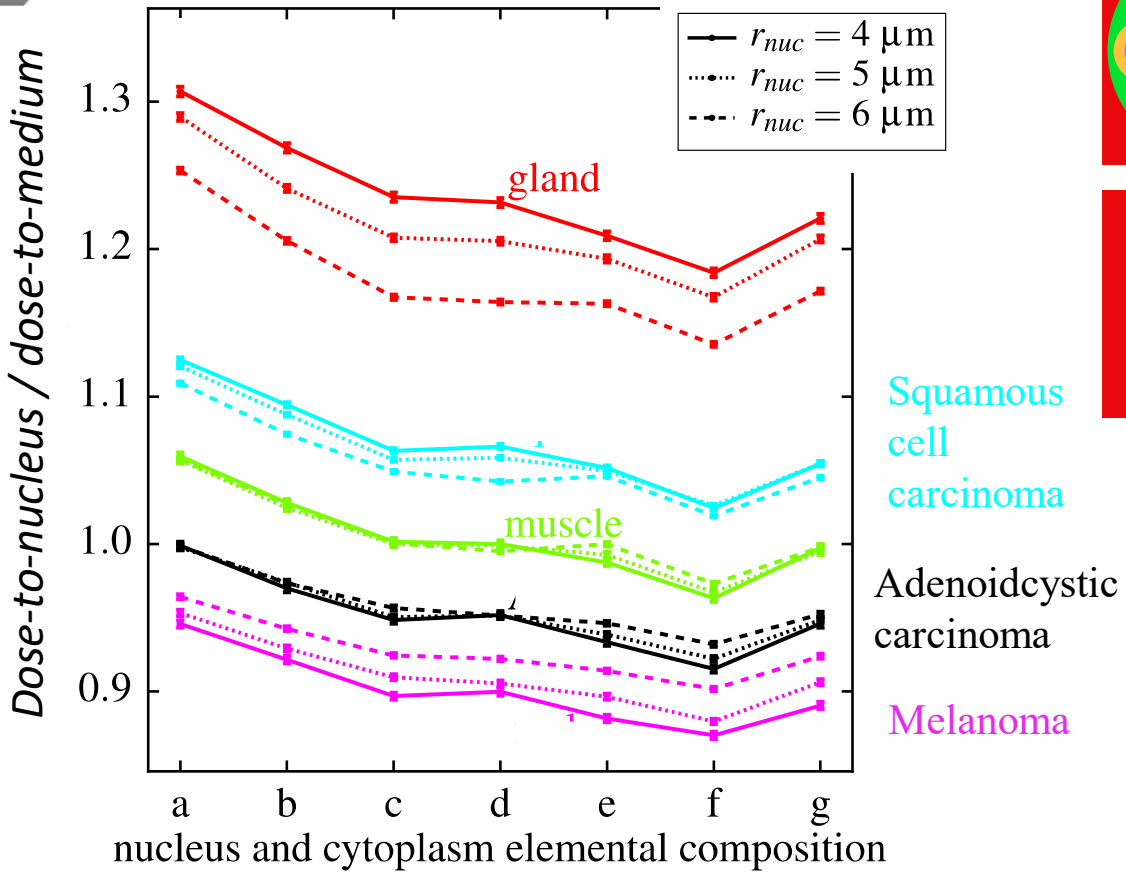


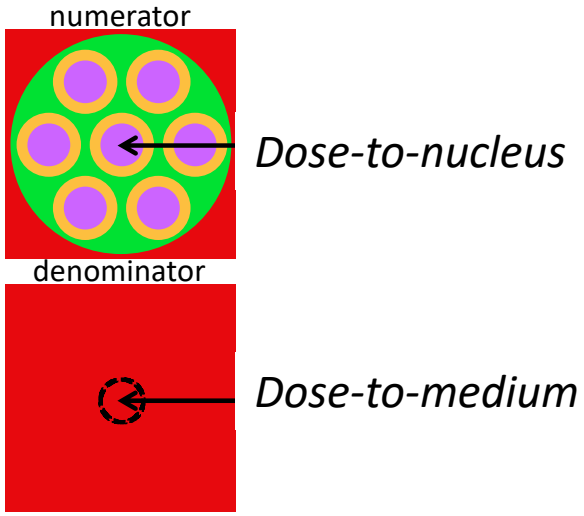


- 10% variation in nucleus doses with varying elemental composition
- Cell, nucleus size matters: 5% variation with nucleus size

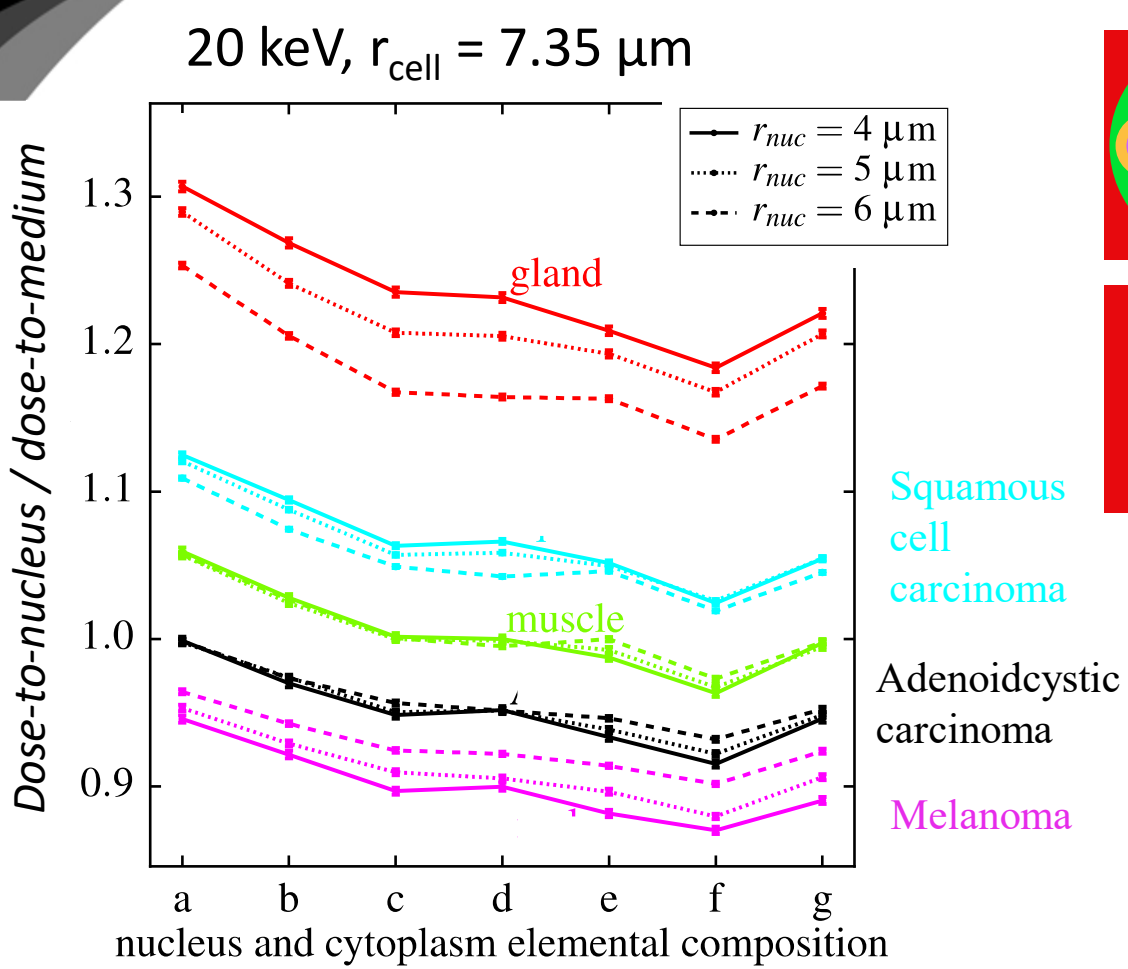
Nucleus dose varies with tissue

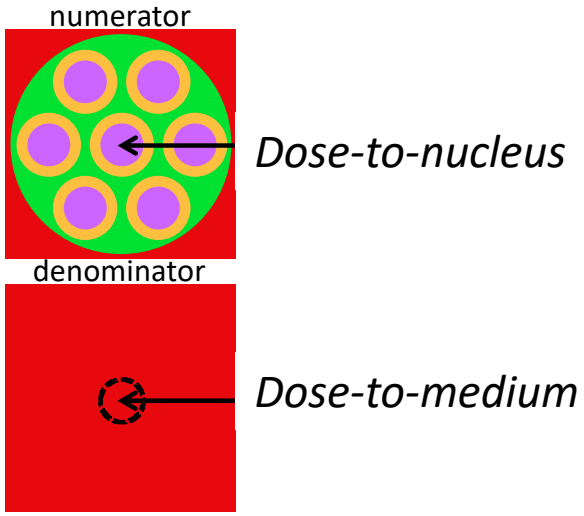
20 keV, r_{cell} = 7.35 µm





Nucleus dose varies with tissue

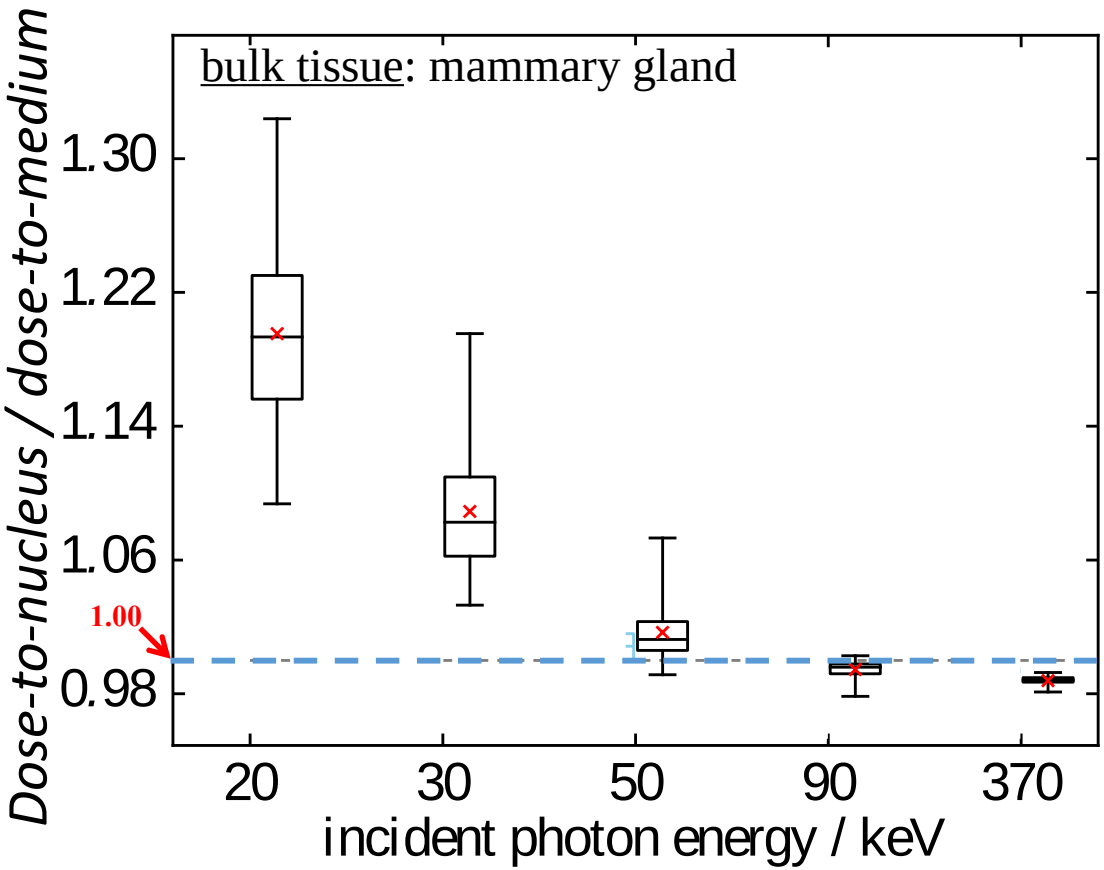




- Considerable variation in nucleus dose with tissue type

Nucleus dose varies with source energy

MC results for 63 different cell models (sizes, elemental compositions)



