Analytical solution of light diffusion and its potential application for light simulation in DUNE

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SB Meeting 08/06/2016

Introduction

Rough Timeline (2) From DUNE GM in South Dakota

- Summer 2016
  - FD Task Force: Consider photon detector optimization studies
  - FD sim/reco WG: Complete implementation of dual-phase simulation in LArSoft (i.e. light readout)
  - FD sim/reco WG: Validation of reconstruction with dual-phase simulation in LArSoft
  - LBL, SN, ND, and Atm Nu WGs : Detector optimization studies with full simulation reconstruction (single-phase)
  - LBL Physics WG: Preliminary full MC-based sensitivity
- September 2016
  - FD Task Force: Preliminary report (September)

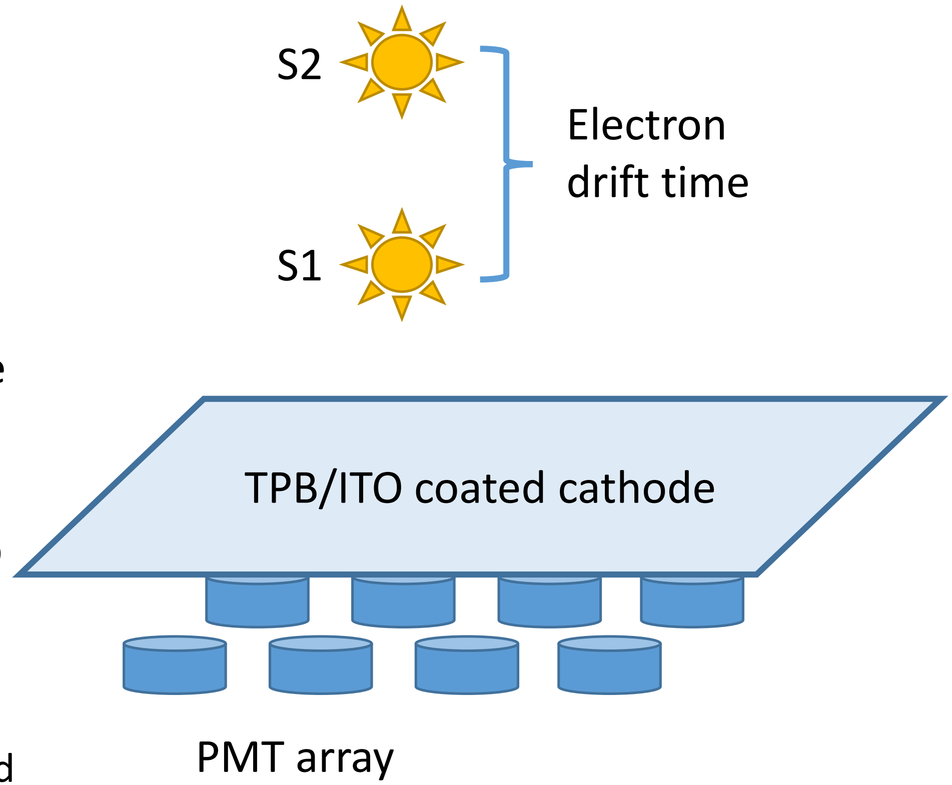
4/14/2016 L. Whitehead - FD TF Monthly Meeting 14

We would like to have fully functional simulation for the dual-phase DUNE detector by the end o this summer

➔ Requires completion of light readout

Some challenges

- Light simulation for dual-phase has to include
  - Generation of S2 in addition to S1
  - Light conversion on the cathode plane
- The challenging aspect is how to populate PMTs with a photons produced along particle tracks
- The solution so far to produce a light map (or light library in larsoft) which defines visibility of a given detector voxel wrt to the photon detectors
  - Note: time spread due to RS is not applied to photon arrival times in larsoft
- Size of the map can quickly become a challenge due to large detector volume
- Simulation of light visibility from each voxel, although to be done once, also becomes a CPU intensive task



Since we are not interested in tracing paths of each photon, but rather the end result, is it possible to find an effective theoretical description?

Photon transport in diffusion media

- Actually there has been a big interest in this question due to its medical applications to evaluate light propagation in tissues (e.g., oxygen meters)
- Also in nuclear physics: neutron transport

Idea: find effective solution for particle propagation in scattering medium using diffusion theory

O_2 meter(image: Wikipedia)

Diffusion equations

- Generally described by Fokker-Plank (FP) PDE:

$$\frac{\partial}{\partial t} p(x,t) = D \frac{\partial^2}{\partial x^2} p(x,t) - v_d \frac{\partial}{\partial x} p(x,t)$$

Where is D is constant diffusion coefficient and v_d is constant drift velocity

- For $v_d = 0$ FP PDE reduces to differential equation describing Brownian motion (Wiener process):

$$\frac{\partial}{\partial t} p(x,t) = D \frac{\partial^2}{\partial x^2} p(x,t)$$

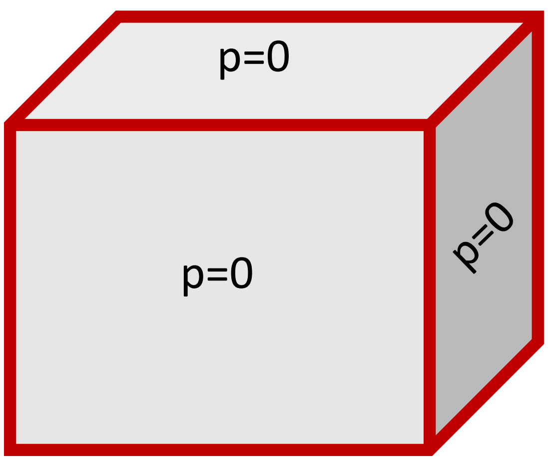
This is the equation one needs to solve for photon diffusion subject to appropriate boundary conditions

Boundary conditions

Photon are absorbed on the cathode → absorption condition for this plane

For other sides of the TPC, the simplest assumption is that photons exiting TPC do not contribute in any significant way → absorption boundary would also be appropriate

But could also consider a quasi-reflective boundary at some point



Absorption boundary condition:

$$p(x,t)\Big|_S = 0$$

Reflective boundary condition:

$$p(x,t)\Big|_S = const$$

$$\Rightarrow \frac{\partial}{\partial x} p(x,t)|_S = 0$$

Diffusion from a point source

In unbound medium solution for diffusion equation for point source at r_0, t_0 is given by Green's function:

$$G(\boldsymbol{r}, t; \boldsymbol{r}_0, t_0) = \frac{1}{[4\pi Dc(t-t_0)]^{3/2}} \exp\left(-\frac{|\boldsymbol{r}-\boldsymbol{r}_0|^2}{4Dc(t-t_0)}\right)$$

Where c is the velocity of light in the medium. For LAr c = 21.7 cm/ns

$$D = \frac{1}{3(\mu_A + (1-g)\mu_S)}$$

For $\mu_S = \frac{1}{55}$ and $\mu_A \sim 0$

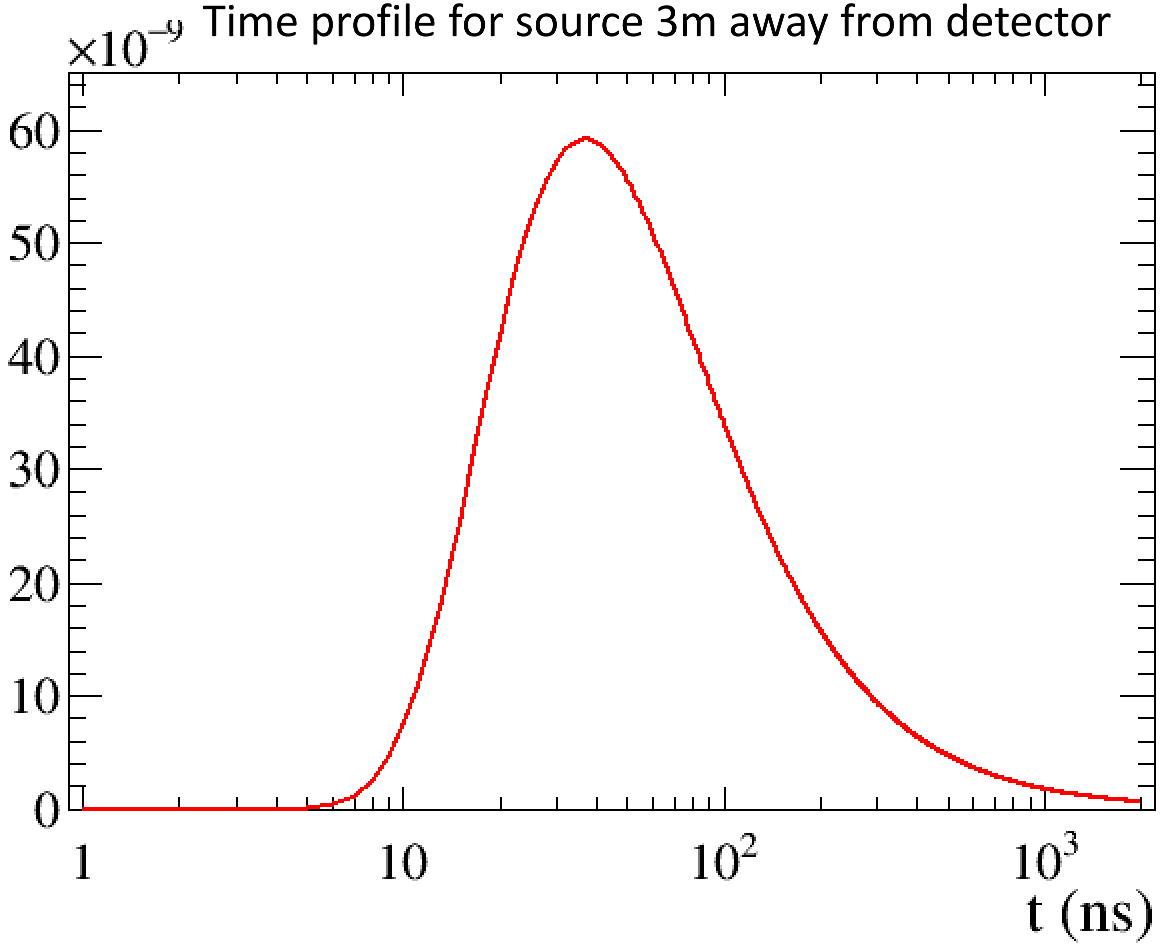
$D = 18.8$ cm
Or cm2/ns if one multiply by velocity to get more familiar units

