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

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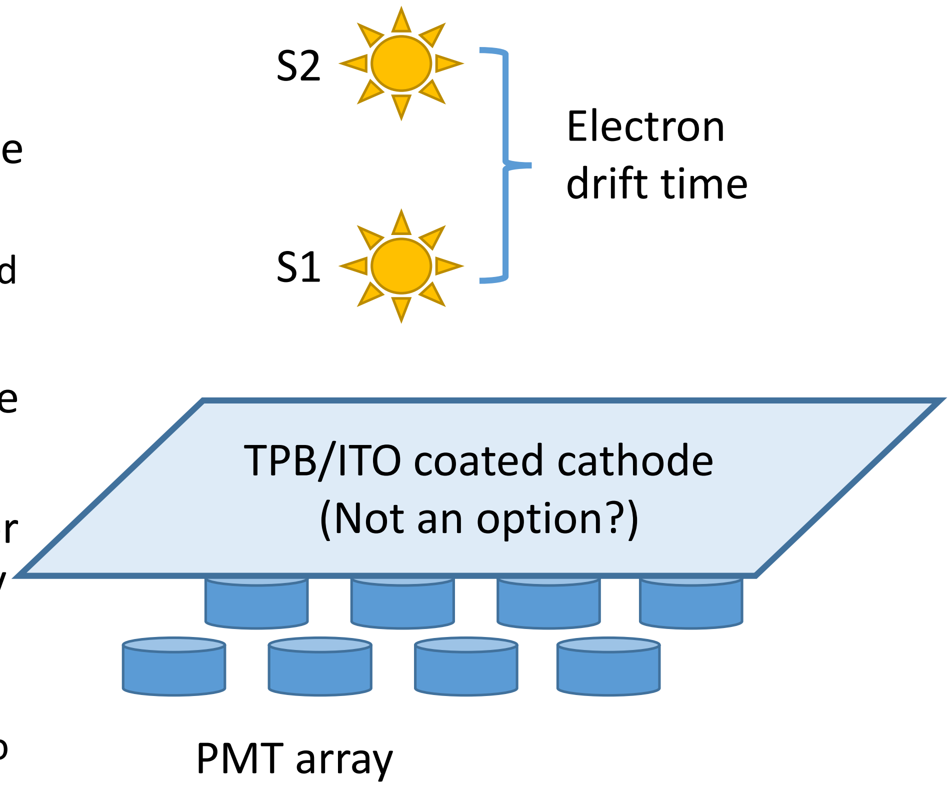
# Some challenges

- Light simulation for dual-phase has to include
  - Generation of S2 in addition to S1
  - Light conversion on the cathode plane if used
- 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

$O_2$ meter(image: Wikipedia)

**Basically find effective solution for particle propagation in scattering medium using diffusion theory**

# 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):

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

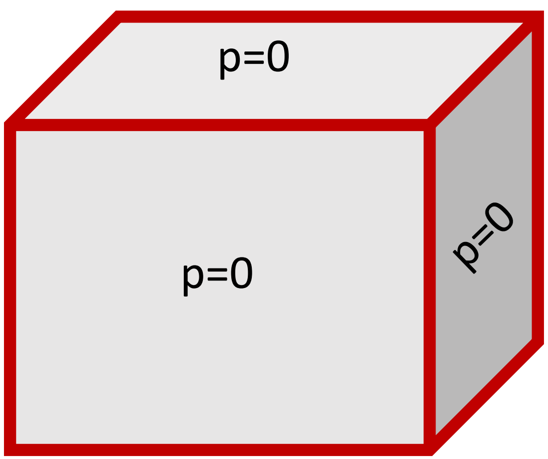
This is the equation one needs to solve for photon diffusion subject to appropriate boundary conditions

# 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 $\mu_A \sim 0$

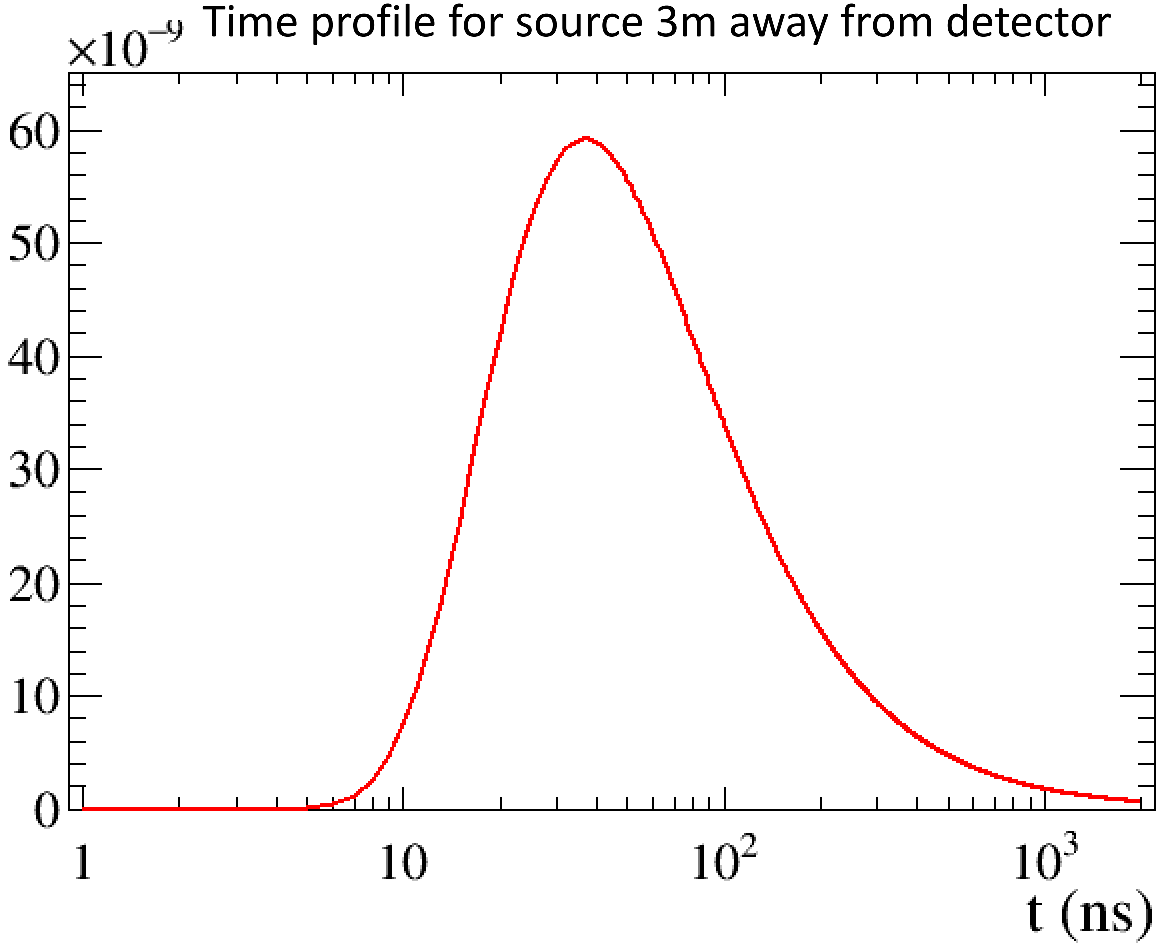
$D = 18.8$ cm
Or cm2/ns if one multiply by velocity to get more familiar units

$\mu_A$ - absorption coefficient [1/units of L]
$\mu_S$ - scattering coefficient [1/units of L]
$g$ – average scattering cosine

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

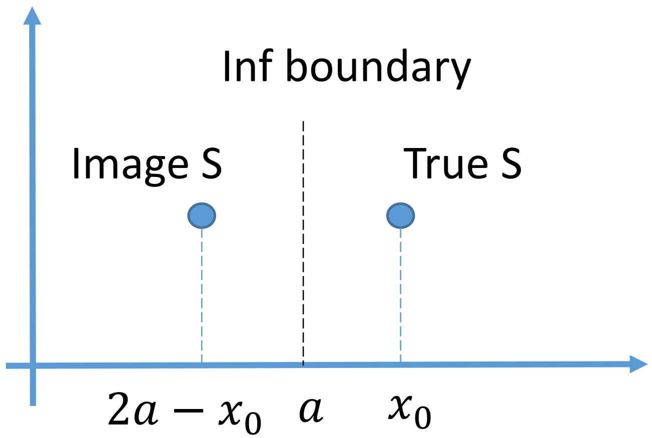
# Unbound solution

Time profile for source 3m away from detector

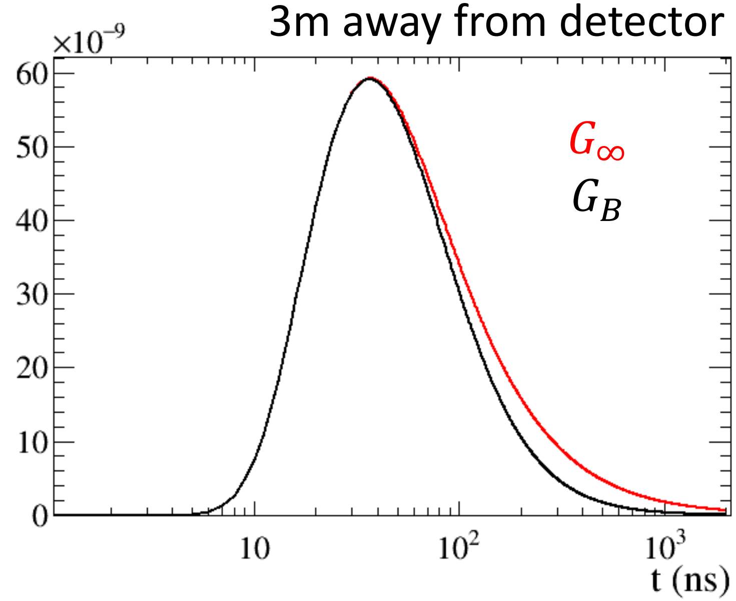



Note the extending tail is due to infinite boundaries ➔ due to scattering photons will keep arriving …