- Whiskers indicate min & max over set of results
- Box extends between upper and lower quartiles
- Line gives median; 'x' is mean

Oliver & Thomson, Phys. Med. Biol. **62** (2017)

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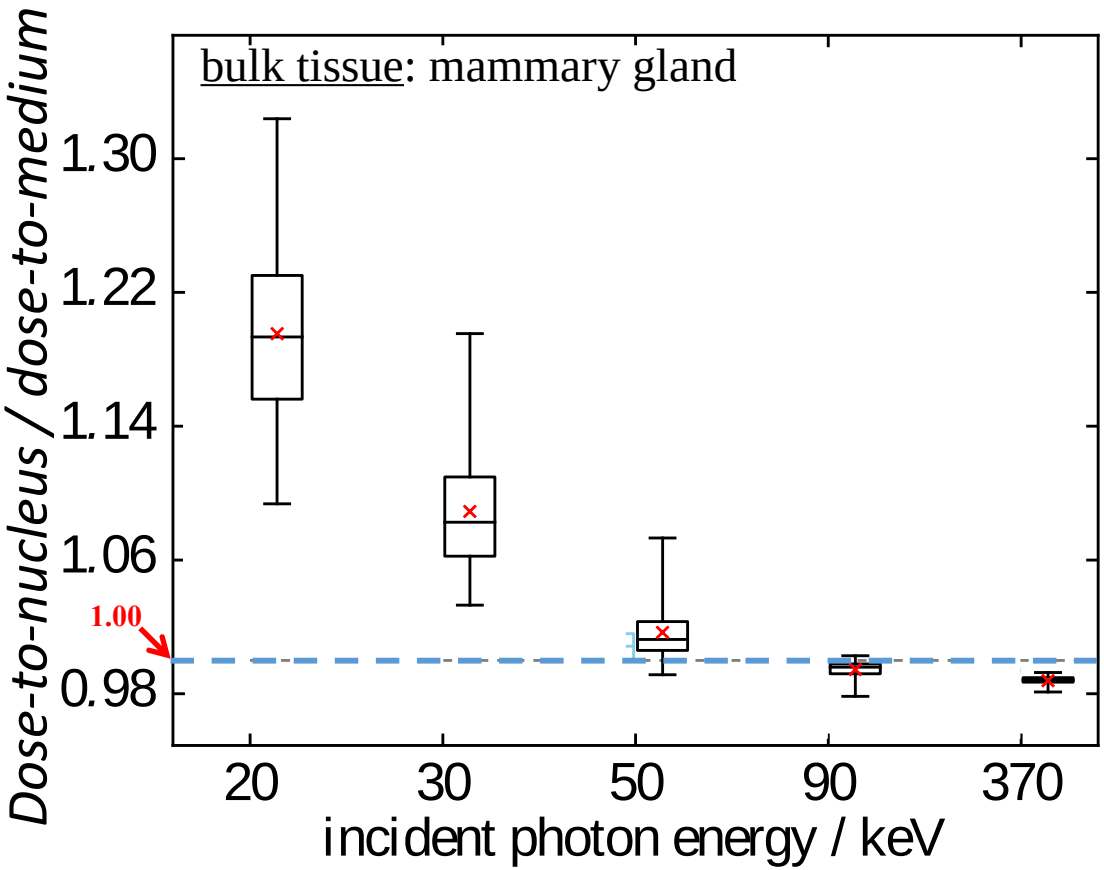

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→ Decreasing sensitivity to cell model with increasing source energy.

Oliver & Thomson, Phys. Med. Biol. **62** (2017)

Populations of cells

Stochastic nature of radiation transport and energy deposition

- Specific energy, z = energy imparted per unit mass
- Absorbed dose = mean specific energy

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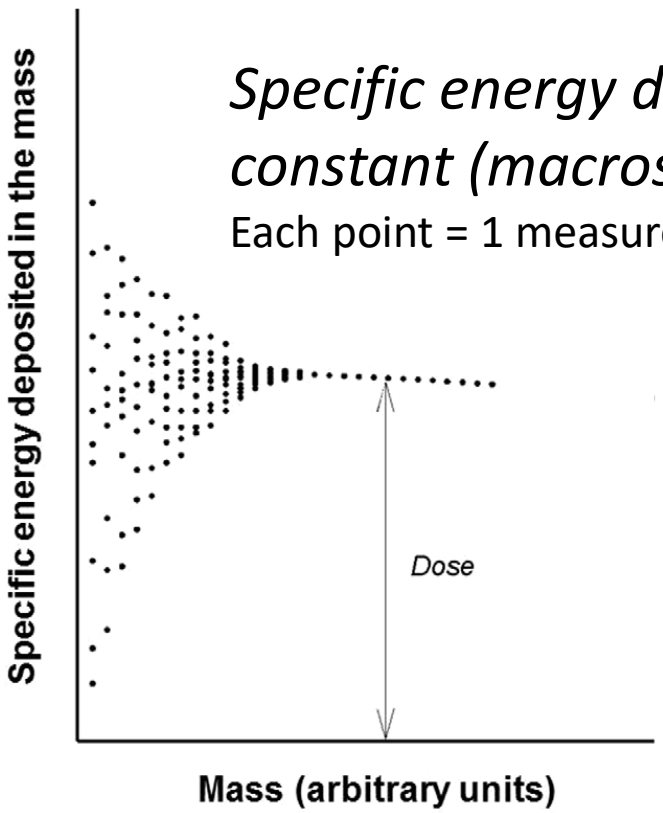
Specific energy deposited as a function of mass for constant (macroscopic) dose.

Each point = 1 measurement



Kron et al, Phys. Med. Biol. **61** (2016)

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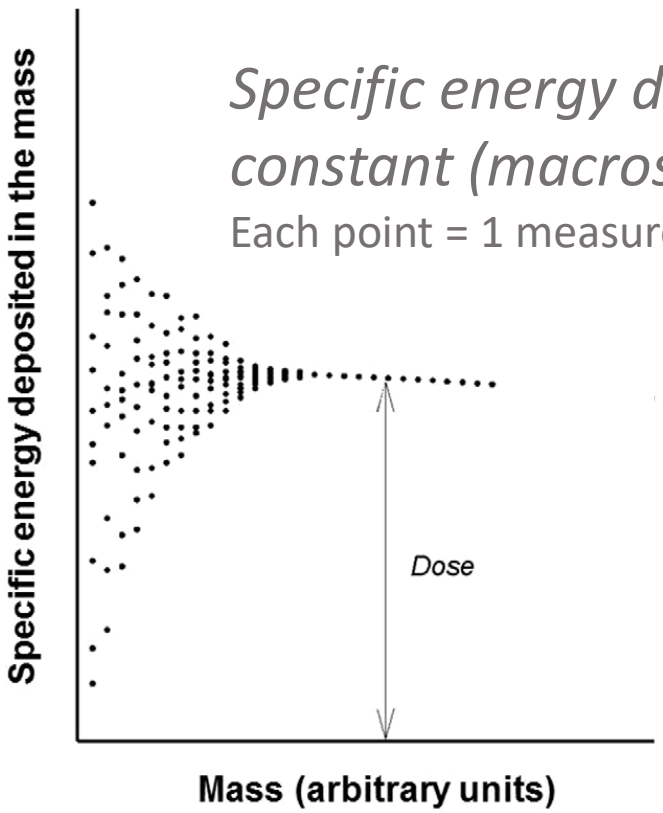

→ For low doses and small targets, specific energy varies over population of targets

Kron et al, Phys. Med. Biol. **61** (2016)

How to model populations of cells?

- Varying cell, nucleus sizes
- Intercellular spacing
- Cell arrangement

- Uncertainty in underlying microscopic structure

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Randomly sampled from normal distribution		
Uniform		

Oliver & Thomson, under review

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Cell arrangement method

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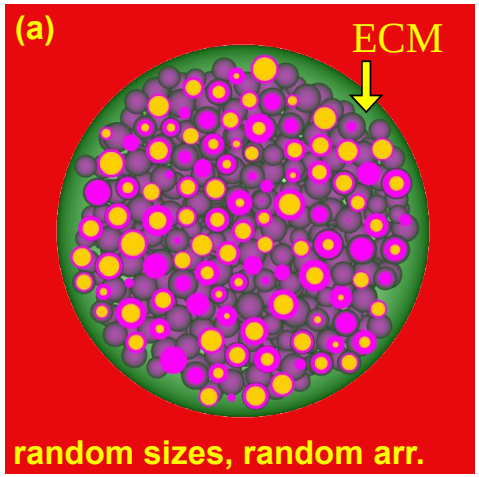
Randomly sampled from normal distribution		
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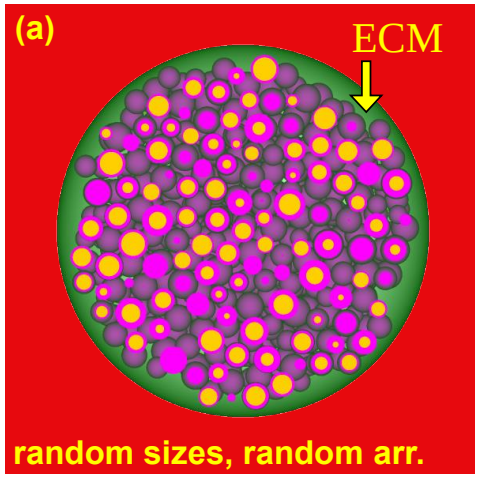
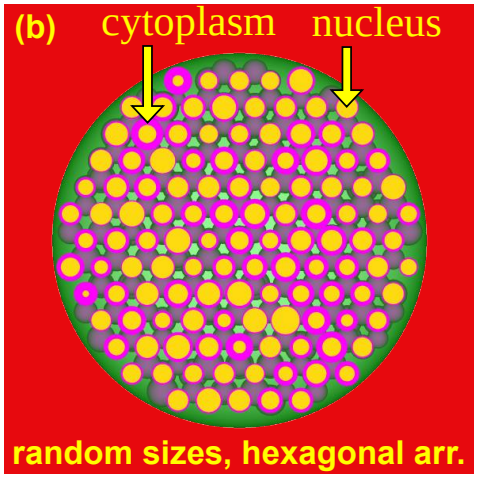
Randomly sampled from normal distribution		
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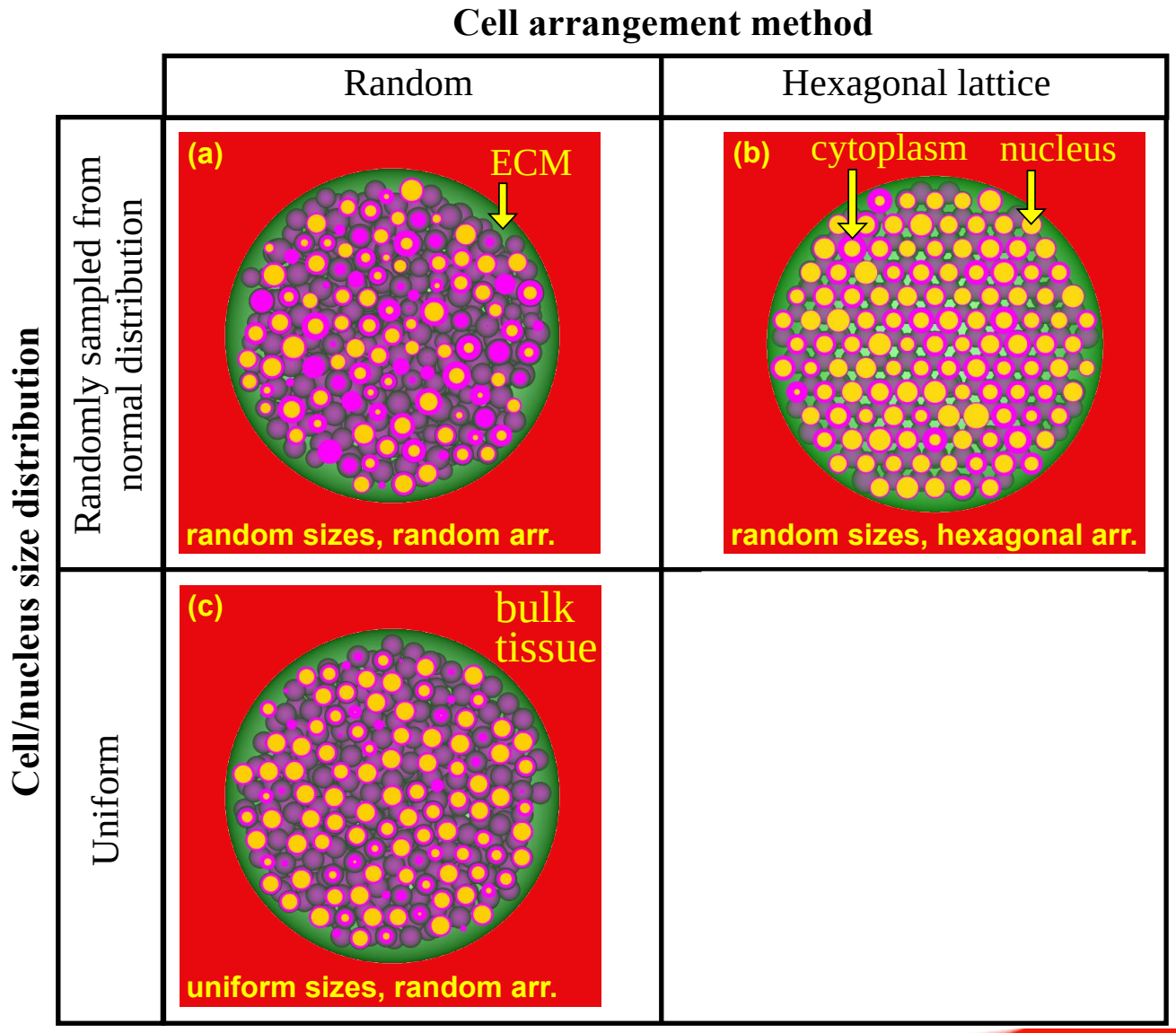