μ_A - absorption coefficient [1/units of L]
μ_S - scattering coefficient [1/units of L]
g – average scattering cosine

- Isotropic scattering $g = 0$
- Including Ar form factors introduces some anisotropy for Rayleigh scattering $g = 0.025$

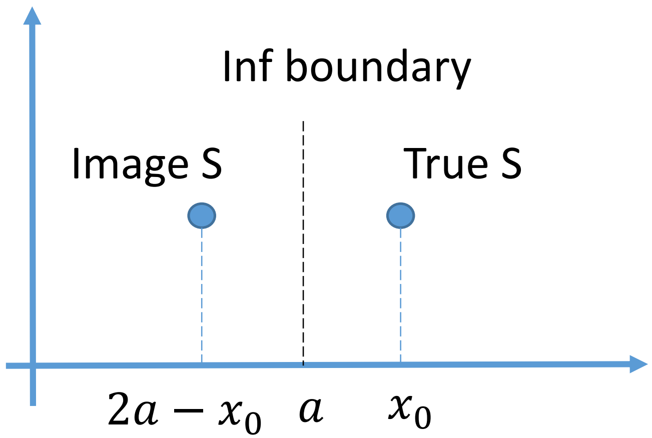
Unbound solution

Time profile for source 3m away from detector



Note the extending tail is due to infinite boundaries ➔ due to scattering photons will keep arriving …

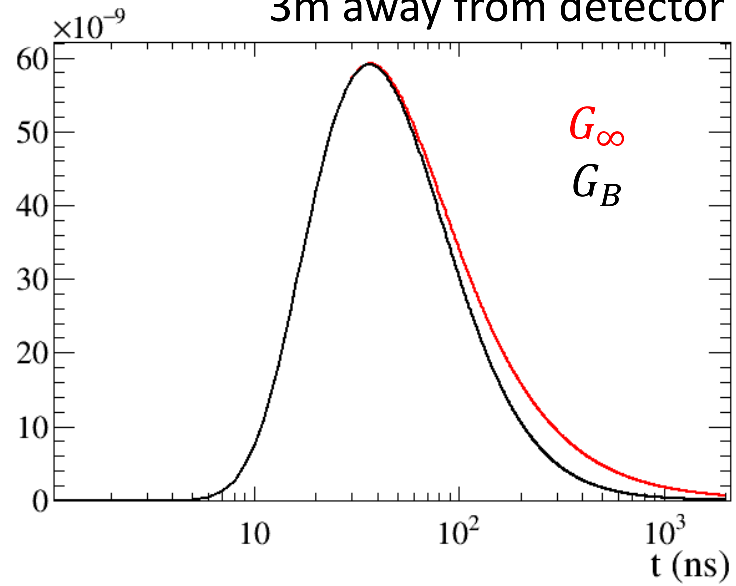
Single absorption boundary



Solution for $x > a$ is simply a difference between two unbound Green's functions for true source x_0 at and its mirror image at $2a - x_0$

$$p(x, x_0, t) = G(x, x_0, t) - G(x, 2a - x_0, t)$$

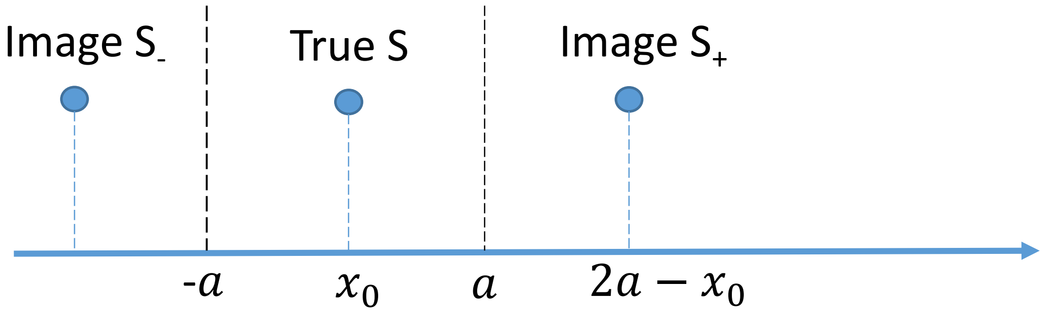
Time profile for source 3m away from detector



The tail is reduced due to photons absorbed at the boundary

Source between two absorbing planes

Source b/w two absorption boundaries at -*a* and *a*



Could use image source method as well, but need to also absorb image sources at further boundary:
in the sketch that would be $S_{-}(-2\mathrm{a} + x_0)$ at boundary a would need an image source at $4a + x_0$ and so on

Just like an image of a mirror reflection in a mirror or a screen capture of a screen capture on a video call

Of course each contribution becomes smaller and smaller correction ➔ truncates the infinite series

Source reflection

Reflection operations:

- Negative boundary at -a: **-2a – x**
- Positive boundary at +a: **2a – x**

First few terms in the series

Image source	Add/Subtract	Img Source 1	Img Source 2
1	-	$-x' - 2a$	$-x' + 2a$
2	+	$x' - 4a$	$x' + 4a$
3	-	$-x' - 6a$	$-x' + 6a$
…	…	…	…

Subtract terms with n/2 = odd, add terms with n/2 = even

Full solution 1D

Diffusion PDE: $$\frac{\partial}{\partial t}p(x,t) = D\frac{\partial^2}{\partial x^2}p(x,t)$$

with absorption at $\mathrm{x} \pm a$

$$p(x,t) \propto \sum_{n=-\infty}^{+\infty} \exp\left[-\frac{(x-x'+4na)^2}{4Dt}\right] - \exp\left[-\frac{(x+x'+(4n-2)a)^2}{4Dt}\right]$$

Solution for point source in 3D

$$\frac{\partial}{\partial t}p = D\left[\frac{\partial^2}{\partial x^2}p + \frac{\partial^2}{\partial y^2}p + \frac{\partial^2}{\partial z^2}p\right]$$

With absorbing boundaries at $x_b = \pm w, y_b = \pm l, z_b = \pm h,$

Take: $p = X(x,t) \times Y(y,t) \times Z(z,t)$

➔ 3D PDE reduces to 1D PDE for each component

$$\left.\begin{aligned} \partial_t X &= \partial_x^2 X \\ \partial_t Y &= \partial_y^2 Y \\ \partial_t Z &= \partial_z^2 Z \end{aligned}\right\}$$

Since 1D has been solved, we have simply to take a product of 1D solutions

Full solution in 3D

$$p(\boldsymbol{r}, t; \boldsymbol{r}_0, t_0) = \frac{1}{[4\pi D(t - t_0)]^{3/2}} \times S_x \times S_y \times S_z$$

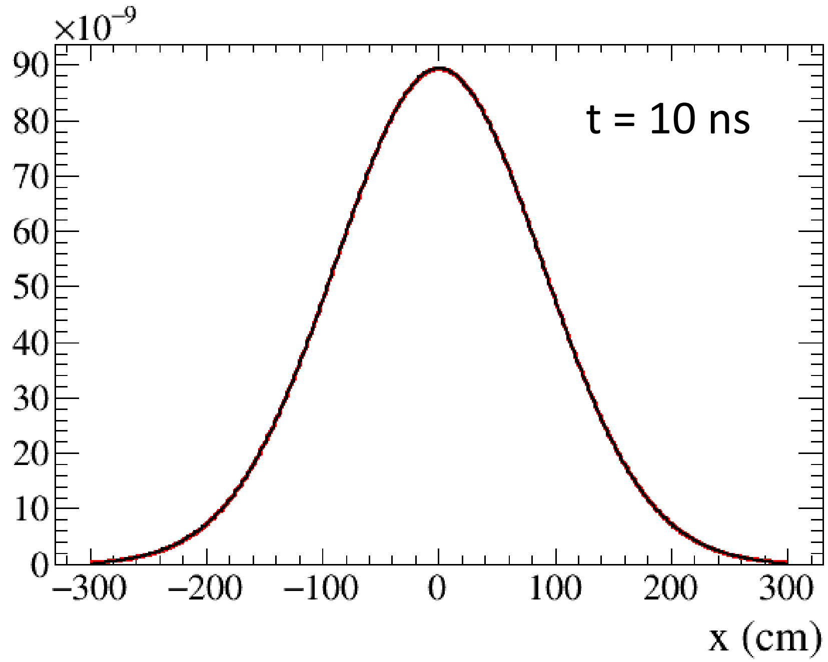
$$S_x = \sum_{n=-\infty}^{+\infty} \exp\left[-\frac{(x - x_0 + 4nw)^2}{4D(t - t_0)}\right] - \exp\left[-\frac{(x + x_0 + (4n - 2)w)^2}{4D(t - t_0)}\right]$$

