Solution of the Boltzmann equation for light transport

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Definitions

Wanted: photon's flux L

Method: transport Boltzman equation

Notations: time (t), position (r), direction ($\hat{s}$)

Flux magnitude

Scattering indicatrix

$$\frac{1}{c}\frac{\partial L(\vec{r},t,\hat{s})}{\partial t} + \hat{s}\cdot\nabla L(\vec{r},t,\hat{s}) + \mu_t L(\vec{r},t,\hat{s}) = S(\vec{r},t,\hat{s}) + \underbrace{\mu_s \int_{\mathbb{S}^2} d\hat{s}\, g(\hat{s},\hat{s}')L(\vec{r},t,\hat{s}')}_{\textbf{Scattering term}}$$

Free propagation term

Source

$$\mu_t = \mu_a + \mu_s,\ \mu_s = 1/l_s,\ \mu_a = 1/l_a$$

Scattering length

Absorption length

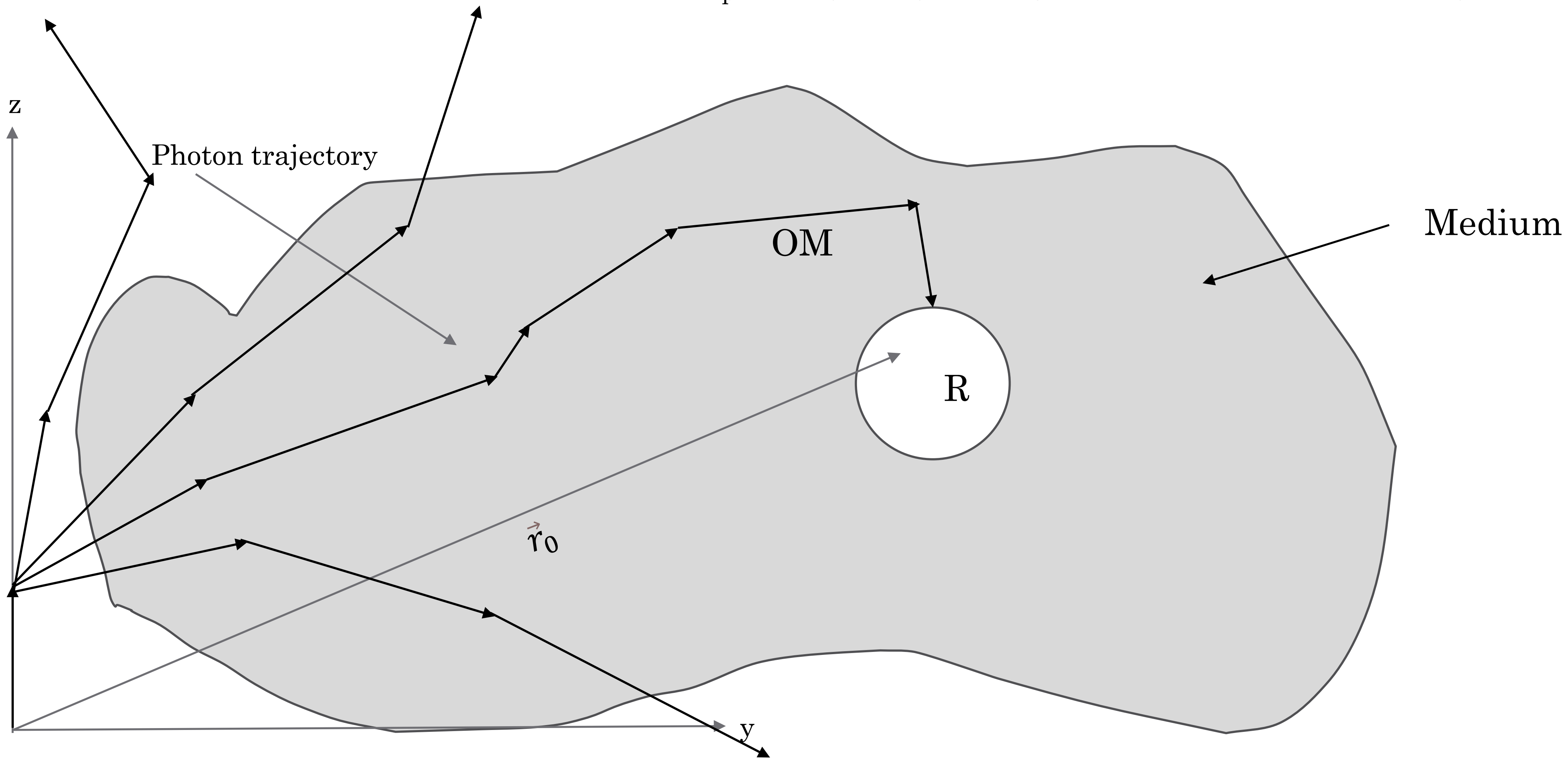
Existing solution schemes

Method	References	Issue
Monte Carlo methods	Standard MC method	extreme CPU for low flux (too few photons hit the detector).
Expansion in spherical harmonics.	[1]	Problem with g = 1-ε (ε – small)
Lattice method (discretisation)	[2]	Memory and time of calculation

- [1] – Andr'e Liemert, Alwin Kienle «Infinite space Green's function of the time-dependent radiative transfer equation»
- [2] – Kausar Banoo «DIRECT SOLUTION OF THE BOLTZMANN TRANSPORT EQUATION IN NANOSCALE SI DEVICES»

Problem with MC method

$N_{ph} \sim N_{tot}(R/r_0)^2 \sim N_{tot}(0.21m/100m)^2=4*10^{-6}N_{tot}$



Our method

- Equivalent integral equation

$$L(r,t,\hat{s}) = c\int_0^t dt' e^{-c\mu_t(t-t')} S(r - c\hat{s}(t-t'), t', \hat{s}) + c\mu_s \int_0^t dt' e^{-c\mu_t(t-t')} \hat{V}_{\hat{s}\hat{s}'} L(r - c\hat{s}(t-t'), t', \hat{s}')$$

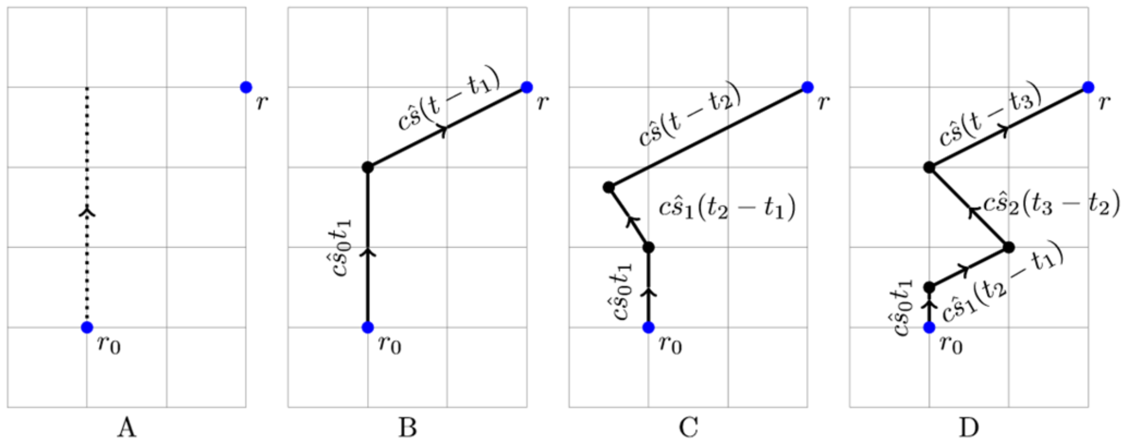
$$\hat{V}_{\hat{s}\hat{s}'} f(\hat{s}') \equiv \int_{4\pi} d\hat{s}' P(\hat{s}, \hat{s}') f(\hat{s}')$$