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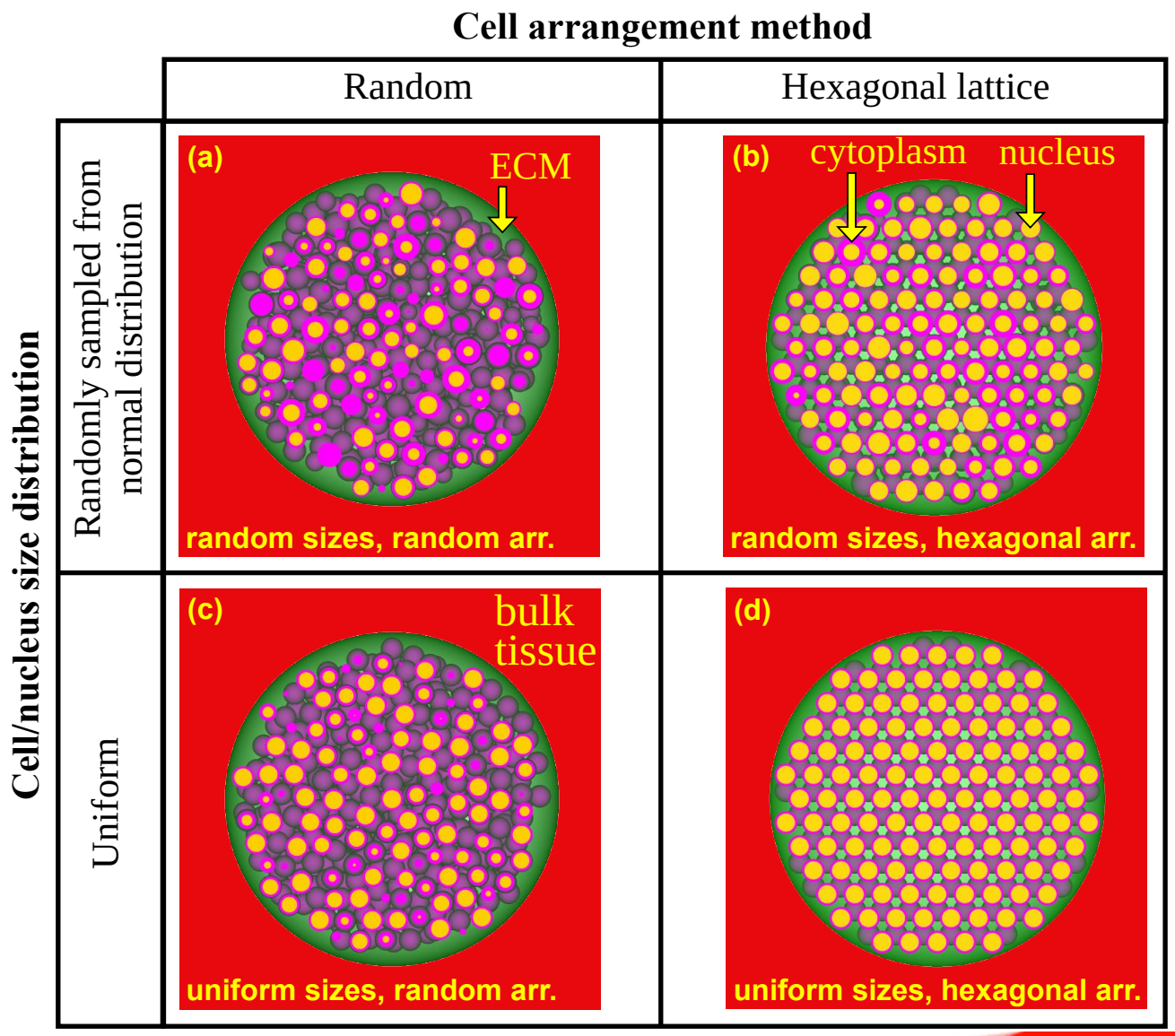

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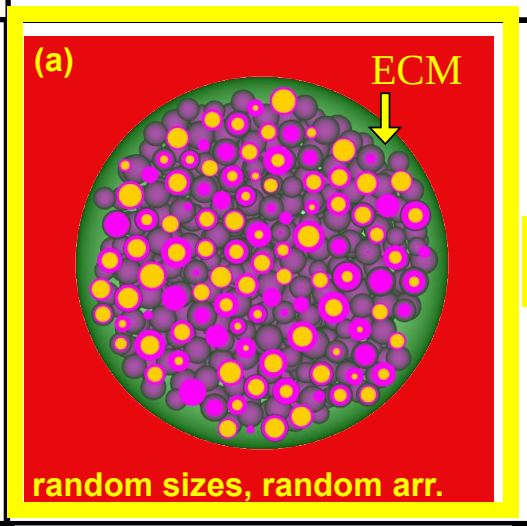
Randomly sampled from normal distribution	 Focus	
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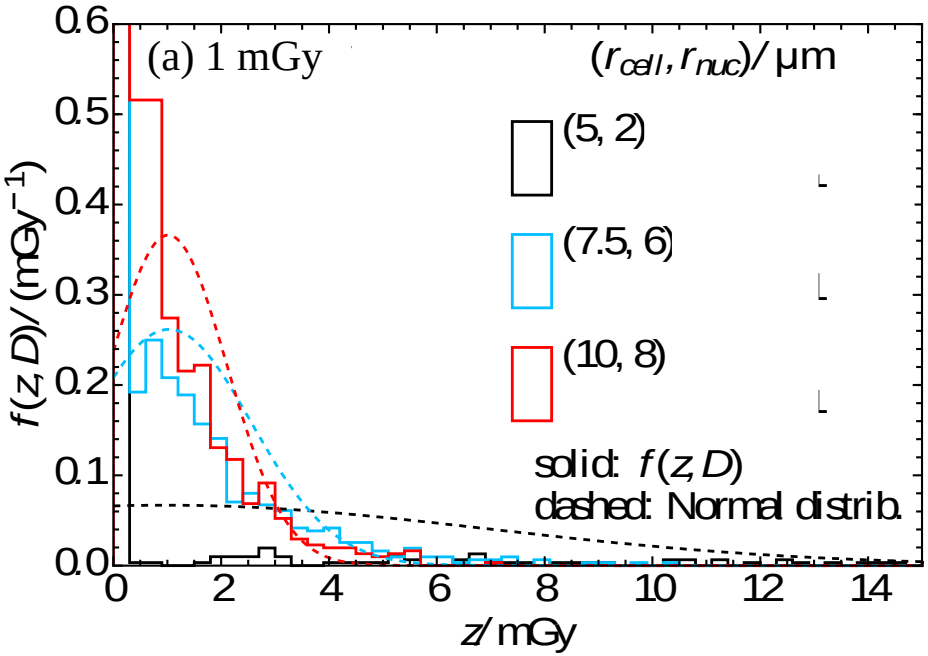
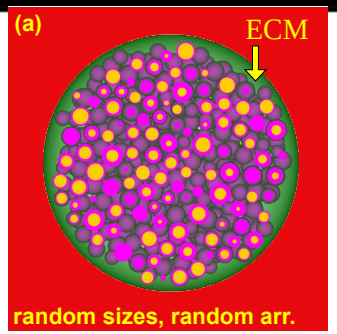
Specific energy distributions for nuclei

Histogram of nucleus specific energies over populations of >1000 cells





50 keV photons, melanoma

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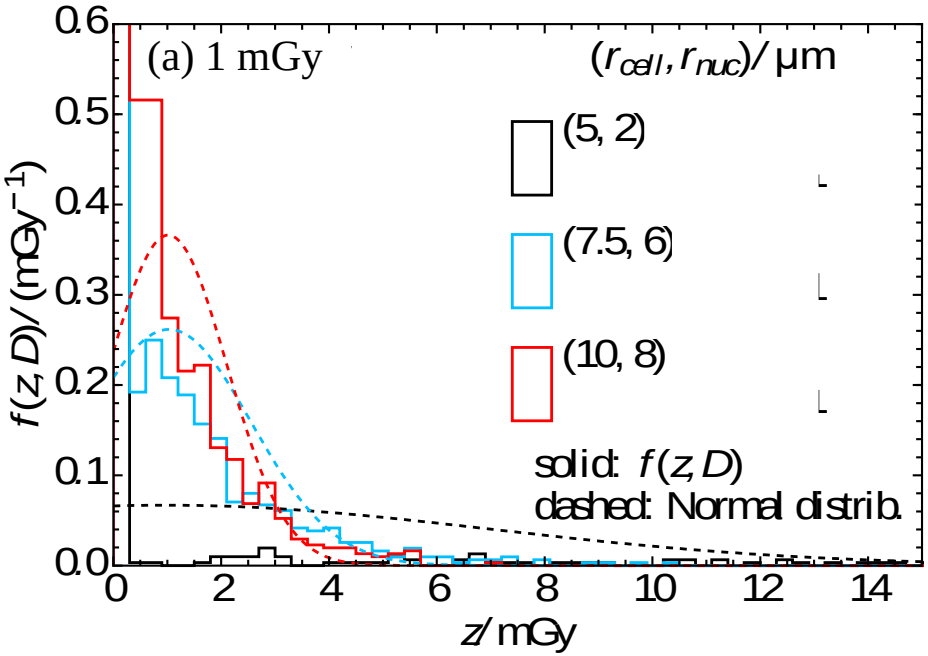

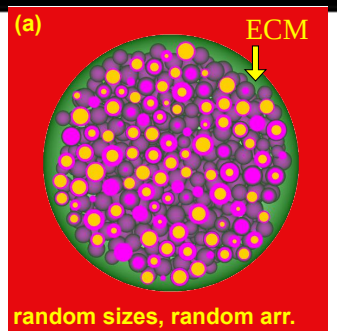

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Low dose:

- Distributions skewed (not-normal)
- Many nuclei receive no energy (1st bin truncated)