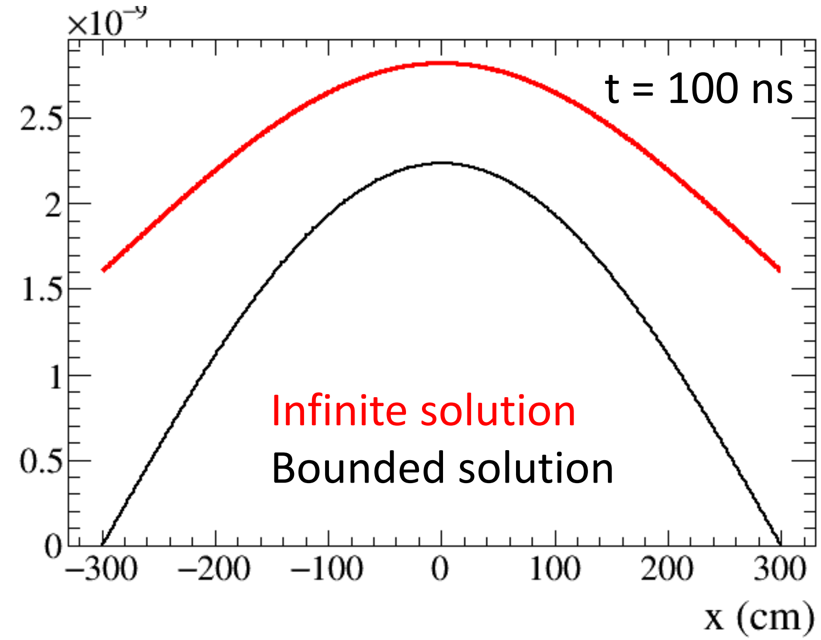
$$S_y = \sum_{n=-\infty}^{+\infty} \exp\left[-\frac{(y - y_0 + 4nl)^2}{4D(t - t_0)}\right] - \exp\left[-\frac{(y + y_0 + (4n - 2)l)^2}{4D(t - t_0)}\right]$$

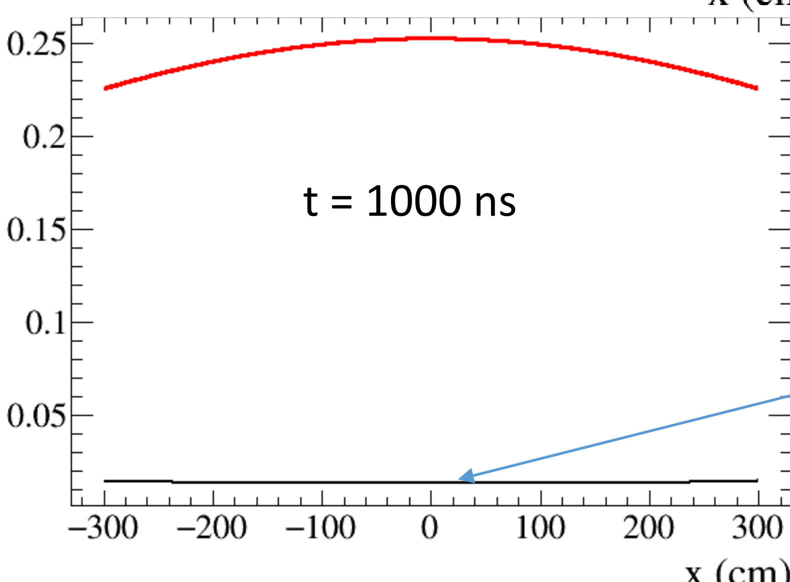
$$S_z = \sum_{n=-\infty}^{+\infty} \exp\left[-\frac{(z - z_0 + 4nh)^2}{4D(t - t_0)}\right] - \exp\left[-\frac{(z + z_0 + (4n - 2)h)^2}{4D(t - t_0)}\right]$$

This gives us photon concentration density in any point at any given time

Source at (0,0,0) in a 6x6x6 box







Particles have diffused to the walls where they were absorbed

Photon flux across the surface

What is of interest to us is the so-called time of first passage

- The time photon hit a given absorptive surface
- The overall integral of this distribution would give us an acceptance probability for this point

Note that by construction $p(\boldsymbol{r},t)|_S = 0$

Fick's law of diffusion relates flux to the concentration density:

$$J(\boldsymbol{r},t;\boldsymbol{r}_0,t_0) = -D\nabla p(\boldsymbol{r},t;\boldsymbol{r}_0,t_0)$$

The change in particle density crossing the surface per unit time:

$$\partial_t P_\Omega(t;r_0,t_0) = \int_\Omega \boldsymbol{dA}\cdot D\nabla p$$

Photon flux PDF at a bounding surface

3D PDF in the volume:

$$p(\boldsymbol{r}, t; \boldsymbol{r}_0, t_0) = \frac{1}{[4\pi D(t - t_0)]^{3/2}} \times S_x \times S_y \times S_z$$

And the Cartesian components of the flux vector are

$$J \sim S_y S_z \partial_x S_x \hat{\imath} + S_x S_z \partial_y S_y \hat{\jmath} + S_x S_y \partial_z S_z \hat{k}$$

Since we are working with a cubical geometry the unit normal to each face would simply be $\pm\hat{\imath}$, $\pm\hat{\jmath}$, $\pm\hat{k}$

So depending on the face the integrand $\boldsymbol{dA} \cdot \boldsymbol{J}$ reduces to one of a the appropriate *J* term

Photon flux PDF at a bounding surface

Consider we are interested at surface z = -300
(e.g., cathode plane in 6x6x6)

$$f(x, y, t; x_0, y_0, z_0, t_0) = \frac{1}{[4\pi D(t - t_0)]^{3/2}} \times S_x \times S_y \times \partial_z S_z \Big|_{z=-300}$$

