Progress on the full Monte Carlo production of IBD-like spectral components and geoneutrino sensitivity studies

JUNO EU-AM Fall Meeting 2022, Ferrara (Italy)

25th October 2022 | Nikhil Mohan[1,3], Anita Meraviglia[1,3], Livia Ludhova[2,3]

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(3) RWTH Aachen University, Aachen (Germany)

OUTLINE

1. Analysis strategy
2. Current status of the MC PDFs
3. Accidental background MC production
4. Geoneutrinos sensitivity studies
5. Conclusions and outlook

1. Analysis Workflow

1. **Massive MC simulations (SNiPER)**
2. **Reference shapes production (PDF)**
3. **Toy data sampling (Fitter)**
4. **Fitting procedure (Fitter)**

Geo-neutrino study →

Signal:
Geo-neutrinos

+

Bkgs:
Reactor IBDs,
$^{9}Li/^{8}He$, Accidentals,
Fast-n, $^{13}C(\alpha,n)^{16}O$.

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2. (a) Reactor IBD MC Simulation

Thanks to Tao !!!

Offline Software: Trunk version

Includes all the relevant standard parameters used in recent NMO release.

- Generator: hepevt (IBD.exe)
- No. of events: 1,006,000 IBD events (unoscillated)
- Rate: 1 Hz (default)

- IBD event: e^+ (prompt) + n (delayed)

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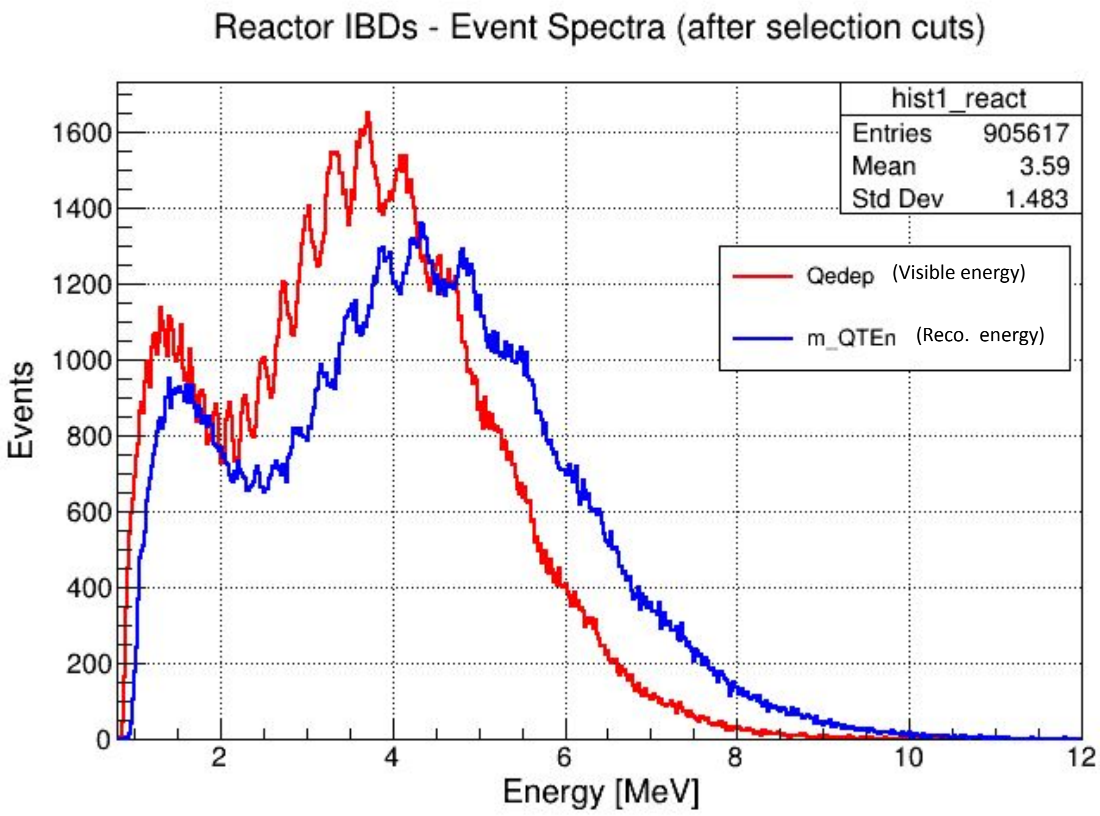

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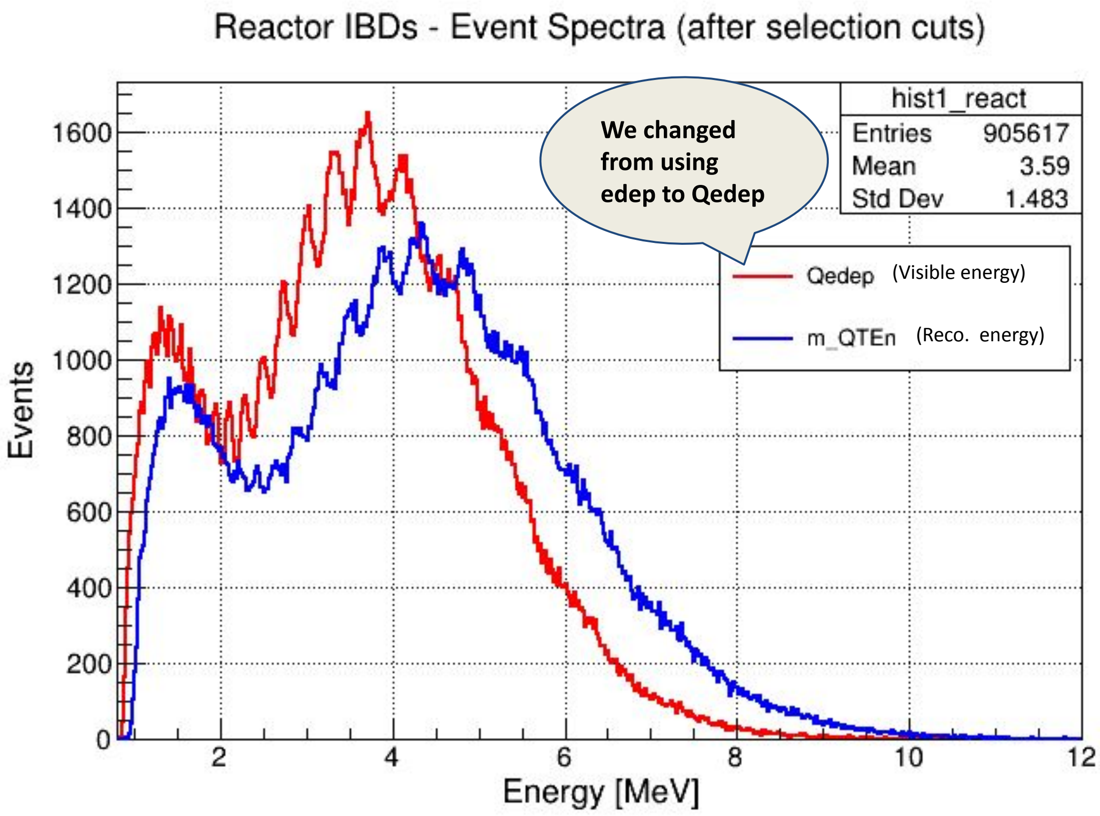

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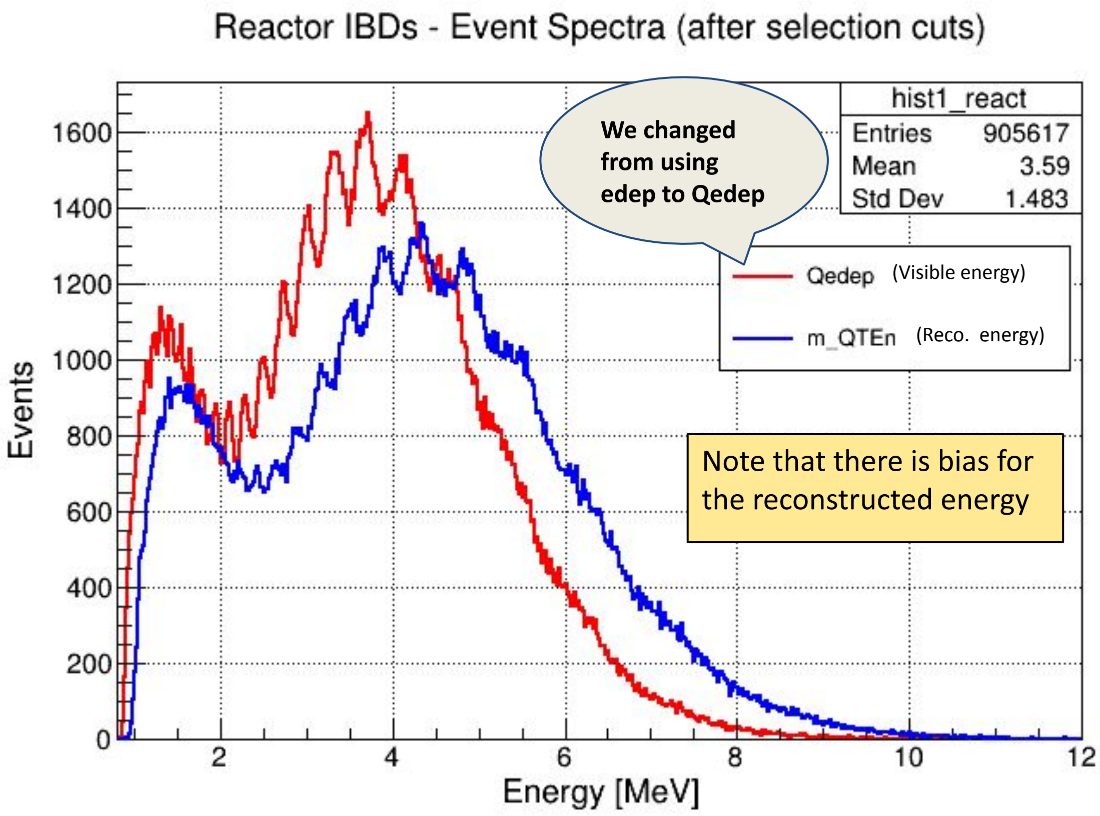

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How to correct the bias in reco energy?

