JUNO detector simulation based on customized Geant4 physics list

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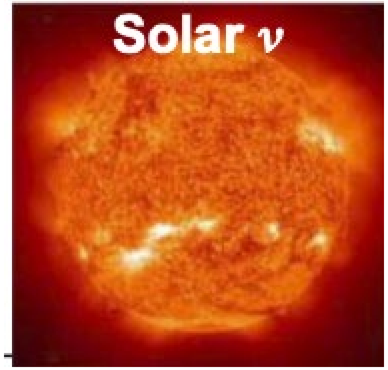
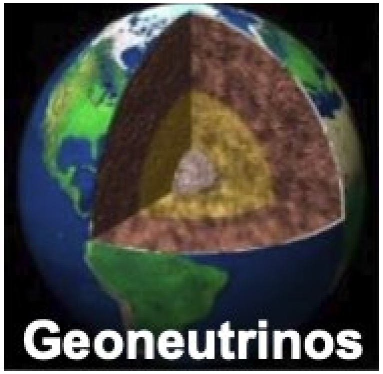
Outline

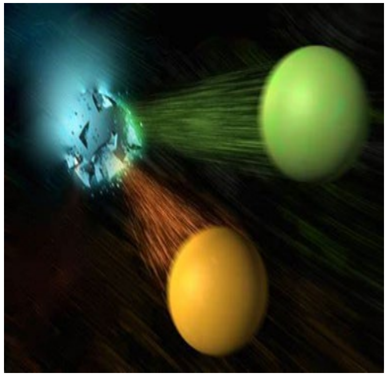
- Introduction
- JUNO Simulation Software
- Modified Geant4 processes for JUNO
- Summary

JUNO physics program

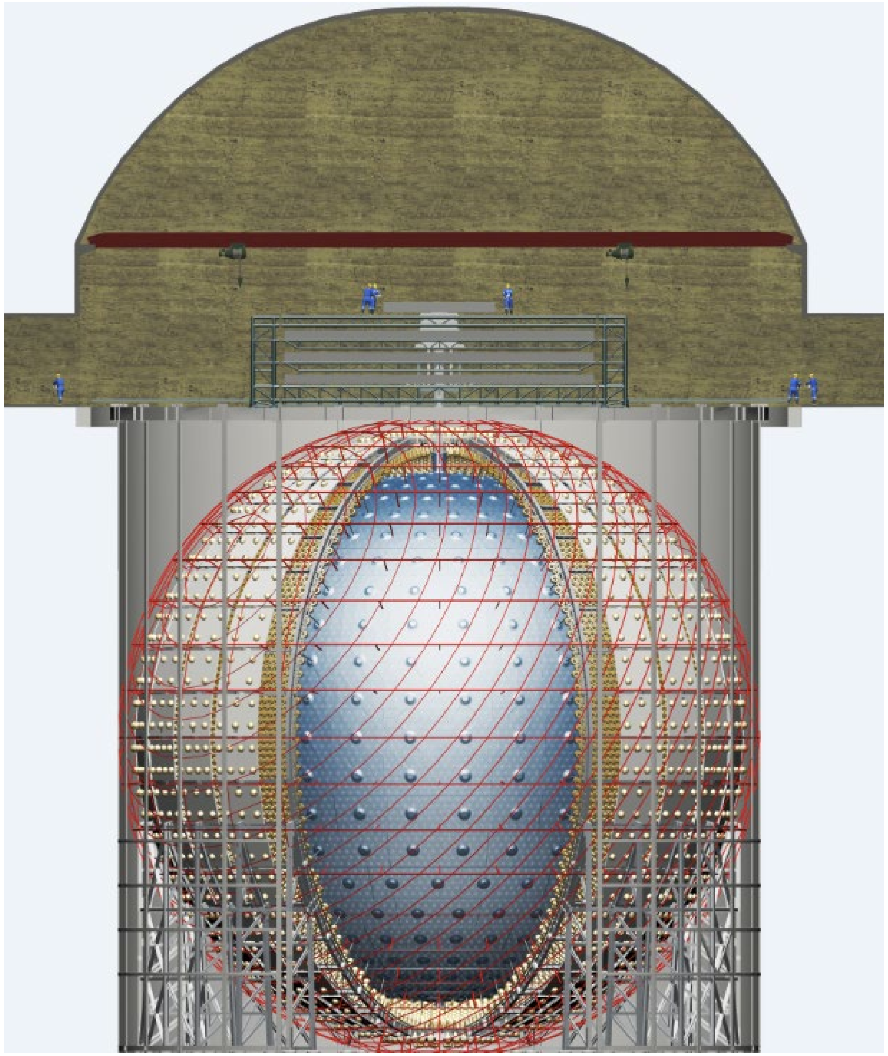
- JUNO is a multipurpose Neutrino Observatory with a rich program in neutrino physics and astrophysics, studying neutrinos in a large energy range.