Independent of z now

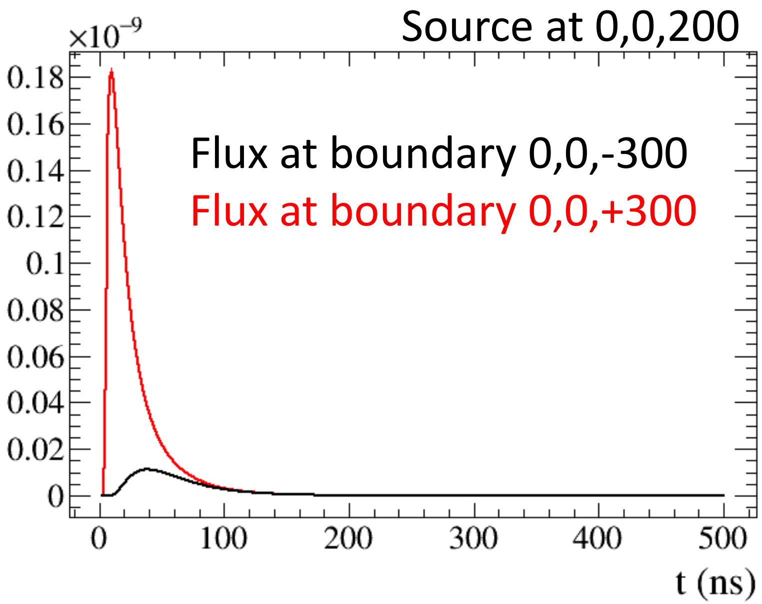
But still depend on of z0

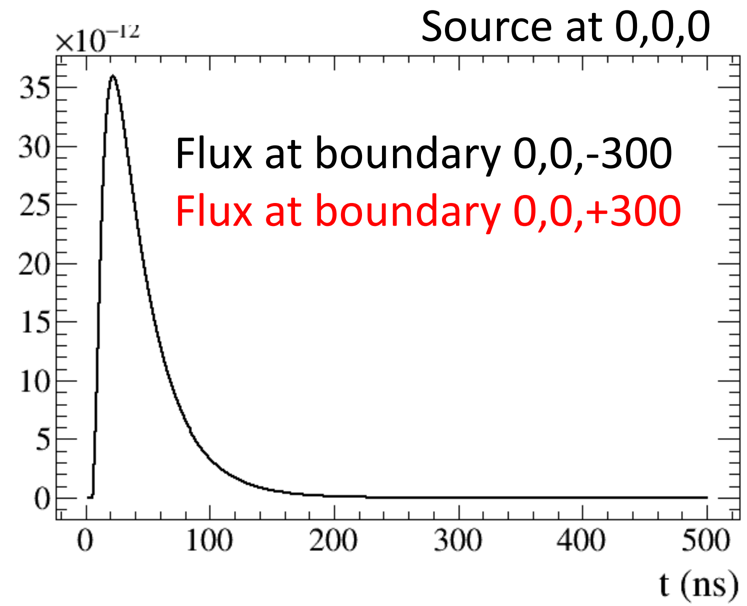
Derivative wrt z
evaluated at z = -300

Since we have a sum of Gaussians of the form

$$G \sim \exp[-s(x - x_0)^2] \Rightarrow \partial_x G = -2s(x - x_0)G$$

Time profiles for single "detection" point at the boundary





Closer the source to the surface higher the overall probability

For a middle point the time distributions are identical

Checking normalization

$$\int dt \int_{\Omega} \boldsymbol{dA} \cdot D\nabla p$$

This gives the acceptance per detector face

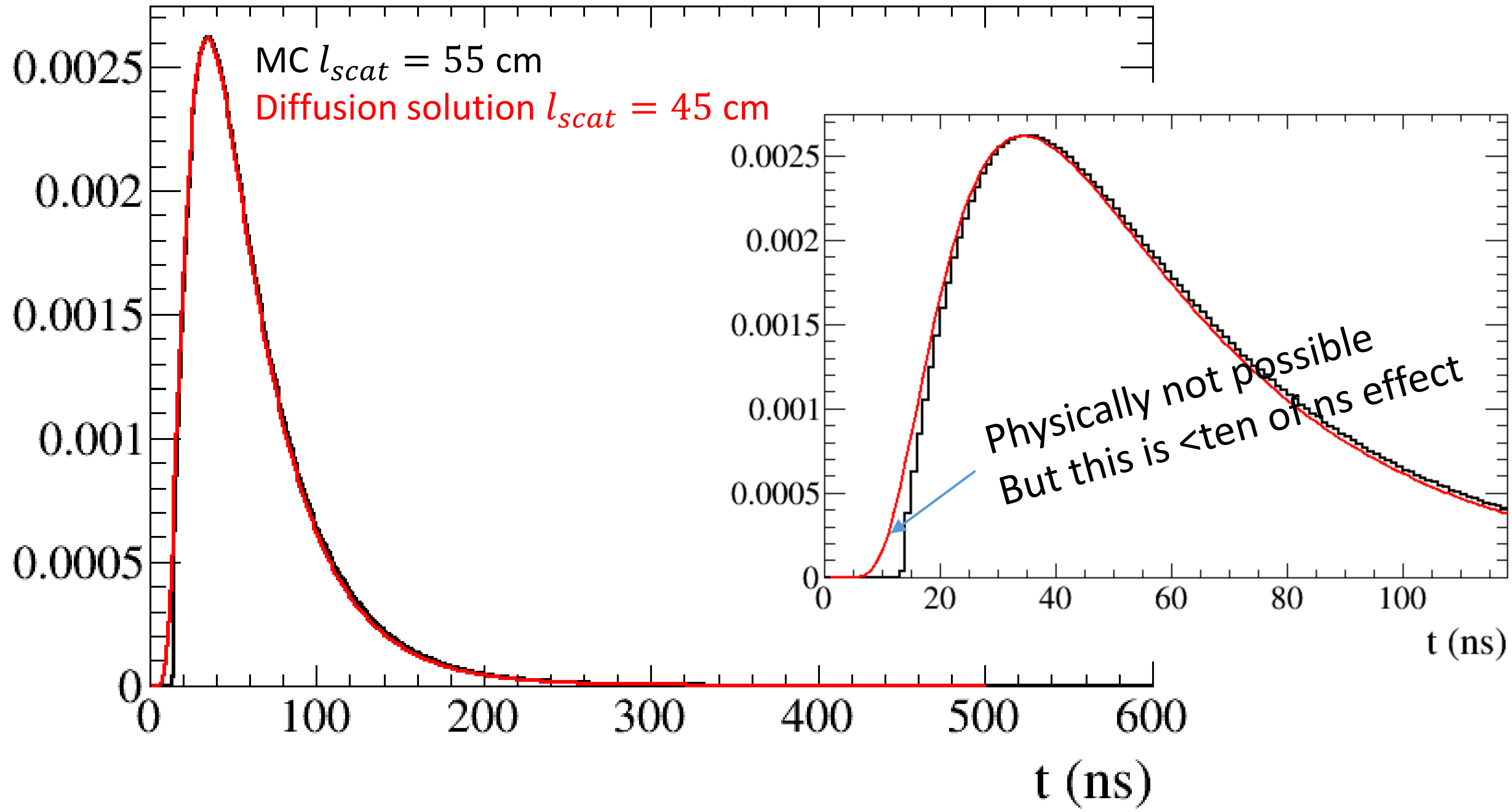
For a cubical boundary and the source at the center the answer is simply : $1/6 \approx 1.666667$

Calculation gives exactly that!

More detailed comparison can be done against MC simulation of photon transport

Comparison with MC

Time distribution for photon arrival integrated over cathode plane



Solution follows quit well MC prediction. No normalization adjustment (in this case)
Another point: rising tail which is earlier than the fastest arrival time of photons given the velocity

When I first made these plots I had to reduce scattering coefficient in the calculation from 1/55 cm to 1/45 cm (this was a symptom of a problem I will discuss next).

Comparison cont'd

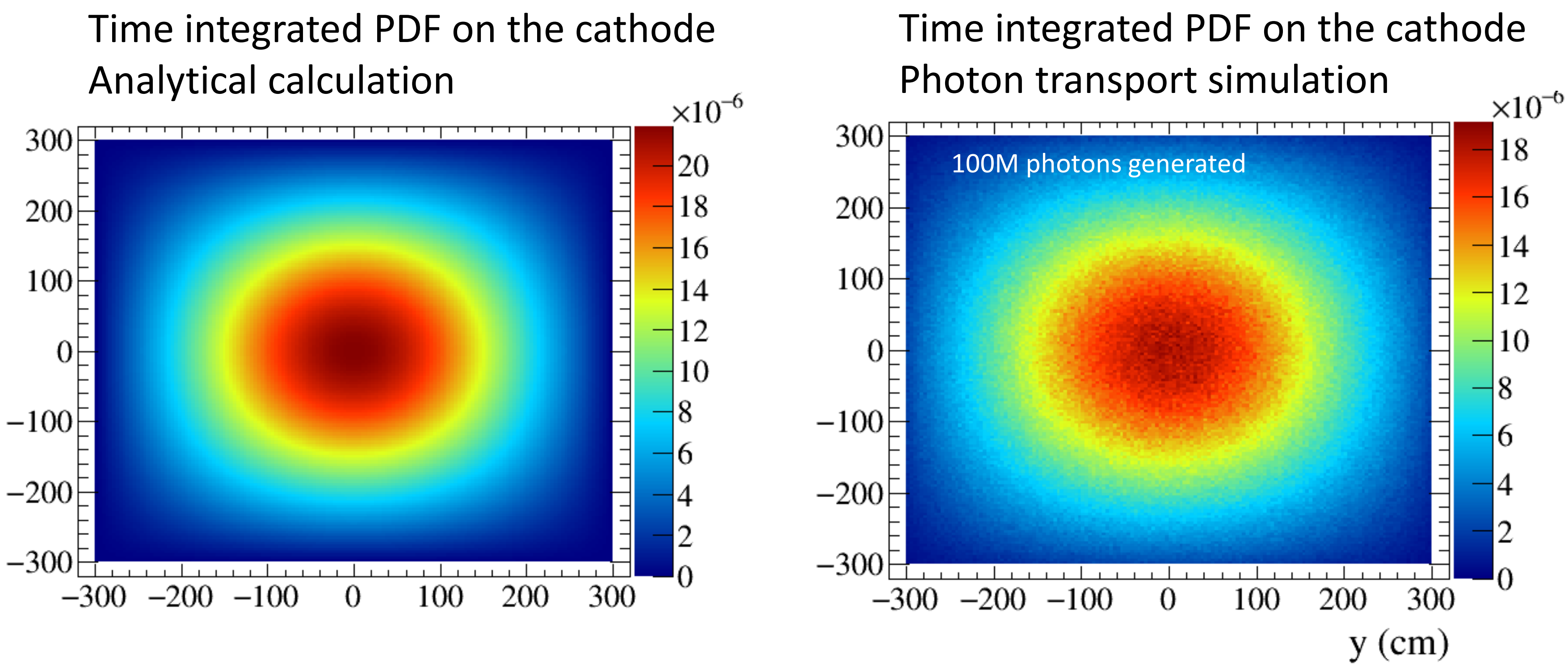
Photon probability at the cathode for MC has been computed with 100M photons tracked

Source point	P Cath MC	P Cath Calc
(0,0,-200)	0.5372	0.6147
(0,0,0)	1/6	1/6
(0,0,200)	0.0395	0.0306
(200,0,-200)	0.4082	0.4369
(200,0,0)	0.1058	0.0887
(200,0,200)	0.02419	0.0155