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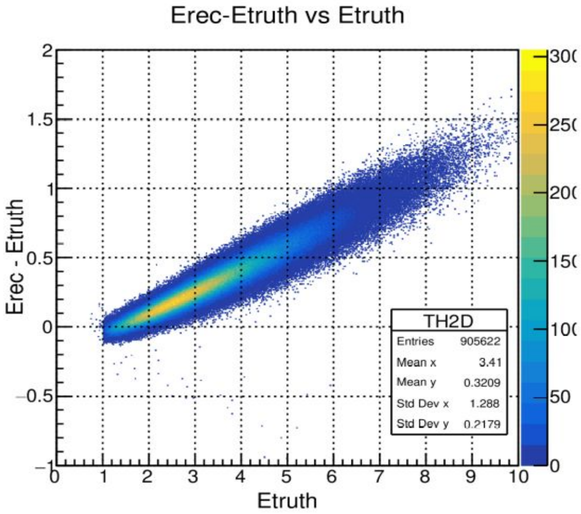
1. Previously, we used the **Erec-Edep** vs **Edep** plot to get the energy correction for the bias.

2. From the comments from last G.M., we realised this is the wrong approach and so switched to Erec-Qedep vs Erec.



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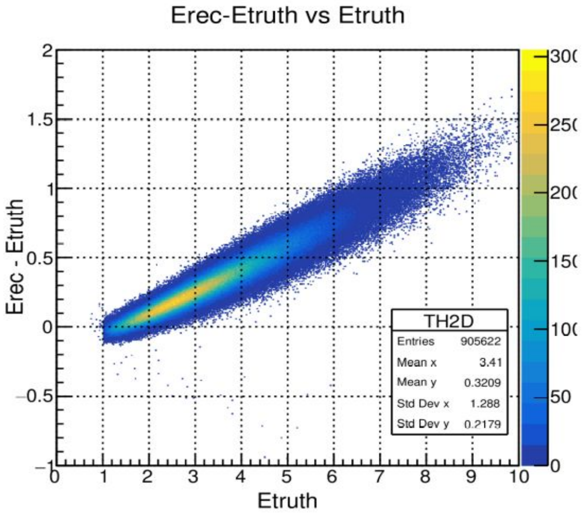
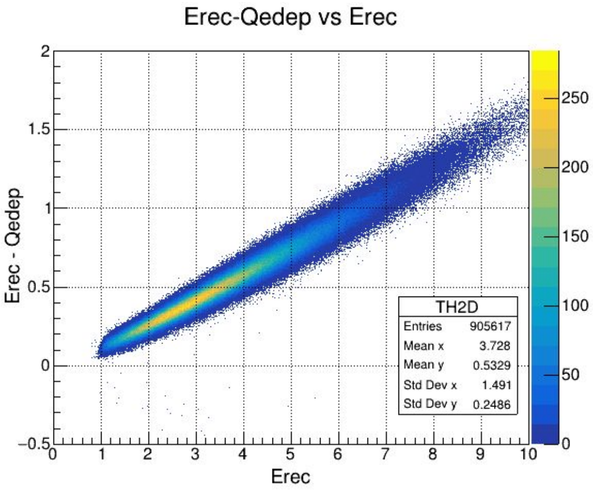
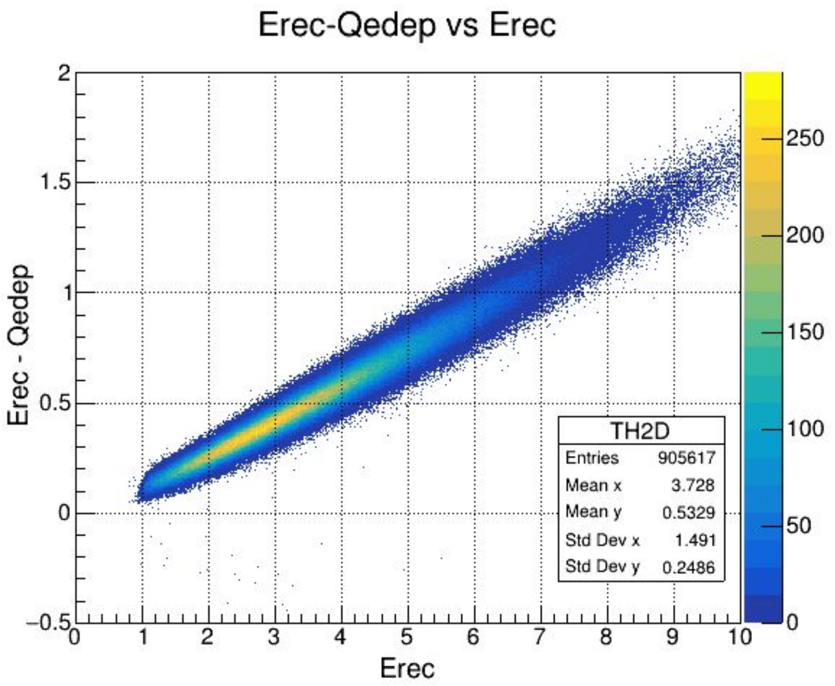
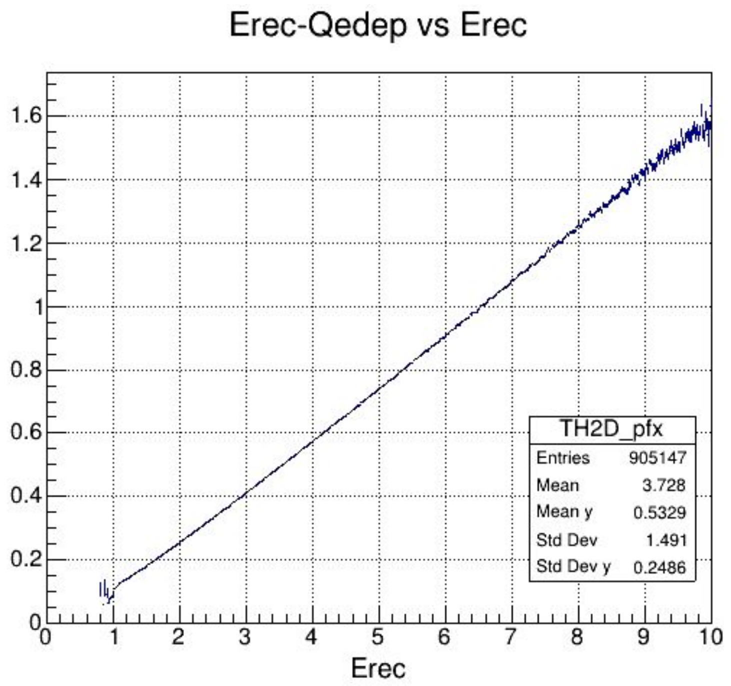