JUNO detector



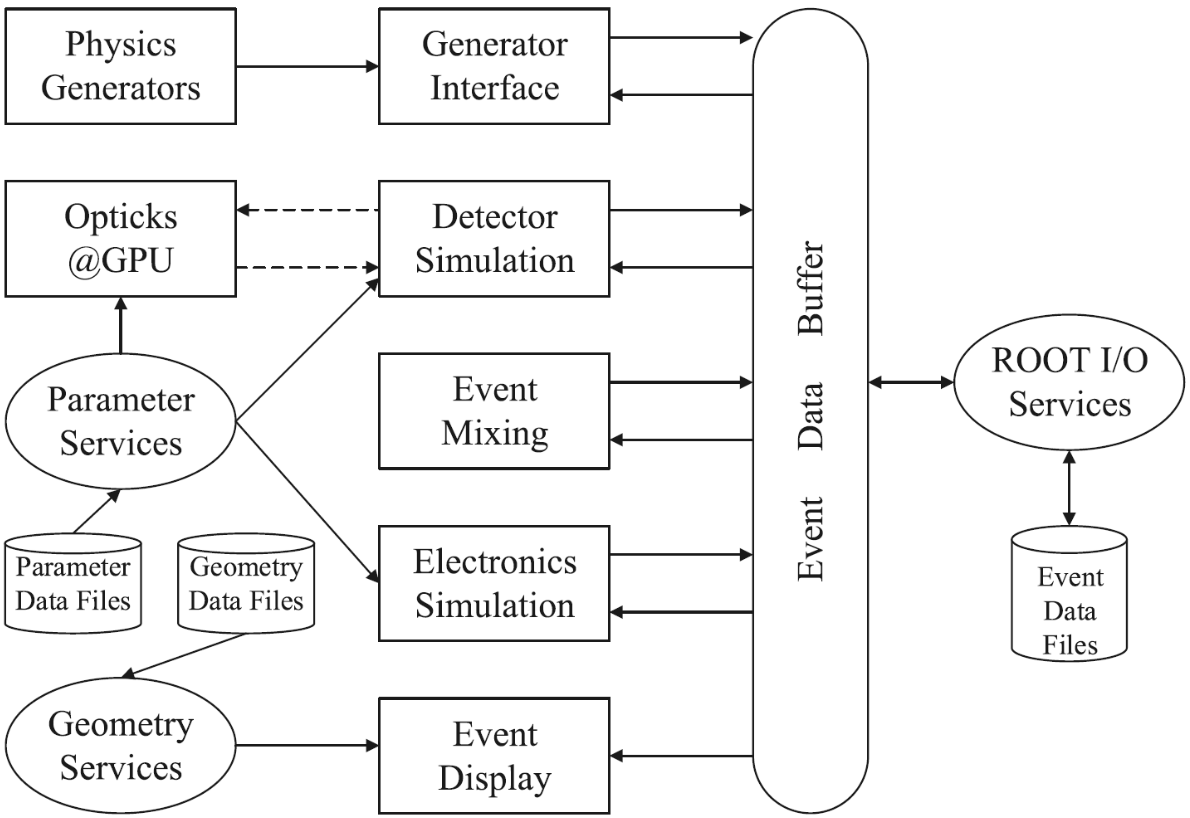
- Central Detector (CD)
  - 20 kilo-ton Liquid Scintillator (LS)
  - 17,612 20inch PMTs
  - 25,600 3inch PMTs
- Water Pool (WP)
  - 2,400 20inch PMTs
- Top Tracker (TT)
  - 3 layers of plastic scintillator

Outline

- Introduction
- JUNO Simulation Software
  - Overview
  - Physics generator interface
  - Detector simulation
  - Electronics simulation
  - Data model and MC truth
- Modified Geant4 processes for JUNO
- Summary

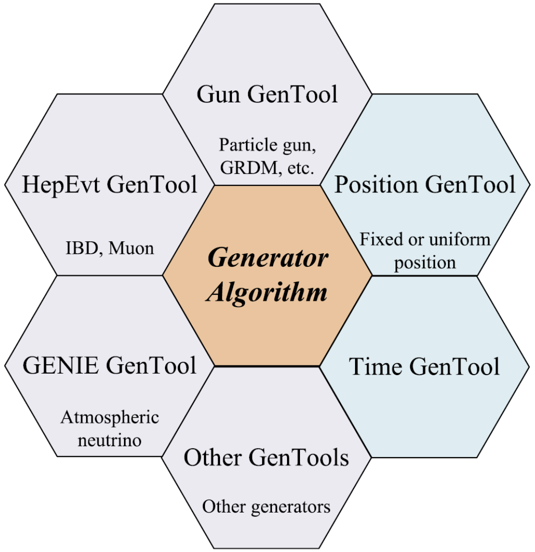
JUNO Simulation Software

- JUNO Simulation software is based on the Geant4 toolkit and the SNiPER (Software for Non-collider Physics Experiment) framework
  - Ref: *Eur.Phys.J.C 83 (2023) 5, 382, Eur.Phys.J.C 83 (2023) 7, 660 (erratum).*



Physics Generator Interface

- Support a variety of physics generators
  - Cosmic ray muons, reactor neutrinos, atmospheric neutrinos, DSNB, natural radioactivities, calibration sources.
  - HepMC 2 as the intermediate data object
  - Multiple converters: HepEvt, GHEP (GENIE)
  - Geant4 Radioactivity Decay Module (GRDM)



- Generator level pre-mixing for data production of radioactivities.