- Successive approximations

$$L^{(n)}(r,t,\hat{s}) = c\int_0^t dt' e^{-c\mu_t(t-t')} S(r - c\hat{s}(t-t'), t', \hat{s})$$
$$+ c\mu_s \int_0^t dt' e^{-c\mu_t(t-t')} \hat{V}_{\hat{s}\hat{s}'} L^{(n-1)}(r - c\hat{s}(t-t'), t', \hat{s}')$$

Each iteration corresponds to additional photon scattering in the medium

Diagrammatic interpretations: A- without scattering, B – a single scattering, C - a double scattering, D – a triple scattering



General expression

- Point-like source: $S(r,t,\hat{s}) = \delta^3(r)\delta(t)\delta^2(\hat{s}-\hat{s}_0)$

- The general formula for an arbitrary order:

$$\Delta L^{(N)} = \frac{(\mu_s ct)^N}{N!} e^{-\mu_t ct} \cdot N! \int_0^1 d\xi_N \ldots \int_0^1 d\xi_1 \int_{\mathbb{S}^2} d\hat{s}_{N-1} p(\hat{s}_N, \hat{s}_{N-1}) \ldots \int_{\mathbb{S}^2} d\hat{s}_1 p(\hat{s}_1, \hat{s}_0) \prod_{k=1}^{N} (1-\xi_k)^{k-1} c\delta^3(r-ct\hat{s}_{eff})$$

where $\hat{s}_{eff} = \sum_{k=0}^{n} \hat{s}_{n-k}(1-\xi_n)\ldots(1-\xi_{n-k+1})\xi_{n-k}$.

- The formula can be read: $\Delta L^{(N)} = \underbrace{e^{-\mu_a ct}}_{absorption} \cdot \underbrace{P_N(\mu_s ct)}_{Poisson} \cdot \underbrace{f_N(r,\hat{s},t)}_{\text{scattering}}$

- The solution is a singular function inappropriate for numerical calculation

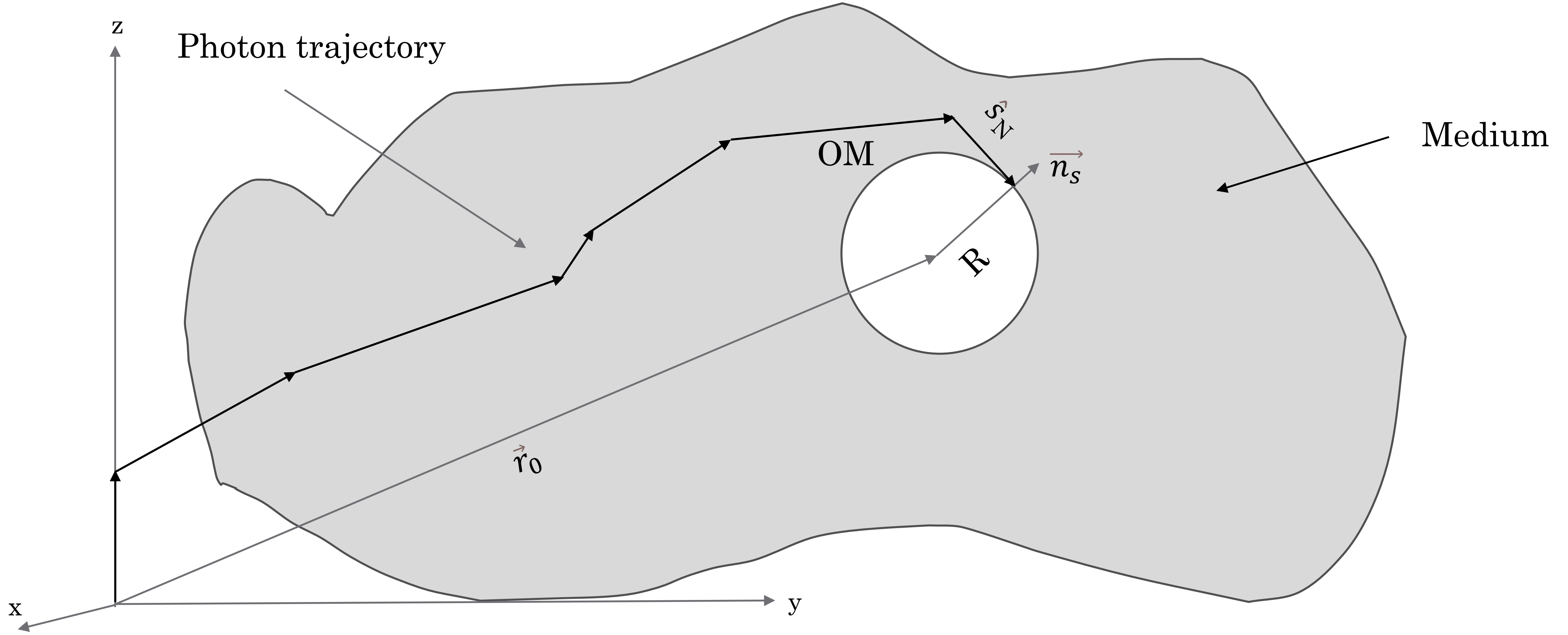
$$L^{(0)}(r,t,\hat{s}) = ce^{-c\mu_t t}\frac{\delta(r-ct)}{r^2}\delta^2(\hat{r}-\hat{s}_0)\delta^2(\hat{s}-\hat{s}_0)$$

Use $\hat{s}_0 = (0,0,1)$

Observed quantities

- Calculate an observable: number of photons hitting a sphere with radius R and acceptance epsilon

$$\Delta F_i^{(N)} = \int_{T_i}^{T_{i+1}} \frac{dt}{T_{i+1} - T_i} \int_{\mathbb{S}^2} d\hat{s}_N \Delta L^{(N)} \cdot \underbrace{\epsilon(\hat{s}_N, n_S, t)}_{acceptance} \cdot \underbrace{\Theta(-(n_S, \hat{s}_N))}_{direction}$$