Correcting the bias in reco energy





- Erec-Qedep vs Erec 2D plot

- Y-profile of the 2D plot

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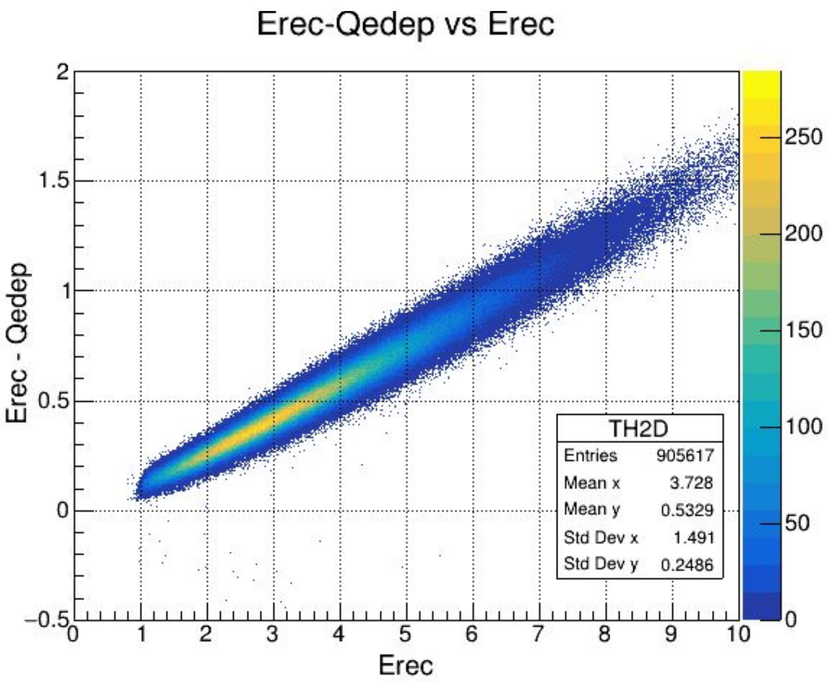
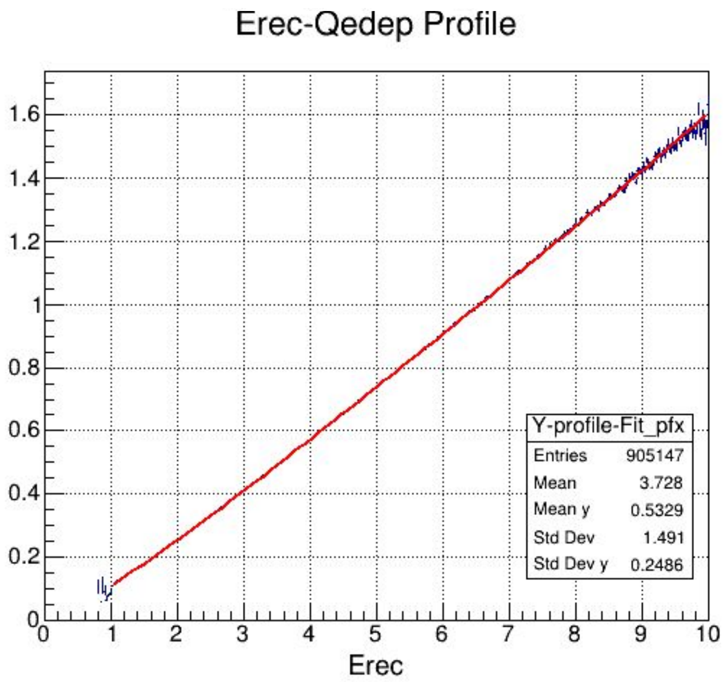




Polynomial fit parameters:

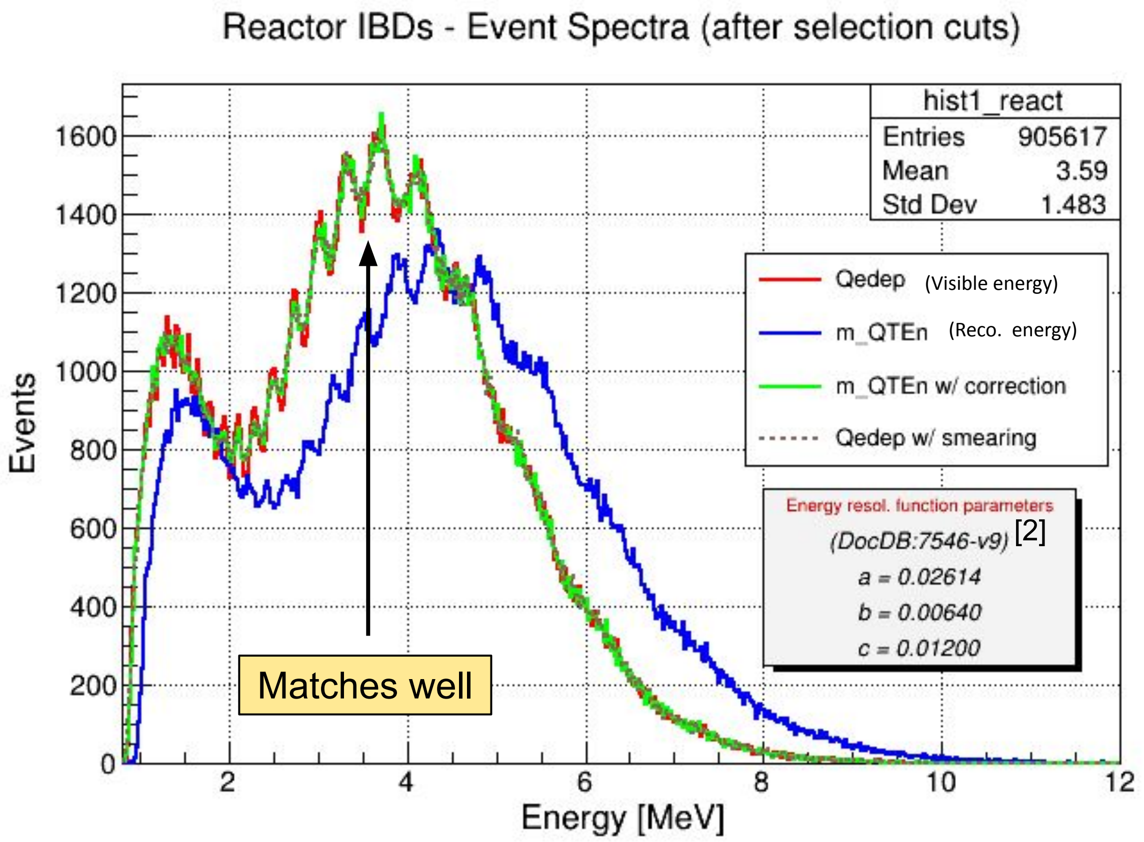
p0= -0.0194
p1= 0.1183
p2= 0.0116
p3=-0.0012
p4= 5.37e-5

This correction is applied to all input PDFs.

- Erec-Qedep vs Erec 2D plot

- Y-profile of the 2D plot

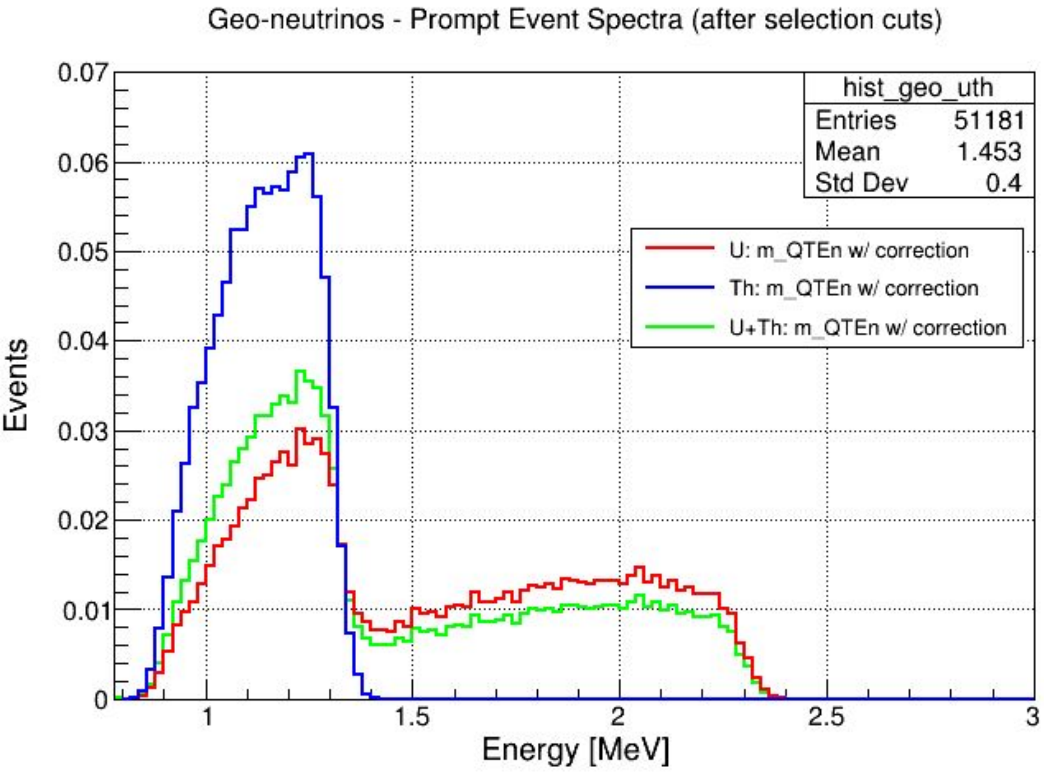
2. (a) Reactor spectra - corrected and Gauss smeared



- Corrected reco. energy = Reco. energy - poly(Reco. energy)
- Corrected reco. spectrum matches very well with the Convoluted spectrum (Qedep smeared with the abc-model)

[2] DocDB: 7546-v9: TechNote on Comparison of JUNO Neutrino Mass Ordering Analysis Results

2. (b) Geo-neutrino MC Simulation (updated)



<u>Offline Software:</u> Trunk version

- Simulated 50,000 Geo-neutrino events from U and Th sources separately (GeoNu.exe).
- IBD event: e^+ (prompt) + n (delayed)

