

Scintillation Light in LArTPCs: Simulation and Reconstruction

Patrick Green

University of Oxford

Adapted from previous slides written by Andrzej Szelc and Diego Garcia-Gamez

UK-LArSoft workshop, Edinburgh, October 2024

Outline

- This talk will give an overview of how LArSoft deals with simulating light and why it's hard
- I will also talk a bit about reconstruction
- Next, we will go through a few hands-on 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 Simulation

• **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, generative neural network

Full optical light simulation

Scintillation yield ∼**24000 photons/MeV**

For GeV-scale interactions in large detectors, the tracking of each individual photon is prohibitively slow -> alternatives needed

(Aside): Using GPUs - NVIDIA Optimal

Some progress using GPUs for full optical simulation, but challenges re

– GPU resources limited + using vendor specific tools (NVIDIA OptiX)

GPU based photon simulation

intensive and limit event by event simulation

often solved with voxel-ized lookup tables

Opticks developed by Simon Blyth for JUNO, now part of GEANT4 releases

CaTS integrate GEANT4+Opticks **LArSoft for simplit LArTPC**

speedup of several times for photon simulation

also report that 1 co could saturate the

Fast optical model: Optical Library

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

- 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 large detectors -- difficult to get working in SBND and DUNE, so different approaches currently used.

Fast optical model: Semi-Analytical

Fast optical model: Neural Networks

Generative neutral network (GENN):

- network trained on Geant4 simulation of voxelized detector, similar to library
- rather than storing visibilities in look-up table, use network to predict at run-time
- avoids memory limitation of library, at some CPU cost; currently used in DUNE

Some ongoing attempts to train similar networks using data rather than simulation:

- no longer have to rely on often poorly known detector properties \rightarrow could be more accurate / closer to data
- but challenging to get well understood training samples

Mach.Learn.S ci.Tech. 3 (20 22) 1, 015033

Full Optical Sim vs FastSim knobs

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

Emission

Scintillation mechanism in LAr

• **Self-trapped excitation luminescence**

Ar + Ar Ar* 2 2Ar + hv*

Scintillation wavelength in LAr

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

In LArSoft this is parameterised in larproperties.fcl

Ph. Rev. B 56 (1997), 6975

lardataalg / lardataalg / Detectorinfo / larproperties.fcl

Fast and slow scintillation emission spectra, from [J Chem Phys vol 91 (1989) 1469] FastScintEnergies: $[7.2, 7.9, 8.3, 8.6, 8.9, 9.1, 9.3, 9.6, 9.7, 9.8, 10, 10.2, 10.3, 10.$

SlowScintEnergies: $[7.2, 7.9, 8.3, 8.6, 8.9, 9.1, 9.3, 9.6, 9.7, 9.8, 10, 10.2, 10.3, 10]$ FastScintSpectrum: $[0.0, 0.04, 0.12, 0.27, 0.44, 0.62, 0.80, 0.91, 0.92, 0.85, 0.70, 0.50, 0.31, 0.1]$ $[0.0, 0.04, 0.12, 0.27, 0.44, 0.62, 0.80, 0.91, 0.92, 0.85, 0.70, 0.50, 0.31, 0.1]$ SlowScintSpectrum:

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 Ar excimer decays characterized by two very different components:

a fast component, $\tau_s \approx 6$ ns, and a slow component, $\tau_{\tau} \approx 1.3 \mu s$

• Implementation in LArSoft:

lardataalg / lardataalg / Detectorinfo / larproperties.fcl

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

sbndcode/sbndcode/LArSoftConfigurations/opticalproperties_sbnd.fcl

Updating the triplet decay-time (Phys. Rev. C 91, 035503). Note that in our simulations we account # independently for the TPB-delay time and the emission (fast and slow) decay times. ScintSlowTimeConst: 1300. # slow scintillation time constant (ns)

*Note: a slow time constant value convolved with the WLS-delay, results in a larger value $\approx 1.5 - 1.6 \mu s$

Scintillation Yields: E-field

Liquid Argon is a prolific scintillator: ∼40000 photons/MeV @ zero electric field

Strength of the electric field applied to the LAr impacts the amount of recombination \rightarrow alters amount of charge (Q) and light (L)

Effect is (anti-)correlated, as electric field increases Q grows, L decreases. At 500 V/cm, energy deposit about equally divided between Q and L

This is modelled in LArSoft ISCalcCorrelated, and enabled in SBND:

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

// calculate scintillation photons double const num_photons = $(Nq - num_electrons)$ * fScintPreScale;

PHYSICAL REVIEW D 101, 012010 (2020)

Phys. Rev. B 20, 3486

Scintillation Yields: Particle Type

Light yield and fast/slow ratio depend on how ionising the particles are:

- electrons: ∼20000 photons/MeV, ∼ 30% prompt light
- alphas: ∼16800 photons/MeV, ∼ 60% prompt light

In LArSoft this is configured in larproperties.fcl, ScintByParticleType:

ScintByParticleType: true

Jpn. J. Appl. Phys. Vol. 41 (2002) pp. 1538–1545; Ph. Rev. B 27 (1983), 5279

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 Argon

Rayleigh scattering length for VUV photons in Ar measured variously between ∼50 – 120 cm

- very hard to measure: small uncertainties in the index of refraction can drastically change the scattering length λ_{RS}
- most recent measurement around 100 cm, adopted by many LArTPC experiments

RS ∼100cm < typical size of LArTPC detectors \rightarrow has significant impact on light seen

In LArSoft, parameterized in larproperties.fcl

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

Modelling in fast optical simulation

Optical library / GENN network:

• Encoded in *visibilities* in each voxel directly from full optical simulation

Semi-analytical model:

- Treated as a correction to the geometric prediction
- Parameterised based on difference between geometric prediction and full optical simulation
- Also correct for border effects in analogous way (reflections/absorption)

Eur. Phys. J. C $(2021) 81:349$

In LArSoft models implemented in larsim:

larsim/PhotonPropagation/PDFastSimPVS_module.cc (Library) larsim/PhotonPropagation/PDFastSimPAR_module.cc (Semi-analytical)

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

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

$$
t_E = \text{emission time}
$$
\n
$$
t_t = \text{transport time}
$$
\n
$$
t_{WLS} = \text{WLS delay time}
$$
\n
$$
t_{det} = \text{detector time}
$$

Time structure of detected signals

In fast optical simulation, modelled using parameterisations of Landau + Exponential fits to distributions from full optical simulation

– developed in conjunction with semi-analytical model, but can be used in combination with any approach to get number of photons (library, etc.)

larsim / larsim / PhotonPropagation / PropagationTimeModel.h

larsim / larsim / PhotonPropagation / PDFastSimPAR.fcl

IncludePropTime: true

Implementation in SBND

Hybrid approach used in SBND:

- semi-analytical model (hits + timing) inside TPC
- slimmed-down optical library outside TPC

Configuration in SBND:

sbndcode/sbndcode/LarSoftConfigurations/opticalsimparameterisations_sbnd.fcl

```
PARAMETERS SETS FOR SEMI-ANALYTIC SIMULATION ARE DEFINED HERE
 # VUV/DIRECT LIGHT: TIMING PARAMETERISATION
# VUV/DIRECT LIGHT: NUMBER OF HITS CORRECTIONS
 VIS semi-analytic model, specific to SBND
# VISIBLE/REFLECTED LIGHT: TIMING PARAMETERISATION
# VISIBLE/REFLECTED LIGHT: NUMBER OF HITS CORRECTIONS
```
(Aside): Enhancing the Light Yield in LArTPCs

(Aside): 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

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

$$
\frac{1}{\pi} \frac{1}{\sqrt{\frac{1}{\pi}}}
$$
\n
$$
\frac{1}{\sqrt{\frac{1}{\pi}}}
$$
\nwith respect to\n
$$
\cos \theta_{\tilde{C}} = \frac{1}{\beta \cdot n_{Ar}(\lambda)}
$$
\n
$$
\frac{1}{\beta \ln \frac{1}{\beta} \cdot \frac{1}{\beta}} = \frac{1}{\beta \cdot n_{Ar}(\lambda)}
$$
\n
$$
\frac{1}{\beta \ln \frac{1}{\beta} \cdot \frac{1}{\beta} \cdot \frac{1}{\beta} \cdot \frac{1}{\beta} \cdot \frac{1}{\beta}} = \frac{1}{\beta \cdot n_{Ar}(\lambda)}
$$

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

 \rightarrow 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

Beware enabling: no fast optical simulation exists, will use very slow full simulation!

Detection

Detecting light in LArTPCs

VUV LAr scintillation light is hard to detect directly, absorbed by most materials

– need to make use of wavelength shifters, most commonly TPB

Photon detectors used:

- PMTs coated with WLS (SBND) or with WLScoated plates in-front of them (MicroBooNE)
- Arapuca/XArapuca wavelength-shifting light traps using SiPMs (DUNE, SBND)

Wavelength shifters emit ∼isotropically, lose 50% of light emitted away from photon-detectors

Arapuca operational principle

Photon detection system module in SBND, mixture of PMTs and XArapucas

Wavelength shifter in LArSoft

Processes handled by G4OpWLS:

- \triangleright 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]

Wavelength shifter time delay

TPB has complex time structure:

- bulk of light emitted promptly, but non-negligible longer components
- would non-negligibly alter time distribution

Geant4 (G4OpWLS class) only simulates Delta or Exponential model (neither is the case)