# Single absorption boundary




Time profile for source 3m away from detector



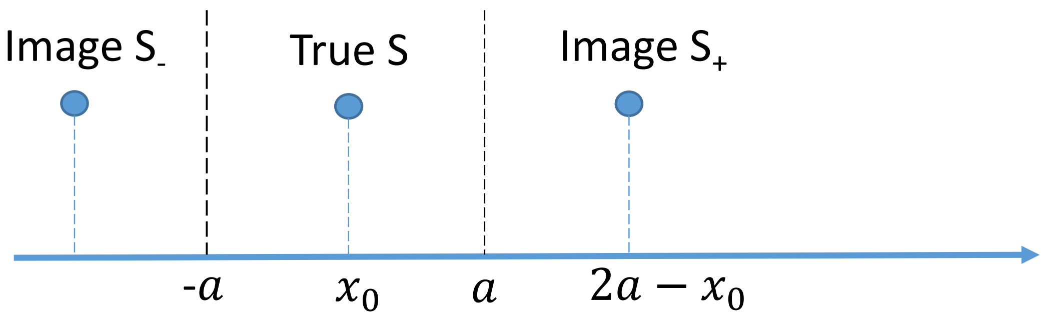

Solution for $x > a$ is simply a difference between two unbound Green's functions for true source $x_0$ at and its mirror image at $2a - x_0$

The tail is reduced due to photons absorbed at the boundary

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

# 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 $S_-(-2a + x_0)$ 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

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

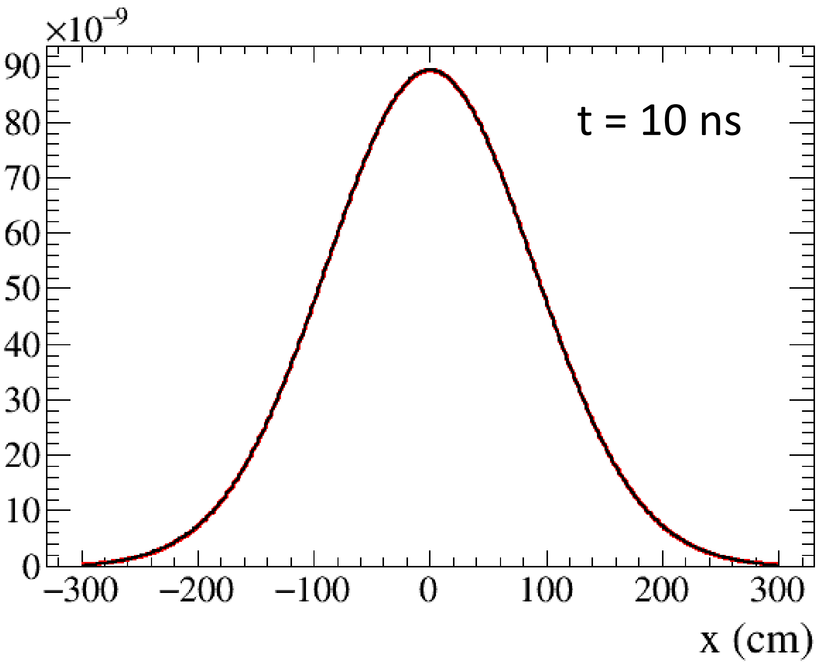
$$S_x = \sum_{n=-\infty}^{+\infty} \exp\left[-\frac{(x - x_0 + 4nw)^2}{4D(t - t_0)}\right] - \exp\left[-\frac{(x + x_0 + (4n - 2)w)^2}{4D(t - t_0)}\right]$$

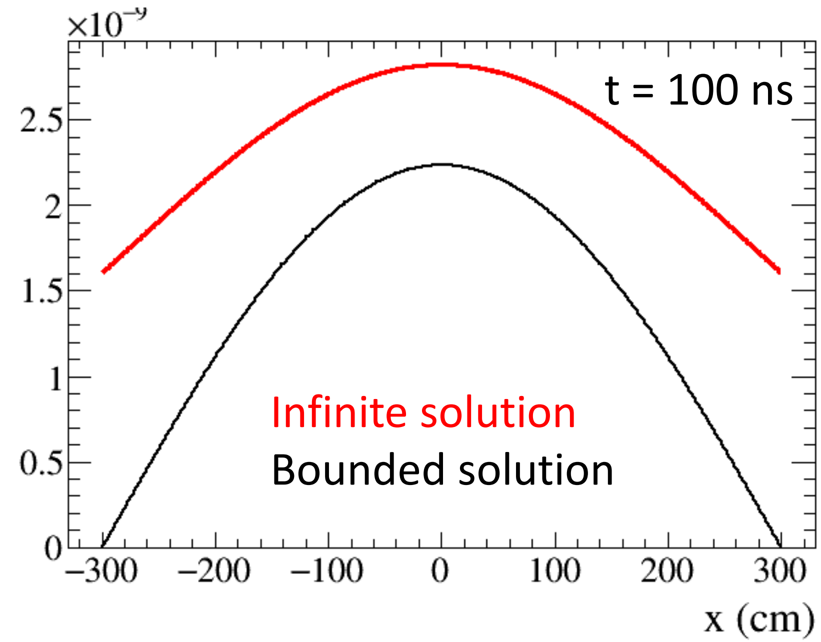
$$S_y = \sum_{n=-\infty}^{+\infty} \exp\left[-\frac{(y - y_0 + 4nl)^2}{4D(t - t_0)}\right] - \exp\left[-\frac{(y + y_0 + (4n - 2)l)^2}{4D(t - t_0)}\right]$$

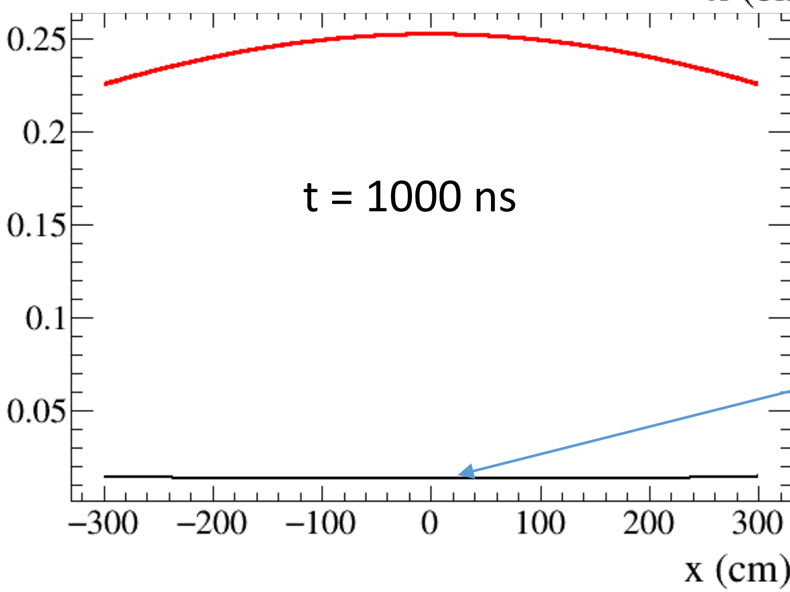
$$S_z = \sum_{n=-\infty}^{+\infty} \exp\left[-\frac{(z - z_0 + 4nh)^2}{4D(t - t_0)}\right] - \exp\left[-\frac{(z + z_0 + (4n - 2)h)^2}{4D(t - t_0)}\right]$$

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 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