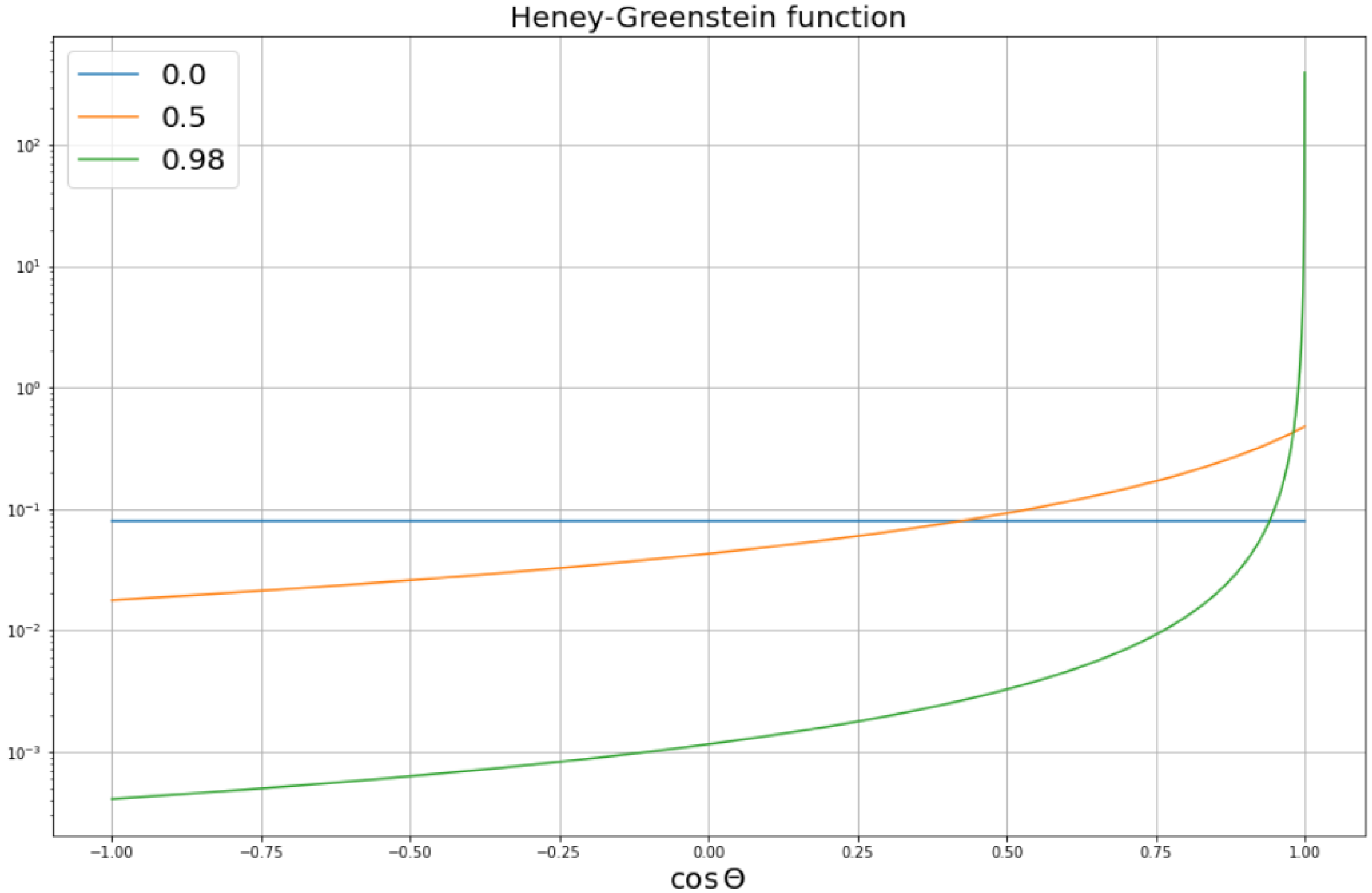


Vegas

- For N^{th} order we had to calculate 3N integrals. For these purposes, we use the VEGAS integration method.
- This is a very powerful method for calculating multivariate integrals.
- Vegas is very effective for cases where we have a function with a sharp peak under the integrals

Scattering indicatrix

- We will use as a scattering function the Henyey-Greenstein function. This is a universal scattering function that describes a huge number of types of scattering, ranging from isotropic (g = 0) to completely anisotropic (g = 1).

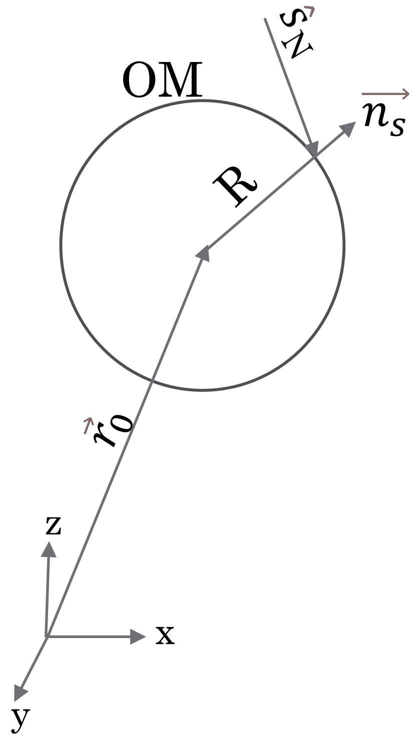


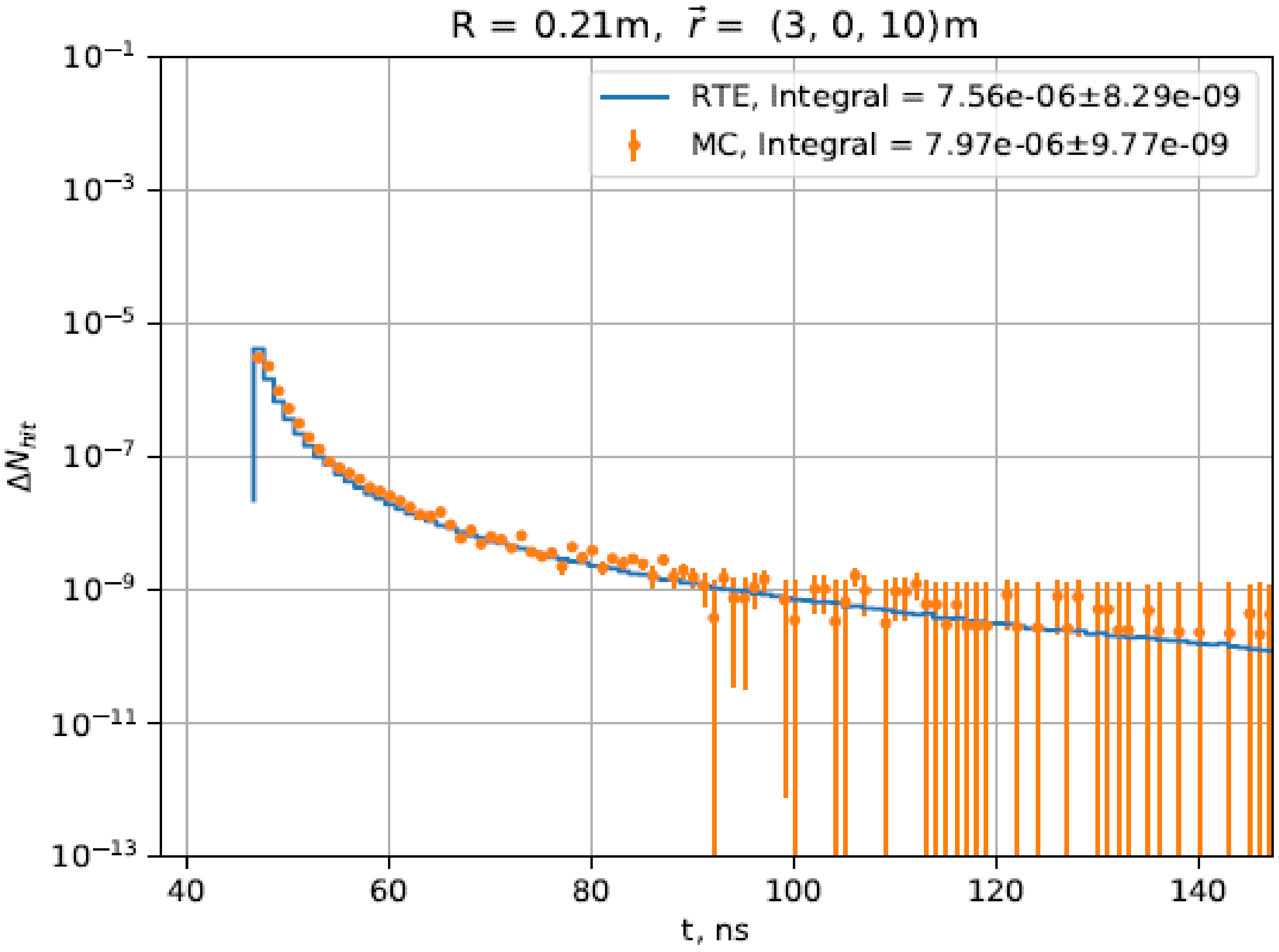
$$g(\hat{s}, \hat{s}') = \frac{1}{4\pi} \frac{1-g^2}{(1+g^2-2g\cos\Theta)^{3/2}}$$

