

Scintillation Light in LArTPCs: Simulation and Reconstruction

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

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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



Bulk absorption

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 OptiX

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

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

GPU based photon simulation



simulation of photons within open detectors can be incredibly CPU intensive and limit event by event simulation

often solved with voxel-ized lookup tables

Opticks developed by <u>Simon Blyth</u> for JUNO, now part of GEANT4 releases



also report that 1 core could saturate the GPU





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 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 → 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

	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

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

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, 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 Ar excimer decays characterized by two very different components:

a fast component, $\tau_s \approx 6ns$, and a slow component, $\tau_T \approx 1.3 \mu s$

• Implementation in LArSoft:



lardataalg / lardataalg / DetectorInfo / larproperties.fcl

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

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 ≈ 1.5-1.6µs

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

# Scintillation yie	elds a	nd 1	fast/slow	ratios
MuonScintYield:		240	000	
MuonScintYieldRatio	0:	0.2	23	
PionScintYield:		240	000	
PionScintYieldRatio	0:	0.2	23	
ElectronScintYield	:	200	000	
ElectronScintYield	Ratio:	0.2	27	
KaonScintYield:		240	000	
KaonScintYieldRatio	0:	0.2	23	
ProtonScintYield:		192	200	
ProtonScintYieldRat	tio:	0.2	29	
AlphaScintYield:		168	300	
AlphaScintYieldRat	io:	0.5	56	



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

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 \sim 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 larsim/PhotonPropagation/PDFastSimPAR_module.cc (Library) (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

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

$$t_T = emission time$$

 $t_{det} = detector time$

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

(Aside): Enhancing the Light Yield in LArTPCs



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(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

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



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

Can be considered a second order effect with respect to scintillation light emission \rightarrow 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:

- 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, 100000.0,0.001,0.0000000001,0.0000000001, 0.0000

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

	Decay time (ns)	Abundance (%)
Instantaneous component	1–10	60 ± 1
Intermediate component	49 ± 1	30 ± 1
Long component	3550 ± 500	8 ± 1
Spurious component	309 ± 10	2 ± 1



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
- •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

	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

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 / OpDetSim / digi_pmt_sbnd.fcl

<pre># Parameters for ideal</pre>	SER simulat	tion
PMTRiseTime:	3.8	#ns
PMTFallTime:	13.7	#ns
PMTMeanAmplitude:	0.9	#in pC
TransitTime:	55.1	#ns
PMTChargeToADC:	-25.97	#charge to adc factor

Parameters for test bench SER simulation

PMTSinglePEmodel:	true	#false	for	ideal	PMT	respons
PMTDataFile:	"OpDetSim	n/digi_p	omt_s	bnd_v2	2int0	.root"



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

undershoot due to AC coupling →
 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



int	f0pChannel;
unsigned short	fFrame;
double	fPeakTime;
double	fPeakTimeAbs;
double	fWidth;
double	fArea;
double	fAmplitude;
double	fPE;
double	fFastToTotal;

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:

double	<pre>fTime { 0.0 };</pre>	///< Time on @ref DetectorClocksHardward
double	fTimeWidth;	///< 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	fXWidth { NoCer	<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:

- Distinguish 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 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: $\rightarrow \frac{\sigma_N^2}{\langle N \rangle^2} = \frac{1}{g_1} + \frac{1}{g_1g_2} + \dots + \frac{1}{g_1g_2\dots g_n}$
 - <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

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
                                                RefIVisibility
                                                                            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 extensions (available)



800

1000

distance [cm]

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