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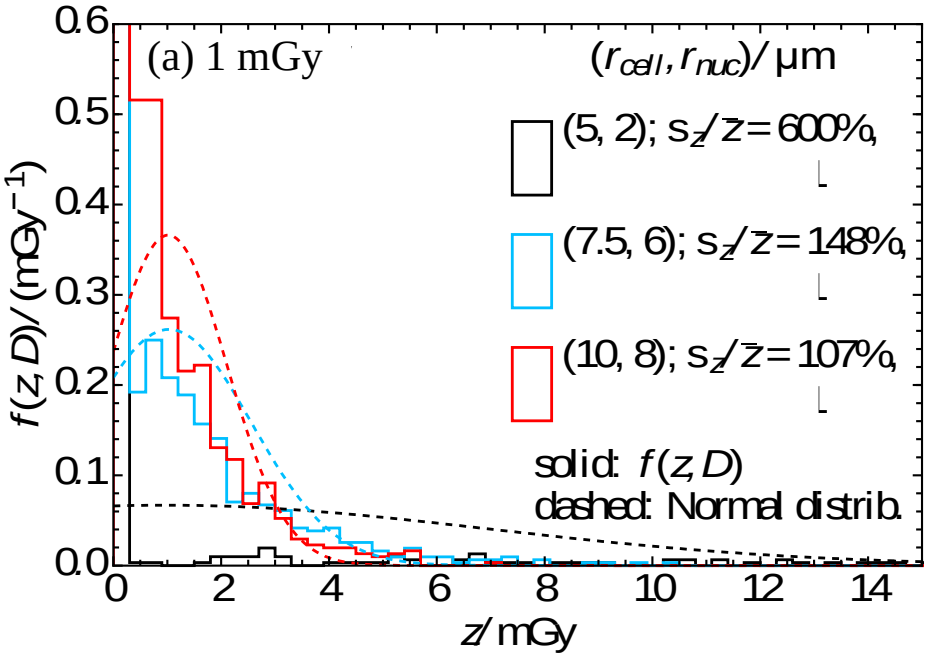
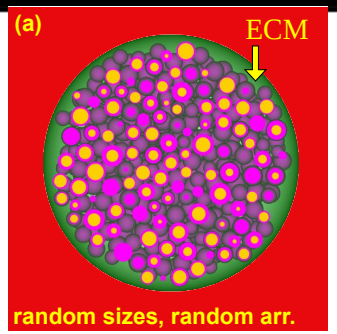




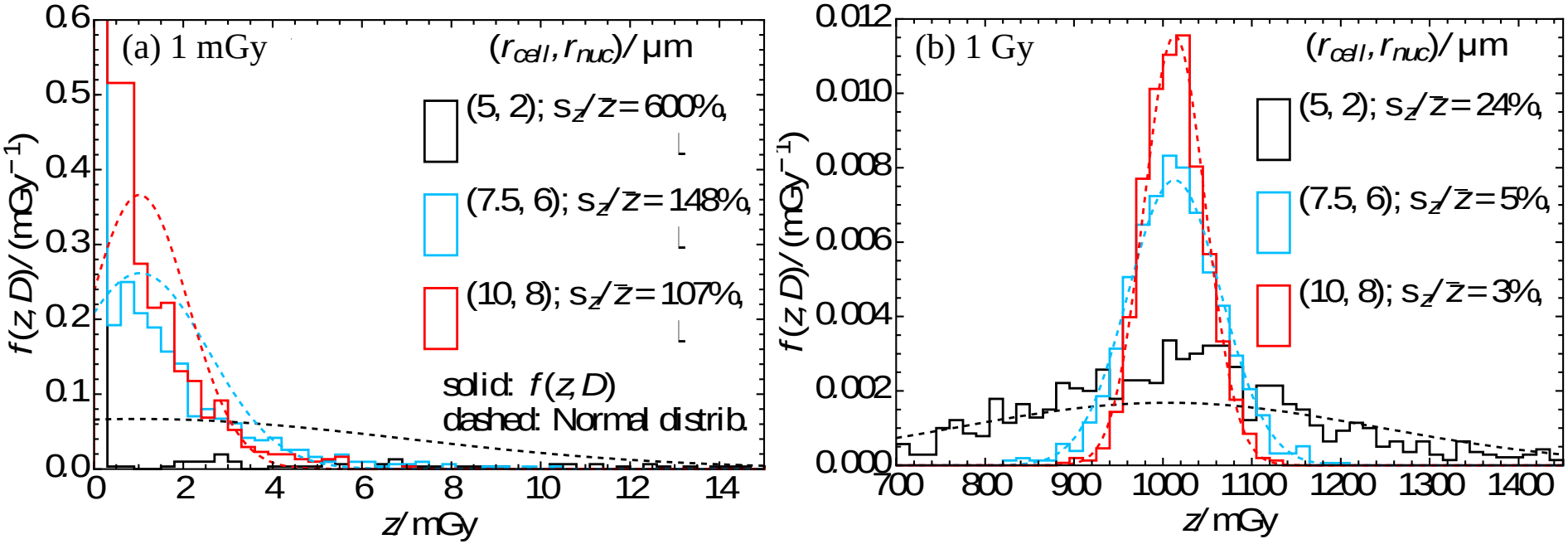
50 keV photons, melanoma

Low dose:

- Distributions skewed (not-normal)
- Many nuclei receive no energy (1st bin truncated)
- Relative variation in specific energy (σ_z/z) is large
- σ_z/z increases as nucleus/cell size decreases

Specific energy distributions for nuclei

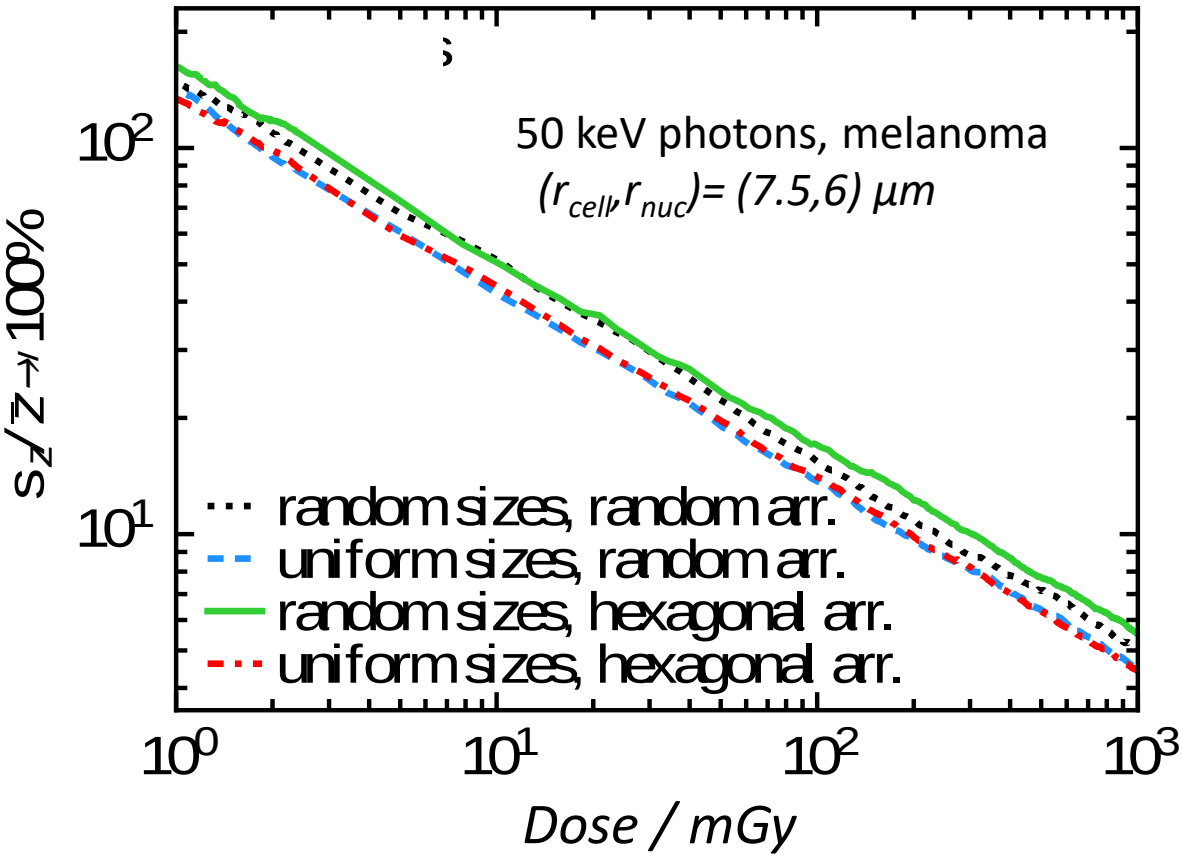
Dose (macroscopic) increases…

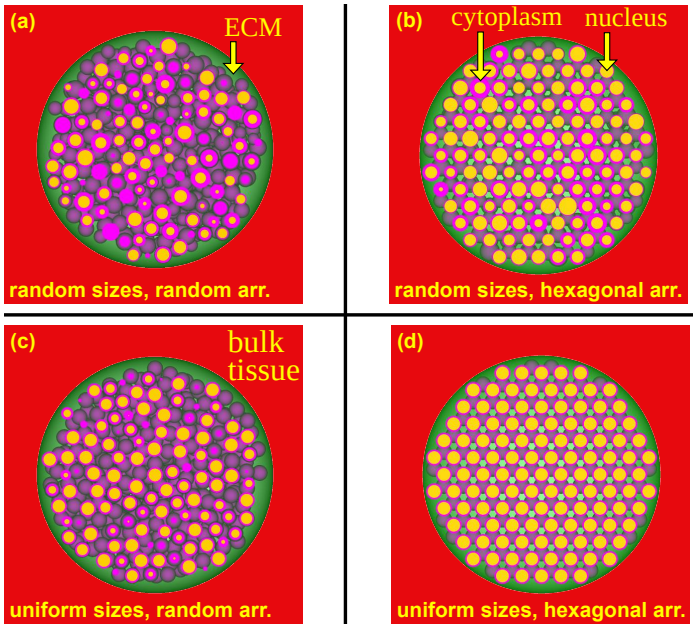


- Specific energy distribution approaches normality
- Relative variation in specific energy (σ_z/z) decreases

