

Scintillation Light in LArTPCs: Simulation and Reconstruction

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UK-LArSoft workshop, Lancaster, October 2023

Outline

- This talk will give an overview of how LArSoft deals with simulating light and why it's hard.
- I will mention a bit about reconstruction
- Next, Jiaoyang will go through a few examples in the tutorial.

Simulation Flowchart



Simulation Flowchart (Legacy Version)

Each stage is a module Each stage passes data products, "objects", to the next stage.



Elements of Light Sim in a Nutshell



Light source:

- How many photons are generated?
- What is their time distribution?
- What is their wavelength?



- Transport:
 - How many photons make it to the detector?
 - How long does it take them?
 - Do they scatter / get absorbed / reflected etc?

- Detection:
 - What is our detection efficiency?
 - Does it depend on position on detector?
 - Are there any extra timing effects?

Different modes of simulation

- Full optical simulation (extremely slow)
 - Requires definition of all optical properties.
- Fast optical simulation (faster, but less precise)
 - Still need to run full optical at least once
 - Majority of optical properties "burned in"
 - Three primary methods exist: optical library, semi-analytical, GANN.

Full optical light simulation



Bulk absorption

In large detectors, the tracking of each individual photon is prohibitively slow \rightarrow alternative approaches are needed





Fast optical model: Optical Library



$$\langle N \rangle_{PMT-hits} = \left(\frac{dE}{dx}_{step} \cdot Length_{step} \right) \cdot LY \cdot visibility_{step}^{PMT}$$

- Resolution depends on voxel sizes: granularity effects at short distances
- Optical library size scales with detector size and number of photon detectors



- Prohibitive memory use for events with large energy depositions (i.e. cosmics)
- Difficult to get working in SBND and DUNE, so different approach currently used.

Fast optical model: Semi-Analytical



Full Optical Sim vs FastSim knobs

| | Full Optical Sim | Fast Optical |
|-----------------------------------|-----------------------------------|---|
| Timing Constants | Tunable | Tunable |
| Energy Spectrum | Tunable | Tunable (although affects transport) |
| Ionization/Scintillation Yield | Tunable (handwavy implemented) | Tunable (handwavy implemented) |
| Rayleigh Scattering | Tunable | "Burned in" |
| Timing Parametrization | Not needed | "Burned in"/but separate |
| Material Properties | Tunable | "Burned In" |
| OnePhoton vs LitePhotons | chooseable | chooseable |

• This table is for reference – we'll come back to it later.



Emission

Scintillation mechanism in LAr



Self-trapped excitation luminescence

 $Ar^* + Ar \longrightarrow Ar^*_2 \longrightarrow 2Ar + hv$

Scintillation wavelength in LAr

Ph. Rev. B 56 (1997), 6975



In liquid argon, the overall spectrum is well represented by a gaussian shape, peaking around $\lambda = 128$ nm (FWHM $\simeq 6$ nm)

lardataalg / lardataalg / DetectorInfo / larproperties.fcl

| # Fast and slow scint | illation | emiss | ion spe | ectra, | from | [J Che | m Phys | vol 9 | 1 (198 | 9) 146 | 9] | | | |
|-----------------------|----------|-------|---------|--------|-------|--------|--------|-------|--------|--------|-------|-------|-------|-----|
| FastScintEnergies: | [7.2, | 7.9, | 8.3, | 8.6, | 8.9, | 9.1, | 9.3, | 9.6, | 9.7, | 9.8, | 10, | 10.2, | 10.3, | 1(|
| SlowScintEnergies: | [7.2, | 7.9, | 8.3, | 8.6, | 8.9, | 9.1, | 9.3, | 9.6, | 9.7, | 9.8, | 10, | 10.2, | 10.3, | 1(|
| FastScintSpectrum: | [0.0, | 0.04, | 0.12, | 0.27, | 0.44, | 0.62, | 0.80, | 0.91, | 0.92, | 0.85, | 0.70, | 0.50, | 0.31, | 0.: |
| SlowScintSpectrum: | [0.0, | 0.04, | 0.12, | 0.27, | 0.44, | 0.62, | 0.80, | 0.91, | 0.92, | 0.85, | 0.70, | 0.50, | 0.31, | 0.: |



Scintillation signal shape in LAr

- In all measurements the overall scintillation light emission exhibits a double exponential behavior in time
- This is a result of excimer decays (at 90 K) characterized by two very different components: a fast component, with a time constant of τ_s ≈ 6ns, and by a slow component, with a time constant of τ_T ≈ 1.3µs

lardataalg / lardataalg / DetectorInfo / larproperties.fcl

ScintFastTimeConst: 6. # fast scintillation time constant (ns) *)ScintSlowTimeConst: 1590. # slow scintillation time constant (ns)