Dataset Name	Generators to be used	Number of Events	Rates (used in elecsim)	Shift persons	Status
Muon	Muon.exe	1,000,000 events (x10)	28.2 Hz	[illegible]	[illegible]
U238@LS	GRDM	1,000,000 events (x13)	3.234 Hz	[illegible]	[illegible]
Th232@LS	GRDM	1,000,000 events (x10)	0.733 Hz	[illegible]	[illegible]
K40@LS	GRDM	1,000,000 events	0.53 Hz	[illegible]	[illegible]
Pb210@LS	GRDM	1,000,000 events (x3)	17.04 Hz	shift	1,000,000 events (x3)
C14@LS	GRDM	1,000,000,000 events	3.3e4 Hz	shift	1,000,000,000 events
Kr85@LS	GRDM	1,000,000 events	1.163 Hz	[illegible]	[illegible]
U238@Acrylic	GRDM	10,000,000 events (x13)	98.41 Hz	[illegible]	[illegible]
Th232@Acrylic	GRDM	10,000,000 events (x10)	22.29 Hz	[illegible]	[illegible]
K40@Acrylic	GRDM	10,000,000 events	161.25 Hz	shift	10,000,000 events
U238@node/bar	GRDM	100,000,000 events (x13)	2102.36 Hz	shift	100,000,000 events (x13)
Th232@node/bar	GRDM	100,000,000 events (x10)	1428.57 Hz	[illegible]	[illegible]
K40@node/bar	GRDM	100,000,000 events	344.5 Hz	[illegible]	[illegible]
Co60@node/bar	GRDM	100,000,000 events	97.5 Hz	[illegible]	[illegible]
U238@PMTGlass	GRDM	1,000,000,000 events (x13)	4.90e6 Hz	[illegible]	[illegible]
Th232@PMTGlass	GRDM	1,000,000,000 events (x10)	8.64e5 Hz	shift	1,000,000,000 events (x10)
K40@PMTGlass	GRDM	1,000,000,000 events	4.44e5 Hz	shift	1,000,000,000 events
Tl208@PMTGlass	GRDM	1,000,000,000 events	1.39e5 Hz	[illegible]	[illegible]
Co60@Truss	GRDM	N events	? Hz	[illegible]	[illegible]
Tl208@Truss	GRDM	N events	? Hz	[illegible]	[illegible]
Rn222@WaterRadon	GRDM	100,000,000 events (x7)	90 Hz	shift	100,000,000 events (x7)

O(1) Hz

O(10^2) Hz

O(10^4) Hz

O(10^6) Hz

```
U238-LS         3.234    $TUTORIALROOT/share/mac/config/U238.conf
U238-PMTGlass   4.90E+6  $TUTORIALROOT/share/mac/config/U238.conf
```

GtPosGeoMapping.yaml

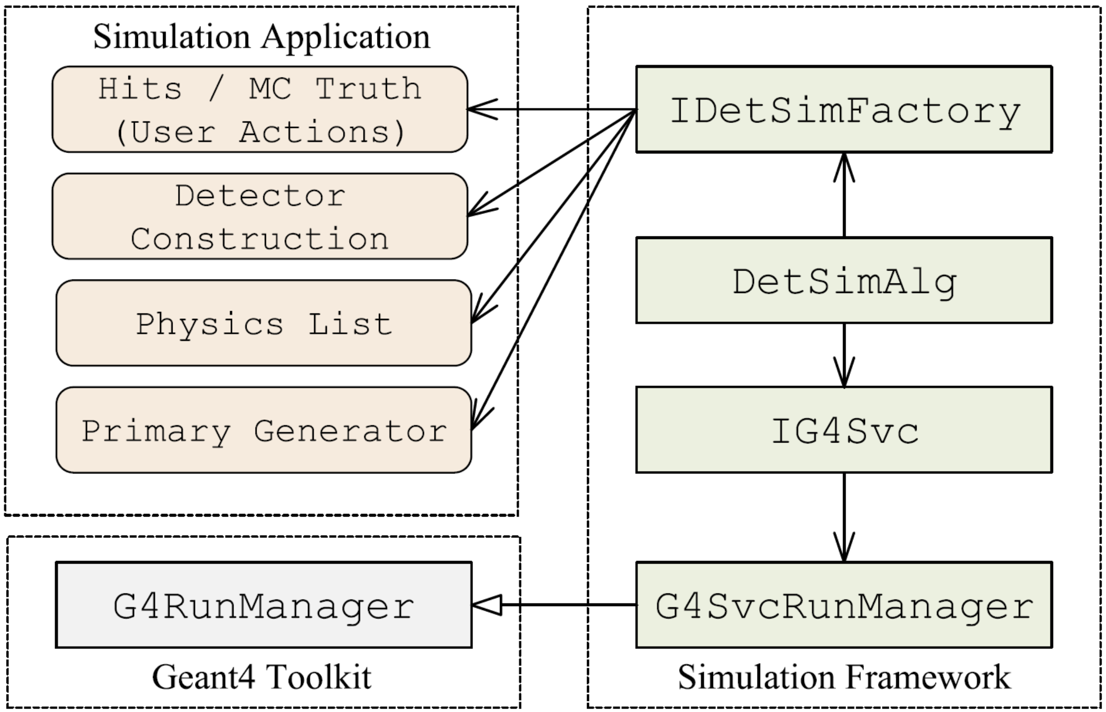
```
LS:
  pTarget: LS

PMTGlass:
  pLPMT_Hamamatsu_R12860: Pyrex
  pLPMT_NNVT_MCPPMT: Pyrex

Water:
  pCentralDetector: Water
```