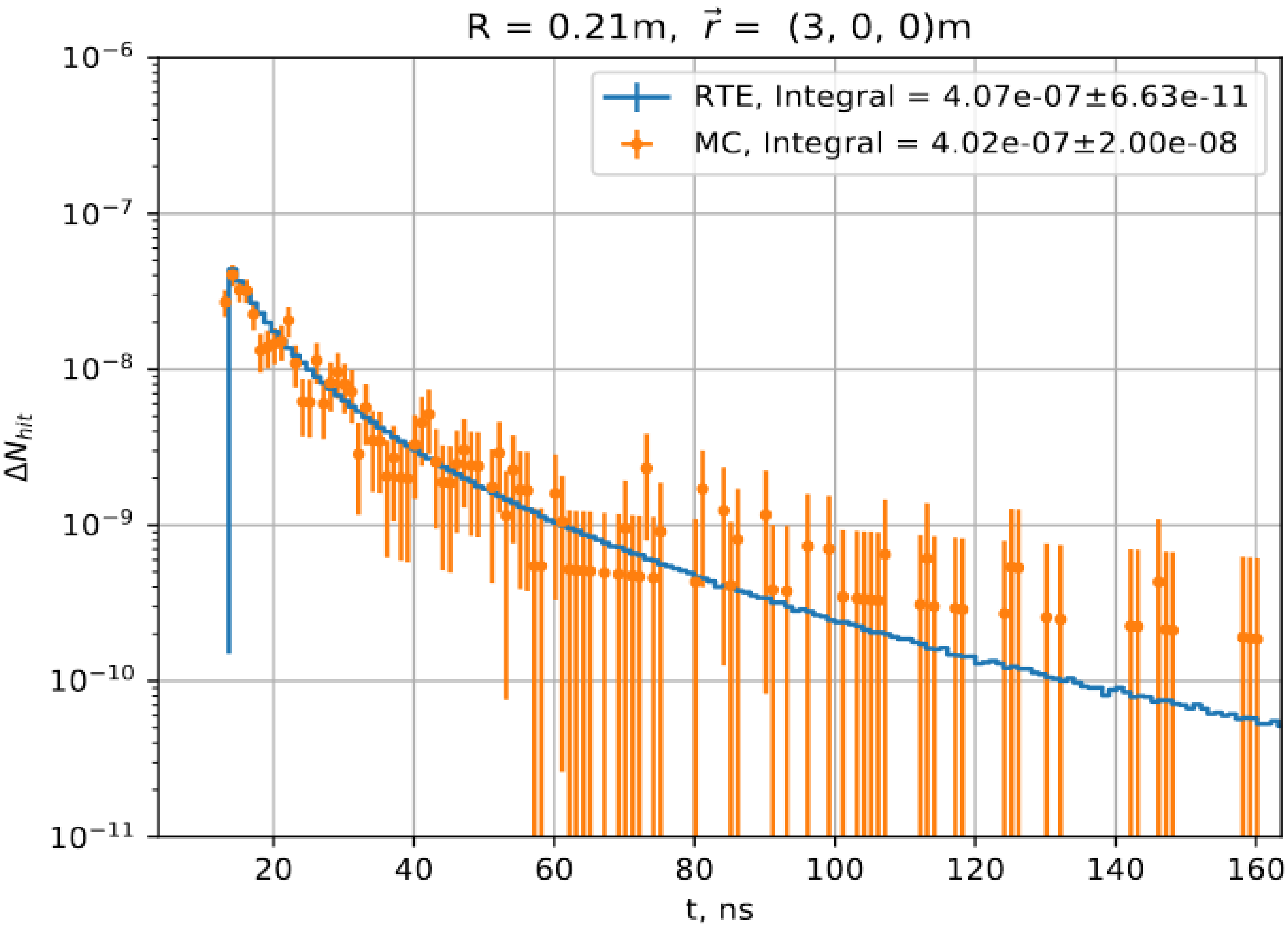
$$\cos\Theta = (\hat{s}, \hat{s}')$$

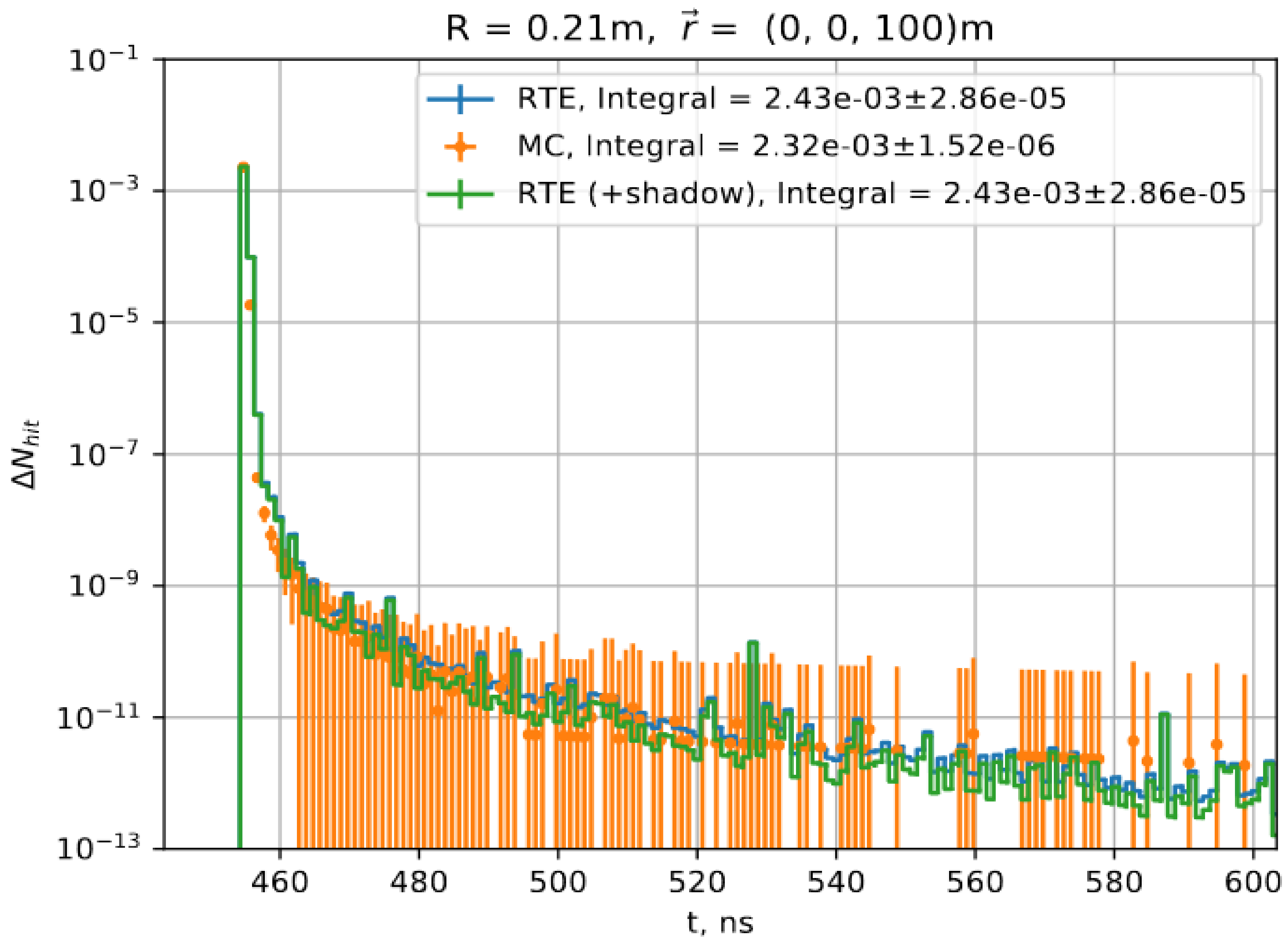
Results

- First, let's compare between RTE and Monte Carlo(photon tracing method) for different points and different asymmetry parameter.

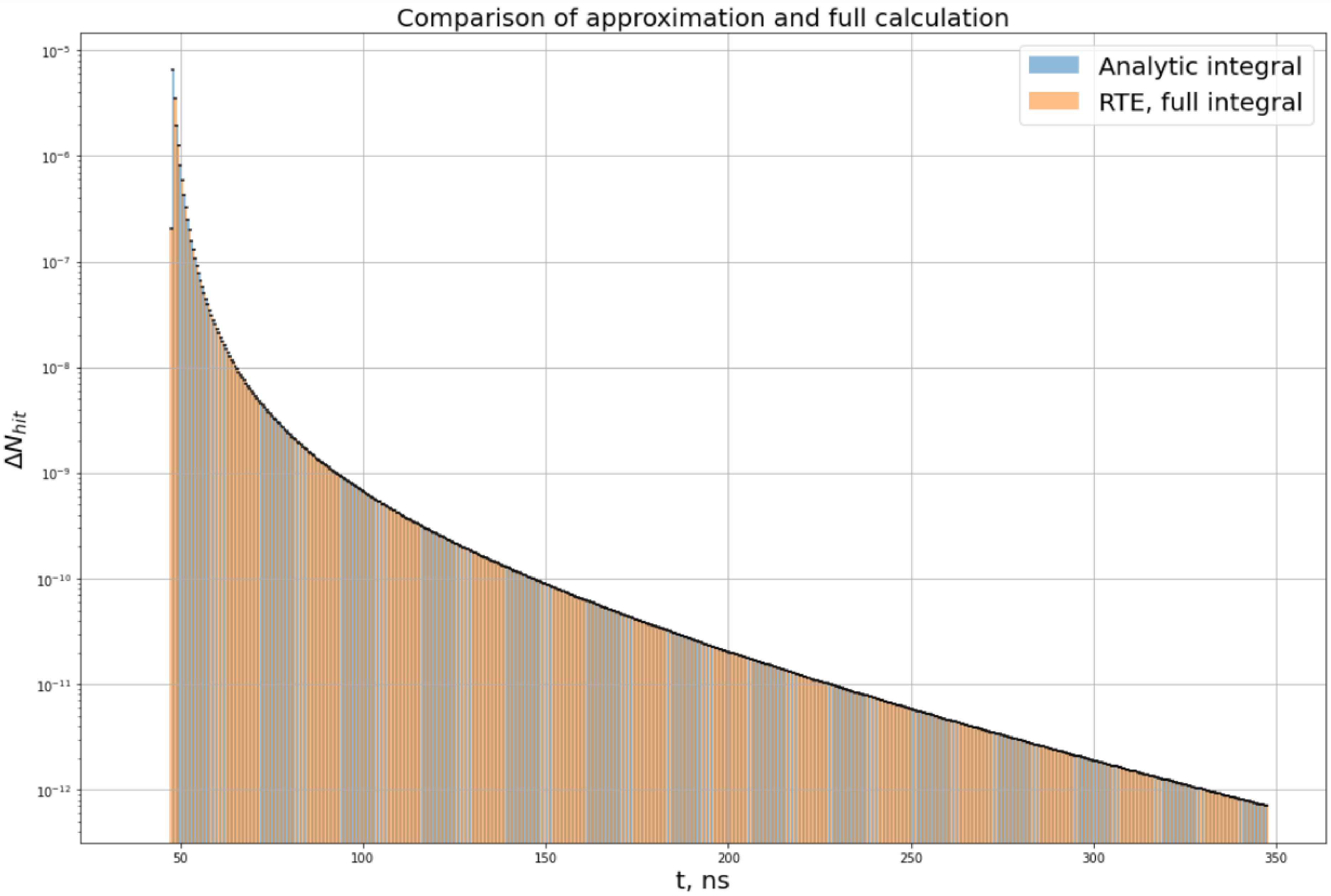





R = 0.21m, $\vec{r}$ = (3, 0, 0)m
RTE, Integral = 4.07e-07±6.63e-11
MC, Integral = 4.02e-07±2.00e-08
ΔN_{hit}
t, ns
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
20
40
60
80
100
120
140
160


R = 0.21m, $\vec{r}$ = (0, 0, 100)m
RTE, Integral = 2.43e-03±2.86e-05
MC, Integral = 2.32e-03±1.52e-06
RTE (+shadow), Integral = 2.43e-03±2.86e-05
ΔN_{hit}
t, ns
10^{-1}
10^{-3}
10^{-5}
10^{-7}
10^{-9}
10^{-11}
10^{-13}
460
480
500
520
540
560
580
600

Good approximation for number of photons



- The zero order is calculated completely analytically.
- For the first and second order, an approximation was obtained that works very well For definiteness, I took the point (3,0,10).