Sensitivity to cell population model

Relative standard deviation of the specific energy versus dose





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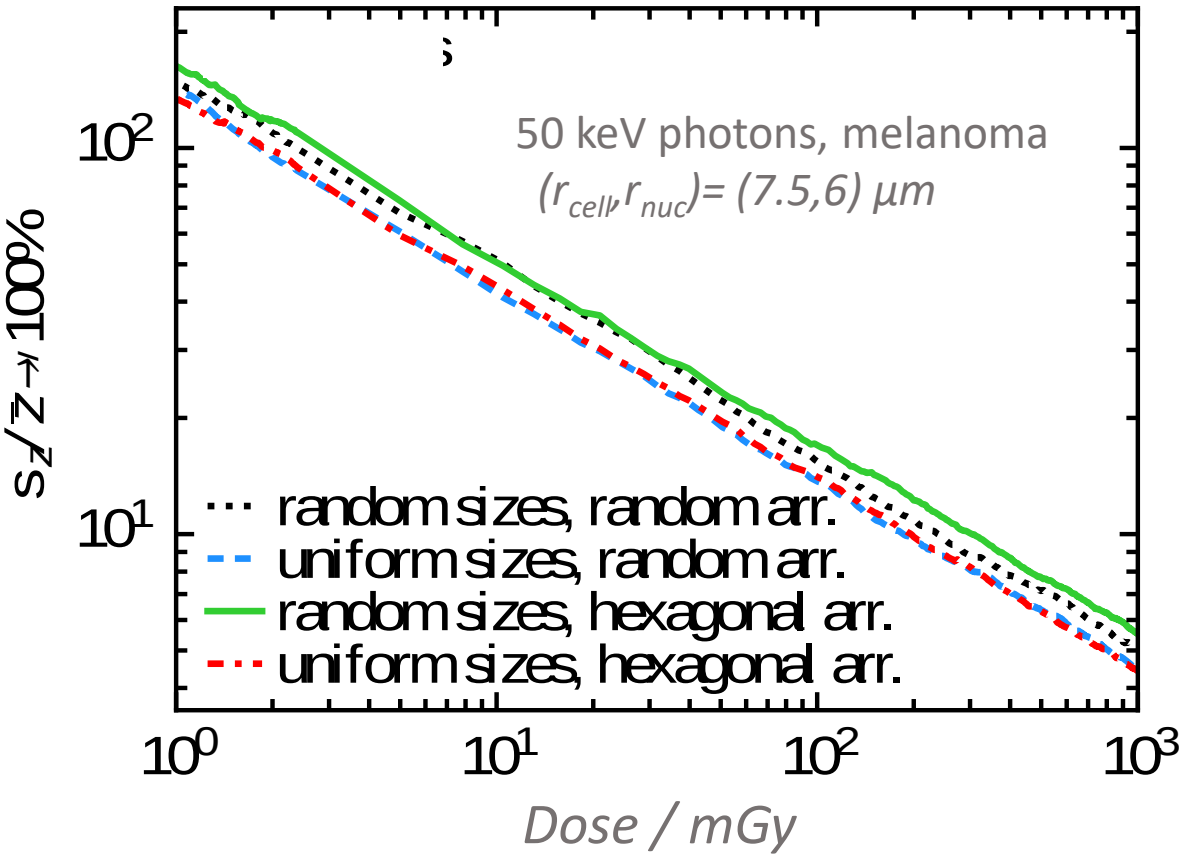
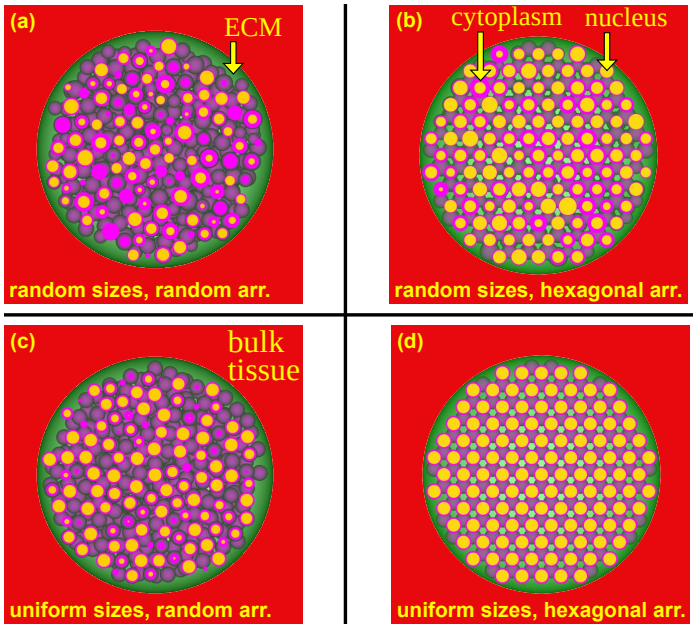
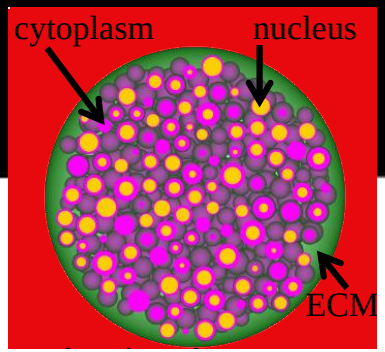




- Sensitive to cell/nucleus size distribution (σ_z/z smaller for "uniform")
- Less sensitive to cell arrangement method

MC simulations of cells



- Considerable variation in cell morphology (size, elemental composition) with tissue type, normal versus cancerous
- Cells are not radiologically water equivalent
- Investigated specific energy distributions within cell populations; sensitivity to cell/nucleus size distribution

Thomson et al, Phys. Med. Biol. **58** (2013)
Oliver & Thomson, Phys. Med. Biol. **62** (2017) X 2

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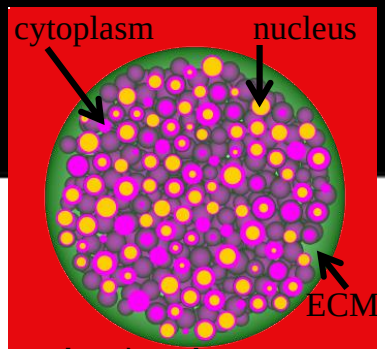

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Challenges:

- Uncertainties in microscopic tissue models – size, shape, composition
- Simulation efficiency – decreases with # of cells
- Verification of results

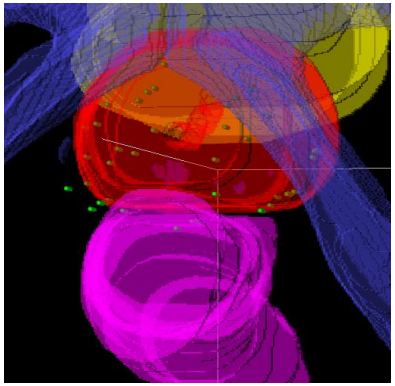
Poster @ CIRMS – Martin Martinov

Today: Monte Carlo simulations

Scale

cm

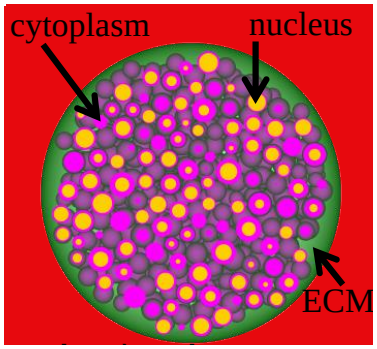
Patient



"Microdosimetry"

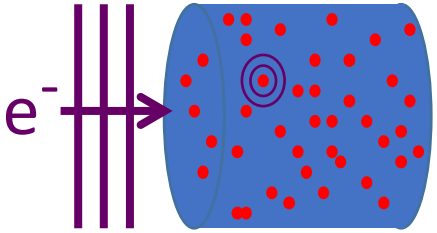
µm

Cells: microscopic tissue models, populations of cells



nm

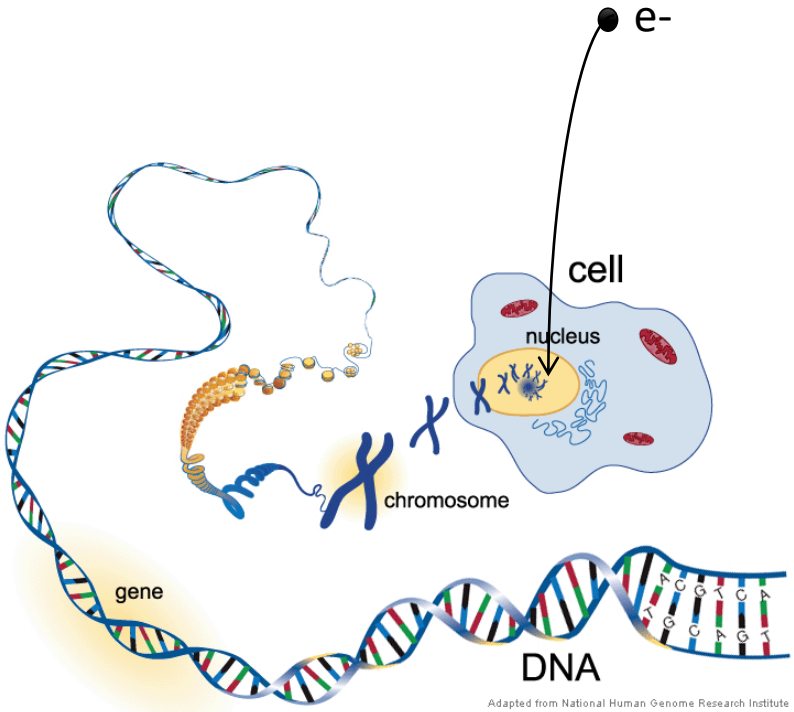
Subcellular, DNA: low-energy electron transport



Low-energy simulations

- Monte Carlo simulations of radiation transport at low (sub-keV) energies of increasing importance

- Understand radiation-induced damage on short length scales (cell components, DNA) → biological response to radiation

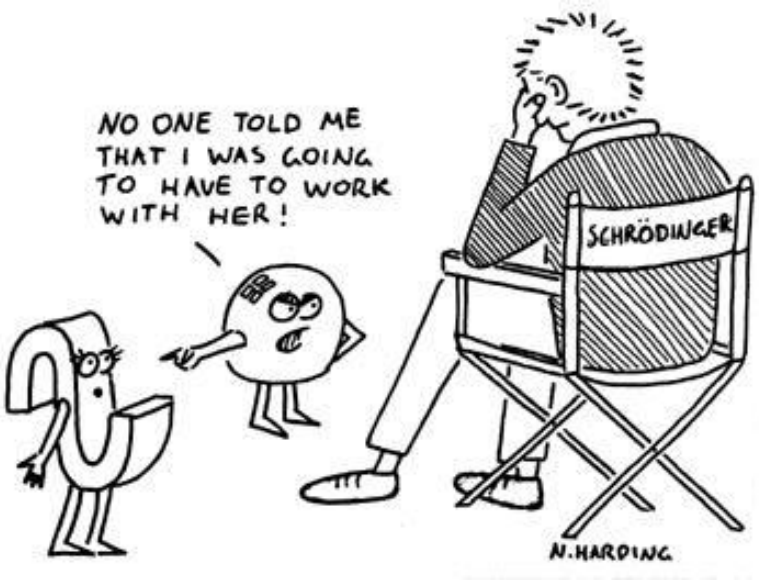


https://elcaminogmi.dnadirect.com/img/content/common/cellsToDNA.gif

Low-energy simulations

- Various MC codes are being applied to eV energies and below, e.g. GEANT4-DNA

- In these “track” or “trajectory” MC codes, electrons are point-like objects → quantum wave nature is ignored.



Potential for quantum effects - MC valid?

Medical Physics Letter Med. Phys. **38** (2011).

On the Monte Carlo simulation of electron transport in the sub-1 keV energy range

Rowan M. Thomson[a)]
Ottawa Carleton Institute for Physics, Carleton University Campus, Ottawa, Ontario K1S 5B6, Canada

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Investigated validity of classical trajectory MC electron transport in the context of quantum theory

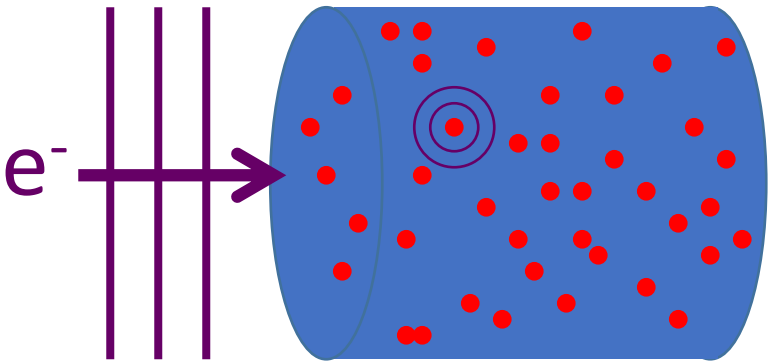
- Quantum effects may be non-negligible for electrons with sub-1 keV energies in condensed media
- Classical trajectory MC technique is questionable for sub- 1 keV energies – research needed…

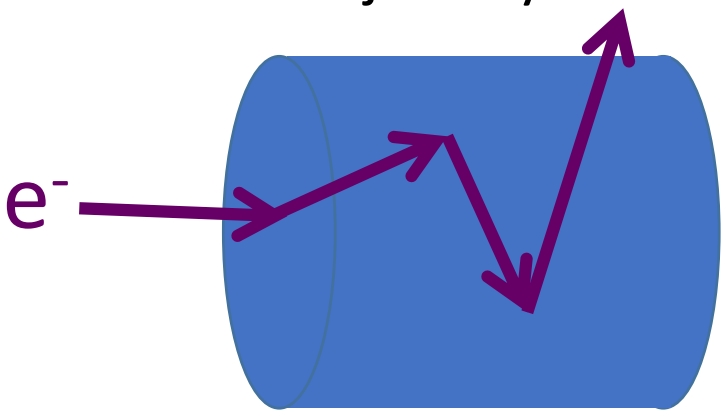
Simplified model of electron transport

Quantum mechanical
QM

versus

Classical
trajectory MC





Point scatterers represent water molecules off which electrons may scatter isotropically