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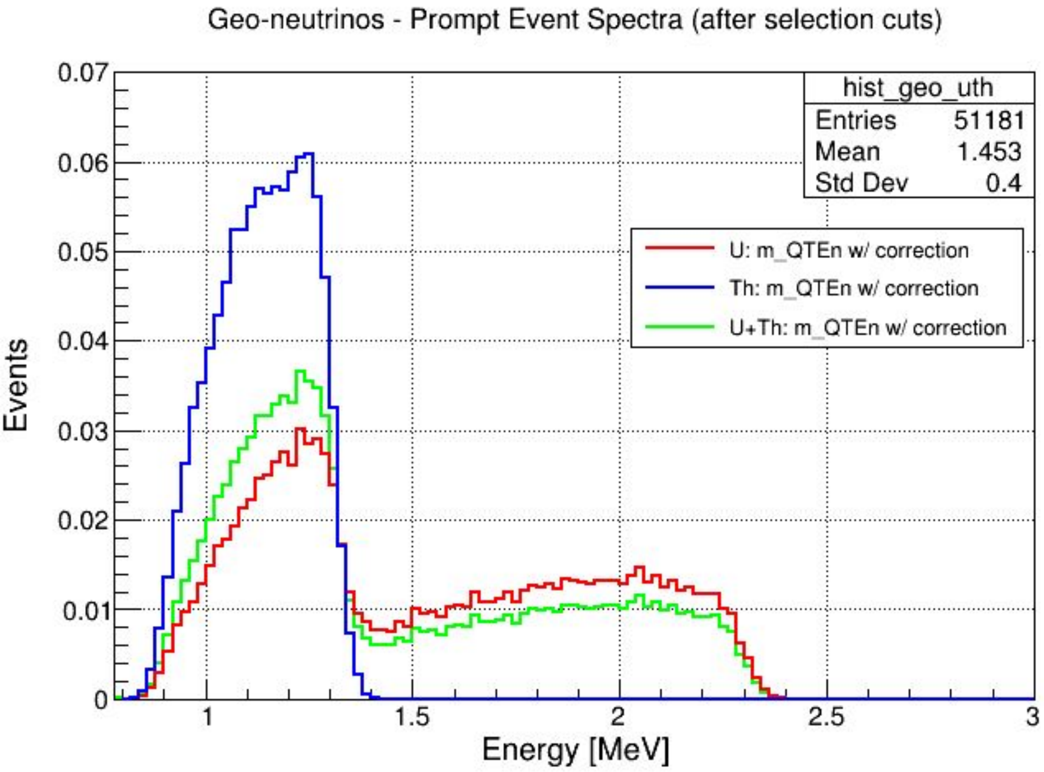

Geo-neutrino spectra updated with the new energy correction!

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2. (c) Li-He MC Simulation (new)

Thanks to Cécile !!!

<u>Offline Software:</u> Trunk version

- Simulated 100,000 Li and He events separately using the gun generator.
- IBD-like event: e^{-}+n+α+γ (prompt) + n (delayed)

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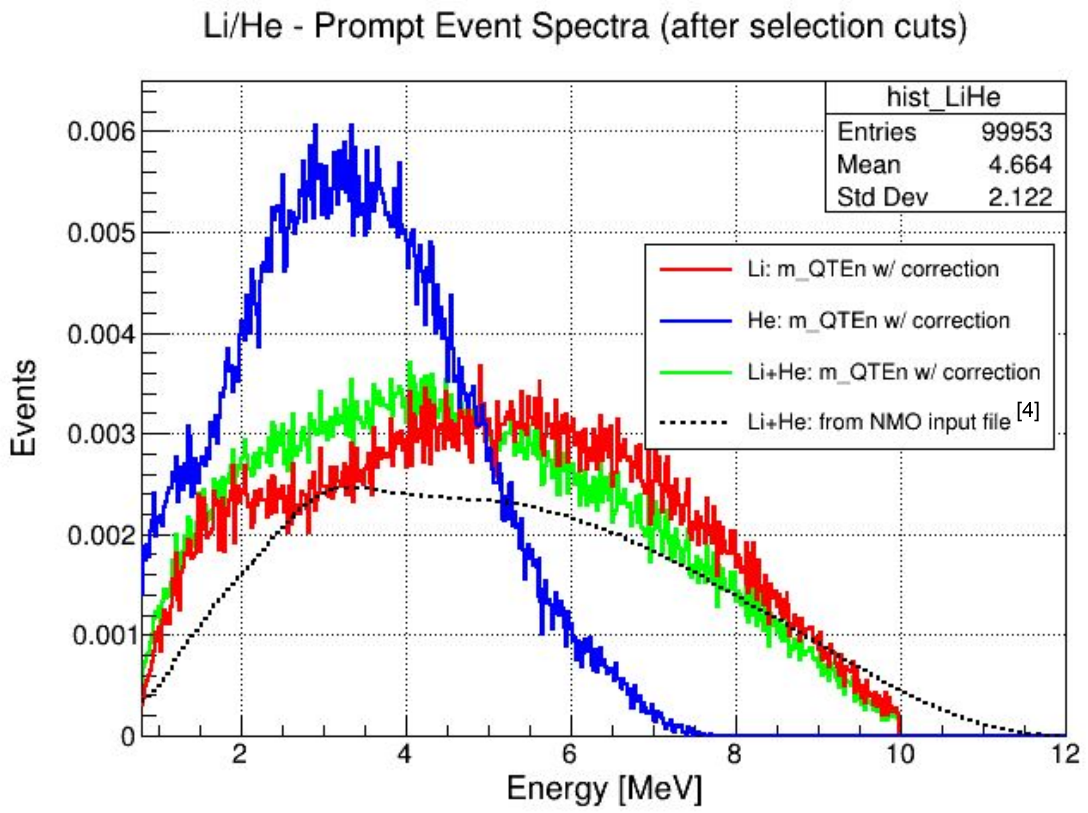

[4]DocDB-5929-v34

Thanks to Cécile !!!

Offline Software: Trunk version

- Simulated 100,000 Li and He events separately using the gun generator.
- IBD-like event: $e^{-}+n+\alpha+\gamma$ (prompt) + n (delayed)

Contributions from Li and He are combined in the ratio 75 to 25 respectively (from KamLAND results).

Ratio of Li-He in the spectrum from NMO under investigation.

2. (c) Li-He MC Simulation (new)

We apply the same energy correction in this case also!

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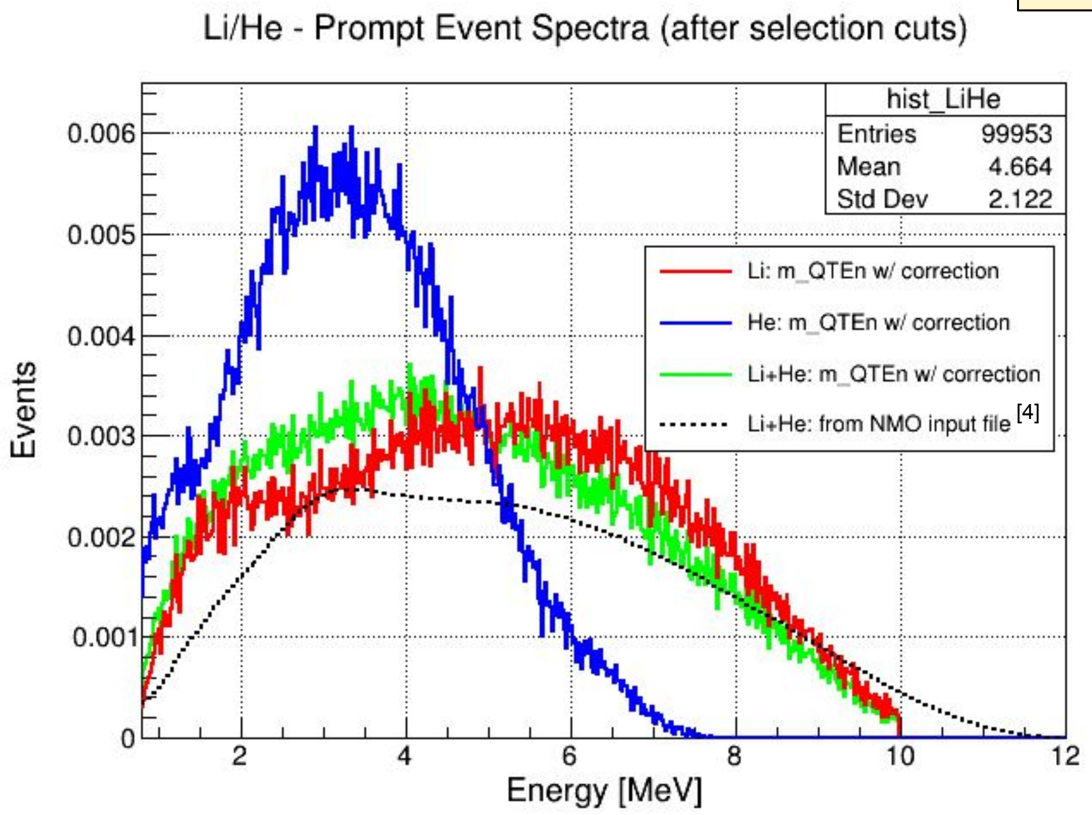

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3. Accidental background MC production

How we obtained the PDF: the logical steps

1. Run the pre-mixed radioactivity datasets until the reco. stage.
2. Build the 4D (E_{rec}, R_x, R_y, R_z) plot from the user-rec rootfile.
3. Extract the prompt energy spectrum of accidentals by considering all the possible pairs of events from the 4D plot, and check whether they pass the IBD selection cuts.
4. Impose the FV ($r < 17.2$ m) cut on the prompt spectrum.