Scintillation yields

- The lifetimes of the fast and slow components agree within experimental uncertainties for different particles
- Light yield and fast/slow ratio depend on how ionising the particles are



| Particle | $	au_{S}$ | $	au_T$ | I_S/I_T | Reference |
|----------|-----------------|----------------|-----------|----------------------------------|
| Electron | 6.3 ±0.2 | 1020±60 | 0.083 | Kubota et al. ^a |
| | (5.0 ± 0.2) | (860 ± 30) | (0.045) | $(E=6 \text{ kV/cm})^{a}$ |
| | 4.6 | 1540 | 0.26 | Carvalho and Klein ^b |
| | 4.18±0.2 | 1000 ± 95 | | Keto et al. ^c |
| | | 1110 ± 50 | | Suemoto and Kanzaki ^d |
| | 6 ±2 | 1590 ± 100 | 0.3 | This work |
| α | ~5 | 1200 ± 100 | | Kubota et al. ^e |
| | 4.4 | 1100 | 3.3 | Carvalho and Klein ^b |
| | 7.1±1.0 | 1660 ± 100 | 1.3 | This work |
| F.F. | 6.8±1.0 | 1550 ± 100 | 3 | This work |

lardataalg / lardataalg / DetectorInfo / larproperties.fcl

ScintYield: ScintYieldRatio: ScintByParticleType; 24000. # total scintillation yield (ph/Mev)
0.3 # fast / slow scint ratio (needs revisitting)
true # whether to use different yields and

Scintillation yields and fast/slow ratios per particle type

MuonScintYield: 0.23 MuonScintYieldRatio: PionScintYield: 0.23 PionScintYieldRatio: 20000 ElectronScintYield: ElectronScintYieldRatio: 0.27 KaonScintYield: KaonScintYieldRatio: 0.23 ProtonScintYield: 19200 ProtonScintYieldRatio: 0.29 AlphaScintYield: AlphaScintYieldRatio: 0.56



L vs Q and Electric Field



$$Q = N_e = N_i R$$

$$L = N_\gamma = N_{\text{ex}} + N_i (1 - R)$$

$$Q + L = N_{\text{ex}} + N_i = \frac{\Delta E}{W_{\text{ph}}}$$
(19.5±1.0) eV

Electric Fields applied to the LAr medium also affect the intensity weights of the decay components by the recombination (R)

larsim / larsim / lonizationScintillation / ISCalcCorrelated.cxx

// calculate scintillation photons

// using this recombination, calculate number of ionization electrons
double const num_electrons = (energy_deposit / fWion) * recomb;



Services.LArG4Parameters.IonAndScintCalculator: "Correlated" (available from v09_09_03)

Propagation



Scintillation light propagation

Scintillation (emission):



- Scintillation photons have energy lower than the first excited state of the Ar atom, therefore pure LAr is transparent to its own scintillation radiation
- However, during propagation through LAr VUV photons may undergo elastic interactions on Ar atoms ⇒ Rayleigh scattering
- Rayleigh Scattering affects, in a non negligible way, the light signals in our detectors in comparison with the "pure" emitted scintillation light
- It is important to understand/model it properly in liquid argon

Rayleigh Scattering in LArSoft

 Elastic scattering of photon with medium of particle ~1/10 size of the wavelength (change angle/direction)



• Small uncertainties in the index of refraction can drastically change the scattering length λ_{RS}



lardataalg / lardataalg / DetectorInfo / larproperties.fcl

Refractive index as a function of energy (eV) from arXiv:2002.09346
RIndexEnergies: [1.18626, 1.68626, 2.18626, 2.68626, 3.18626, 3.68626, 4.18626, 4.68626, 5.18626,
RIndexSpectrum: [1.24664, 1.2205, 1.22694, 1.22932, 1.23124, 1.23322, 1.23545, 1.23806, 1.24116, 1
RayleighEnergies: [1.18626, 1.68626, 2.18626, 2.68626, 3.18626, 3.68626, 4.18626, 4.68626, 5.18626,
RayleighSpectrum: [1200800, 390747, 128633, 54969.1, 27191.8, 14853.7, 8716.9, 5397.42, 3481.37, 23

Fast optical model: Semi-Analytic



Transport corrections to light signals



Fast optical model: Semi-Analytic

sbndcode/sbndcode/LarSoftConfigurations/opticalsimparameterisations_sbnd.fcl

VUV/DIRECT LIGHT: TIMING PARAMETERISATION

VUV/DIRECT LIGHT: NUMBER OF HITS CORRECTIONS

SBND Gaisser-Hillas

Includes Wires

VIS semi-analytic model, specific to SBND

VISIBLE/REFLECTED LIGHT: TIMING PARAMETERISATION

VISIBLE/REFLECTED LIGHT: NUMBER OF HITS CORRECTIONS



More configurations below.