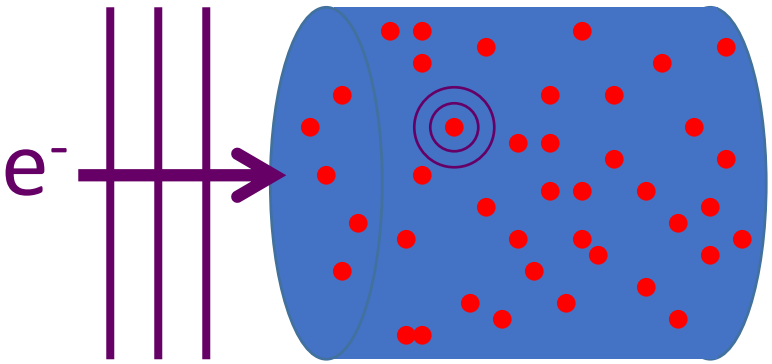
Water droplet is homogeneous

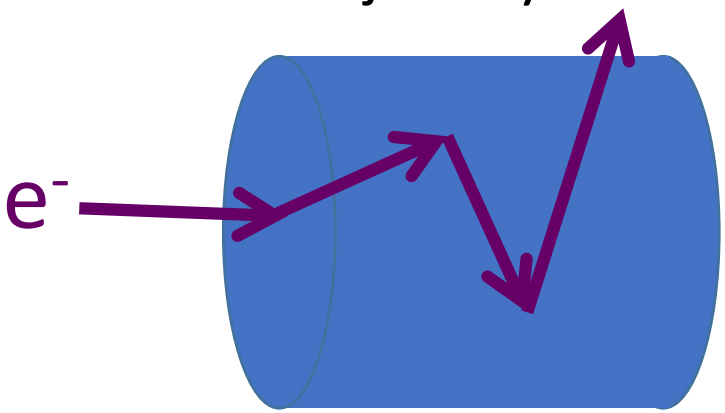
Simplified model of electron transport

Quantum mechanical QM

versus

Classical trajectory MC





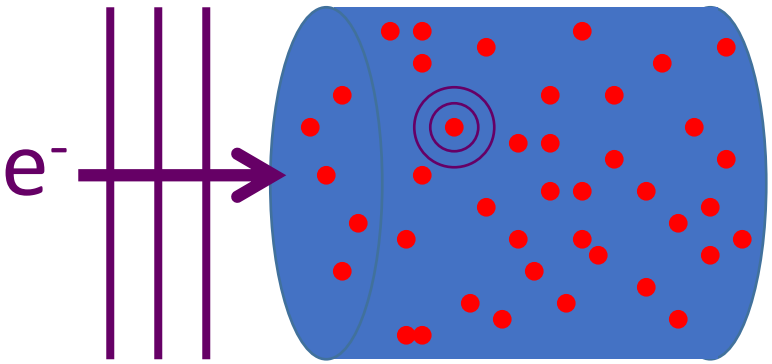
- Consider elastic isotropic scattering and inelastic scattering via absorption
- Mean free path is same for QM and MC calculations
- Vary droplet size (few nm), shape, number of scatterers

Today: radius, length 2.124 nm cylinder 1000 scatterers

QM calculations

$0.05\ \text{nm} \leq \lambda \leq 0.47\ \text{nm}$

600 eV 7 eV



- Random numbers determine point scatterer positions
- Average scatterer separation: d_{av}=0.311 nm
- Structure: 0.001 nm < d_{min} < 0.28 nm

Head-Gordon and Hura, Chem. Rev. **103,** 2651 (2002)

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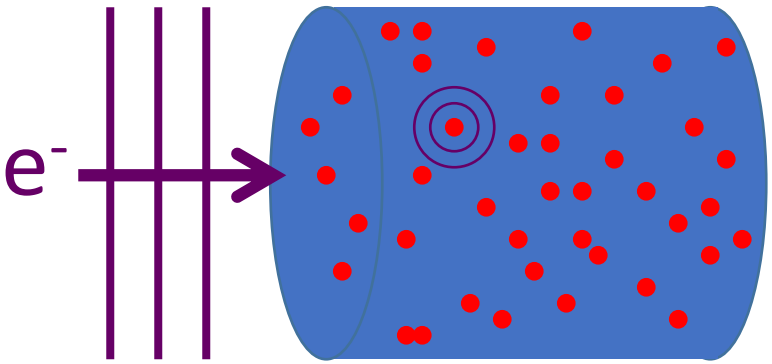

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Head-Gordon and Hura, Chem. Rev. **103,** 2651 (2002)

- Numerically solve ~10^3 coupled equations to find electron wavefield incident on each scatterer
- For each set of model parameters, simulate ~10^5 water droplets each having different scatterer positions and average results over all droplets

Foldy, Phys. Rev. **67**, 107 (1945).
Liljequist, Rad. Phys. Chem. **77**, 835 (2008)

Calculations

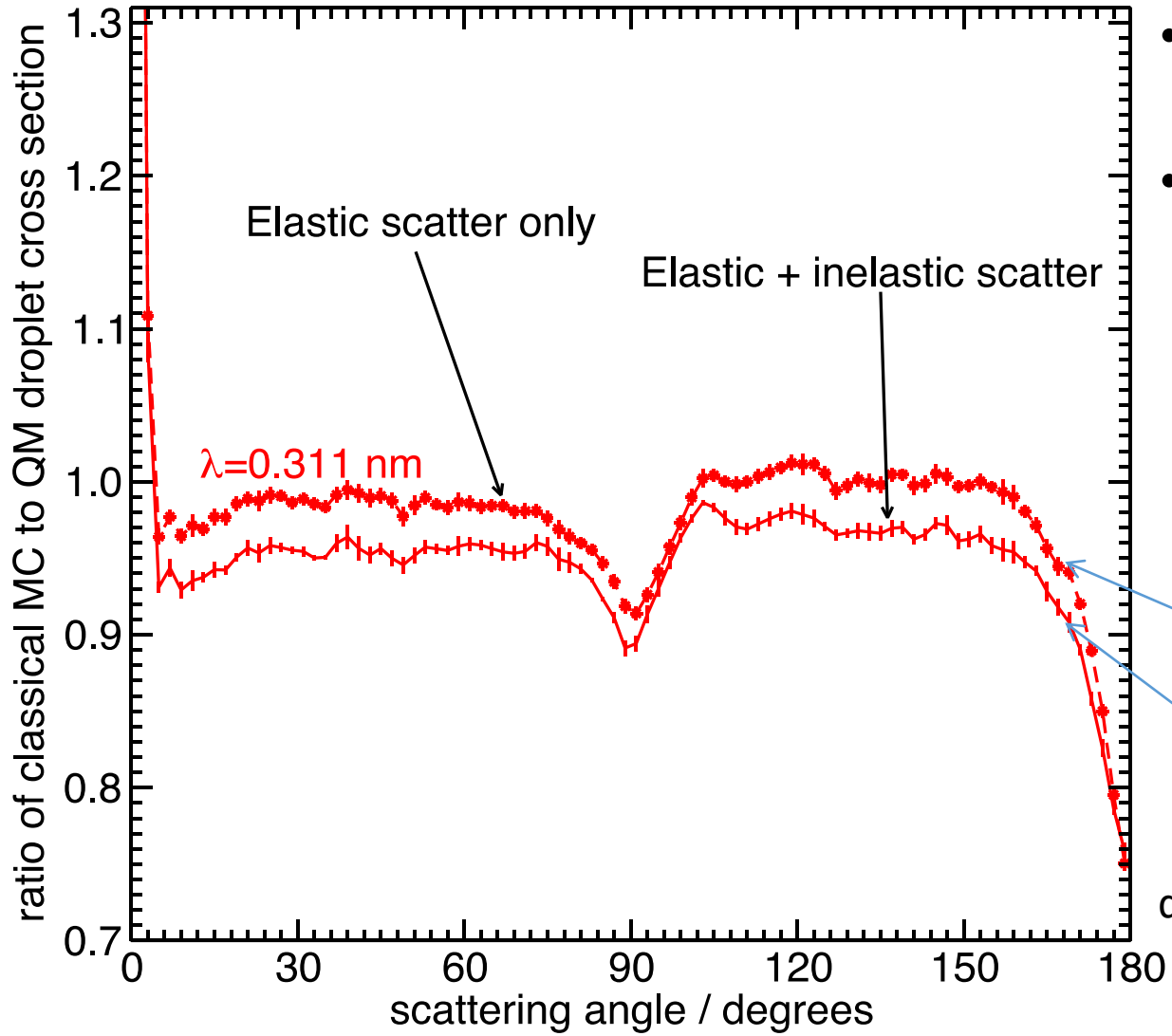
Within each of the QM and MC frameworks, compute Droplet Cross Section (*CS*)

$$CS(i) = \frac{\#\text{ of electrons escaping water droplet in polar angle interval } i}{\#\text{ of incident electrons per unit area}}$$

Compute Relative Error on classical trajectory MC results (relative to QM results):

$$\text{Relative Error (CS)} = \frac{\sum_i |CS_{QM}(i) - CS_{MC}(i)|}{\sum_i CS_{QM}(i)} \text{ (sum over polar angle intervals } i\text{)}$$

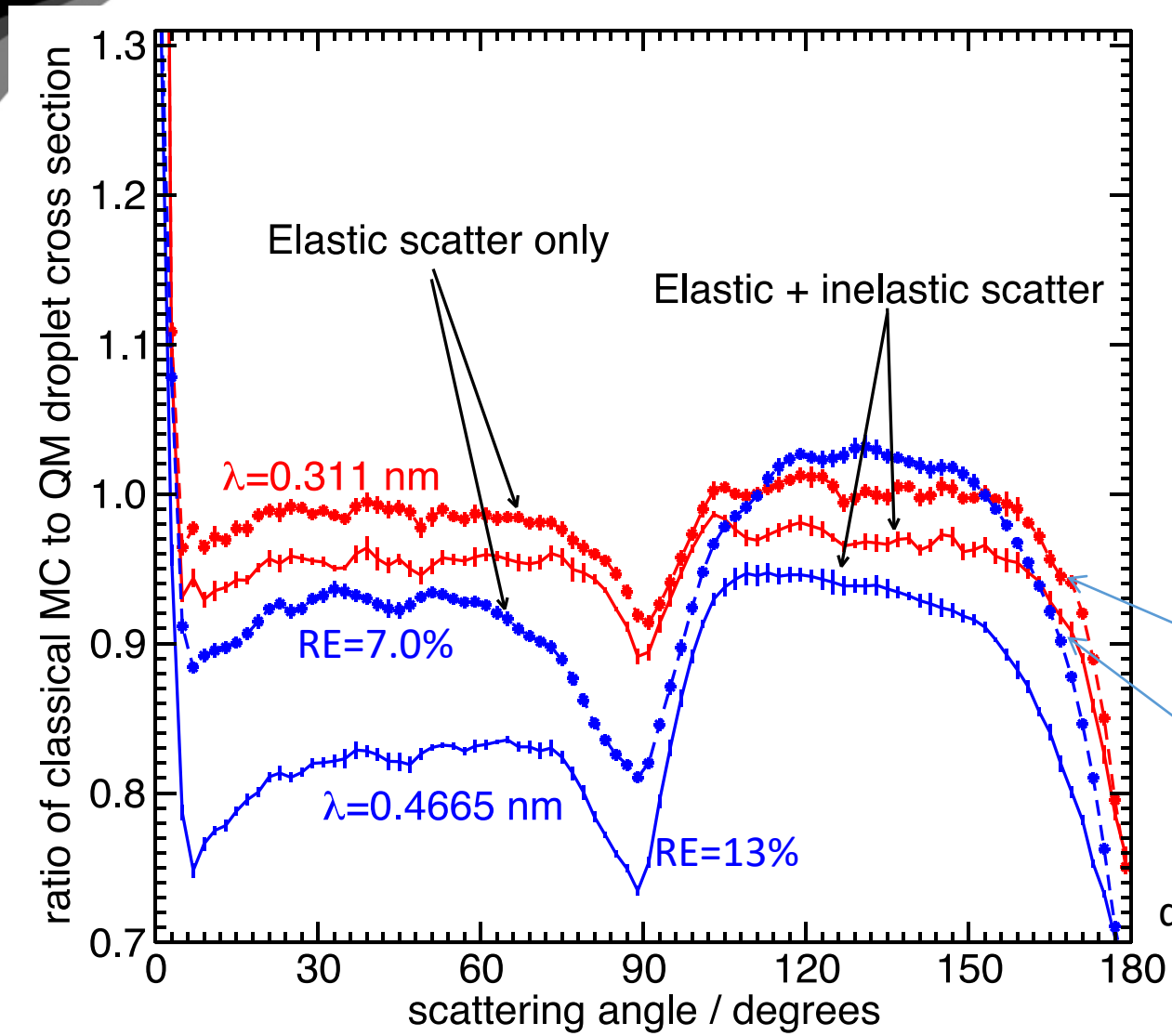
Effect of inelastic scatter



- Maintain same elastic cross section
- Inclusion of inelastic scatter generally increases disagreement between MC and QM