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

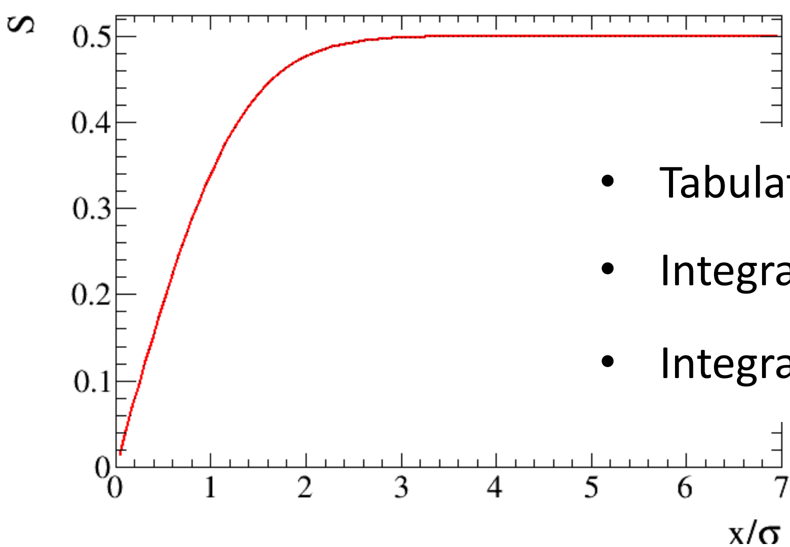
# Integration

Spatial integrals can be done quickly

For the acceptances calculation need to integrate Gaussians in the expansion series of the type

$$\int_a^b dx \exp[-s(x - x_0)^2] \sim \mathrm{erf} \ldots$$

Interpolate error function table computed in advance → fast and independent of integration range, since only need two end-points




- Tabulate $0.5\,\mathrm{erf}\left(\frac{x}{\sigma\sqrt{2}}\right)$ up to $\mathrm{N}\sigma(=1) = N$
- Integral for any interval [x+D, x] → $S\left(\frac{x+D}{\sigma_x}\right) - S\left(\frac{x}{\sigma_x}\right)$
- Integral for an interval [-a, b] → $S\left(\frac{|a|}{\sigma_x}\right) + S\left(\frac{b}{\sigma_x}\right)$

# Acceptance calculation: basic sanity check

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

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*

# Fast MC simulation of photon transport

Necessary to verify analytical solution against full MC simulation of photon transport

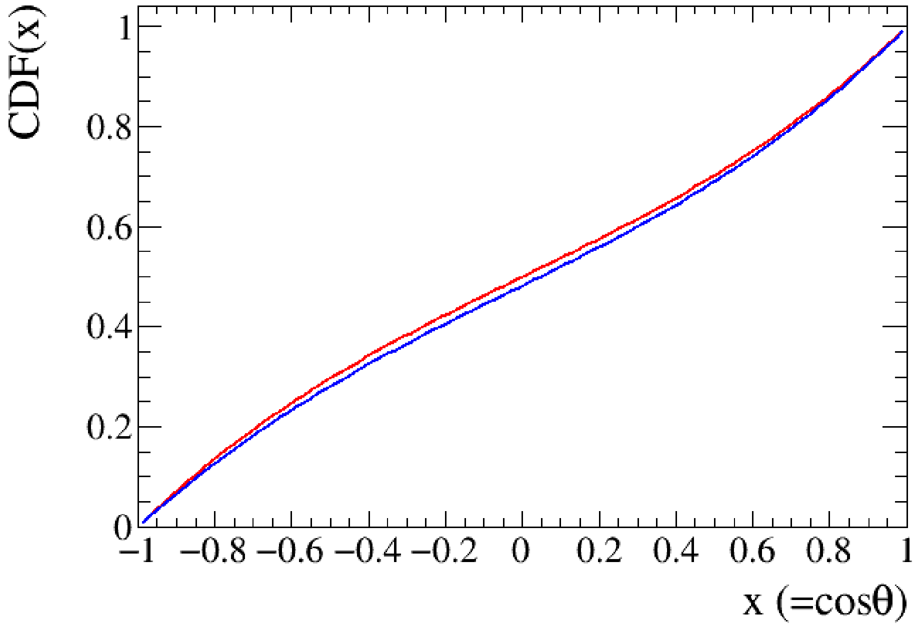
Made simple random walk MC for this

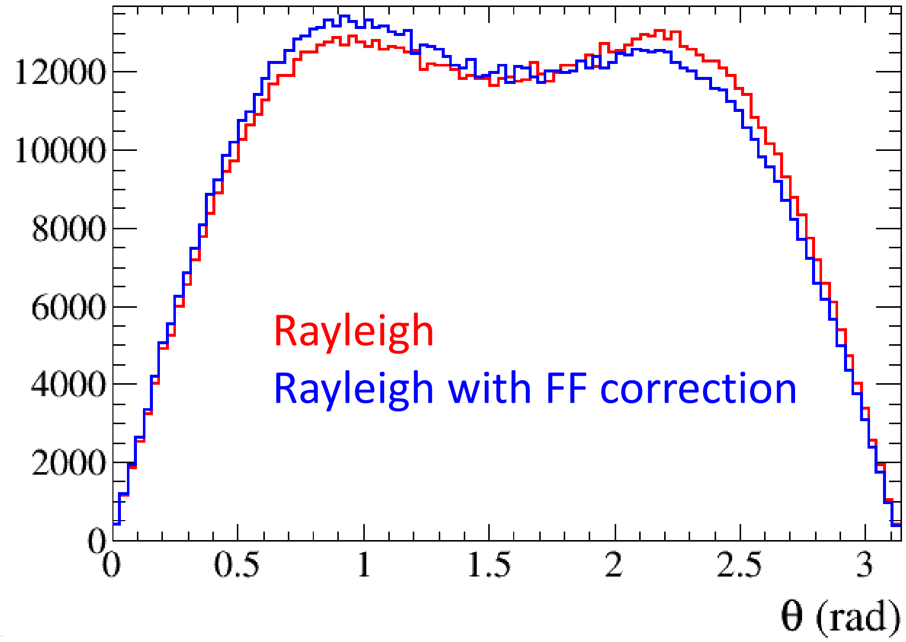
- Given Rayleigh scattering (RS) length, step size is sampled from: $e^{-s/\lambda_{RS}}$
- At the end of the step photon angle is randomized according RS distribution
- Detector is modelled as cuboid and photons crossing the boundary are scored (boundaries are perfect absorbers)

$$\frac{d\sigma_{RS}}{d\Omega} \propto (1 + \cos^2\theta) \quad \Rightarrow \quad CDF(x = \cos\theta) = \frac{3}{8}\left(\frac{4}{3} - \frac{x^3}{3} - x\right)$$

Form factors for argon introduce some anisotropy so they are also included
Hubbel & Overbo: J. Phys. Chem. Ref. Data, Vol. 8, No. 1, 1979