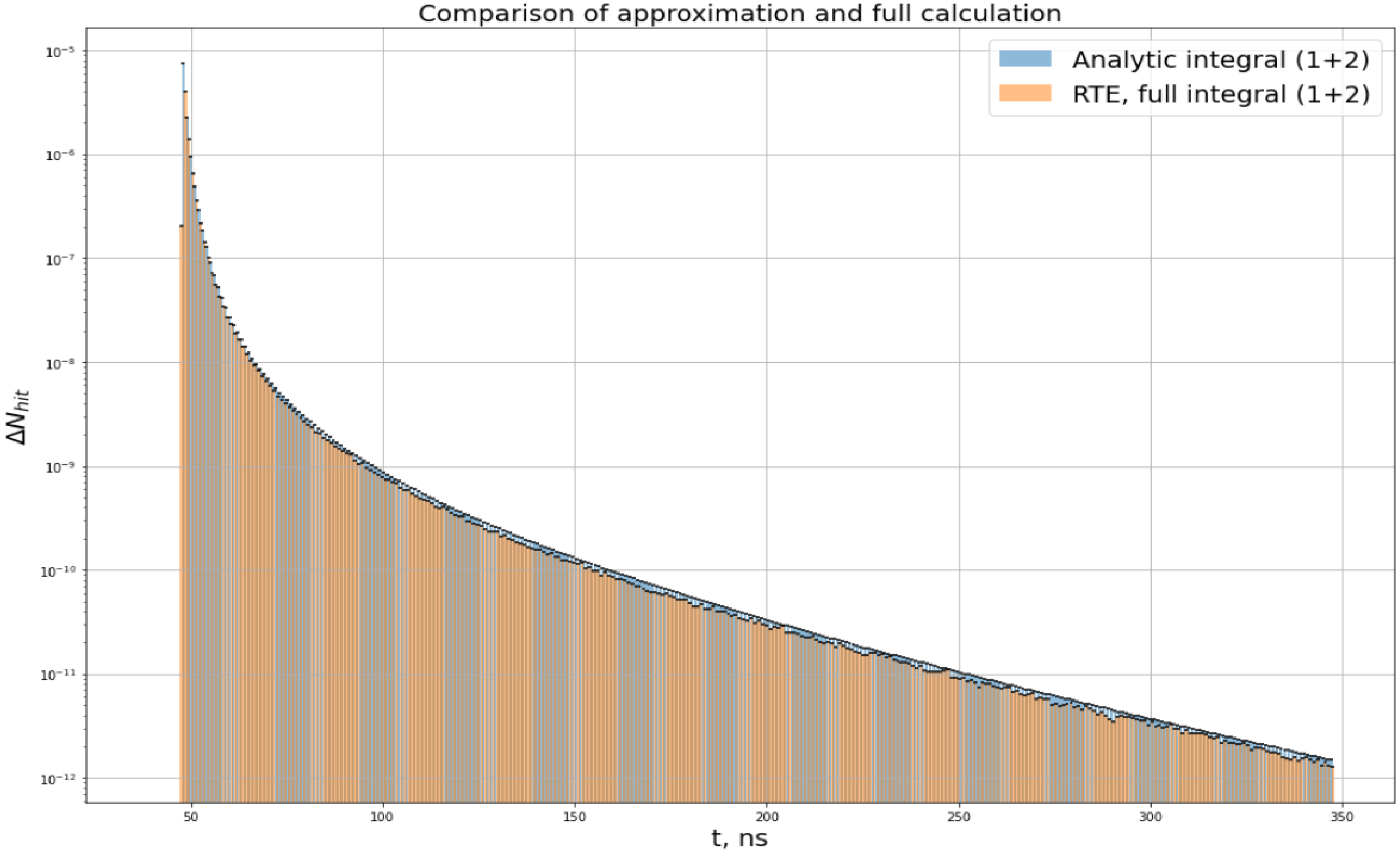
$$\Delta N_{hit}^{(1)} = 2\frac{\mu_s}{\mu_t} \cdot (e^{\mu_s ct_i} - e^{\mu_s ct_{i+1}}) \cdot p(x_0) \cdot \frac{1}{d \cdot y^2} \cdot \Theta(t_i - r/c)$$

$$\Delta N_{hit}^{(2)} = 2\frac{\mu_s}{\mu_t} \cdot (e^{\mu_s ct_i} - e^{\mu_s ct_{i+1}}) \cdot p(x_0) \cdot \frac{1}{d \cdot y^2} \cdot (\mu_s ct_i) \cdot \Theta(t_i - r/c)$$