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Step 1: the pre-mixed radioactivity dataset

- It has been built starting from the single radioactive isotope produced for the **Mock Data Challenge (MDC)**

Dataset Name	Generators to be used	Number of Events	Rates (used in elecsim)	Shift persons	Status	Document	Notes
Muon	Muon.exe	1,000,000 events (x10)	28.2 Hz	Jilei Xu	1,000,000 (x10)	Link to gitlab	Total 4 days
U238@LS	GRDM	1,000,000 events (x13)	3.234 Hz	Cailian Jiang	1,000,000 events (x13)	Link to gitlab	Notes
Th232@LS	GRDM	1,000,000 events (x9)	0.733 Hz	shift	1,000,000 events (x9)	Links	Notes
K40@LS	GRDM	1,000,000 events	0.53 Hz	shift	1,000,000 events	Links	Notes
Pb210@LS	GRDM	1,000,000 events (x3)	17.04 Hz	shift	1,000,000 events (x3)	Links	Notes
C14@LS	GRDM	1,000,000,000 events	3.3e4 Hz	shift	1,000,000,000 events	Links	Notes
Kr85@LS	GRDM	1,000,000 events	1.163 Hz	shift	1,000,000 events	Links	Notes
U238@Acrylic	GRDM	10,000,000 events (x13)	98.41 Hz	shift	10,000,000 events (x13)	Links	Notes
Th232@Acrylic	GRDM	10,000,000 events (x9)	22.29 Hz	shift	10,000,000 events (x9)	Links	Notes
K40@Acrylic	GRDM	10,000,000 events	161.25 Hz	shift	10,000,000 events	Links	Notes
U238@node/bar	GRDM	100,000,000 events (x13)	2102.36 Hz	shift	100,000,000 events (x13)	Links	Notes
Th232@node/bar	GRDM	100,000,000 events (x9)	1428.57 Hz	shift	100,000,000 events (x9)	Links	Notes
K40@node/bar	GRDM	100,000,000 events	344.5 Hz	shift	100,000,000 events	Links	Notes
Co60@node/bar	GRDM	100,000,000 events	97.5 Hz	shift	100,000,000 events	Links	Notes
U238@PMTGlass	GRDM	1,000,000,000 events (x13)	4.90e6 Hz	shift	1,000,000,000 events (x13)	Links	Notes
Th232@PMTGlass	GRDM	1,000,000,000 events (x9)	8.64e5 Hz	shift	1,000,000,000 events (x9)	Links	Notes
K40@PMTGlass	GRDM	1,000,000,000 events	4.44e5 Hz	shift	1,000,000,000 events	Links	Notes
Tl208@PMTGlass	GRDM	1,000,000,000 events	1.39e5 Hz	shift	Not start	Links	Notes
Co60@Truss	GRDM	N events	? Hz	shift	Not start	Links	Notes
Tl208@Truss	GRDM	N events	? Hz	shift	Not start	Links	Notes
Rn222@WaterRadon	GRDM	100,000,000 events (x7)	90 Hz	shift	100,000,000 events (x7)	Links	Notes

We did several cross-checks to understand the numbers given here and found the following:

Thanks to Tao, Jie and Cailian !!!

https://juno.ihep.ac.cn/mediawiki/index.php/Analysis_Foundation_Groups/Data_production/Mock_Data_Challenges

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Step 1: the pre-mixed radioactivity dataset

What we found:

- The Number of events do not match the actual number simulated.
  - For the external bkg, the Number of events actually simulated is larger because at least 1 hour needed to be generated for the pre-mixing.
- We verified that the Rates shown here matches with the rates calculated from the inputs given in the JUNO radioactivity paper*

*https://arxiv.org/abs/2107.03669

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After having understood the structure, we run all the 3600 pre-mixed detsim files until the reco stage (J22.1.0-rc2)

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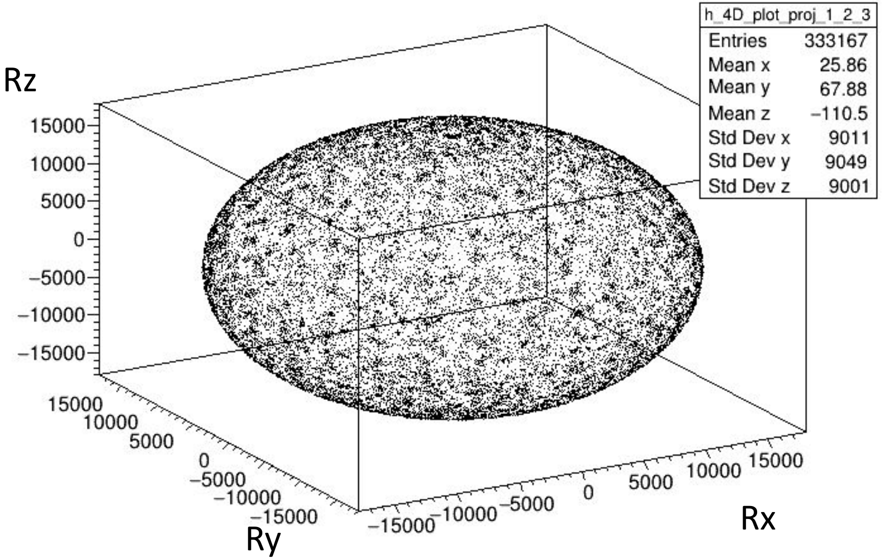
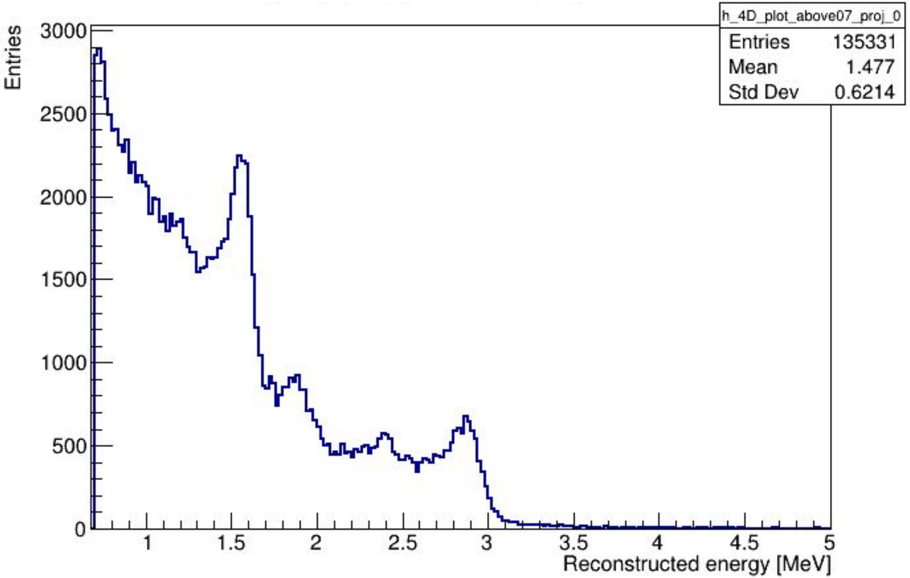
Step 2: build the 4D (Erec, Rx, Ry, Rz) plot



Distribution of the reconstructed energy (>0.7 MeV)



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Being **N** the number of events of the 4D plot, we consider all the **N(N-1) ~ 10^{10} combinations** between every possible p-d pairs and check whether they pass the IBD cuts:

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- 1.9 MeV < $\mathbf{E}_{\mathbf{delayed}}$ < 2.9 MeV and