# Cumulative & Angular Distributions for RS

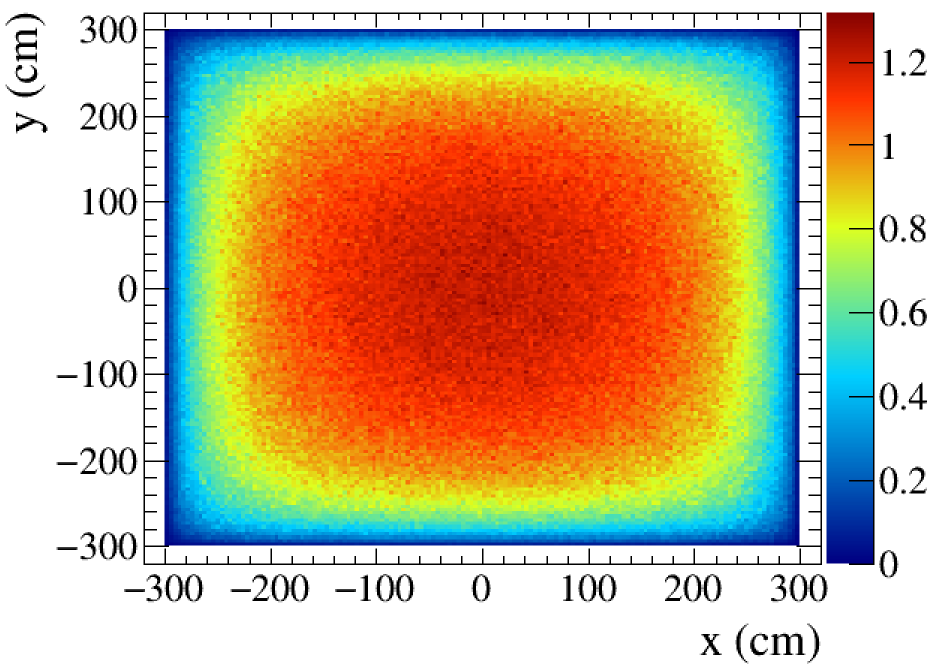


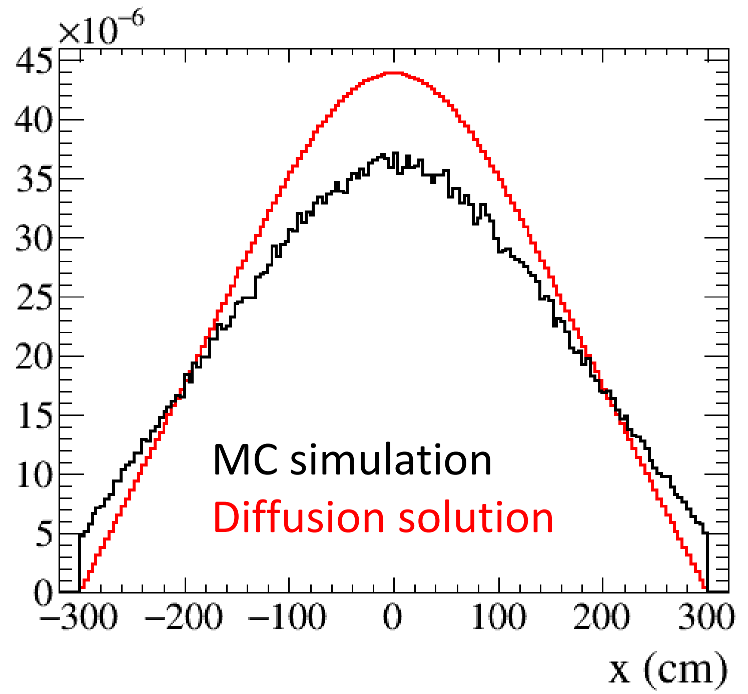
# Problems at the edges

*Example: source at 0,0,0*

Ratio Calculation/MC




View through central slice in X

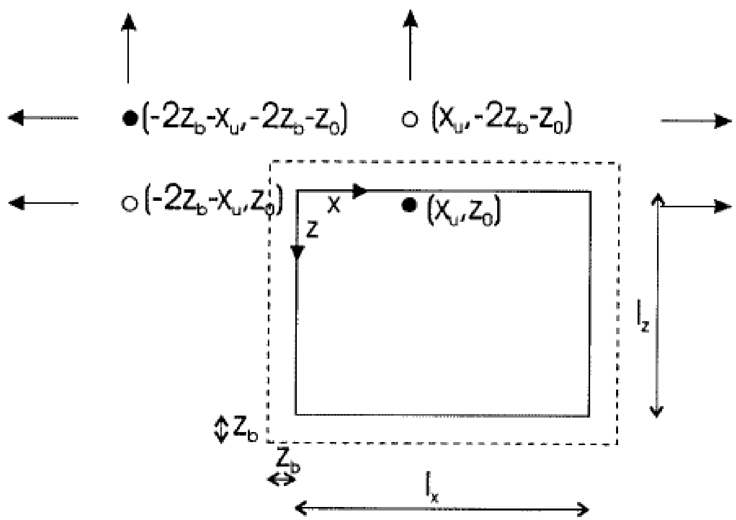



The spatial distribution is squeezed from the borders due to boundary absorption conditions on $\pm x$ and $\pm y$: $S_x \to 0, S_y \to 0$

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 $\lambda_{RS} = 55$ cm | P Cath Calc $L_{ext} = 0$ | P Cath Calc $L_{ext} = 2.143 \times D$, $\lambda_{RS} = 55$ cm |
|---|---|---|---|
| (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 if extrapolated boundary is used

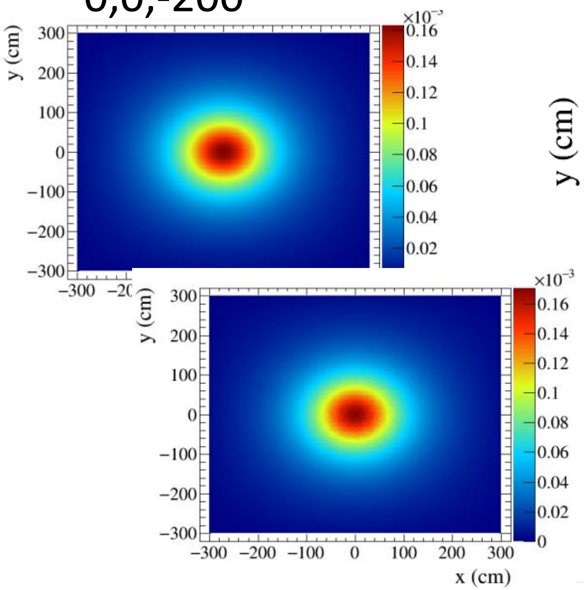
Agreement could be further improved by tuning the extrapolated boundary factor to more significant digits