$$\vec{y} = \vec{r} - c\hat{s}_0 t_i$$

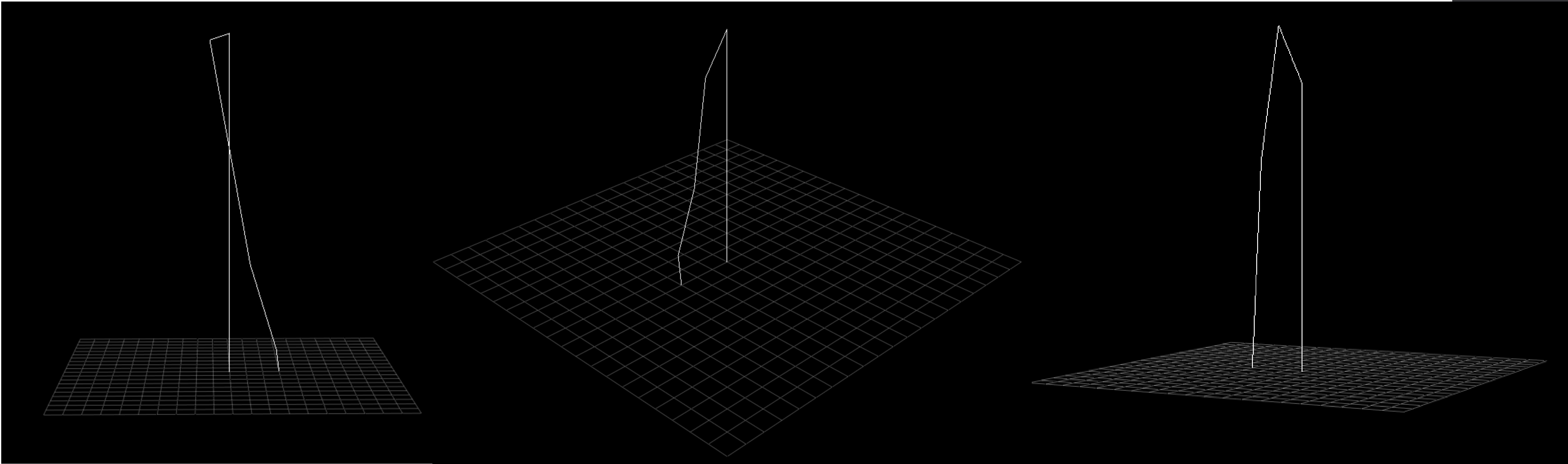
$$d = t_{i+1} - t_i$$

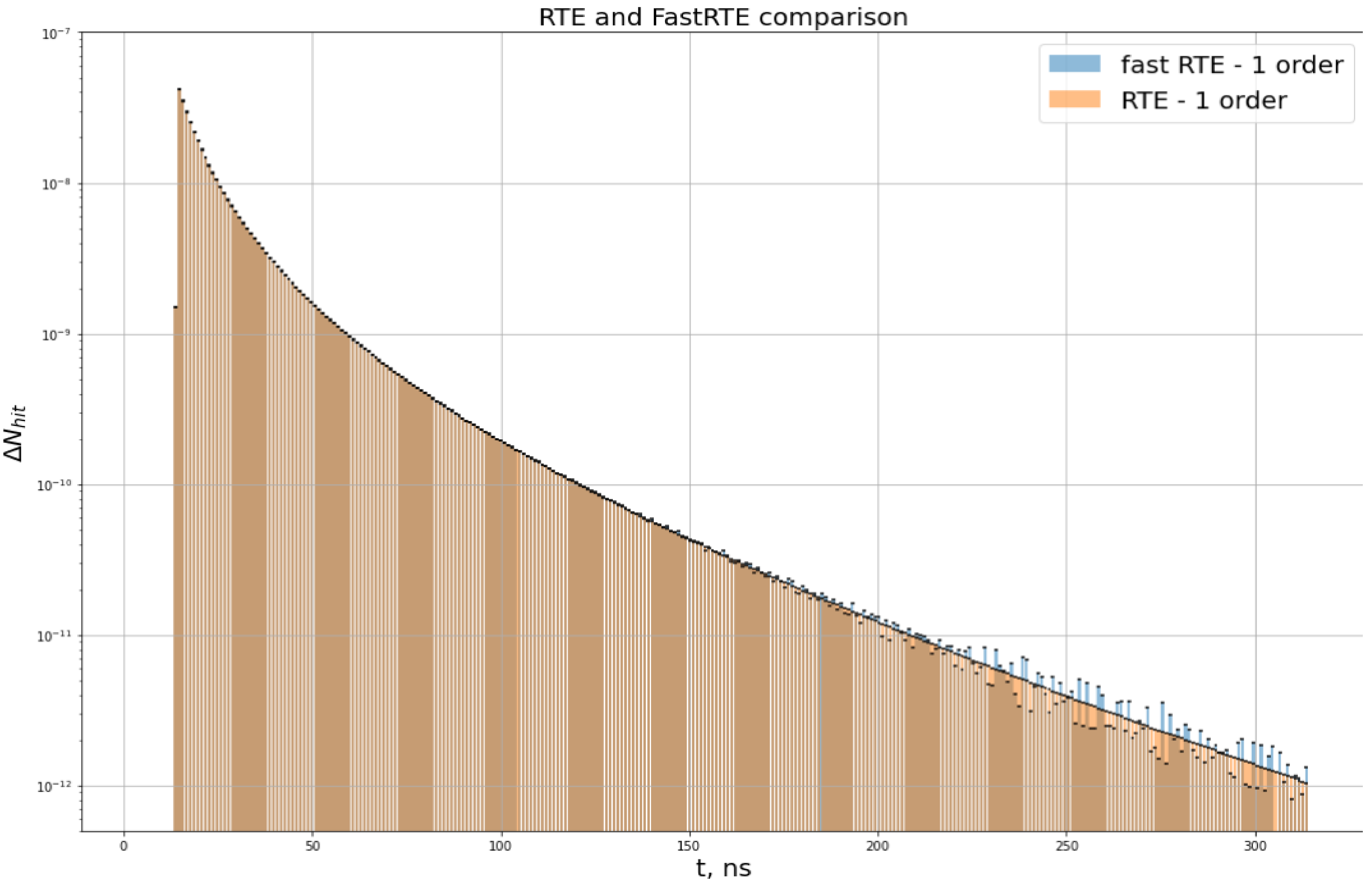
$$x_0 = 1 - (\vec{y}, \hat{s}_0)/y^2$$



Monte Carlo method with fixed start and end points (FastRTE)

- We can use Vegas like Monte Carlo generator
- Vegas, after integration, stores all the photon trajectories (and the corresponding weights) for which it calculated the value of the integral.
- We can integrate our entire function not in narrow bins, but in one large bin, and then recalculate the result using only those trajectories whose time is in the bin we need.
- So essentially, thanks to Vegas, we have a Monte Carlo method that drags a photon from one fixed point to another FIXED point (so we can remove problem of MC method from slide 3).




RTE and FastRTE comparison
fast RTE - 1 order
RTE - 1 order
ΔN_{hit}
t, ns
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
0
50
100
150
200
250
300

Calculation time

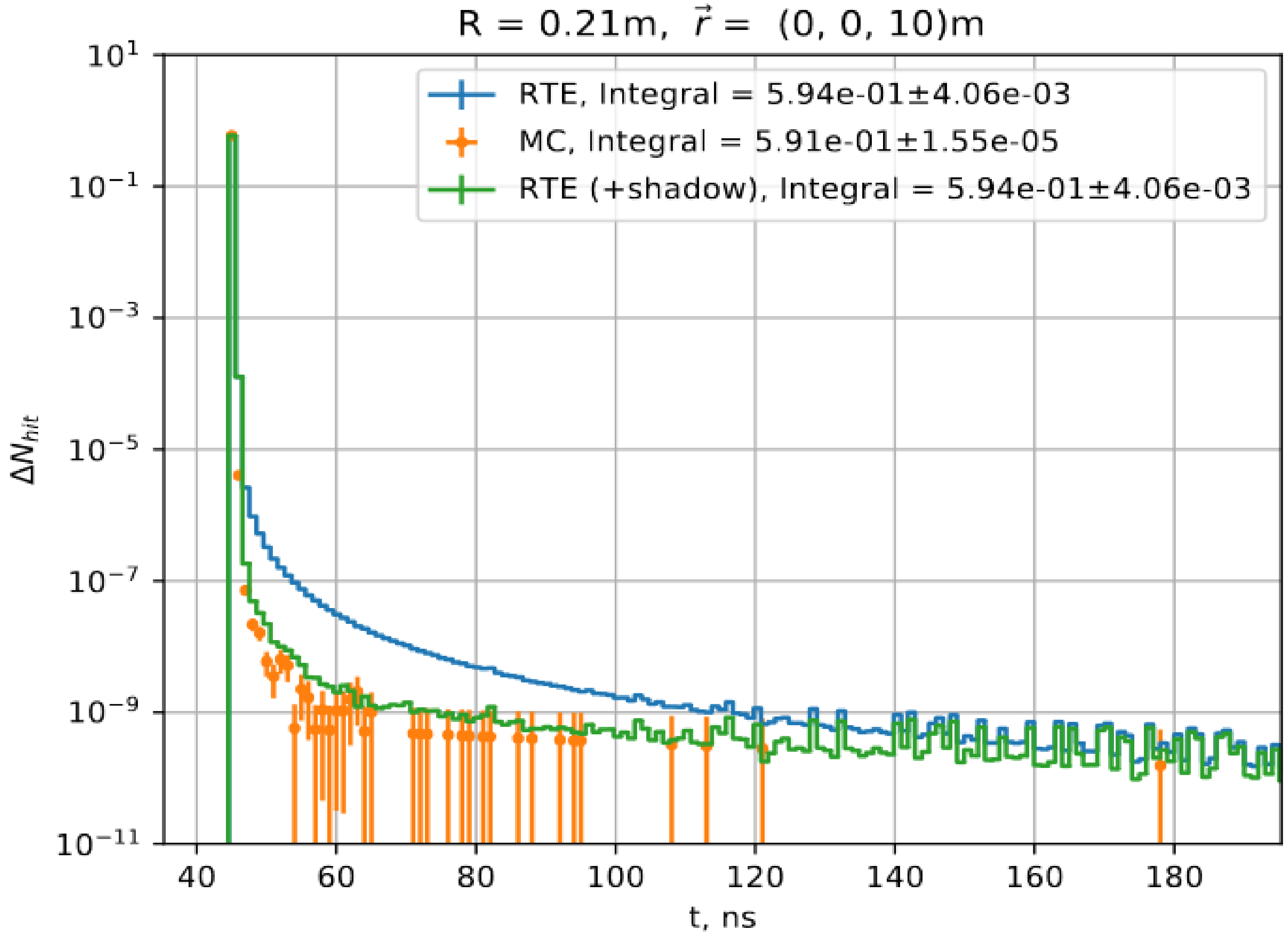
Method	Monte Carlo	RTE (full integration)	Approximation
Time (for relative error = 0.001)	Depends on calculation accuracy 10^9 events– 1h 43m	Depends on calculation accuracy (about 1.5 half for higher orders)	instantly