\+

```
IndexUFNs:
  - LS
  - Acrylic
  - node-bar
  - PMTGlass
```

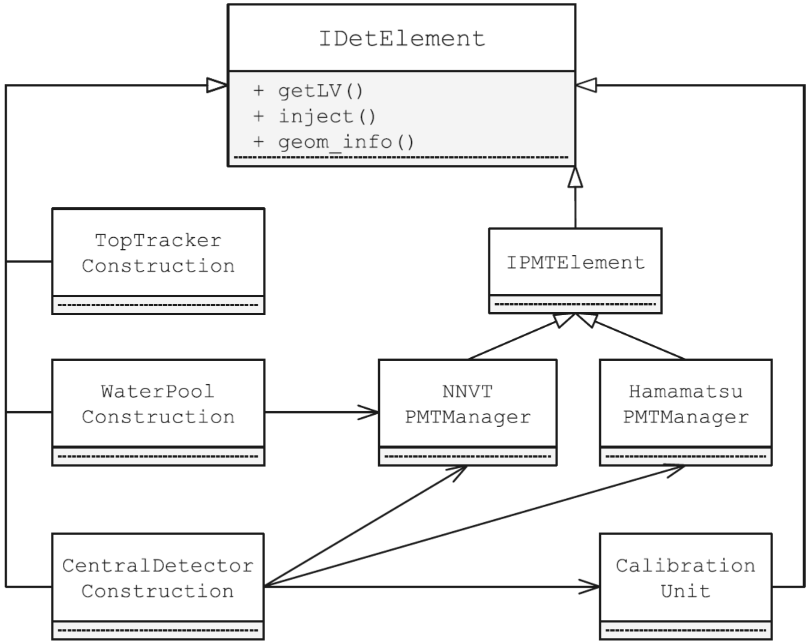
Detector Simulation (1)

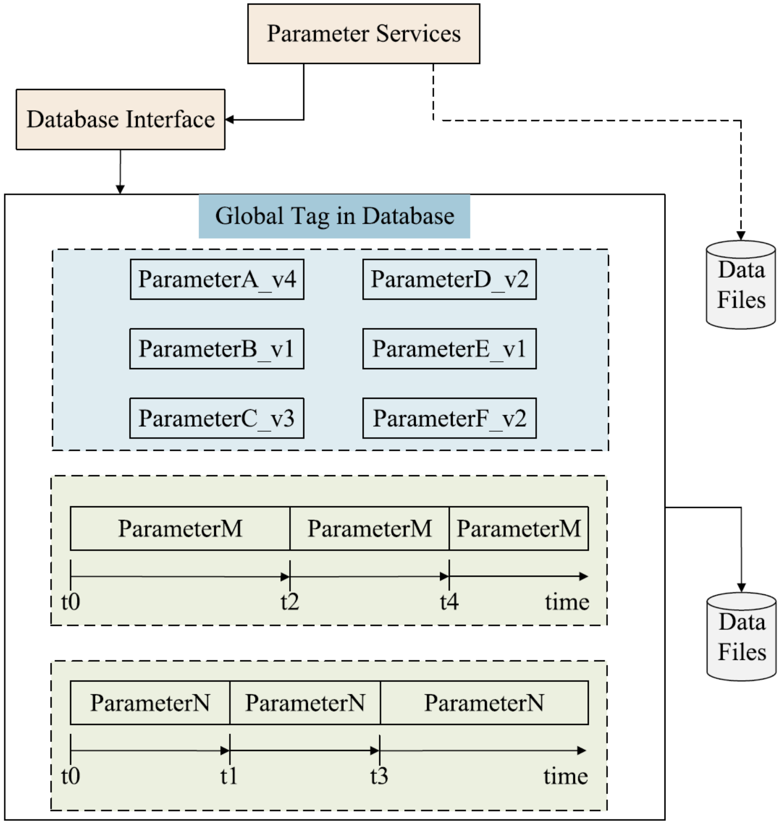
- A lightweight simulation framework is developed to adapt the original Geant4 workflow in the SNiPER framework.
  - The event loop is controlled by the framework instead of Geant4.
  - Multi-threading is supported.



Detector Simulation (2)

- Flexible geometry and parameter management
  - Geometries are grouped into different IDetElements.
  - Parameters are accessed from a unified interface.





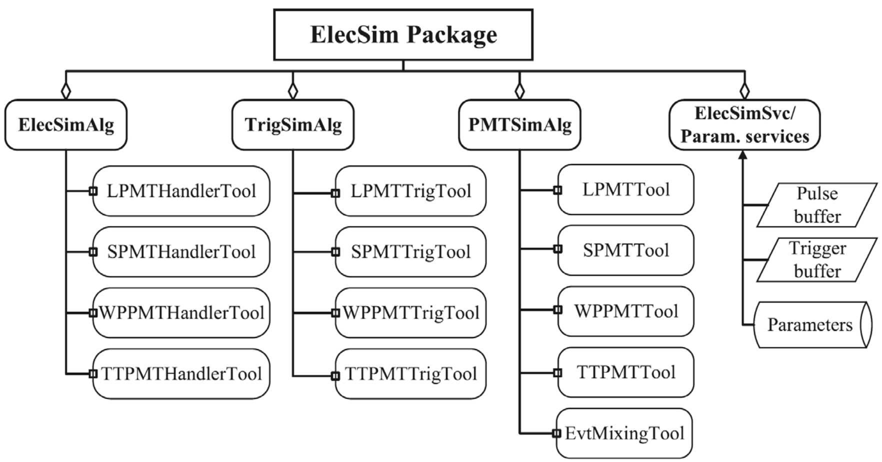
Detector Simulation (3)