Note the discrepancy between MC transport and diffusion calculation is actually part of the same problem as the previous slide

Acceptance on the cathode

Example: source at 0,0,0



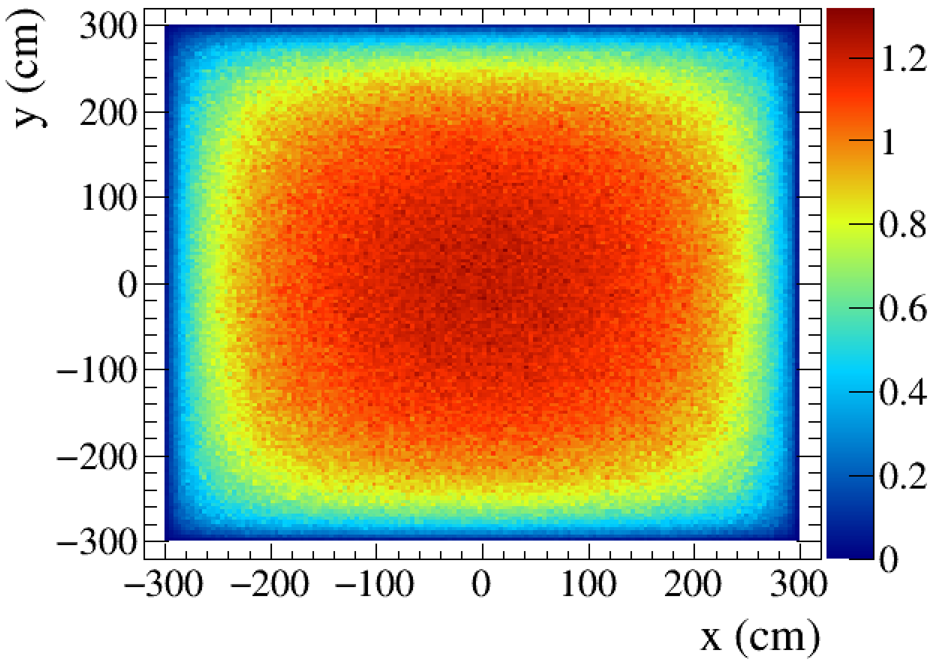
For analytical calculation was performed on 4x4cm2 grid on a cathode, so PDF and time integral was calculated at 25600 point

Approximate time of execution is ~30.0s ← not fast enough to execute this per each step during actual MC transport, but this would be a brute force approach

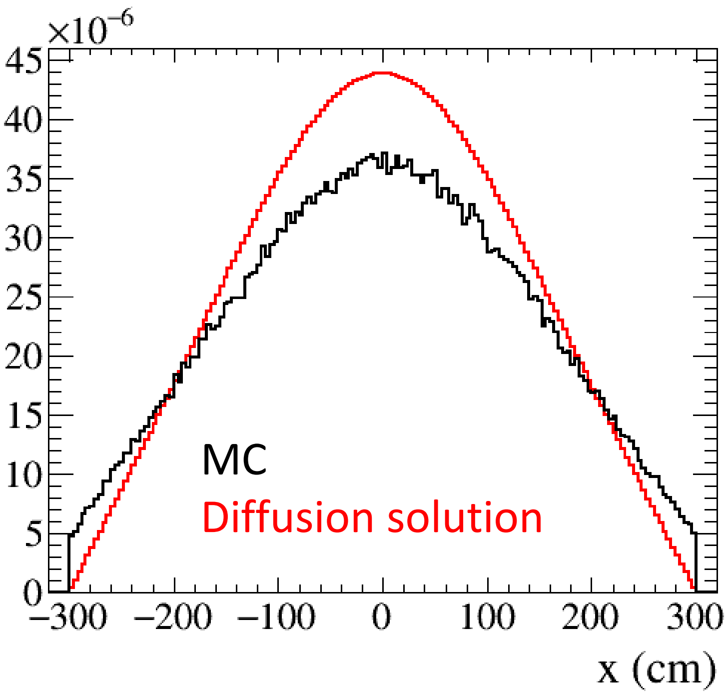
Acceptance on the cathode

Example: source at 0,0,0

Ratio Calculation/MC



View through central slice in X

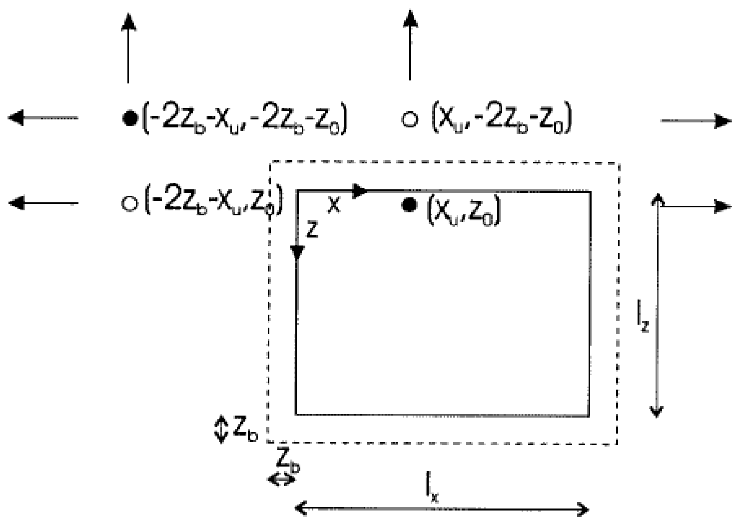


The spatial distribution is squeezed from the borders due to boundary absorption conditions on $\pm x$ and $\pm y$: $S_x \rightarrow 0, S_y \rightarrow 0$

These drive solution to zero along the cube edges

Solution to the problem

From A. Kienle
Vol. 22, J. Opt. Soc. Am. A 1883 (2005)



Apply so-called extended boundary condition, where the absorption boundary is displaced by some amount from the real detector boundary.
Introduced by Duderstadt and Hamilton, in *Nuclear Reactor Analysis (1976)* for neutron diffusion analysis

The size of the extension depends on the diffusion constant D and could be tuned for given problem (~2xD works)

$$z_b = \frac{1 + R_{eff}}{1 - R_{eff}} 2D \qquad (1)$$

Some of the detector surface could also act as a partial reflectors
Full solution can be found in A. Kienle Vol. 22, J. Opt. Soc. Am. A 1883 (2005)

Solution with extrapolated boundary condition

The position of the extrapolated boundary from the actual boundary is parametrized as $\boldsymbol{L_{ext} = f_{ext} \times D}$

For an interface between with non-scattering medium with the same index of refraction $f_{ext} = 2.1312$ (Patterson *et al* (Vol 28, J. Appl. Op. p2331 (1989)) quote this from A. Ishimaru "*Wave Propagation and Scattering in Random Media*")

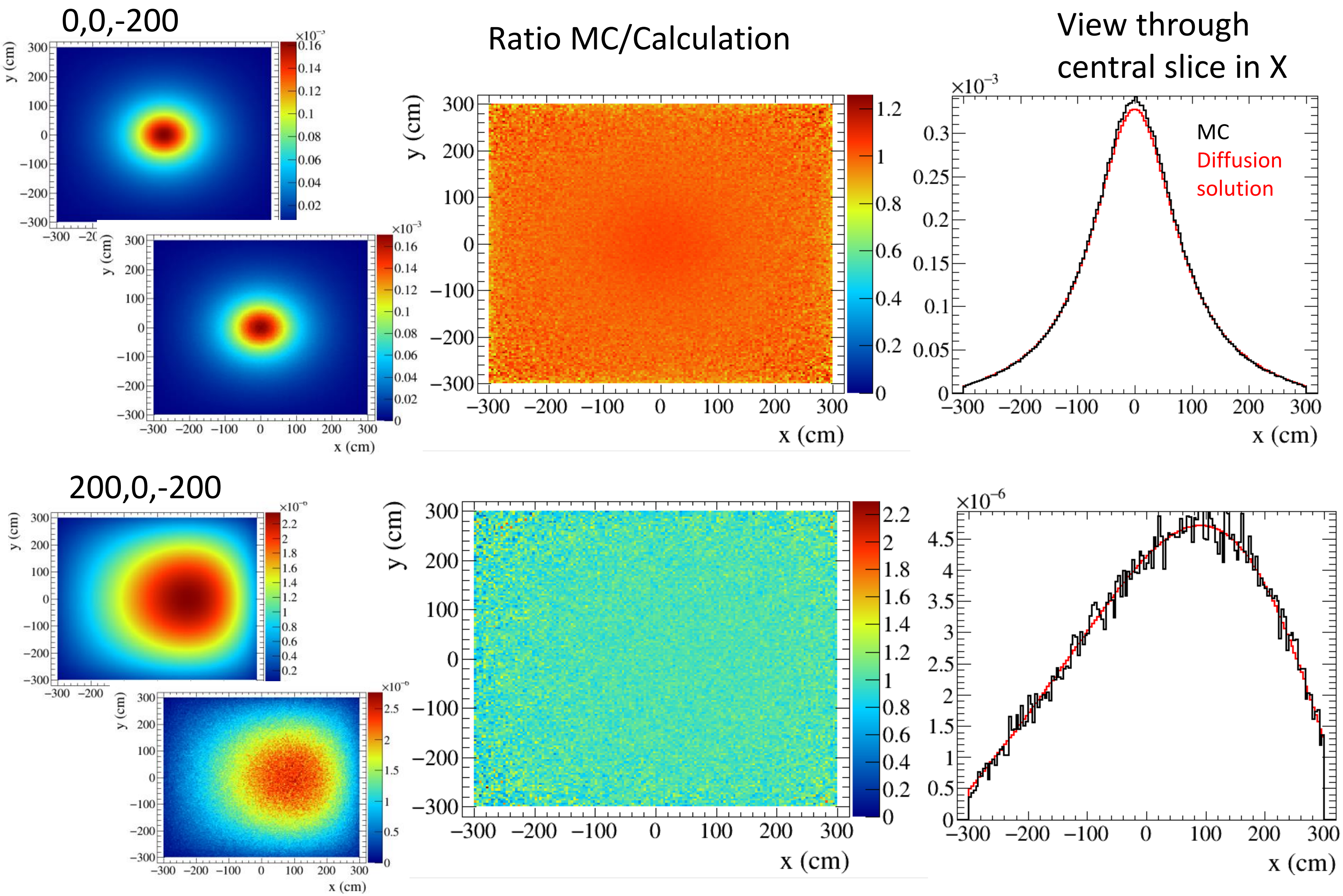
An empirical approach is to tune this parameter to match MC