Time structure of detected signals



Propagation:

Direct transportation + Rayleigh Scattering



In "large" detectors transport effects will affect the effective time structure of the detected scintillation light

$$t_{\gamma} = t_E + t_t(d, \theta) + t_{WLS} + t_{det},$$

$$t_T = emission time$$

 $t_{det} = detector time$

Time structure of detected signals



larsim / larsim / PhotonPropagation / opticalsimparameterisations.fcl

larsim / larsim / PhotonPropagation / PDFastSimPAR.fcl

IncludePropTime:

true

(Digression): Enhancing the Light Yield in LArTPCs



Semi-Analytic model extensions (available)



- - LArSoft semi-analytic model simulation can also model these the extensions:
 - LAr and LXe wavelengths (doping)
 - Direct and Reflected light (foils)

(Digression): Cherenkov radiation in LAr

- A particle propagating in a medium with velocity greater than that of light in the medium produces an electromagnetic shock-wave with conic wavefront
- Photons are emitted with a precise angle with respect to particle direction $\cos \theta_{\check{C}}$

$$\frac{d^2 N}{d\nu dx} = \frac{2\pi\alpha}{c}\sin^2\theta_{\check{C}}$$

than
$$\frac{c}{n} t$$

$$\theta$$

$$\beta ct$$

$$1$$

$$\beta \cdot n_{Ar}(\lambda)$$

•

NIM A 516 (2004) 348–363

$$\Rightarrow \int_{109nm}^{600nm} (hard to detect) \\ \Rightarrow \int_{109nm}^{600nm} (LAr absorbed) \qquad R_{\check{C}} = \frac{dN_{\check{C}}/dx}{dN_{scint}/dx + dN_{\check{C}}/dx} = 2.4\%$$

→ Can be considered a second order effect with respect to scintillation light emission sbndcode/sbndcode/LArSoftConfigurations/opticalproperties_sbnd.fcl

EnableCerenkovLight: false # Cerenkov light OFF by default

Detection



Wavelength shifter in LArSoft

Processes handled by G40pWLS:

- Initial photon killed and a new one created with different wavelength
- User must provide:
- Absorption length as function of photon energy
- Emission spectrum as function of photon energy
- Time delay between absorption and re-emission

The **WLSABSLENGTH** defines the absorption length which is the average distance travelled by a photon before it is absorbed by the TPB.



lardataalg / lardataalg / DetectorInfo / larproperties.fcl

WLS - TPB properties original tpb [0.0, 0.0, 0.0, 0.0588,0.235, 0.853, 1.0,1.0,0.9259,0.704 TpbEmmisionEnergies: [0.05,1.0,1.5, 2.25, 2.481, 2.819, 2.952,2.988,3.024, 3.1, 3.14,3.1807, TpbEmmisionSpectrum: [0.0, 0.0, 0.0, 0.0588,0.235, 0.853, 1.0,1.0,0.9259,0.704,0.0296,0.011, TpbAbsorptionEnergies: [0.05,1.77,2.0675, 7.42, 7.75, 8.16, 8.73, 9.78,10.69, 50.39] TpbAbsorptionSpectrum: [100000.0,100000.0, 100000.0,0.001,0.0000000001,0.000000001, 0.0000

Wavelength shifter time delay

Geant4 (G4OpWLS class) only simulates Delta or Exponential model (none is the case for TPB)

PHYSICAL REVIEW C 91, 035503 (2015)

time simulation.