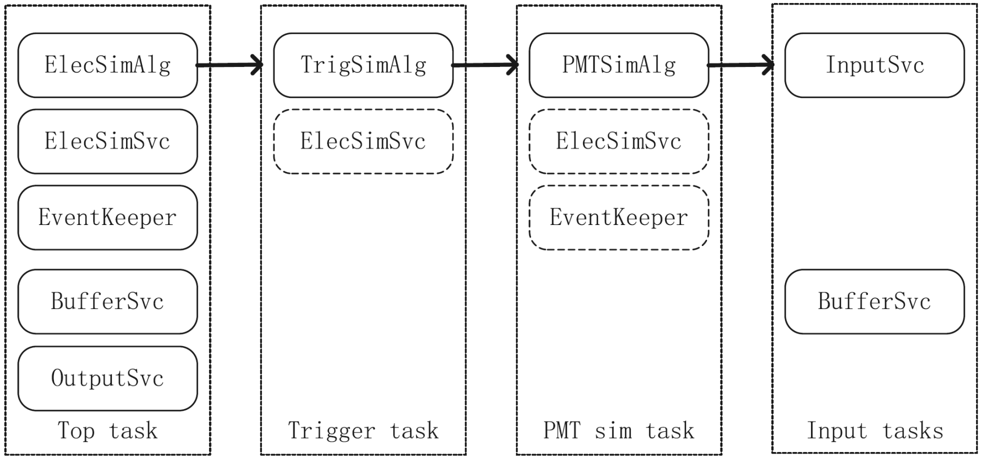
- Several processes have been changed in **Geant4 10.04.p02** in order to better fit with the requirements of the experiment.
  - Most of the physics processes are unchanged.
  - For details of modifications, see the next section.
- JUNO PMT optical model
  - Develop a package to use transfer matrix method (TMM) to consider the interference effects within the thin layers of anti-reflection coating and photocathode between the PMT glass and interior vacuum.

Physics constructors	Status
G4EmLivermorePhysics	Customized
G4EmExtraPhysics	Unchanged
G4DecayPhysics	Unchanged
G4RadioactiveDecayPhysics	Customized
G4HadronPhysicsQGSP_BERT_HP	Customized
G4StoppingPhysics	Unchanged
G4IonPhysics or G4IonPhysicsPHP	Unchanged
G4OpticalPhysics	Customized

Electronics Simulation

- The ElecSim package implements the PMT response and readout electronics of CD, WP and TT.
- A pull based workflow is implemented using SNiPER incidents.
  - The event mixing is invoked on demand. It could avoid the excessive memory usage.



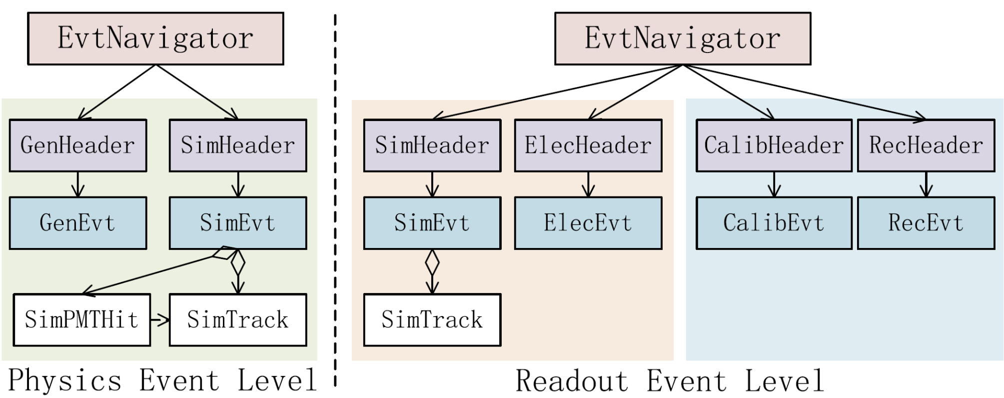


Data Model and MC truth

- Two-level design
  - The event data model is implemented following Header-Event design.

Stage	Header object	Event object	Contained objects	Default EDM path
Generator	GenHeader	GenEvt	Tracks	/Event/Gen
Simulation	SimHeader	SimEvt	Tracks and hits (CD/TT/WP)	/Event/Sim
Trigger	CdTriggerHeader	CdTriggerEvt		/Event/CdTrigger
	WpTriggerHeader	WpTriggerEvt		/Event/WpTrigger
	TtTriggerHeader	TtTriggerEvt		/Event/TtTrigger
Readout	CdWaveformHeader	CdWaveformEvt	Waveforms (CD)	/Event/CdWaveform
	CdLpmtElecHeader	CdLpmtElecEvt	t/q pairs (CD LPMT)	/Event/CdLpmtElec
	CdSpmtElecHeader	CdSpmtElecEvt	t/q pairs (CD SPMT)	/Event/CdSpmtElec
	WpElecHeader	WpElecEvt	t/q pairs (WP)	/Event/WpElec
	WpWaveformHeader	WpWaveformEvt	Waveforms (WP)	/Event/WpWaveform
	TtElecHeader	TtElecEvt	t/q pairs (TT)	/Event/TtElec

- Event Navigator
  - An event navigator consists of a list of lightweight header objects.
  - The header object points to the event object and the event object is loaded on demand.