Instead, we simulate this separately in LArSoft:

- in SBND this is done in the at the optical detector digitizer stage (slightly hacky)
- sbndcode/sbndcode/OpDetSim/ DigiPMTSBNDAlg.cc

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
                                                               SimPhotonsLife();
                                                               SimPhotonsLite(int chan)
public:
                                                                 : OpChannel(chan)
  OnePhoton();
                                                               \{ \}bool
                 SetInSD:
                                                                      OpChannel;
                                                               int
  TVector3
                 InitialPosition:
                                                               std::map<int, int> DetectedPhotons;
  TVector3
                 FinalLocalPosition; // in cm
  float
                 Time:
  float
                                                               SimPhotonsLite& operator+=(const SimPhotonsLite &rhs);
                 Energy;
                 MotherTrackID:
  int
                                                               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
- •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

• Hopefully should make more sense now.

PMT digitisation (SBND example)

Finally, we simulate the resulting waveforms we'd see on the photo-detectors:

- each PE gets swapped for an electronics response, either constructed from parameters (idealised) or from a measured response
- the expected noise is also added to the waveforms

sbndcode / sbndcode / OpDetSim / digi_pmt_sbnd.fcl

Parameters for test bench SER simulation

Example PMT waveform in SBND compared with MC photon arrival times:

> undershoot due to AC coupling \rightarrow bipolar single electron response

Reconstruction

Optical Hits

- First, we look for pulses raw (or deconvolved) waveforms
- The light pulses in LArSoft are stored in objects called OpHits
- OpHits are found when the waveform goes above a certain threshold and are held while it continues to be so
- The OpHit Time is decided by the first arriving photon
- This can lead to the merging of visible separate optical signals, especially in the case of SiPMs (in the Arapucas)

lardataobj / lardataobj / RecoBase / OpHit.h

Optical Flashes

Optical hits from different photon detectors that are time-coincident are combined into Optical Flashes:

> – these are analogous to clusters in the charge reconstruction, but matched in time rather than space

Having a flash allows us to reconstruct the position of the particles 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:

Flash Matching: OpT0Finder example

Flash matching goals:

- Distinguish a neutrino interaction from cosmic backgrounds
- Provide T₀ 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) \Rightarrow 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 with reasonable resource usage (size, number of photons -> Memory, CPU).
- Corners are cut, so there is always room for improvement.
- Applications of scintillation light in LArTPCs 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: $\frac{\sigma_N^2}{\sqrt{N}} = \frac{1}{g_1} + \frac{1}{g_1 g_2} + ... + \frac{1}{g_1 g_2 ... g_n}$ fluctuations at first dynode:
	- <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

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)

▶

sbndcode / sbndcode / OpDetReco / OpDeconvolution /

 Ω

500

1000 1500

 PE_{true}

42

2000

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:

```
ſ
    @table::sbnd library vuv vis prop timing photonvisibilityservice
                                                                                                                            Detector
    LibraryFile: "OpticalLibrary/SBND OpLibOUT v2.00.root"
                                                                                                                             specificNX: 66
    NY: 56
    N7: 71
                                                                                                          OpChannel
                                                7 S
                                                         Draw Option:
                                                                           \overline{\phantom{a}}UseCryoBoundary: false
                                                                                                                                      htemp
                                                                            \blacktriangleoroot
                                                                                                                                       3.114135e+08
                                                                                                                                  Entries
                                                                            \equiv3500
                                             PROOF Sessions
                                                                                                                                           162.9
    # IF UseCryoBoundary is so
                                                                                                                                  Std Day
                                                                                                                                           92.48
                                             ROOT Files
                                                                                  3000
                                             白<sup>。</sup>gOpLibSBNDv1.5.root
    XMin:
              -264白 ·· <sup>#</sup> |pmtresponse/PhotonLibraryData;
                                                                                  2500
    XMax:
                                                    Voxel
               264
                                                     OpChannel
                                                                                  2000
    YMin: -280
                                                    Visibility
                                                    ReflVisibility
                                                                                  1500
    YMax:
              280
                                             8/
                                             ⊟⊹⊜जUsers
                                                                                  1000
    ZMin:
               -60Shared
                                               diegogarciagamez
                                                                                   500
    ZMax:
              650
                                                    Applications
                                                    Desktop
                                                                                             50
                                                                                                    100
                                                                                                            150
                                                                                                                   200
                                                                                                                           250
                                                                                                                                   300
ł
                                                                                                                                   OpChannel
                                                    Documents
```
Semi-Analytic model extensions (available)

- **DUNE-Xe** 200 400 600 800 1000 distance [cm]
	- LArSoft semi-analytic model simulation can also model these the extensions:
		- LAr and LXe wavelengths (doping)
		- Direct and Reflected light (foils)

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 \Rightarrow **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** 47