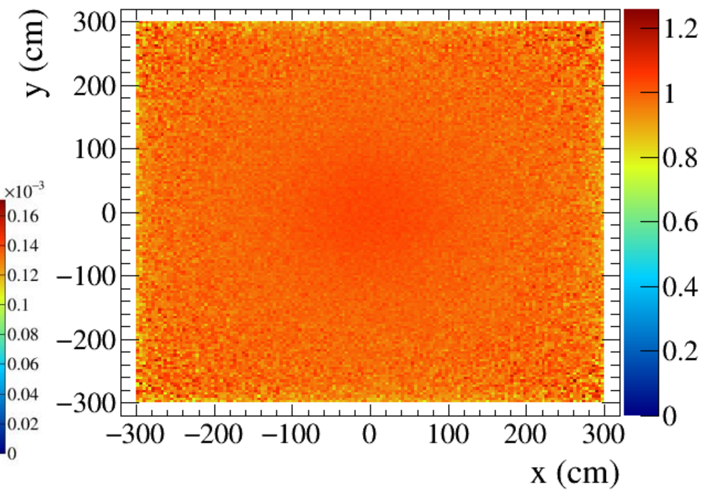
# Comparison of spatial profiles

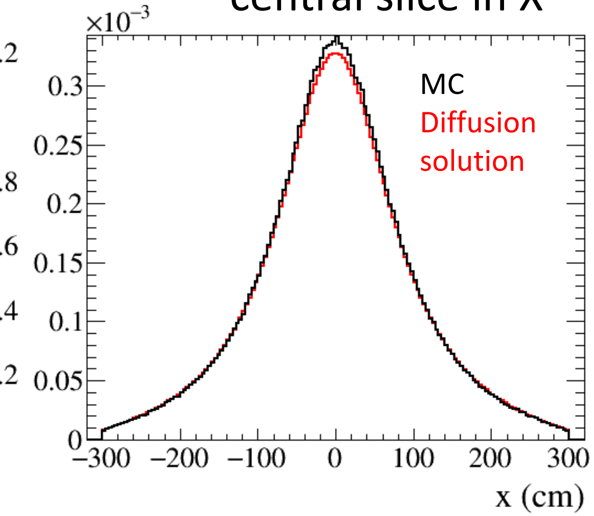
0,0,-200

Ratio MC/Calculation

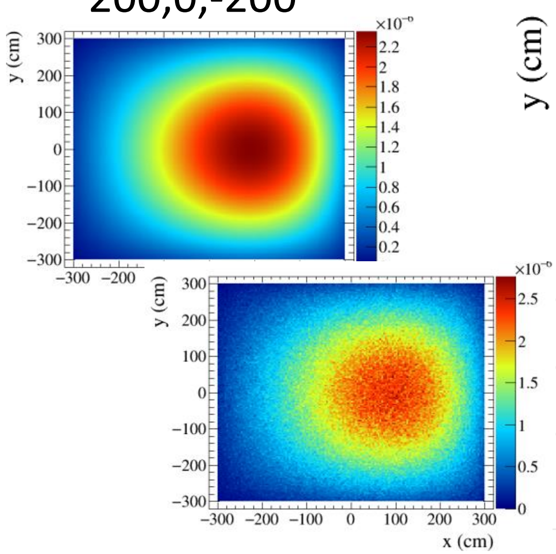
View through central slice in X

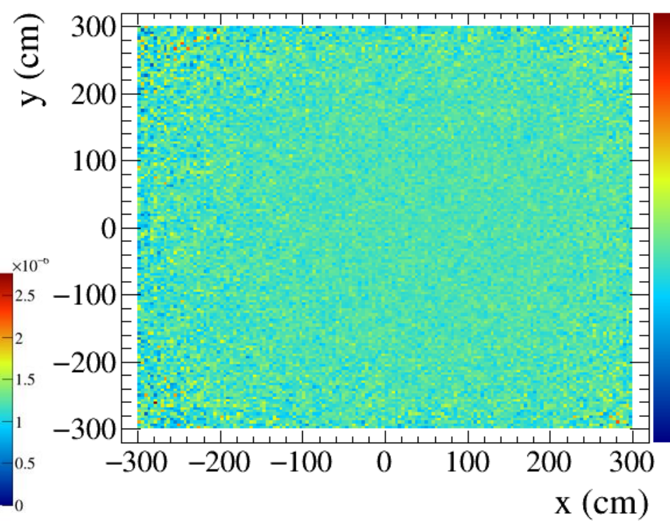


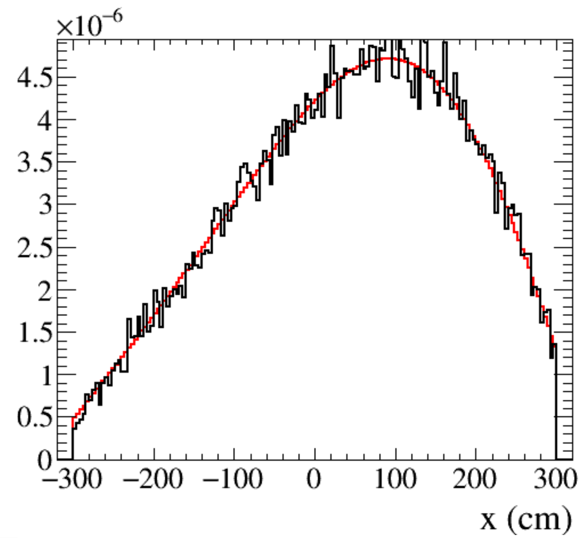



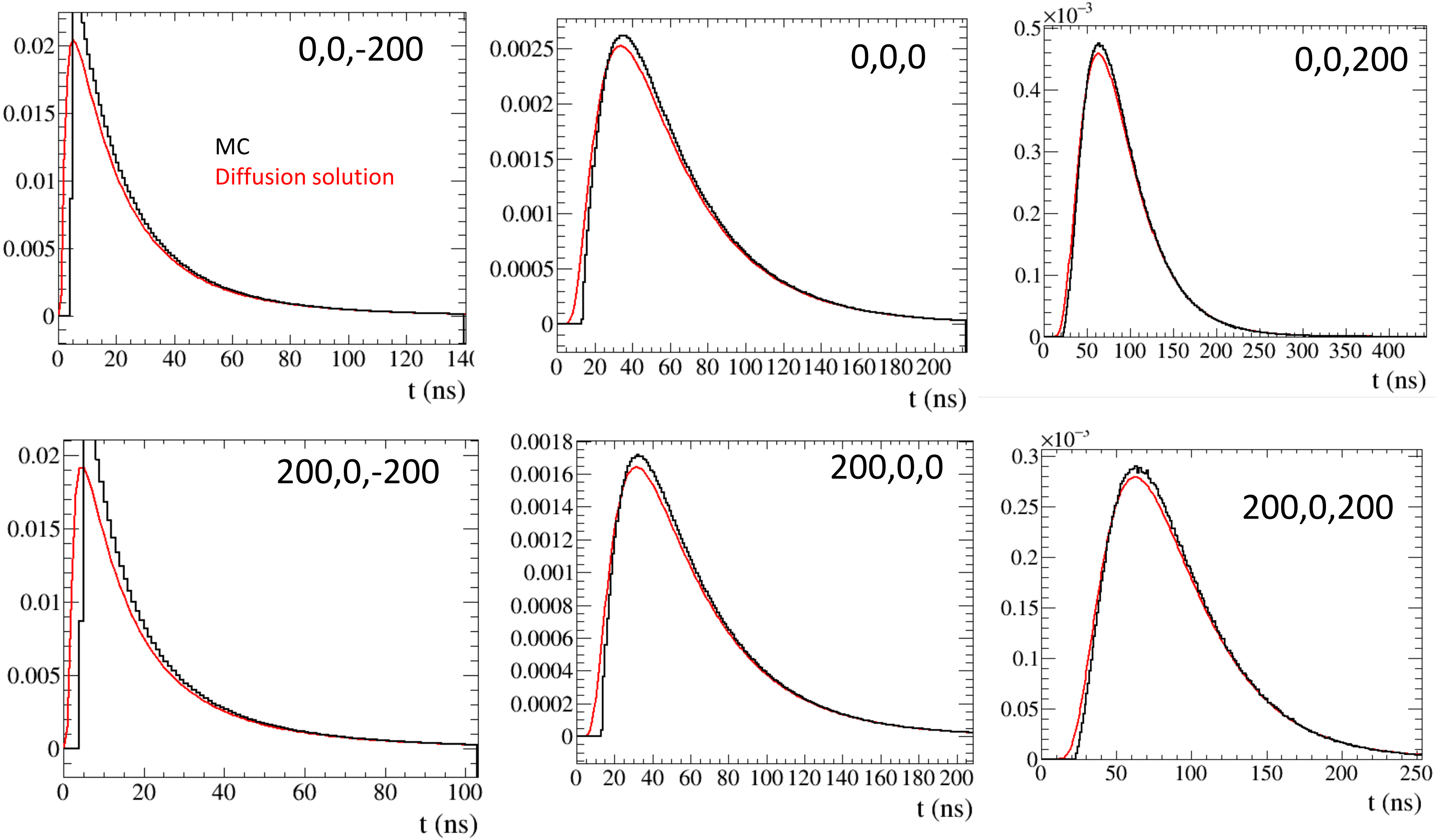

200,0,-200



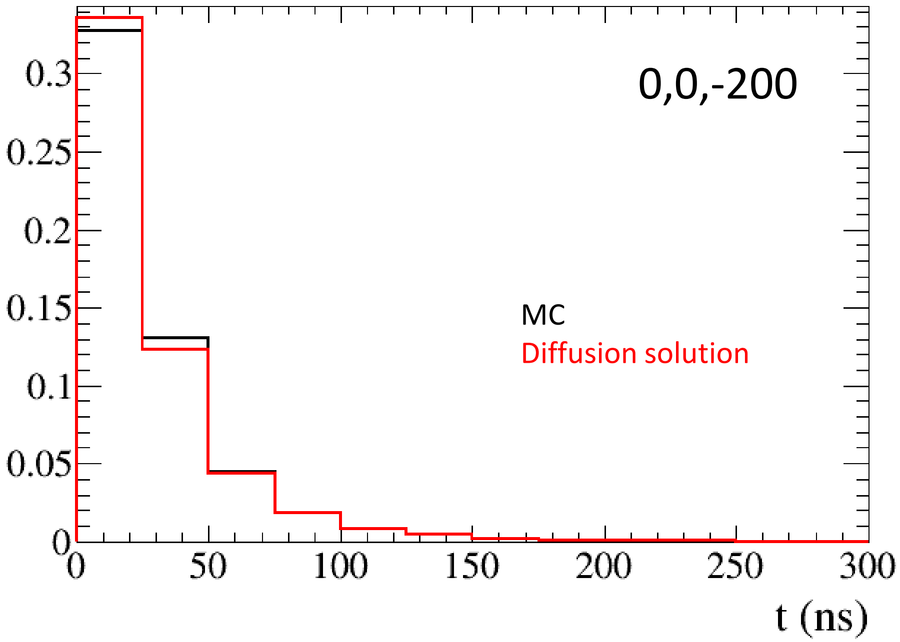



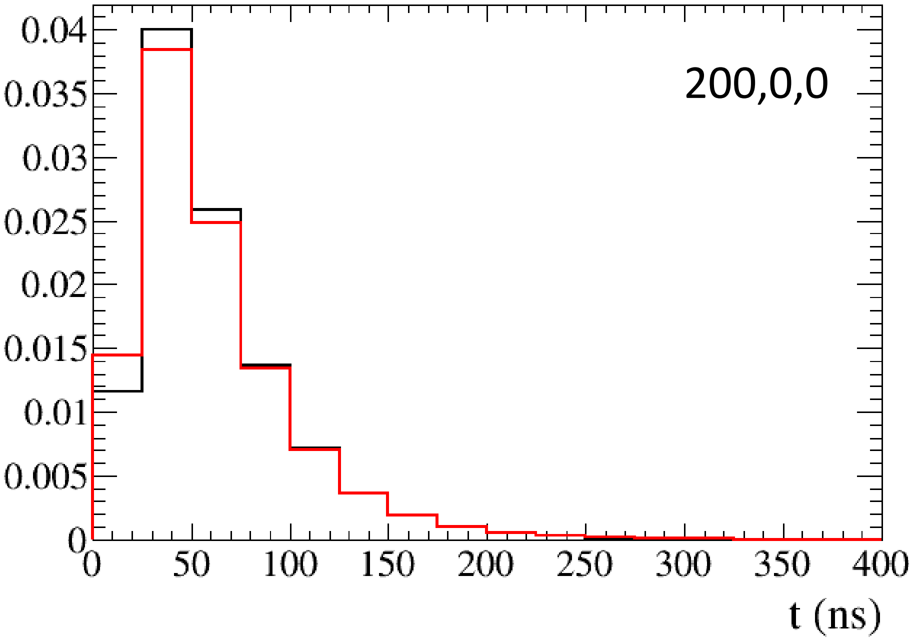
# Comparison of arrival time distribution at the cathode plane