- Event correlation
  - For the event split or mixing in ElecSim, a new EvtNavigator is created and the SimEvt is recreated with the tracks from mixed events.

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- Introduction
- JUNO Simulation Software
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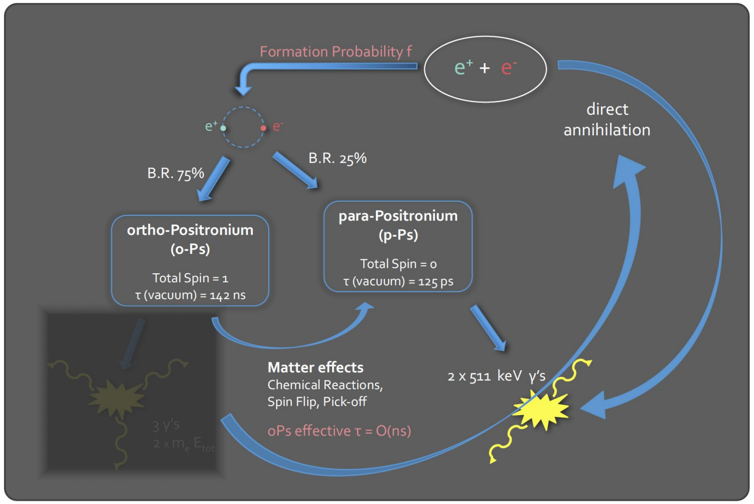
  - Positronium
  - Nuclei radioactive decay
  - Neutron capture
  - Scintillation process
  - Cerenkov process
  - OP boundary process
- Summary

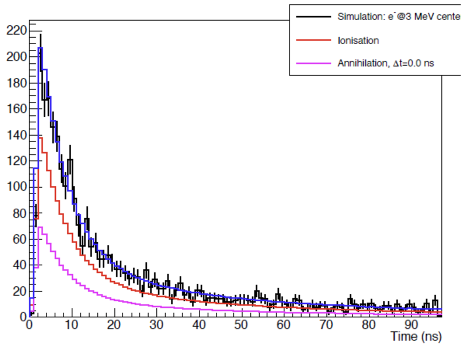
Positronium

- The positronium process is made of 4 classes
  - G4PositroniumFormation: the formation of positronium.
  - G4Positronium: the particle.
  - G4PositroniumDecayChannel2G, G4PositroniumDecayChannel3G: the decay channel.

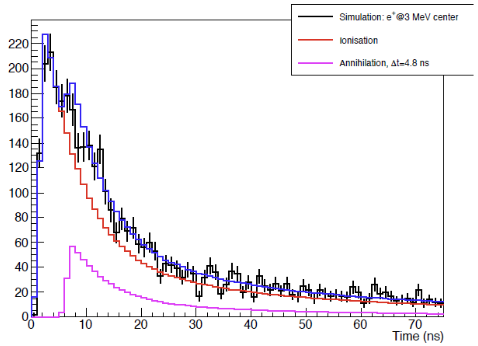


  - In the case of JUNO, the formation probability of 0.545 and lifetime of 3.08 ns from *Phys.Rev.C 88 (2013) 065502*

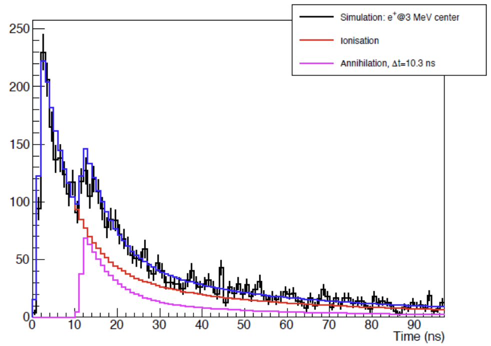
Time distribution of the p.e. on the PMT



e+ without positronium



e+ with positronium and annihilation delayed by ~4.8 ns



e+ with positronium and annihilation delayed by ~10.5 ns

Nuclei radioactive decay

- One important background of reactor anti-neutrinos experiment is the decay of two cosmogenic isotopes: ^{9}Li and ^{8}He.
  - Their spectra have been measured by nuclear spectroscopy and their decay is accompanied by neutrons and alpha emission.
  - In previous Geant4 versions the excited states decayed by gamma emission.
  - The RadioactiveDecay files are modified and the decay with the emission of triton is added (*NIM A 949, 162904 (2020)*).
  - These modifications have been implemented officially in the Geant4 10.6.