d_{min}=0.001 nm→ no structure

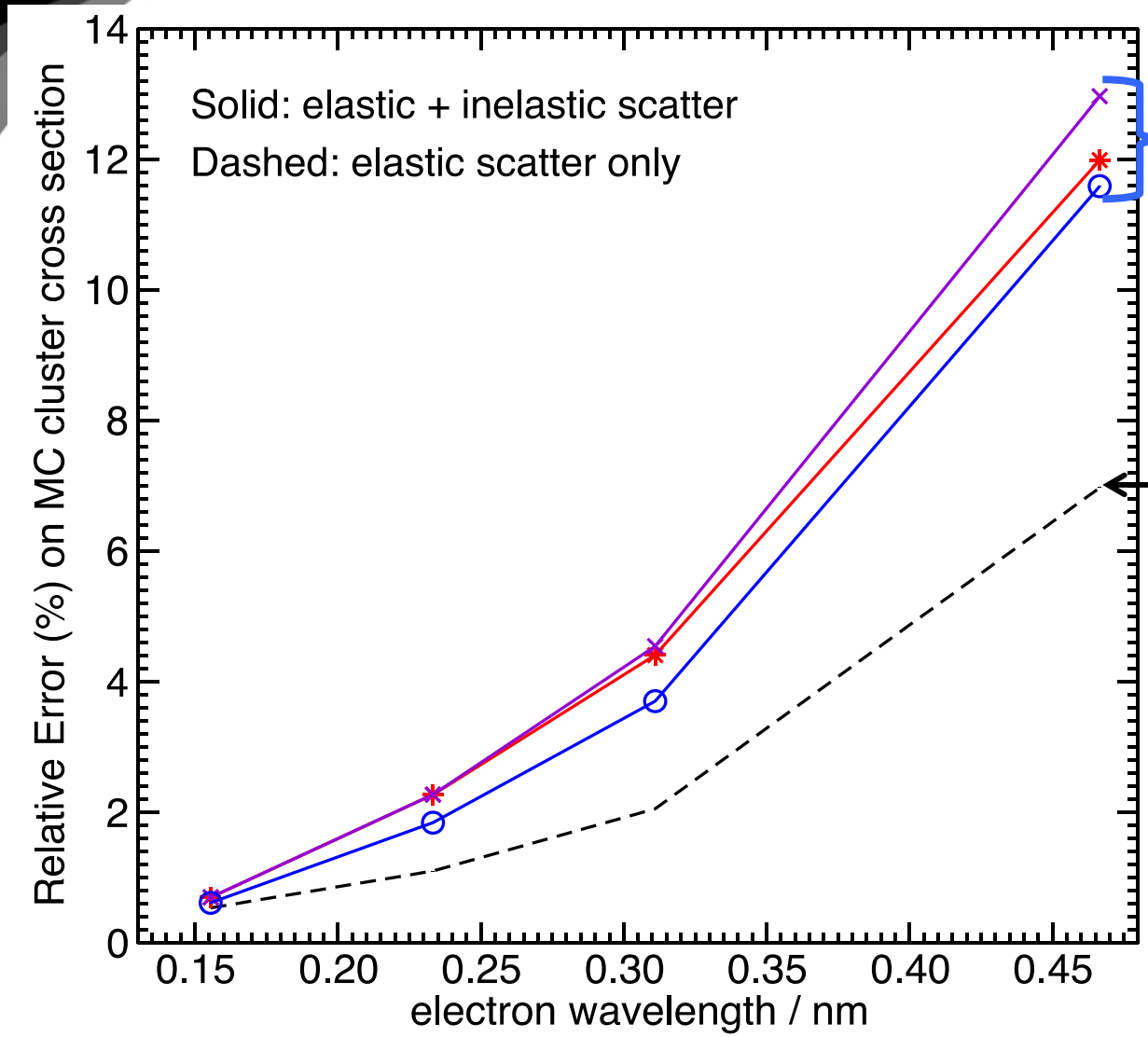
Effect of inelastic scatter



- Increase wavelength: differences between MC and QM increase
- Results depend on inelastic cross section

d_{min}=0.001 nm→ no structure

Effect of inelastic scatter



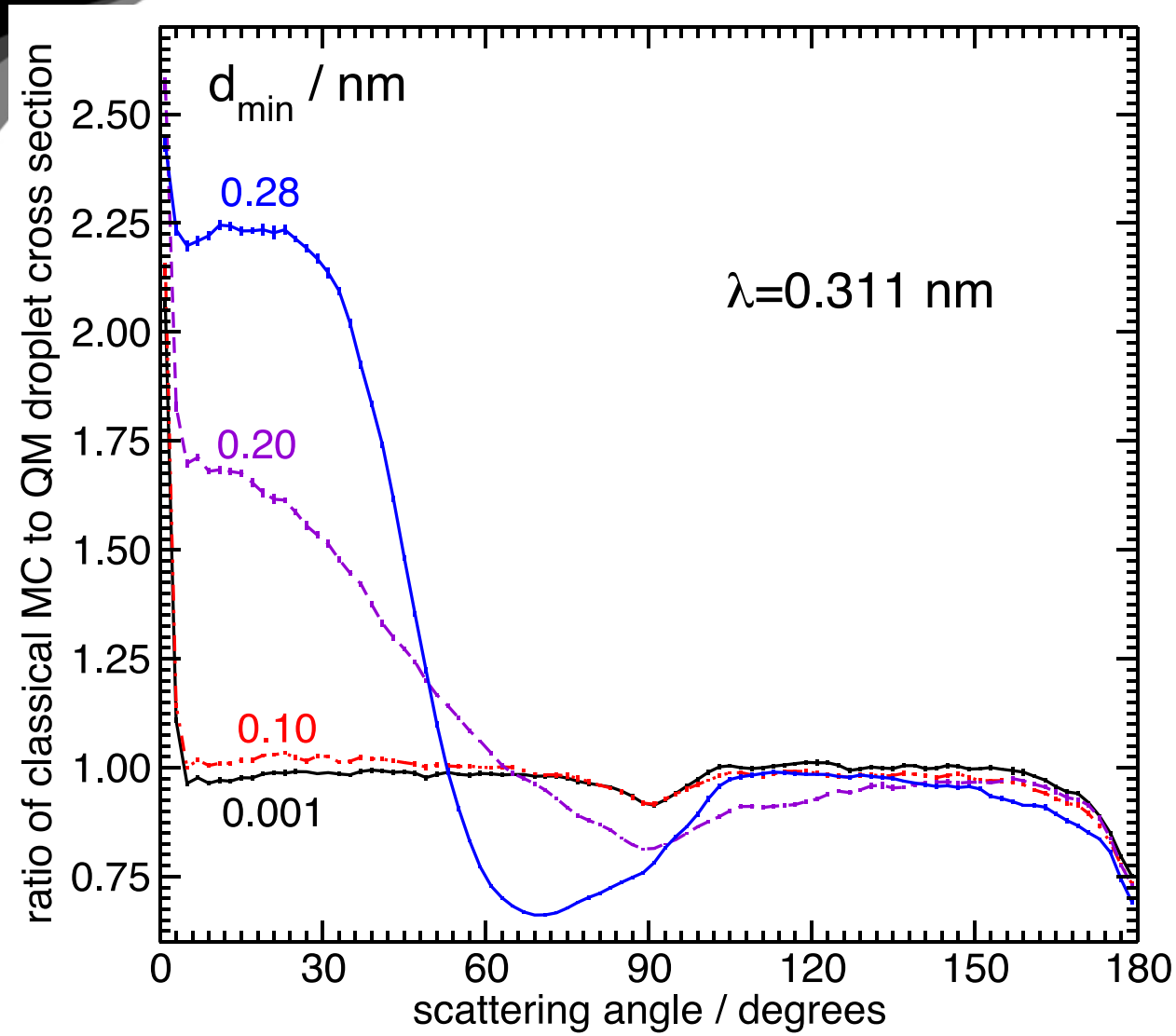
Elastic + Inelastic scatter: different colours correspond to different inelastic cross sections