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 too significant for coarser 25 ns time sampling

Add to that the spread due to scintillation lifetimes and I do not think this discrepancy would matter that much

# Photon simulation: method 1

## During GEANT stepping action:

- Accumulate photon counters in some reasonable voxel: two counters $N_S$ and $N_T$ for singlet and triplet or total $N_\gamma$ and sum of Triplet/Singlet ratios from each step
- Process voxel as soon as the particle leaves it

## Processing photons:

- Loop over photon detectors and find appropriate acceptance factor for a given detector

$$f_{acc,i} = \int_{t_0}^{\infty} dt \int_{S} dxdy\, p(x, y, t; \boldsymbol{r}_0, t_0)$$

- For rectangular detection areas spatial integral is easy and time integral done numerically
  - Also gives CDF(t) for sampling arrival time distribution
- Number of photons seen by this detector is then: $f_{acc,i} \times N_\gamma$
- Their times could be distributed according S/T ratio and lifetimes

# Photon simulation: method 2

## Same actions as Method 1 during GEANT stepping action:

## Processing photons:

- Calculate total acceptance from voxel to the plane of the cathode to get number of photons reaching $N_{cath} = f_{acc} \times N_\gamma$
- Draw photon positions at cathode plane $N_{cath}$ times

  Prescription:

  - Calculate marginal CDF for x

$$CDF(x) = \int_0^\infty dt \int_{-w}^{x} dx \int_{-l}^{+l} dy\, p(x, y, t)$$

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

$$CDF(y|x_i) = \int_0^\infty dt \int_{-l}^{y} dy \int_{x_i-0.5\Delta}^{x_i+0.5\Delta} dx\, p(x, y, t)$$

- Use pre-calculated cathode plane acceptance map for each PMT to assign PMT acceptance weight $\Delta\Omega_{PMT,i}$ for each generate photon
- Randomize times of photon arrival times as before

# Some numbers

| Source position | Phot to simulate | Exec time |
|---|---|---|
| 0,0,-200 | 10740 | ~5s |
| 0,0,0 | 3333 | ~3s |
| 0,0,200 | 792 | ~3s |

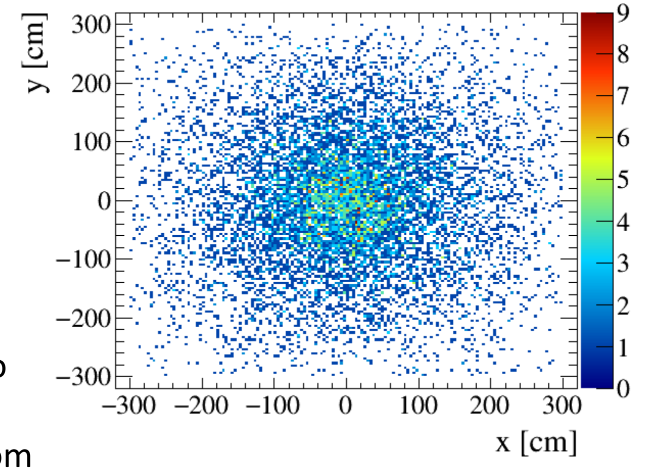
System specs
CPU: i7, 2.90GHz

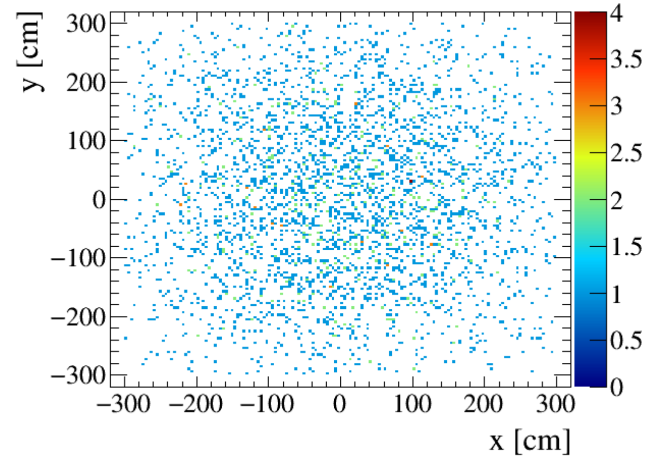
The numbers correspond to generating photons on the plane w/ times sampled from time profile distribution
Could be reduced by choosing coarser time bins for numerical integration

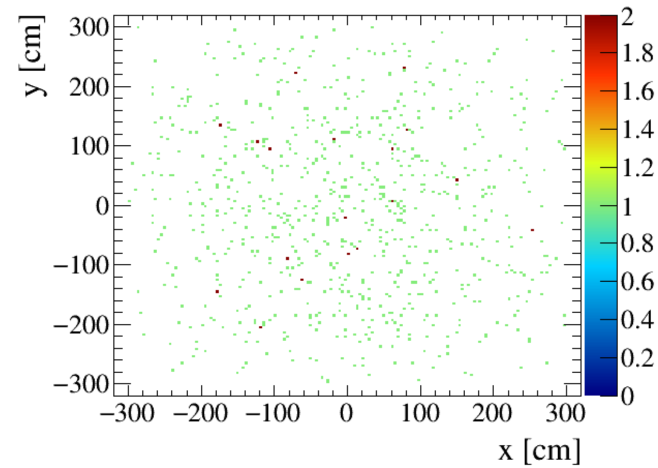
Source: 20,000 photons ~ 2 MeV/cm deposited by MIP
Binning used to calculate CDFs at the cathode plane is 10x10 cm2

For extended charge depositions (neutrino events) need to optimize a size of the step before performing light propagation, e.g,. 1 cm would certainly be too fine

For low energy events should also optimize the voxel size, but since the spatial extension is not large it is less critical



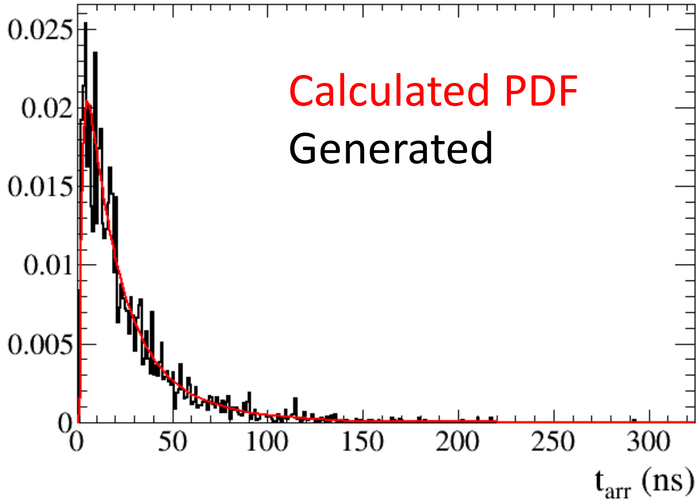



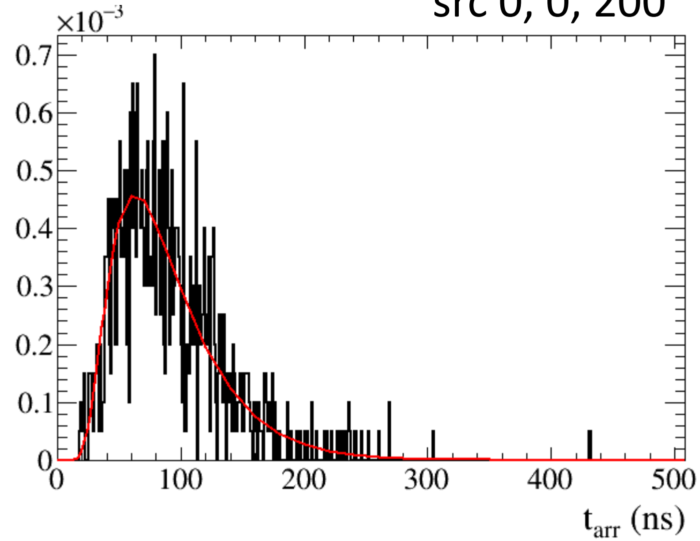
# Distribution of arrival time

- The arrival time (apart from S/T lifetimes) is randomly sampled to account for delayed photons due to RS
  - Since one does numerical integral in time, one calculates CDF(t) in the same step
  - Alternatively can return the time corresponding to the peak of the distribution (already implemented)
  - Or even <t> (just need to add another sum counter $\sum t_i \Delta t f(t_i)$)