z4.a9

#	9BE (8.1814e-17)							
#	Excitation	Flag	Halflife	Mode	Ex	flag	Intensity	Q
P	11810	-	4.22e-21					
				Alpha	0		0.75	
				Alpha	0	-	28.	9340
				Alpha	0	-	47.	8070
				Neutron	0		0.25	
				Neutron	0	-	2.	10140
				Neutron	3030	-	11.	7110
				Neutron	11350	-	12.	10
P	11282	-	4.22e-21					
				Alpha	0		0.76	
				Alpha	0	-	76.	8812
				Neutron	0		0.24	
				Neutron	0	-	3.	9612
				Neutron	3030	-	21.	6582
P	7940	-	4.22e-21					
				Alpha	0		0.8	
				Alpha	0	-	80.	5470
				Neutron	0		0.2	
				Neutron	0	-	10.	6270
				Neutron	3030	-	10.	3240
P	2780	-	4.22e-21					
				Alpha	0		0.25	
				Alpha	0	-	25.	310
				Neutron	0		0.75	
				Neutron	0	-	15.	1110
				Neutron	3030	-	60.	10
P	2429.4	-	4.22e-21					
				Alpha	0		0.025	
				Alpha	0	-	2.5	10
				Neutron	0		0.975	
				Neutron	0	-	11.	759.4
				Neutron	3030	-	86.5	10

z4.a8

#	8BE (8.1814e-17)							
#	Excitation	Flag	Halflife	Mode	Ex	flag	Intensity	Q
P	0	-	8.181436e-17					
				Alpha	0		1.	
				Alpha	0	-	100.	91.84
P	3030	-	1.3e-22					
				Alpha	0		1.	
				Alpha	0	-	100.	3121.84
P	11350	-	1.3e-22					
				Alpha	0		1.	
				Alpha	0	-	100.	11441.84
P	16626	-	4.22e-21					
				Alpha	0		1.	
				Alpha	0	-	100.	16717.84

Neutron capture

- The multiplicity and energy of gammas emitted after neutron capture is important for reactor antineutrinos experiment.
  - Using Geant4.9, some issues are found in the gamma emission for neutron capture on these different nuclei : Gd, Fe, Ni, Si, P, Mn, S, Cr, O, N and C.
  - For all these nuclei, 32 .txt files with the gamma lines from NNDC are generated in total.
  - A class DsG4NNDCCaptureGammas is created to read the files and generate the gammas.

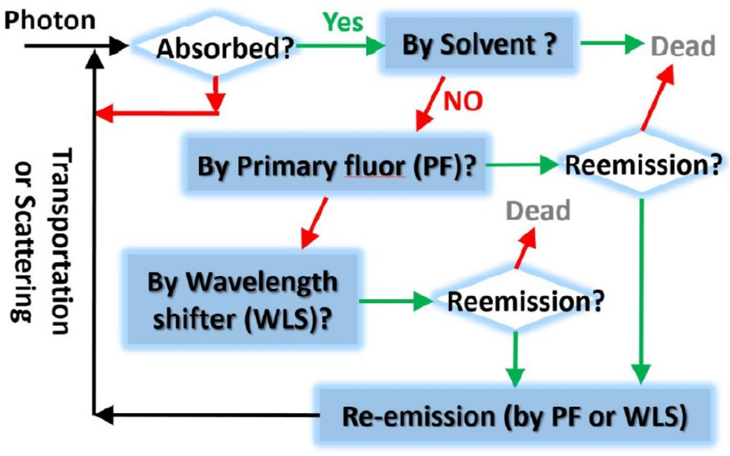
```
# Neutron capture gammas for O-17 generated by sums.py from data obtained from
# NNDC capture gamma tables at http://www.nndc.bnl.gov/capgam/indexbyn.html
#
# Number of gammas in a decay chain limited to 10
#
# First column lists probability for decay scheme; second column lists number of gammas
# in decay scheme; gamma energies (in keV) are then listed separated by a space.
#
0.244492673801 3 3588.0 2473.0 1982.0
0.349320808975 4 3588.0 1982.0 1652.0 822.0
0.257347797328 3 3396.0 2666.0 1982.0
0.17008505995 4 2473.0 1982.0 1938.0 1652.0
```

Scintillation process

- G4Scintillation process is modified in several ways
  - Support different Birks constants for different particles

```
if(aParticleName == "gamma" || aParticleName == "e+" || aParticleName == "e-"){
    birk1 = birksConstant1[11];
    birk2 = birksConstant2[11];
}else if(abs(aParticle->GetCharge())<1.5){
    birk1 = birksConstant1[2212];
    birk2 = birksConstant2[2212];
}else{
    birk1 = birksConstant1[1000020040];
    birk2 = birksConstant2[1000020040];
}
```

  - Different emission time constants and exponential decay components were used for different particles.
  - Photon reemission in LS is implemented.
    - Optical photons from both scintillation and Cerenkov processes can be absorbed in LS and then re-emitted with different wavelength.
    - The reemission probability depends on waveform.



Cerenkov process

- Due to the RINDEX of the LS is not a monotonic function, the default G4Cerenkov cannot be applied.
  - G4Cerenkov is modified to able to calculate the Cherenkov Angle Integral (CAI) according to the energy ranges where RINDEX>1/β.