Source point (cm)	P Cath MC $\lambda_{RS} = 55$	P Cath Calc $L_{ext} = 0, \lambda_{RS} = 45$	P Cath Calc $L_{ext} = 2.143 \times D,$ $\lambda_{RS} = 55$
(0,0,-200)	0.5372	0.6147	0.5370
(0,0,0)	1/6	1/6	1/6
(0,0,200)	0.0395	0.0306	0.0396
(200,0,-200)	0.4082	0.4369	0.4083
(200,0,0)	0.1058	0.0887	0.1058
(200,0,200)	0.02419	0.0155	0.2419

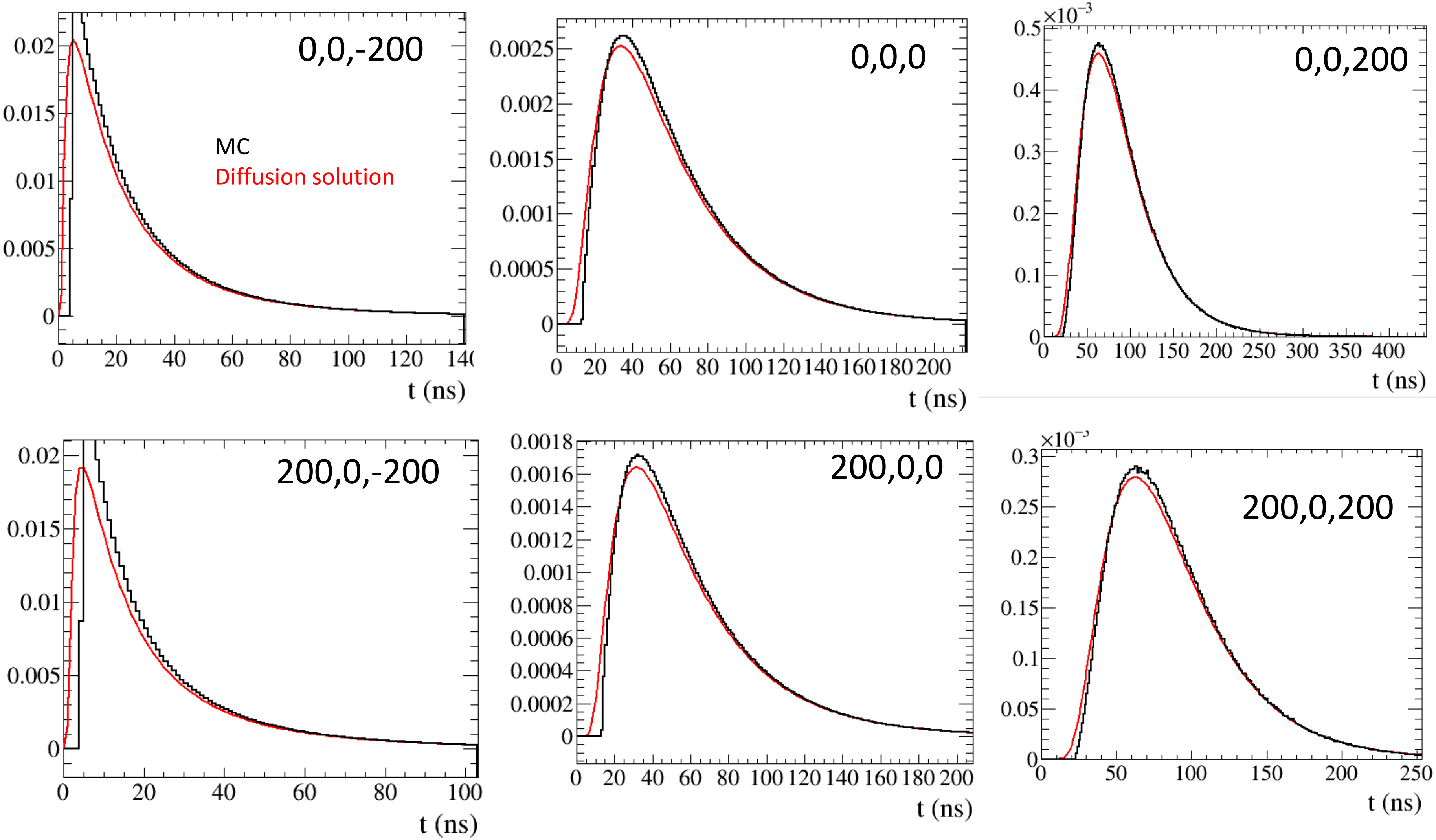
The numbers for overall normalization are essentially in agreement for the <u>same</u> value of Rayleigh scattering length $\lambda_{RS} = 55$ cm

Agreement could be further improved by tuning the extrapolated boundary factor, $f_{ext} = 2.143$, which multiplies the diffusion coefficient to higher significant digits

Comparison of spatial profiles

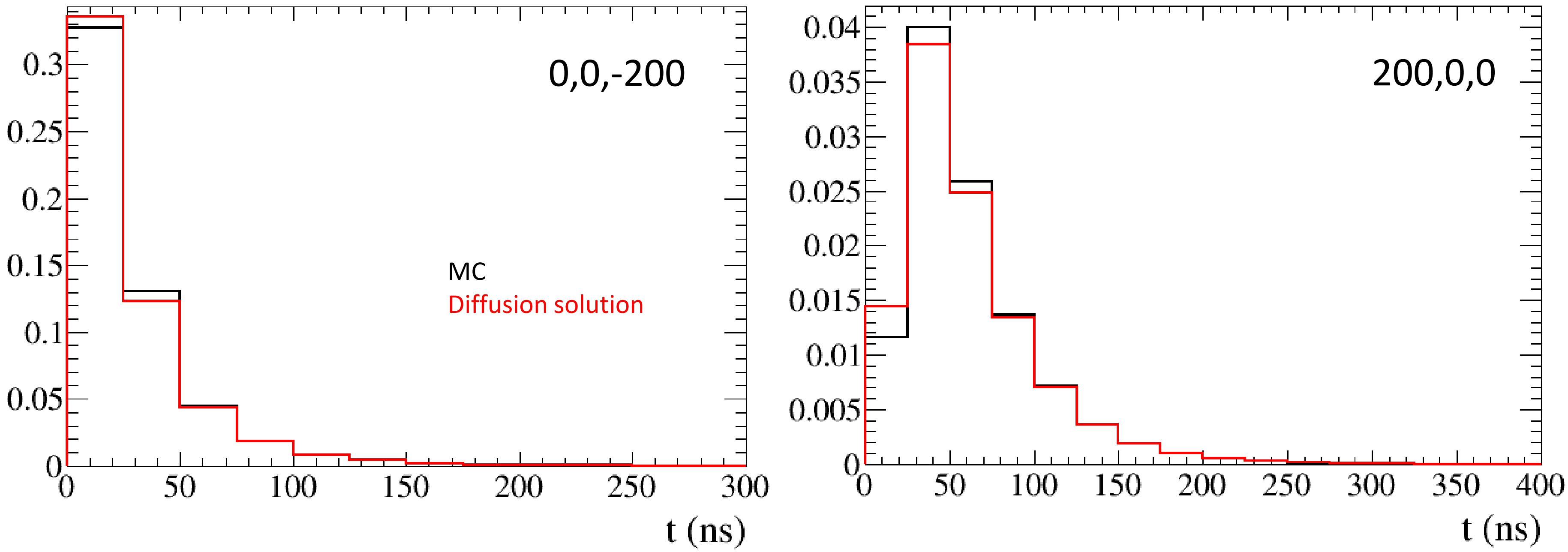


Comparison of arrival time distribution at the cathode plane



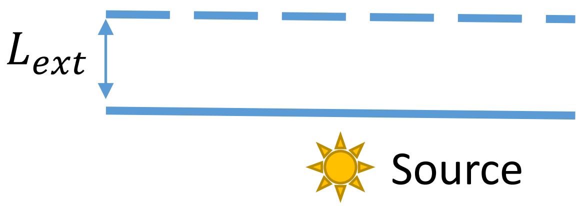
There is some discrepancy for the time distribution (especially for the source near the plane). Calculation could be fine tuned a little by adjusting the scattering length, since this is what affects the time profile the most.