Elastic scatter only

Elastic cross section constant

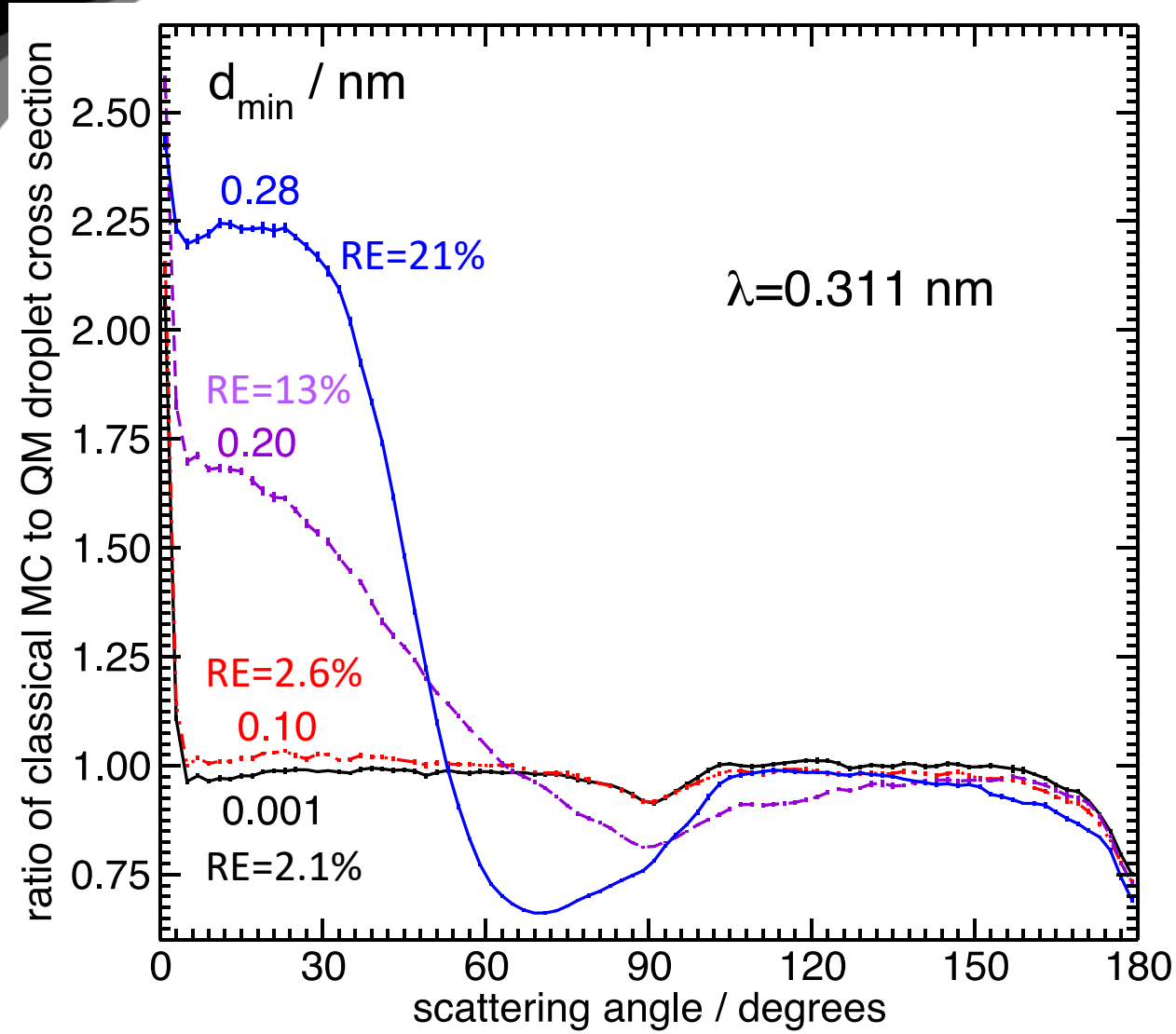
d_{min}=0.001 nm→ no structure

Effect of structure



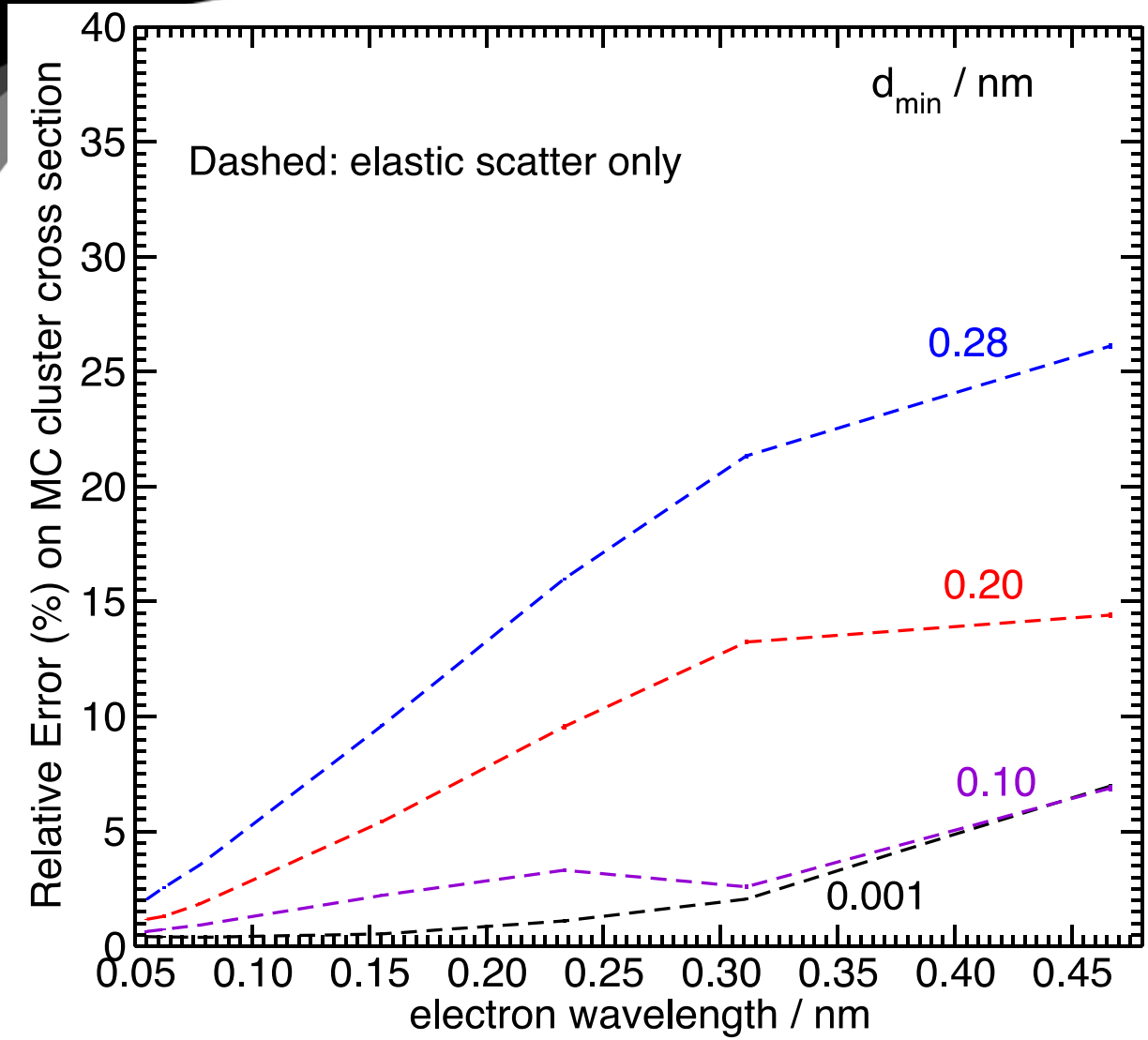
- Elastic scattering only
- Inclusion of structure increases disagreement between MC and QM

Effect of structure



- Elastic scattering only
- Inclusion of structure increases disagreement between MC and QM

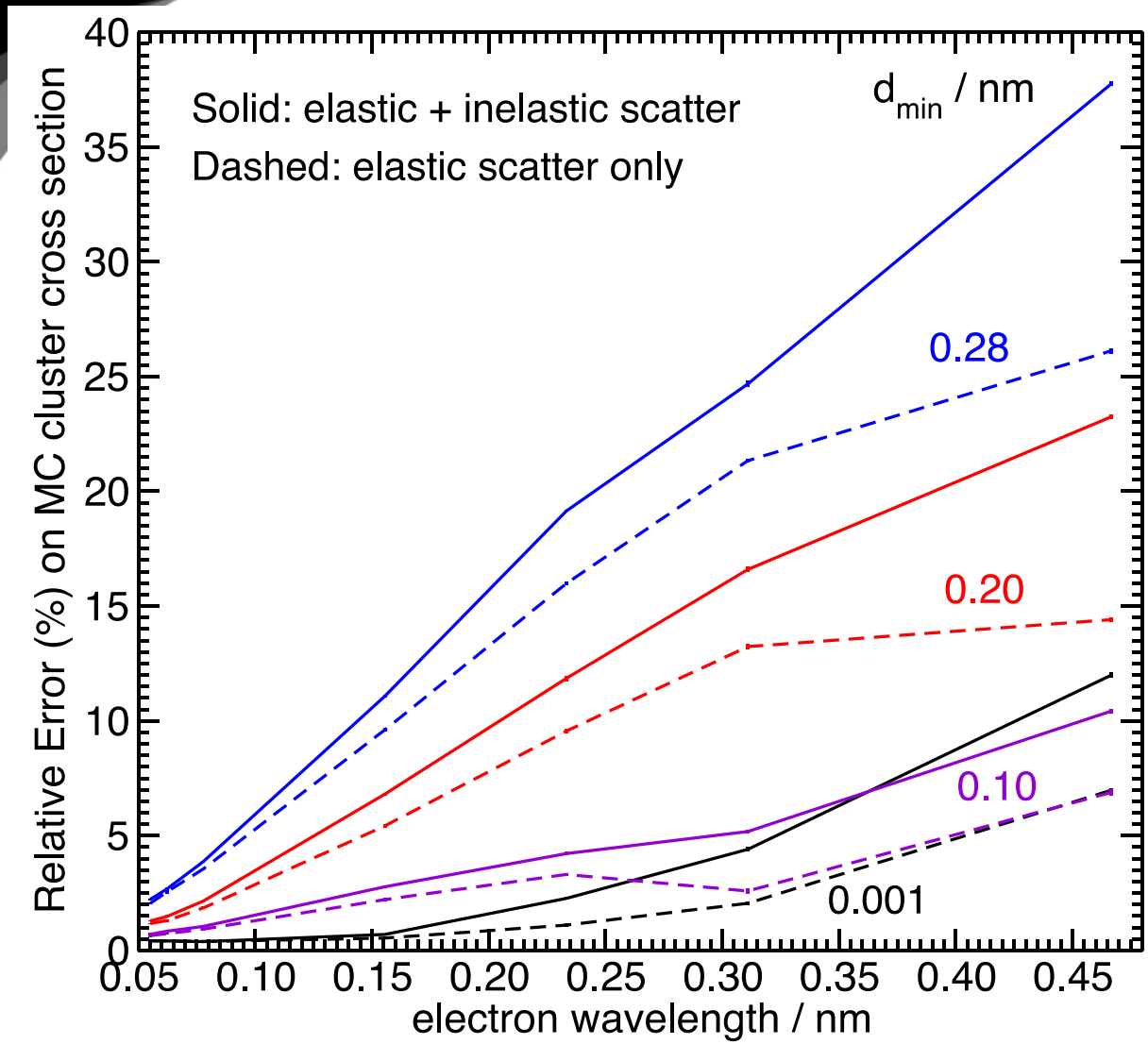
Effect of structure



- Relative errors substantially increase with increasing d_{min} corresponding to an increasingly structured medium
- 0.28 nm = realistic centre-to-centre distance between water molecules

Head-Gordon and Hura, Chem. Rev. **103,** 2651 (2002)

Effect of structure + inelastic scatter



- As before, elastic cross section remains the same; introduce inelastic scatter
- Inelastic scatter increases relative error

→ Inclusion of inelastic scatter and structure generally result in substantial increases in relative error compared with elastic scatter alone

Low energy e- transport

- Quantum wave nature of electrons should be considered for simulation of sub-1 keV electron transport in condensed media → Classical trajectory MC approach questionable

Low energy e- transport

- Quantum wave nature of electrons should be considered for simulation of sub-1 keV electron transport in condensed media → Classical trajectory MC approach questionable

- Simplified model of electron transport in water droplets including elastic and inelastic scattering, medium structure:
  - Results sensitive to electron wavelength, droplet structure, elastic and inelastic cross sections
  - Relative Error on classical MC increases substantially with inclusion of inelastic scatter, structure

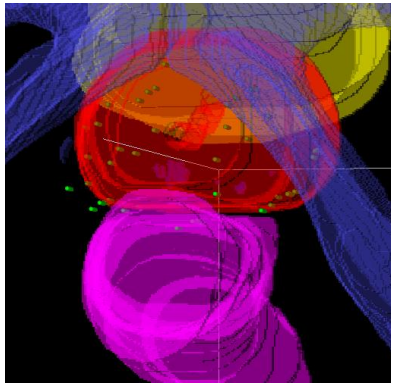
- Future: work towards more realistic QM models

Thomson and Kawrakow, Phys. Med., accepted (2018)

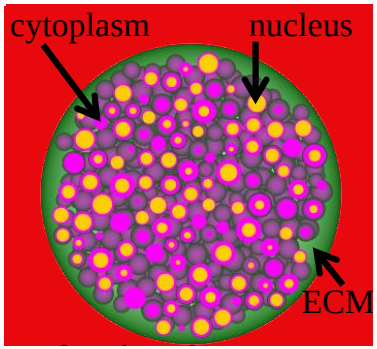
Summary & outlook

Scale

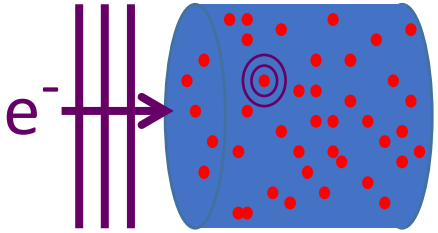
cm Patient



µm Cells



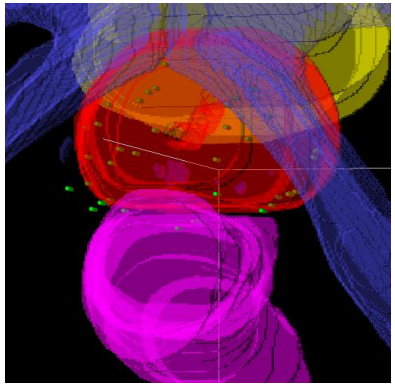
nm Subcellular, DNA



Summary & outlook

Scale

cm Patient



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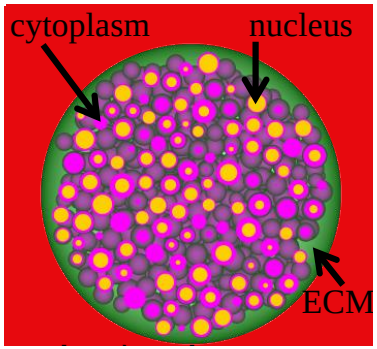

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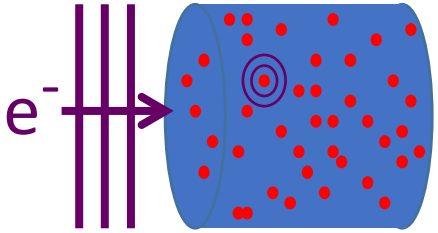

→ MC simulations to advance radiation therapy

- Improve existing treatment methods
- Advance understanding of biological response to radiation
- Develop new treatment approaches -nanoparticles for radiation therapy

Poster @CIRMS – M. Martinov

Thanks

Carleton UNIVERSITY
Canada's Capital University

Patricia Oliver, Martin Martinov, Iwan Kawrakow

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