Photons emitted with an energy beyond a certain value are immediately re-absorbed by the material; this is the window of transparency of the radiator. As a consequence, all photons are contained in a cone of opening angle $\cos\theta_{max} = 1/(\beta n(\epsilon_{max}))$. The average number of photons produced is given by the relations:

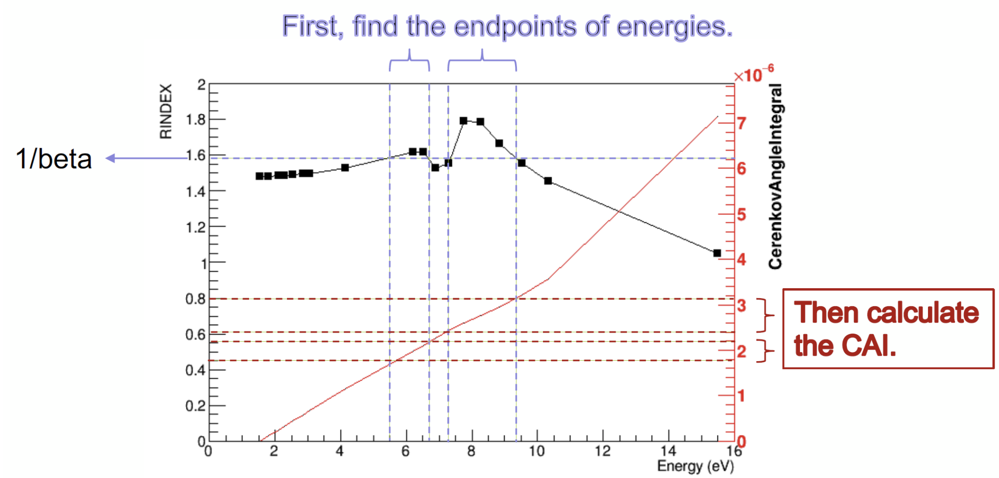
$$dN = \frac{\alpha z^2}{\hbar c}\sin^2\theta d\epsilon dx = \frac{\alpha z^2}{\hbar c}(1 - \frac{1}{n^2\beta^2})d\epsilon dx$$
$$\approx 370 z^2 \frac{\text{photons}}{\text{eV cm}}(1 - \frac{1}{n^2\beta^2})d\epsilon dx$$

and the number of photons generated per track length is

$$\frac{dN}{dx} \approx 370 z^2 \int_{\epsilon_{min}}^{\epsilon_{max}} d\epsilon \left(1 - \frac{1}{n^2\beta^2}\right) = 370 z^2 \left[\epsilon_{max} - \epsilon_{min} - \frac{1}{\beta^2}\int_{\epsilon_{min}}^{\epsilon_{max}} \frac{d\epsilon}{n^2(\epsilon)}\right].$$

where n(E)>1/β

In GEANT4, n(E) is assumed as an increasing function of energy.



https://geant4-userdoc.web.cern.ch/UsersGuides/PhysicsReferenceManual/html/electromagnetic/xray_production/cerenkov.html

OP boundary process

- To support the transverse matrix method (TMM) in PMT optical model (POM), the standard boundary process is modified in a way that reuses as much of standard Geant4 as possible.

README.rst

Custom4 : Geant4 Customizations

This Custom4 mini-package was created to avoid circular dependency between opticks and junosw by splitting off classes/struct that depend only on Geant4 so as to allow high level communication between opticks and junosw in the "language" provided by Custom4.

Classes/Structs

C4OpBoundaryProcess.hh
: modified G4OpBoundaryProcess with customized calculation of absorption, reflection, transmissing coefficients using C4CustomART.h

C4CustomART.h
: integrates between the boundary process and the TMM calculation

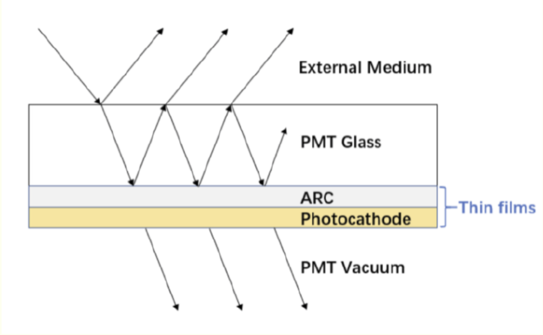
C4MultiLayrStack.h
: TMM (transfer-matrix method) calculation of absorption, reflection and transmission (ART) coefficients based on complex refractive indices and layer thicknesses

C4IPMTAccessor.h
: pure virtual protocol interface for providing PMT information including layer refractive indices and thicknesses to the boundary process

C4CustomART_Debug.h
: debug struct with serialization to std::array

https://github.com/simoncblyth/customgeant4/

TMM : Transfer Matrix Method



multi-layer thin films, coherent calc:

- complex refractives indices, thicknesses
- => (A,R,T) (Absorb, Reflect, Transmit) + E (Efficiency)
- Used from **C4OpBoundaryProcess**

header-only GPU/CPU : C4MultiLayrStack.h

- `Custom4` depends only on Geant4
- Dependency of JUNOSW and Opticks

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Summary

- The JUNO Simulation Software is developed based on Geant4 10.04.p02 with customized physics processes.
  - We implemented the positronium generator instead of standard e+ annihilation. The lifetime and the probability of positronium are dependent of the material.
  - We would be also interested in a more precise of radioactive nuclei taking into account of the width of the energy states.
  - We created several files to reproduce the multiplicity and the energy of gammas for neutron radiative captures.
  - We extended the Scintillation process to support the reemission of photons.
  - We customized the Cerenkov process in order to take into account of the dependance of the refractive index with the photons energy.
  - We developed a complex optical model to better reproduce the photons interactions with the PMTs. This has been accompanied by a customization of the boundary processes.

Thank you for your attention