Time distributions with 25ns bin



The effect may be noticeable at level of 1ns resolution, but not significant for coarser 25 ns time sampling

One point about extrapolated boundary distance



If the source is close to the boundary (~few mm distance) one needs to shrink L_{ext} to avoid contributions from the regions between real and extrapolated boundaries

I have not had time to investigate in detail, but some preliminary results showed that it may be possible to parametrize this as some variation of the scaling parameter as a function distance to the closest boundary

To give some numbers:

Source 1mm from boundary → $f_{ext}/f_{ext}^{0} \sim 0.8$

Source 5mm from boundary → $f_{ext}/f_{ext}^{0} \sim 0.9$

Possible implementation for photon propagation in DUNE DP detector simulation

1. Accumulate photons in some reasonably sized voxel: two counters N_S and N_T for singlet and triplet (or total N and sum of Triplet/Singlet from each step in a voxel)
2. Once the charge particle leaves the voxel process the collected photons and the start a new voxel accumulator
3. Repeat …

- Processing of voxel photons
  1. Calculate/get total acceptance from the voxel to the cathode plane (a scale factor to apply to the total number of photons produced): $N_{cath} = f_{acc} \times (N_S + N_T)$
  2. Randomize times of N_{cath} photons according to singlet / triplet lifetime constants
  3. Draw photon positions at cathode N_{cath} times ← critical point is to figure out how to do this step efficiently
  4. Use pre-calculated cathode plane acceptance map for each PMT to assign PMT acceptance weight $\Delta\Omega_{PMT,i}$ for each photon
     - There is a list of PMTs for each segment of the cathode, which should be already sorted in decreasing order of detector acceptances (i.e., PMTs with highest acceptance for this point are first in the list)
     - Then one goes through this list and draws from Poisson distribution with $\lambda = QE \times \Delta\Omega_{PMT,i}$ until one gets a first non-zero number and accepts this as PE for that PMT at the time given by singlet/triplet + travel time (which could also be drawn randomly from the time profile generated by RS for this point)
- Processing of S2 component goes through the same steps, the only technical aspect to understand is at which step the electron drift time and projected position becomes available in LArSoft

I think steps 1, 2, and 4 need to be done in any schemed adopted from light propagation

Another approach

- Perform convolution with the PMT acceptance directly similar to what is currently implemented in Qscan

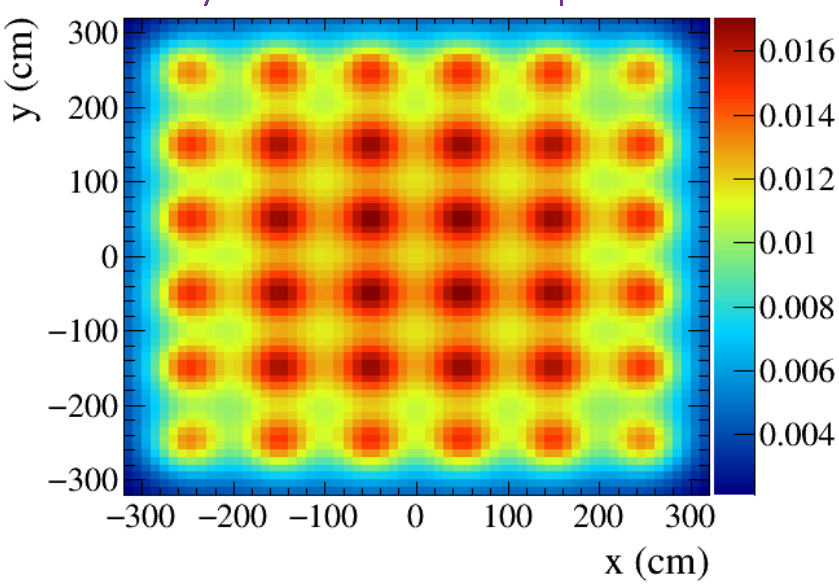
1. Calculate total acceptance from the voxel a ith region on the cathode plane to get $N_i = f_{acc,i} \times (N_S + N_T)$
2. Randomize times of N_i photons according to singlet / triplet lifetime constants
3. Loop over sorted list of PMTs acceptances in each cathode region and assign N_{ij} photons to a given PMT according to

$$N_{ij} = \frac{w_j}{\sum_{all\ PMTs} w_k} N_i$$

PMT acceptances in cathode plane

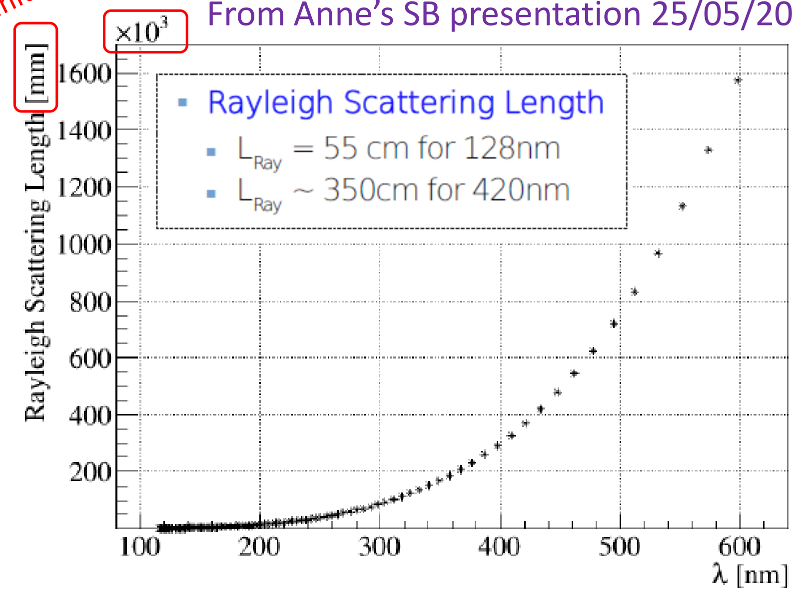
- The acceptance of PMTs from cathode plane points could be computed analytically if one is willing to ignore RS effects (not so bad since distance to PMTs is less than scattering length)
- Otherwise it would be calculated with full simulation of photon transport

Sum of all PMT weights with the array 50 cm below cathode plane



Not sure about this unit though

From Anne's SB presentation 25/05/2016



Acceptances are computed analytically on a grid of 10x10cm^2 ~ PMT radius

Sampling points on the cathode plane

- PDF for photons on the cathode plane is

$$p(x,y,t) = \frac{1}{[4\pi D(t-t_0)]^{3/2}} S_x S_y \partial_z S_z$$

- Is it possible to write down analytical form for *p(x,y)*? Otherwise one has to perform numeric integration over *t*
- Prescription:
  - Calculate marginal CDF for x

This integral is fast by interpolating erf tables

$$CDF(x) = \int_{-w}^{x} dx \int_{0}^{\infty} dt \int_{-l}^{+l} dy\, p(x,y,t)$$

  - Sample it N_{cath} times to generate x_i positions and then sample y from conditional CDF at each x_i

$$CDF(y|x_i) = \int_{-l}^{y} dy \int_{0}^{\infty} dt \int_{x_i-0.5\Delta}^{x_i+0.5\Delta} dx\, p(x,y,t)$$

The speed of execution depends how many bins in x are populated, since this is what determines if one needs to compute new $CDF(y|x_i)$

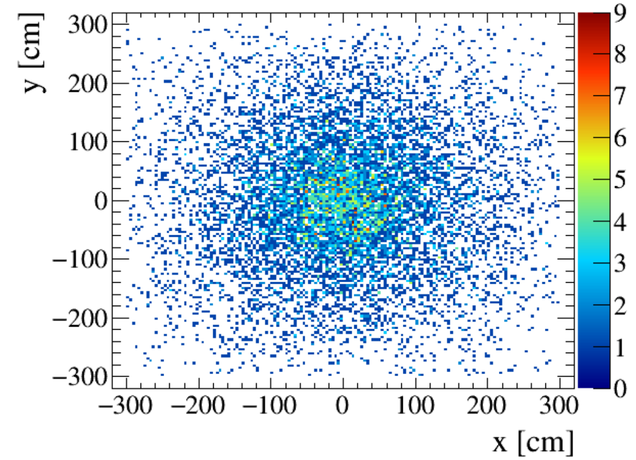
Some numbers

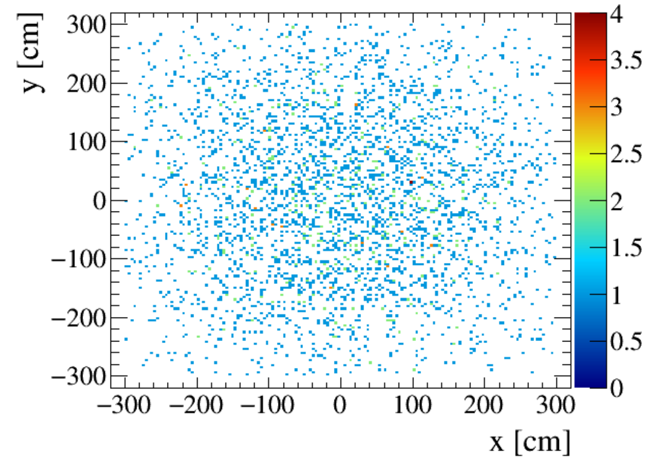
Source position	Phot to simulate	Exec time
0,0,-200	10740	~6s
0,0,0	3333	~5s
0,0,200	792	~2s