Photon simulation output objects

lardataobj / lardataobj / Simulation / SimPhotons.h

```
// This structure contains all the information per photon
                                                           class SimPhotonsLite
// which entered the sensitive OpDet volume.
                                                             public:
class OnePhoton
                                                               SimPhotonsLite();
                                                               SimPhotonsLite(int chan)
public:
                                                                 : OpChannel(chan)
  OnePhoton();
                                                               {}
  bool
                 SetInSD:
                                                                     OpChannel;
  TVector3
                 InitialPosition;
                                                               int
                                                               std::map<int, int> DetectedPhotons;
  TVector3
                 FinalLocalPosition; // in cm
  float
                 Time:
                                                               SimPhotonsLite& operator+=(const SimPhotonsLite &rhs);
  float
                 Energy;
  int
                 MotherTrackID:
                                                               const SimPhotonsLite operator+(const SimPhotonsLite &rhs) const;
};
                                                               bool operator==(const SimPhotonsLite &other) const;
                                                          };
class SimPhotons : public std::vector<OnePhoton>
                                                           // Define a OpDet Hit as a list of OpDet photons which were
                                                           // recorded in the OpDet volume.
                                                           class SimPhotons : public std::vector<OnePhoton>
```

- •SimPhotons objects (collections of OnePhoton) save detailed information about each detected photon
- while SimPhotonsLite objects reduce memory and size at the price of keeping only the number of photons at a time-slot.
- The kind of object you want to save in your simulation is specified in the configuration file by the line:

services.LArG4Parameters.UseLitePhotons: true # false to save SimPhotons

Full Optical Sim vs FastSim knobs

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| Material Properties | Tunable | "Burned In" |
| OnePhoton vs LitePhotons | chooseable | chooseable |

• Hopefully should make more sense now.

PMT digitisation: SBND case example

The PMT features included are: SER, electron transit time, transit time spread, saturation, baseline, dark noise, baseline noise, and pre-trigger.

sbndcode / Sbndcode / OpDetSim / digi_pmt_sbnd.fcl

8" Hamamatsu PMT - R5912



Reconstruction

Optical signal reconstruction: OpHits

- The first stage of the optical reconstructions looks for pulses in the raw waveforms.
- The light pulses in LArSoft are stored in objects called OpHits.

- OpHits are found when the waveform is above certain threshold and held until continues to be so.
- Especially for SiPM signals this can lead to merging of visibly separate optical signals.
- OpHit Time is decided on the first arriving photon.



OpHit(); // Default constructor

private:

| int | f0pChannel; |
|----------------|--------------------------|
| unsigned short | fFrame; |
| double | fPeakTime; |
| double | fPeakTimeAbs; |
| double | fWidth; |
| double | fArea; |
| double | fAmplitude; |
| double | fPE; |
| double | <pre>fFastToTotal;</pre> |
| | |

lardataobj / lardataobj / RecoBase / OpHit.h

Optical signal reconstruction: OpFlash

- OpHits from different photon detectors are combined into Flashes. These are analogous to clusters in the charge reconstruction, but matched in time rather than space
- Having a flash allows us to try to reconstruct the position of the particle that generated the light (roughly)
- This can then be used to match the light signals to the reconstructed TPC tracks – Flash Matching

lardataobj / lardataobj / RecoBase / OpFlash.h

private:

| double | $fTime \{ 0, 0 \}$ | ///< Time on Gref Detector(locksHardward |
|--|----------------------------|--|
| | fTimeldidth : | /// Width of the fleek in time [we] |
| double | Tlimewidth; | ///< width of the flash in time [us] |
| double | fAbsTime; | ///< Time by PMT readout clock |
| unsigned int | fFrame; | ///< Frame number |
| <pre>std::vector< double ></pre> | fPEperOpDet; | ///< Number of PE on each PMT |
| <pre>std::vector< double ></pre> | fWireCenters; | ///< Geometric center in each view |
| <pre>std::vector< double ></pre> | fWireWidths; | ///< Geometric width in each view |
| double | fXCenter { NoCe | <pre>enter }; ///< Estimated center in x [cm]</pre> |
| double | <pre>fXWidth { NoCer</pre> | <pre>nter }; ///< Estimated width in x [cm]</pre> |
| double | fYCenter; | ///< Geometric center in y [cm] |
| double | fYWidth; | ///< Geometric width in y [cm] |
| double | fZCenter; | ///< Geometric center in z [cm] |
| double | fZWidth; | ///< Geometric width in z [cm] |
| double | fFastToTotal; | ///< Fast to total light ratio |
| bool | <pre>fInBeamFrame;</pre> | ///< Is this in the beam frame? |
| int | <pre>fOnBeamTime;</pre> | ///< Is this in time with beam? |
| | | |

Flash Matching: OpTOFinder example

Flash matching goals:

- Identify a neutrino interaction from cosmic backgrounds
- Provide To for each TPC interaction

The two ingredients for flash matching:

- Reconstructed Flashes
- TPC Objects (reconstructed objects in the TPC, i.e. Pandora's recob::Slice) ⇒ The flash matching code should match a TPC Object with its flash



Summary

- Optical simulation is tricky, need to cut some corners to get it working in LArSoft (size, number of photons -> Memory, CPU).
- Corners are cut, so there is always room for improvement.
- Applications of scintillation light are not fully developed – always lots of opportunities to do new things.