src 0, 0, -200



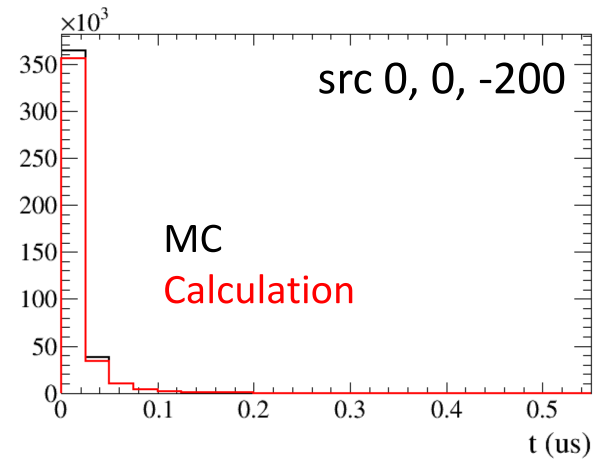

src 0, 0, 200

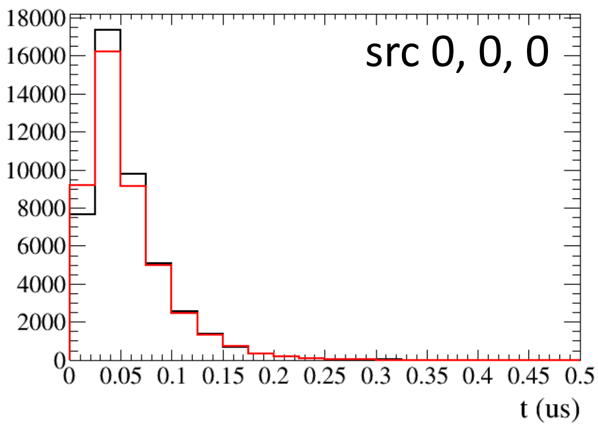



Of course, the precision of sampling is also affected by how coarse the spatial bins are. But if one has ~40-50MHz sampling this does not play a big role

# Visibility and arrival times: method 1

Comparison with MC for voxel visibility and arrival times
For simplicity (and lack of time) only one "detector" with area of 10x10cm$^2$ at the center of the cathode plane. Source 100M photons (<0.02 s to process normally )




Ratio = Visibility calculation/MC

| src | R visibilities |
|---|---|
| 0,0,-200 | 0.97 |
| 0,0,0 | 0.99 |
| 0,0,200 | 1.01 |
| 200,0,-200 | 1.02 |
| 200,0,0 | 1.01 |
| 200,0,200 | 1.00 |
| 0,0,-299 | 0.93 |

Need to tune boundary conditions for source so close

The statistical uncertainty on the number of photons ~0.2-1.0% depending on the distance from the source

# 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
- The calculation can provide a quick answer to visibility of a point inside TPC to a given optical detector as well as reasonable description of arrival times
- It can also give spatial distribution of photons in a given scoring plane
- It is reasonable fast to execute at runtime (without pre-calculated massive photon libraries)
  - Some disagreement with MC exists, but probably can be improved by fine-tuning parameters
- The necessary code has been written for performing calculations
  - Can make it available to anyone interested in its current state
- No attempt at integration in the larsoft framework has been made

# Extra …

# 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 integrals are fast by interpolating erf tables

$$CDF(x) = \int_0^{\infty} dt \int_{-w}^{x} dx \int_{-l}^{+l} dy \, p(x,y,t)$$

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

$$CDF(y|x_i) = \int_0^{\infty} dt \int_{-l}^{y} dy \int_{x_i-0.5\Delta}^{x_i+0.5\Delta} dx \, p(x,y,t)$$

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

# Effect of bin size for CDF calculation

CDFs are calculated on a grid of $10 \times 10 cm^2$, but the x,y values are then linearly interpolated between the bins

Examples:

Source 100M photons

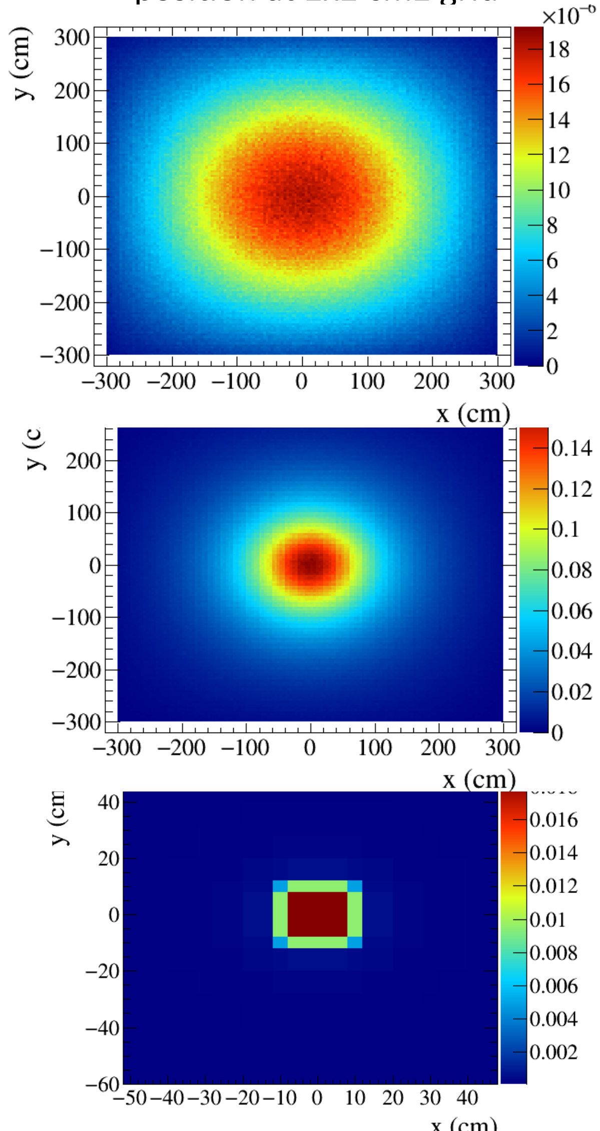
Top: 0,0,0: ~15s exec (17M phot to map)

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

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

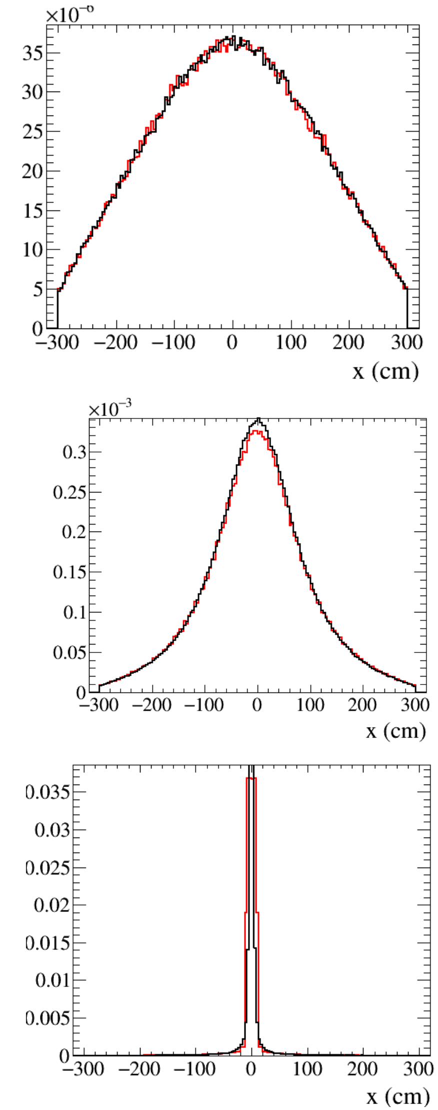
For a source at 1 mm above the plane the binning effect of the CDF becomes more apparent, but we are not looking at the position measurement with light (not ~tens of cm at least)

2D distribution of photon position at 2x2 cm2 grid




Photon light simulation

Generation with RTE solution



# PMT acceptance calculation

THE REVIEW OF SCIENTIFIC INSTRUMENTS VOLUME 30, NUMBER 4 APRIL, 1959

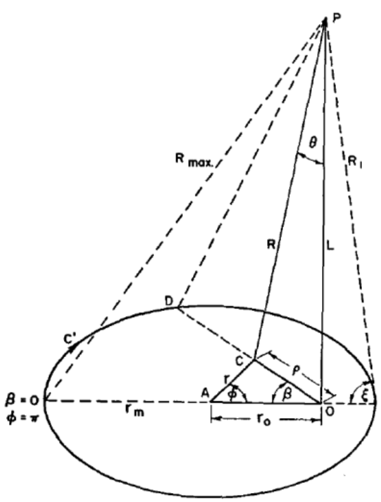
**Solid Angle Calculation for a Circular Disk**

F. PAXTON
*Nuclear Power Department, Research Division, Curtiss-Wright Corporation, Quehanna, Pennsylvania*
(Received April 14, 1958; and in final form, December 31, 1958)

A general expression for the solid angle subtended by a circular disk is derived in terms of complete elliptic integrals of the first and third kind. The elliptic integral of the third kind is reduced in terms of Heuman's lambda function, which has been tabulated. By transformation of the double integral $\Omega=\int\int \sin\theta d\theta d\beta$ into a single line integral, the solid angle can be conveniently determined. Since the solution involves only tabulated functions, it is well suited for desk calculation.