Conclusions

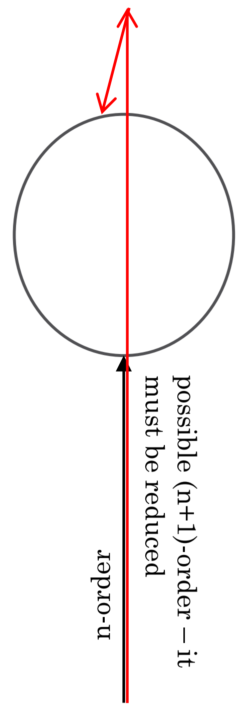
- A semi-analytical method for calculating the light flux has been obtained.
- A way to perform Monte Carlo calculation with fixed ends is obtained.
- Approximations for the light flux for the first and second order in scattering are obtained

Thank you for your attention

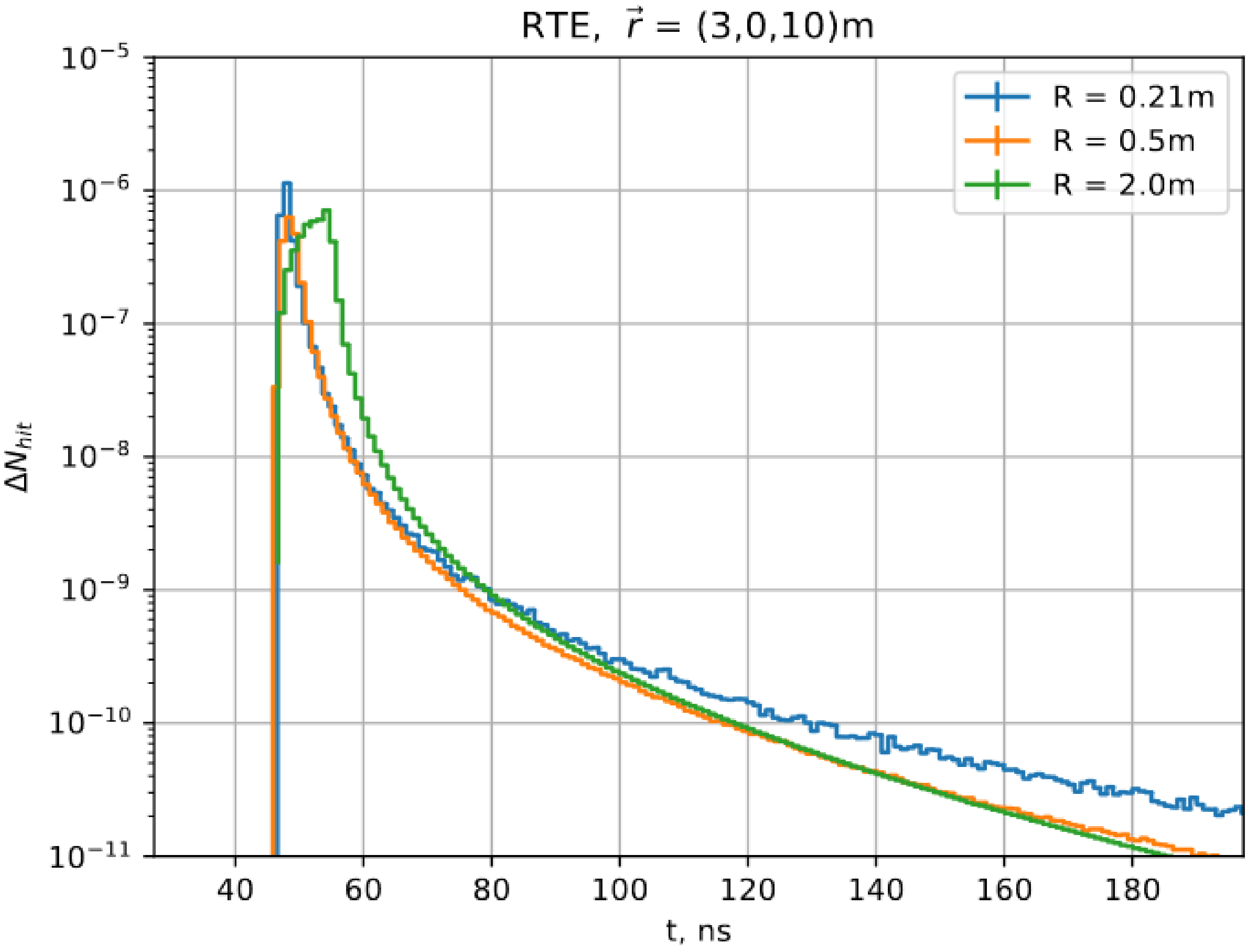
Shadow effect



- In fair photon transport, explicit absorption is taken into account (the photon is absorbed and is not taken into account in further dragging).
- In RTE this effect is not explicitly taken into account (due to the fact that the calculation scheme does not allow it to be taken into account explicitly)



Spectrum broadening.



- If the radius of the OM is small, then a very large number of photons is required
- To increase statistics, the radius of the OM is increased, then the resulting flows are recalculated to a smaller radius. As a result, there is a broadening of the spectrum, which was not originally.