Backups

PMT Gain fluctuation

(Slide from F.J. Nicolás)

- Number of secondary electrons generated at each dynode: random variable
- Toy example:
 - Consider 1e hits one of the dynode (with gain gi)
 - On average $< m >= g_i$ with a standard deviation $\sigma = \sqrt{g_i}$
 - This leads to fluctuations in the SER



- Approximations (approach directly taken from icaruscode) \Rightarrow Only takes into account fluctuations at first dynode: $\rightarrow \frac{\sigma_N^2}{\langle N \rangle^2} = \frac{1}{g_1} + \frac{1}{g_1g_2} + \dots + \frac{1}{g_1g_2\dots g_n}$
 - <N>: average number of electrons at the end of the multiplication chain (anode)
 - σ_N^2 : fluctuations in the total number of electrons at the anode



sbndcode / sbndcode / OpDetSim / PMTAlg / pmtgainfluctuations_config.fcl

(Parenthesis): Light Signal Deconvolution

 In SBND we have PMT (and XARAPUCA) readout with AC coupling: bipolar SER ⇒ This makes accurate light reconstruction a challenge (by F.J. Nicolás)



Optical Library parameters: voxelization scheme

sbndcode / sbndcode / LArSoftConfigurations / photpropservices_sbnd.fcl

(Re)Defining the Optical Library information/files for the PD-fast HYBRID optical mode sbnd_library_for_hybrid_mode_photonvisibilityservice:

```
{
   @table::sbnd library vuv vis prop timing photonvisibilityservice
                                                                                                                  Detector
                                                                                                                   specific
   LibraryFile: "OpticalLibrary/SBND_OpLibOUT_v2.00.root"
   NX: 66
   NY: 56
   NZ: 71
                                                                                                  OpChannel
                                            7 🔁
                                                    Draw Option:
                                                                     •
   UseCryoBoundary: false
                                                                                                                            htemp
                                          root
                                                                      ۰
                                                                                                                             3.114135e+08
                                                                                                                        Entries
                                                                            3500
                                         PROOF Sessions
                                                                                                                                162.9
                                                                                                                        Mean
   # IF UseCryoBoundary is se
                                                                                                                                92.48
                                                                                                                        Std Dev
                                         ROOT Files
                                                                            3000
                                          OpLibSBNDv1.5.root
   XMin:
             -264
                                            E pmtresponse/PhotonLibraryData;
                                                                            2500
                                                🏷 Voxel
   XMax:
             264
                                                🐚 OpChannel
                                                                            2000
   YMin: -280
                                                🐌 Visibility
                                                ReflVisibility
                                                                            1500
   YMax:
             280
                                         / 📥
                                          🗄 🕞 Users
                                                                            1000
   ZMin:
             -60
                                              Shared
                                            🗄 🔄 diegogarciagamez
                                                                            500
             650
    ZMax:
                                                Applications
                                                Desktop
                                                                                     50
                                                                                            100
                                                                                                   150
                                                                                                          200
                                                                                                                  250
                                                                                                                         300
}
                                                                                                                         OpChannel
                                                Documents
```

Semi-Analytic model performance

- Solves the problems of other approaches
- Photon propagation with no impact on memory (RAM) or simulation (CPU) time
- It models both (N_{γ} , time)
 - used in SBND and DUNE-SP simulations





Hybrid model for the photon propagation

- Semi-Analytic model has a limitation: only applicable inside the active volume (geometric approach)
- Simple idea to overcome the problem ⇒ Hybrid model: Semi-Analytic model inside the TPC + Op-Library outside
 ZProjection



E-Field map in a TPC (SBND case example)

Warning: Light yield strongly depends on the Electric Field value



- Inside the active volume EF is constant @ 0.5 kV/cm (nominal)
- In the top of the TPC EF values range from few kV/cm at the CPA location decreasing to ~0 at the APA.
- Behind APA (PD-plane) EF = 0 is a good approximation (almost constant)

E-Field x Visibility map in a TPC (SBND case example)



Only behind APA visibilities are significant

 Current EF model in the hybrid approach: 500V/cm inside the TPC & 0V/cm anywhere else