## Full treatment

Source inside the disk contour




Solid angle acceptance is given in terms of elliptical integrals of 1st and 3rd kind (K and Pi)

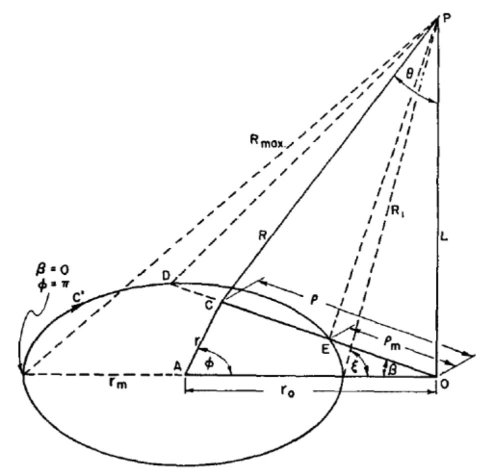
Numerical computation in GSL

Or

ROOT::Math::comp_ellpt_1

ROOT::Math::comp_ellpt_3

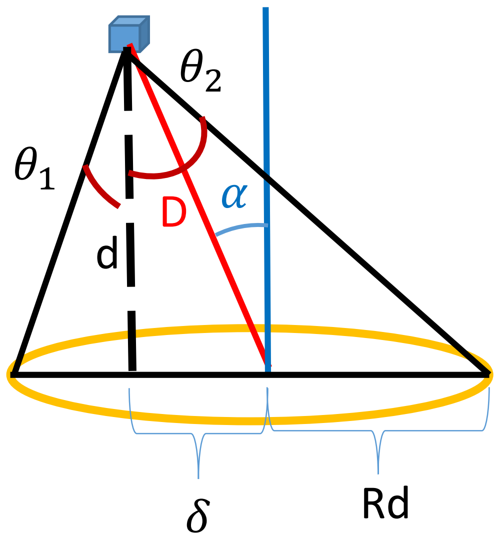
Source outside the disk contour




$$\Omega=2\beta_{\max}-\frac{2L}{R_{\max}}K(k)+\frac{2L}{R_{\max}}\frac{r_0-r_m}{r_0+r_m}\pi(\alpha^2,k). \qquad (14)$$

$$\Omega=-\frac{2L}{R_{\max}}K(k)+\frac{2L}{R_{\max}}\frac{r_0-r_m}{r_0+r_m}\Pi(\alpha^2,k). \qquad (27)$$

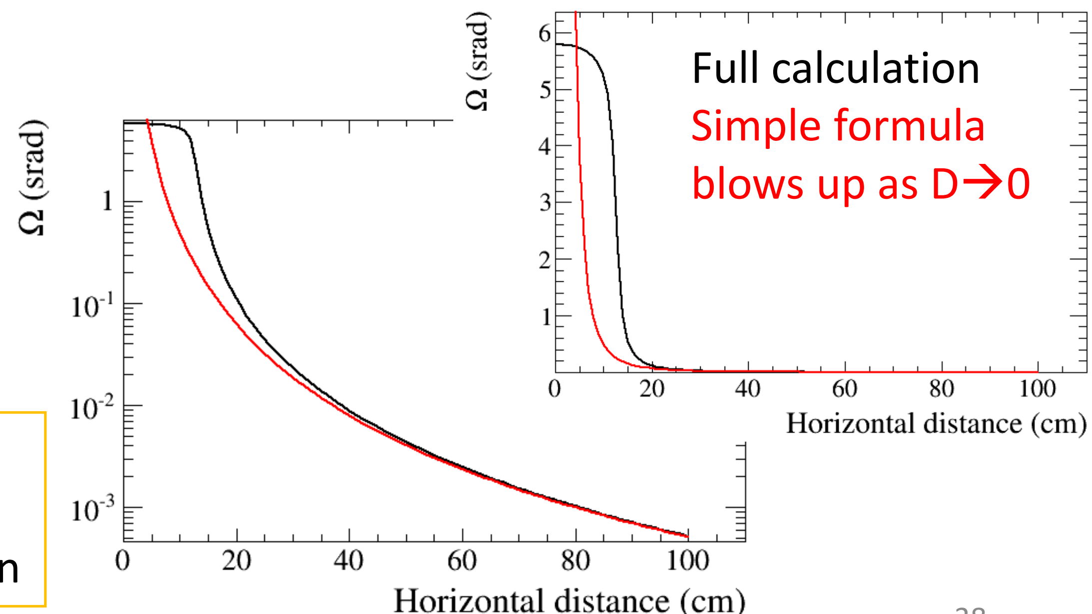
# PMT acceptance: far away




Usual solid angle subtended by disk area:

$$\Omega = \frac{1}{D^2}\pi R_d^2 \cos\alpha$$

Source at 1cm above PMT and moved horizontally
The horizontal distance is varied from 0 to 100 cm




Combine full with approximate treatment. For distances greater than 7xRd of PMT use approximation

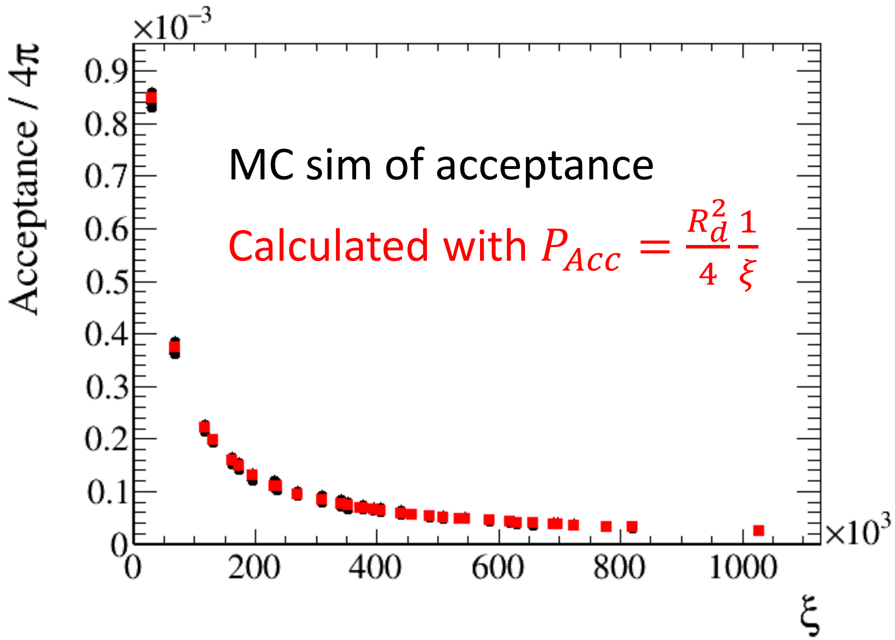
# PMT acceptance (no RS)

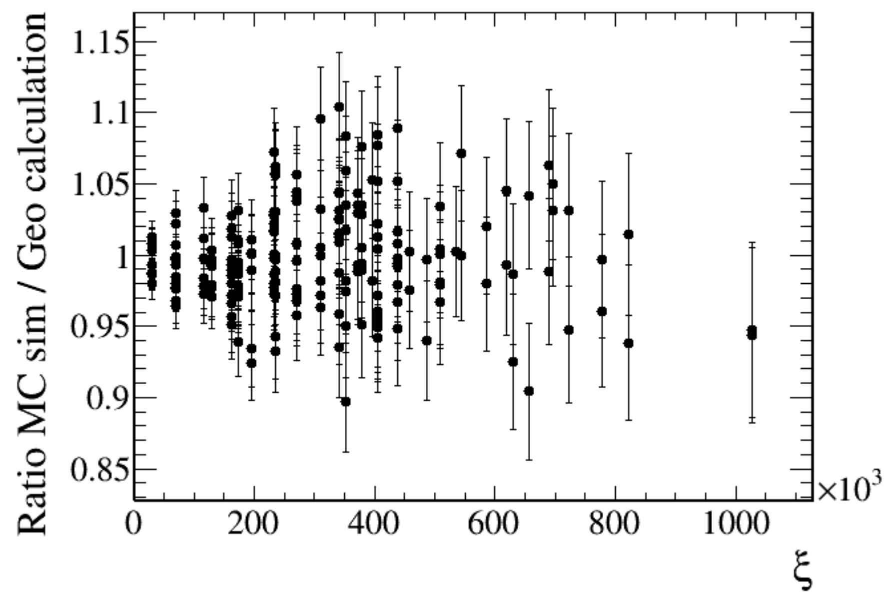
Validation of acceptance probability calculation

One can define $\xi = D^2/\cos\alpha$,

Where D is distance to PMT from source

And $\alpha$ is the angle of PMT normal with direction to source




Without RS acceptance is simply $\sim\frac{1}{\xi}$

Can use geo acceptance to estimate $\Omega_i$ for PMT if RS can be ignored