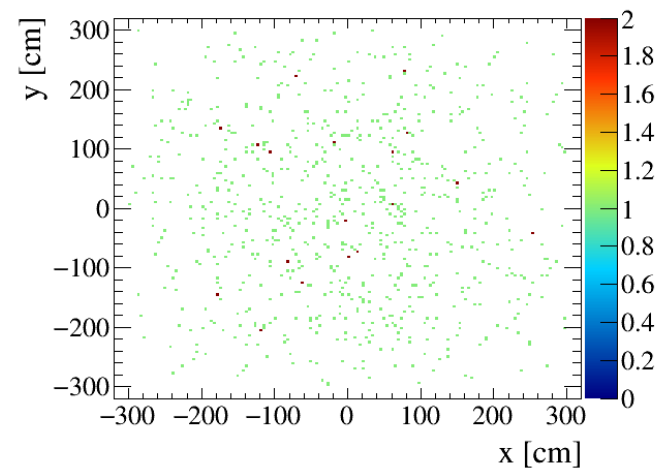
System specs
CPU: i7, 2.90GHz
RAM: 8.0GB

Source: 20,000 photons ~ 2 MeV/cm deposited by MIP
Binning used to calculate CDFs at the cathode plane is 10x10 cm2

Still too slow to perform such calculations at run-time for neutrino events (extended charge depositions)
On the other-hand one should optimize a size of the step before performing light propagation
e.g,. 1 cm would be too fine
➔ Looks promising







Effect of bin size for CDF calculation

CDFs are calculated on a grid of 10x10cm2, but the x,y values are then linearly interpolated between the bins

Examples:

Source 100M photons

Top: 0,0,0: ~15s exec (17M phot to map)

Middle: 0,0,-200: ~40s (54M phot to map)

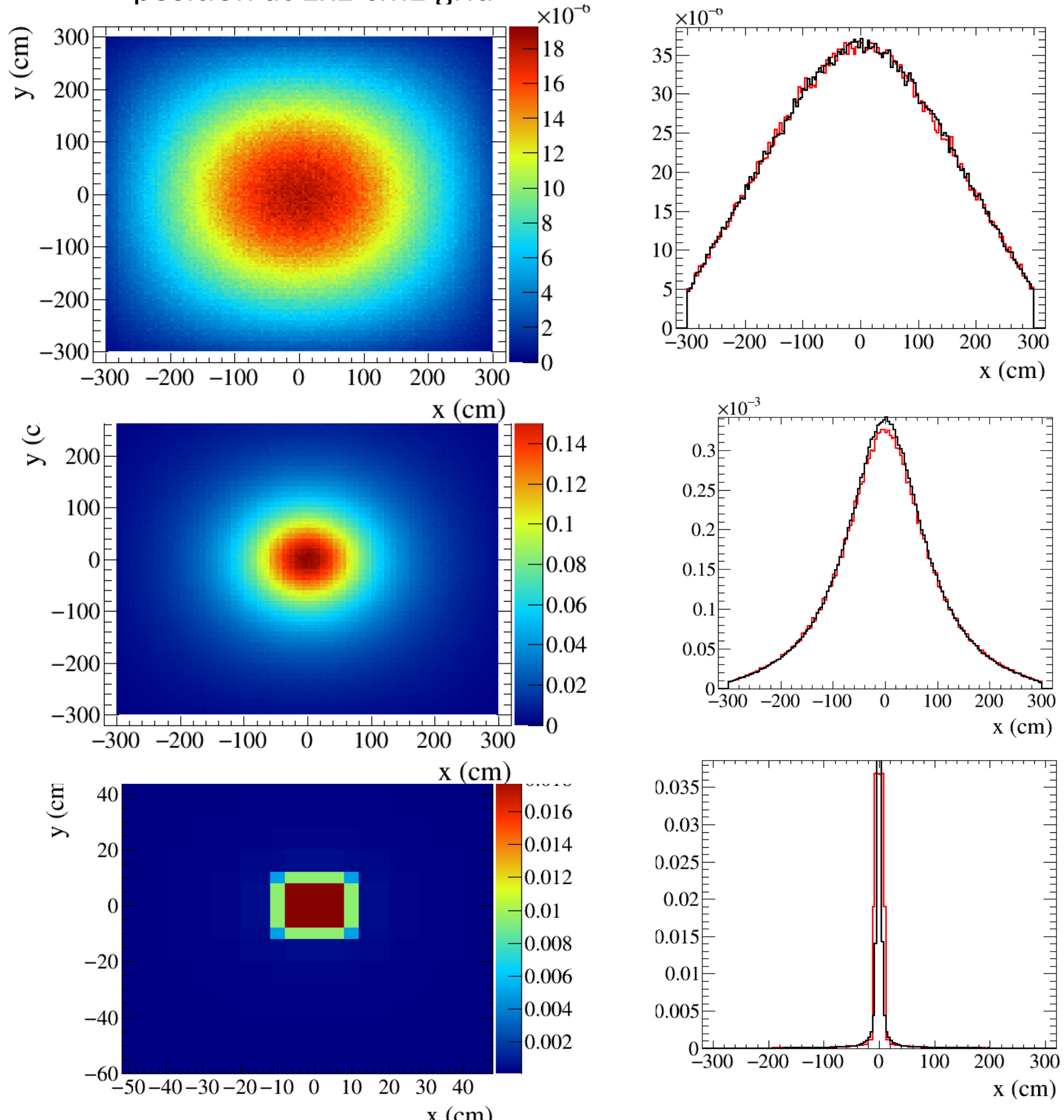
Bottom: 0,0,-299: ~57s (85M phot to map)

For a source at 1 mm above the plane the binning effect of the CDF becomes more apparent, but we are not looking at the position measurement with light (not ~tens of cm at least)

2D distribution of photon position at 2x2 cm2 grid

Photon light simulation

Generation with RTE solution



Some improvements (maybe)

- Possible to write down analytical solution for steady-state (i.e., with t integrated out)
  - It is not a simple expression as one need to multiply the three expansion series (e.g., N terms in each series → N^3 terms after multiplication)
  - This would give a total time integrated probability for given point without need for numerical integration
- To sample time distribution interested in CDF for a given point
  - Need to compute integrals for terms of the form:

$$\int_0^t dt \frac{1}{\sqrt{t^5}} \exp\left[-\frac{r^2}{t}\right]$$

There is actually a close form solution to this integral according to Wolfram Alpha

$$\Rightarrow \quad \sqrt{t^5} \times \frac{\left(\sqrt{\pi t}\,\operatorname{erfc}\frac{r}{\sqrt{t}} + 2r \exp -\frac{r^2}{t}\right)}{2t^3 r^3}$$

Better solution form?

One could re-write solutions on p. 14 using Poisson's summation formula as:

$$p(\boldsymbol{r}, t; \boldsymbol{r}_0, t_0) = \frac{1}{w \times l \times h} \times \Phi_x \times \Phi_y \times \Phi_z$$

$$\Phi_x = \sum_{n \geq 1}^{\infty} \exp\left[-\frac{n^2 \pi^2 D t}{4 w^2}\right] \sin \frac{n\pi(x - w)}{2w} \sin \frac{n\pi(x_0 - w)}{2w}$$

And similarly for Φ_y and Φ_z …

The partial derivatives and the spatial integrals are still easy since it is just a sum of $\sin(ax)$ and then can be computed quickly by building sin/cos lookup table

The advantage is the time dependence is factored out and the temporal integral could be done analytically: it is now a sum of terms $\int dt \exp(-at)$

Another possible advantage could be only terms which depend on source position in the series, $\sin n\pi(x_0 - w)/2w$, need to be recomputed

The problem with periodic functions, however, is ringing in the solution due to truncation of higher order harmonics and this is not a trivial issue to address

Conclusions

- Diffusion equations can be solved to give a reasonable description of the time evolution of photon densities in homogeneous scattering medium
  - It is impressive that collective behavior of the diffusing photons can be described so well by the theory
- Some thought is still needed to improve the execution time in order to consider calculating photon propagation at runtime
  - It would be good to develop and effective approximation which are easy to compute for any point in the detector volume
- Another point to stress: some solution for light simulation has to be implemented soon in order to meet deadline set by DUNE FD TF report
  - Two problems: most effective way to do light propagation for dual-phase detector and how feasible to actually do it in the larsoft framework
- Please let me know if you have other solutions / interesting ideas / proposals