  4.4 MeV < $\mathbf{E}_{\mathbf{delayed}}$ < 5.5 MeV.
- $\mathbf{R}_{\mathbf{prompt\text{-}delayed}}$ < 1.5 m.

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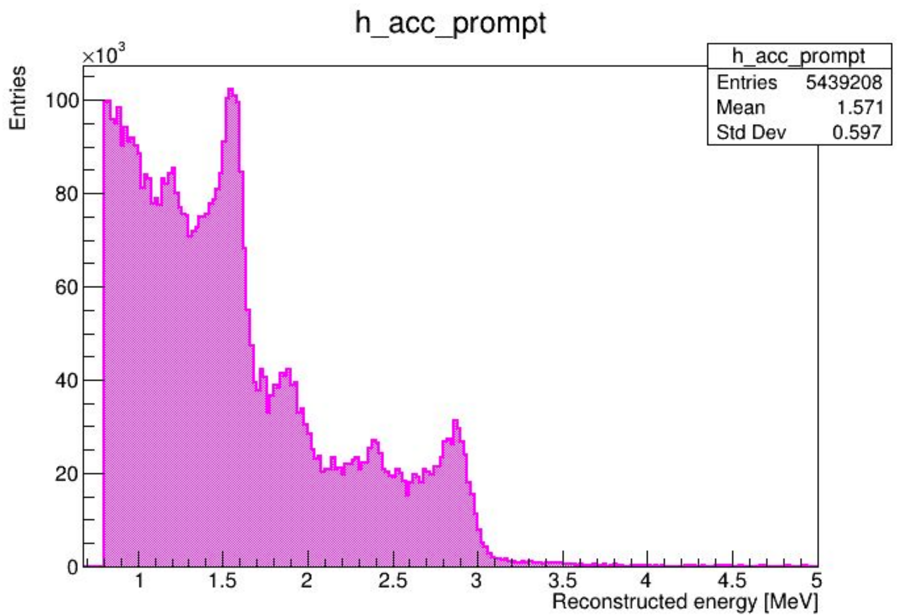
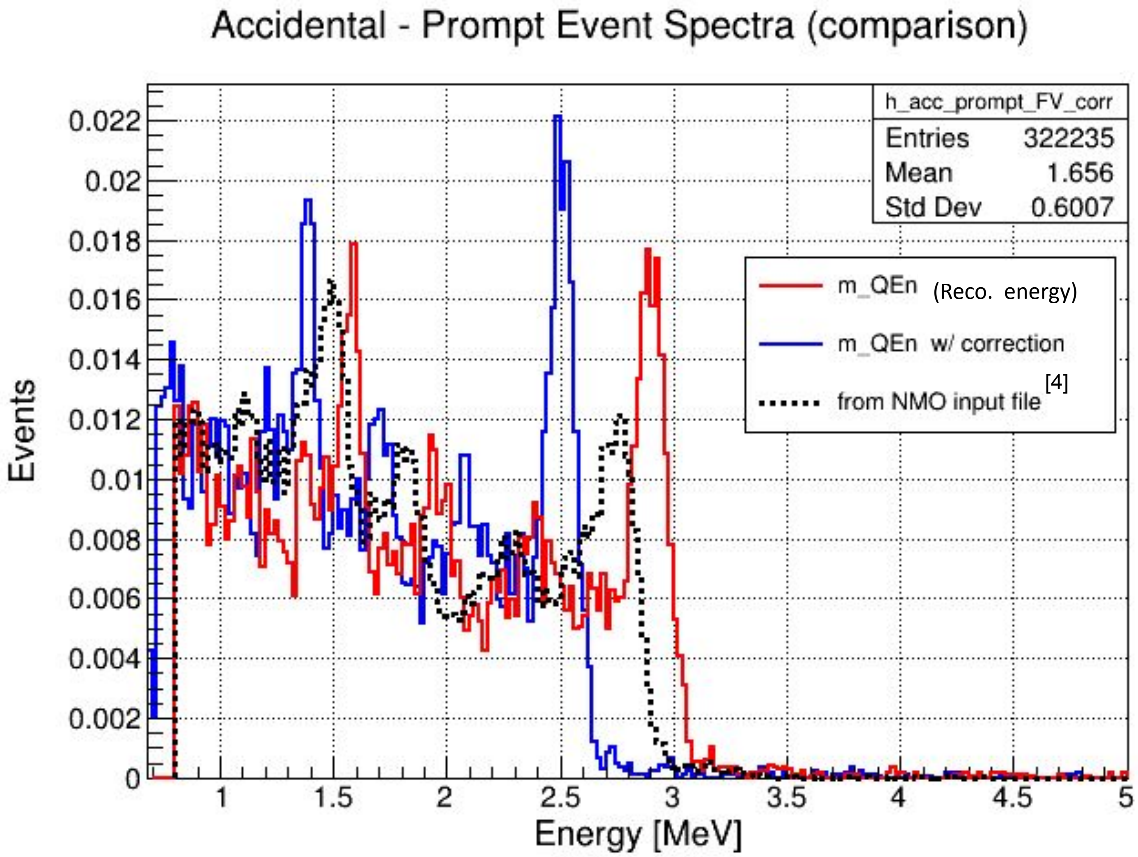


Step 4: FV cut on the accidentals prompt energy spectrum



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[4]DocDB-5929-v34

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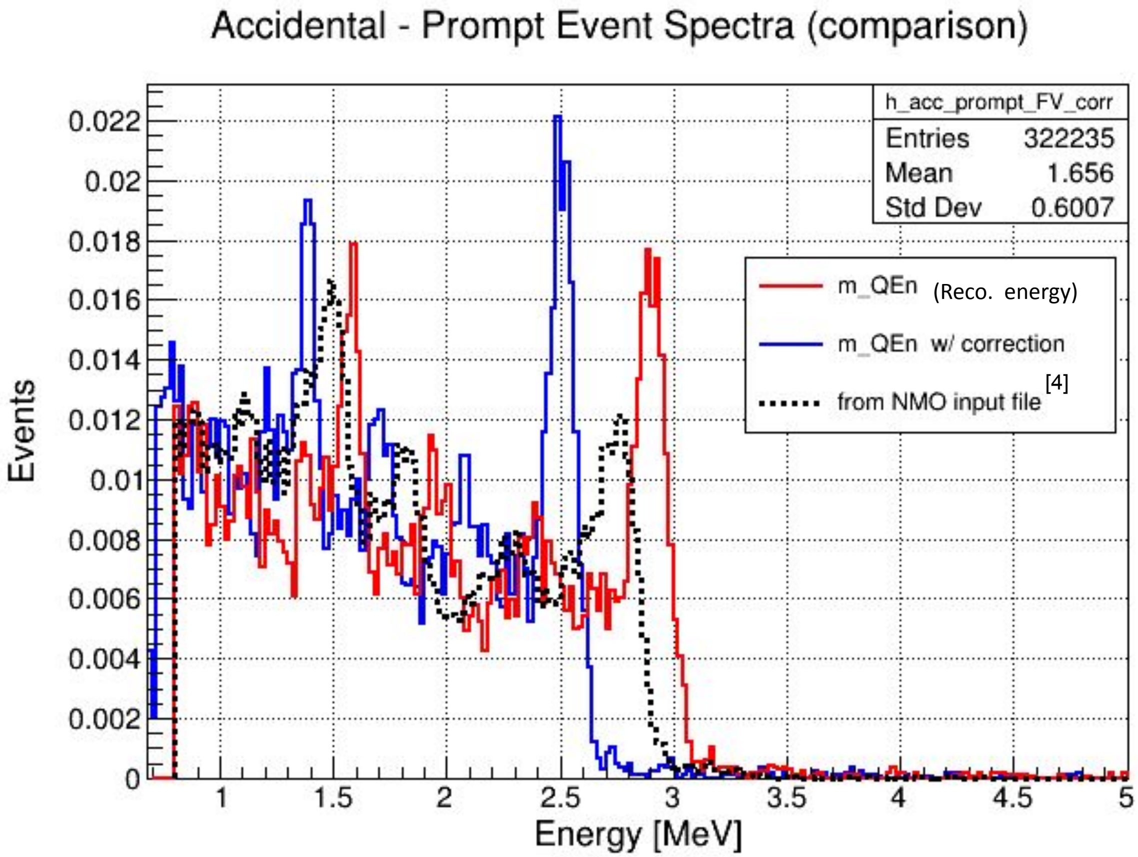

- After applying the **R < 17.2 m FV cut** and adding energy correction on the prompt.
- Reco. spectrum w/ correction and the NMO input spectra have similar shape but is shifted.

[4]DocDB-5929-v34

Evaluation of the rate of accidentals

$$R_{acc} = R_p \cdot R_d \cdot \Delta T_{p-d}$$

(ΔT_{p-d} → 1 ms)

- First we evaluated an upper limit for accidental, considering both $\mathbf{R_p = R_d = R_{int+ext}}$, where

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⇩

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scaling factor from MC

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$R_{acc,\ upper} = 0.5184$ Hz

scaling factor from MC

~1.76×10^{-5}

$R_{acc} = 0.78$/day

Agreement with the current value of 0.8/day

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Analysis Workflow

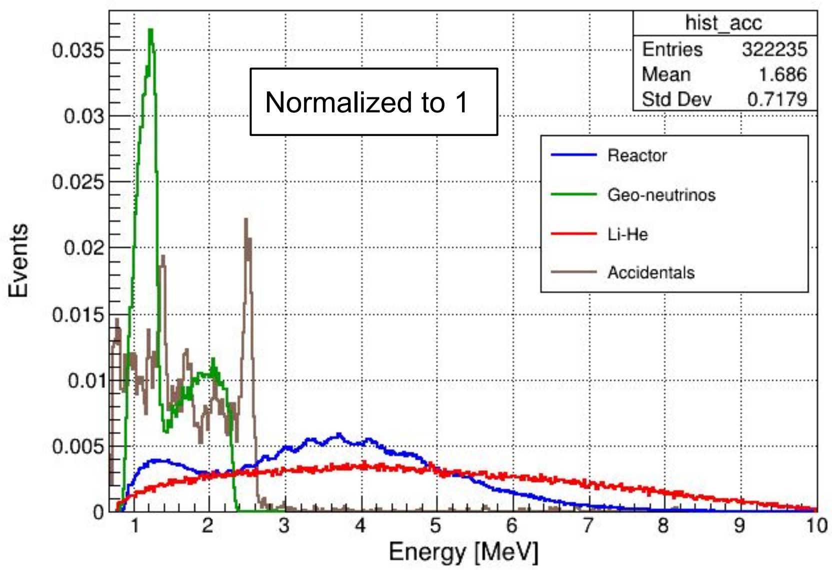
1 Massive MC simulations (SNiPER)

2 Reference shapes production (PDF)

3 Toy data sampling (Fitter)

4 Fitting procedure (Fitter)

PDFs we generated



Analysis Workflow

1 — Massive MC simulations (SNiPER)

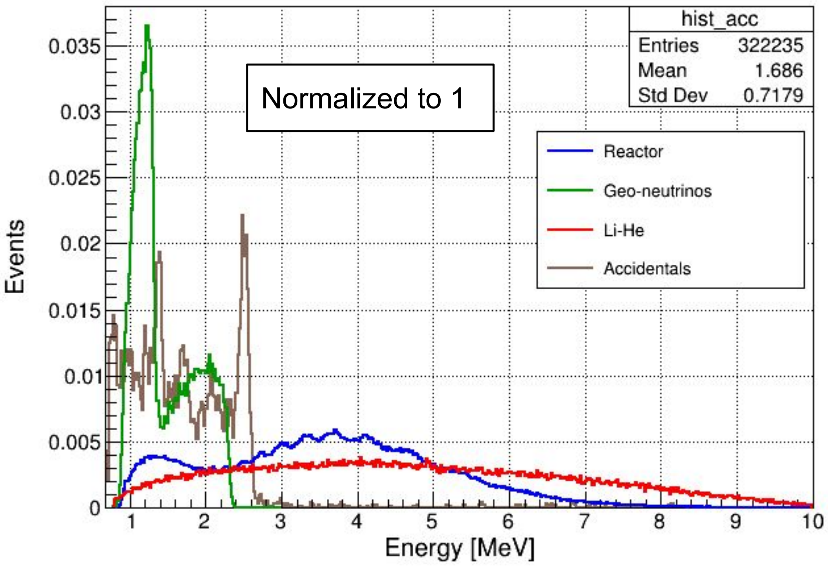
2 — Reference shapes production (PDF)

3 — Toy data sampling (Fitter)

4 — Fitting procedure (Fitter)

The pdfs of the rest of the bkgs are taken from the common inputs root file (JUNOInputs2022_01_06.root)[4]

PDFs we generated



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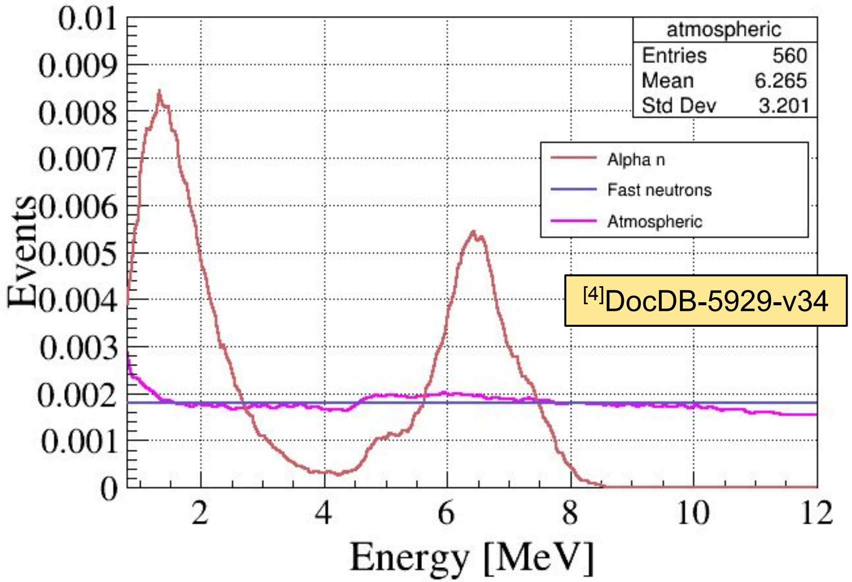
PDFs from NMO input file



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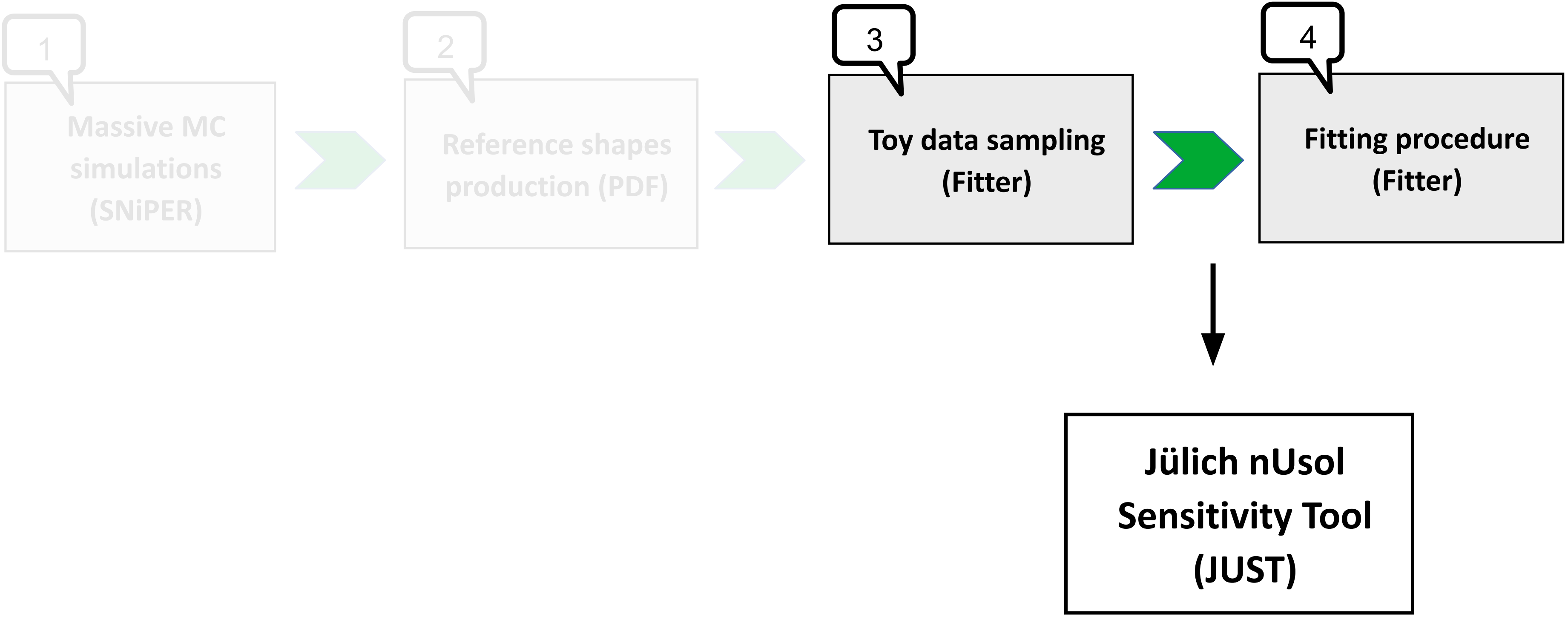
Analysis Workflow



4. Geoneutrinos sensitivity studies

JUST fitter configurations

- General config:

- Fitting range: 0.8 - 12 MeV
- Bin Width: 0.02 MeV
- Exposure fraction: 0.916 (after veto)
- IBD efficiency: 82.2%
- FV Mass: 18.31 kton
- Time: 1 year
- No. of fits: 10k

- Species: $^{9}Li/^{8}He$ (constraint 20%), Acc. (constraint 1%), Fast-n (constraint 100%), Alpha-n (constraint 50%), Atm. neutrinos (constraint 50%).

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Species	Events/day/kton	Uncertainty (%)
Reactors	3.4093	-
Geo-neutrinos	0.0870	-
$^{9}Li/^{8}He$	0.0477	20
Accidentals	0.0477	1
Alpha-n	0.0030	50
Fast-n	0.0060	100
Atm. neutrinos	0.0095	50

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✓ new PDFs from full MC simulations

✓ newly calculated event rate

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✓ Reactors	3.4093	-
✓ Geo-neutrinos	0.0870	-
✓ ^{9}Li/^{8}He	0.0477	20
✓ Accidentals	✓ 0.0426	1
Alpha-n	0.0030	50
Fast-n	0.0060	100
Atm. neutrinos	0.0095	50

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Fit results:

	Median of error/rate distbn.	**Sigma left**	**Sigma right**
Case 1 (old PDFs w/o updated energy correction)	14.00	1.63	2.11
Case 2 (old PDFs w/ updated energy correction)	14.02	1.63	2.10
Case 3 (new Li-He PDF w/ energy correction)	14.02	1.64	2.07
Case 4 (new Acc. PDF w/ energy correction)	13.96	1.58	2.17
Case 5 (new Li-He + Acc. PDF w/ energy correction)	13.97	1.58	2.16

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Conclusions and outlook

- ✔ Updated the energy correction for the reco. bias from the new 2D plot.
- ✔ New PDFs from the full MC simulations of Accidentals (using MDC data) & Li-He, and are used in template fits.

- New shapes do not change the results of the the Geoneutrino sensitivity of 1 year, but the effect on NMO should be checked.
- Study of the background from the correlated Bi-Po events planned.
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Conclusions and outlook

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Thank you !!!

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Backup slides

Step 1: the pre-mixed radioactivity dataset

Where do the rates come from?

Dataset Name	Rates (used in elecsim)
Muon	28.2 Hz
U238@LS	3.234 Hz
Th232@LS	0.733 Hz
K40@LS	0.53 Hz
Pb210@LS	17.04 Hz
C14@LS	3.3e4 Hz
Kr85@LS	1.163 Hz
U238@Acrylic	98.41 Hz
Th232@Acrylic	22.29 Hz
K40@Acrylic	161.25 Hz
U238@node/bar	2102.36 Hz
Th232@node/bar	1428.57 Hz
K40@node/bar	344.5 Hz
Co60@node/bar	97.5 Hz
U238@PMTGlass	4.90e6 Hz
Th232@PMTGlass	8.64e5 Hz
K40@PMTGlass	4.44e5 Hz
Tl208@PMTGlass	1.39e5 Hz
Co60@Truss	? Hz
Tl208@Truss	? Hz
Rn222@WaterRadon	90 Hz

We compared them with the **JUNO radioactivity paper***. Starting from the **concentrations in ppb** (from Table 4 of the paper):

Material	Mass	Target impurity concentration					Singles	
	[t]	^{238}U [ppb]	^{232}Th [ppb]	^{40}K [ppb]	^{210}Pb [ppb]	^{60}Co [mBq/kg]	DV [Hz]	FV [Hz]
LS-reactor	20000	10^{-6}	10^{-6}	10^{-7}	10^{-13}		2.5	2.2
Acrylic	610	10^{-3}	10^{-3}	10^{-3}			8.4	0.4
SS structure	1000 65	1 0.2	3 0.6	0.2 0.02		20 1.5	15.9	1.1
PMT glass	33.5 100.5 2.6	400 200 400	400 120 400	40 4 200			26.2	2.8
PMT readout	125 16.3	68 93	194 243	5 12		16 14	3.4	0.4
Other							2.5	0.3
Sum							59	7.2

Table 4: Final background budget for the main materials used in the JUNO detector with reconstructed energy E_{rec} larger than 0.7 MeV. The expected count rates are given both in the full DV ($r_{LS} = 17.7$ m) and in the default FV ($r_{LS} = 17.2$ m). The "Other" components include all materials that have relatively smaller contribution to the background (compare with Table 3), such as the calibration parts, the LPMT cover, the rock, and the radon in water. These results include energy resolution, optical propagation, charge reconstruction, and non-uniformity corrections.

*https://arxiv.org/abs/2107.03669

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We calculate the rates as:

$$R[Hz]=\frac{c[g/g]\cdot N_A[1/mol]}{\tau[s]\cdot M[g/mol]}\cdot Material\,mass[g]$$

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Step 1: the pre-mixed radioactivity dataset

Results

Radioactivity paper							MDC table
Isotope	c [ppb]	c [g/g]	Half life [y]	Mean lifetime [s]	Molar mass [g/mol]	R [Hz]	R [Hz]
238U @ LS	1.00E-06	1.00E-15	4.47E+09	2.03E+17	238.0507882	3.234	3.234
232Th @ LS	1.00E-06	1.00E-15	1.41E+10	6.39E+17	232.0380553	0.731	0.733
40K @ LS	1.00E-07	1.00E-16	1.25E+09	5.69E+16	39.96399817	0.530	0.53
210Pb @ LS	1.00E-13	1.00E-22	2.23E+01	1.01E+09	209.9841885	16.960	17.04

Liquid scintillator

Radioactivity paper							MDC table
Isotope	c [ppb]	c [g/g]	Half life [y]	Mean lifetime [s]	Molar mass [g/mol]	R [Hz]	R [Hz]
238U @ acrylic	1.00E-03	1.00E-12	4.47E+09	2.03E+17	238.0507882	98.643	98.41
232Th @ acrylic	1.00E-03	1.00E-12	1.41E+10	6.39E+17	232.0380553	22.290	22.29
40K @ acrylic	1.00E-03	1.00E-12	1.25E+09	5.69E+16	39.96399817	161.500	161.25

Acrylic vessel

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232Th @ SS structure	6.00E-01	6.00E-10	1.41E+10	6.39E+17	232.0380553	1,425.09	1428.57
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SS structure

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Step 1: the pre-mixed radioactivity dataset

Results

Very good agreement!

Liquid scintillator

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IBD Event Selection Strategy - Elecsim stage

Using the eventindex tree to align between MC and reconstructed events.

5 IBDs simulated becomes 10 elecsim events.

Elecsim ID (eventid.e) — Detsim ID (entries)

Row	Instance	eventid.e	nevents.n	tags	filenames	entries	nhits
0	0	0	1	default	./output/	0	4413
1	0	1	1	default	./output/	0	3668
2	0	2	1	default	./output/	1	3938
3	0	3	1	default	./output/	1	3704
4	0	4	1	default	./output/	2	4314
5	0	5	1	default	./output/	2	3634
6	0	6	1	default	./output/	3	12334
7	0	7	1	default	./output/	3	3954
8	0	8	1	default	./output/	4	5319
9	0	9	1	default	./output/	4	3612
10	0	10	1	default	./output/	5	7062
11	0	11	1	default	./output/	5	3781
12	0	12	1	default	./output/	6	3437

1) The prompt and delayed are triggered in 2 separate readouts at elecsim stage.

2) The prompt is always the first entry and the corresponding delayed is the next entry.

→ Events with 2 readouts gets selected.

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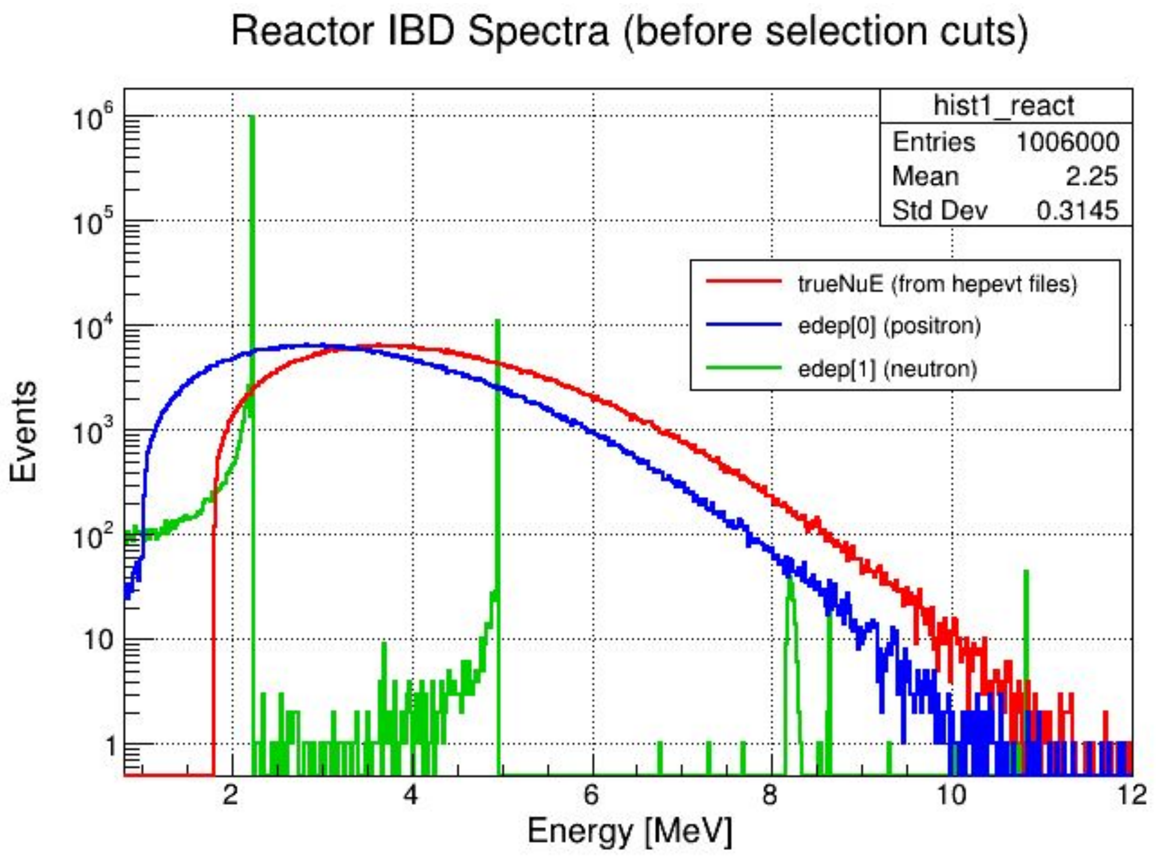
Reactor IBD MC Simulation Spectra



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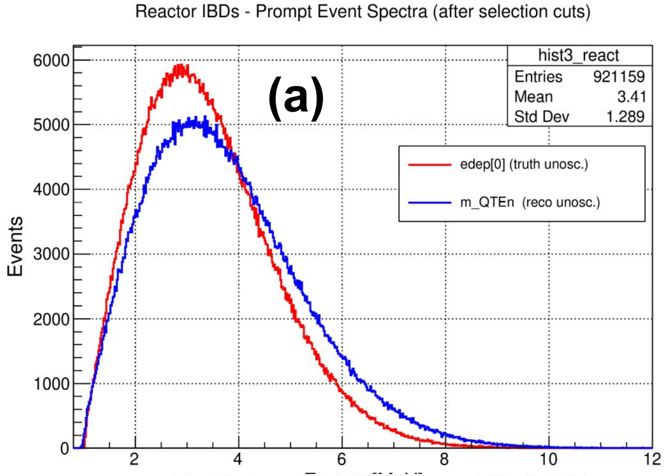
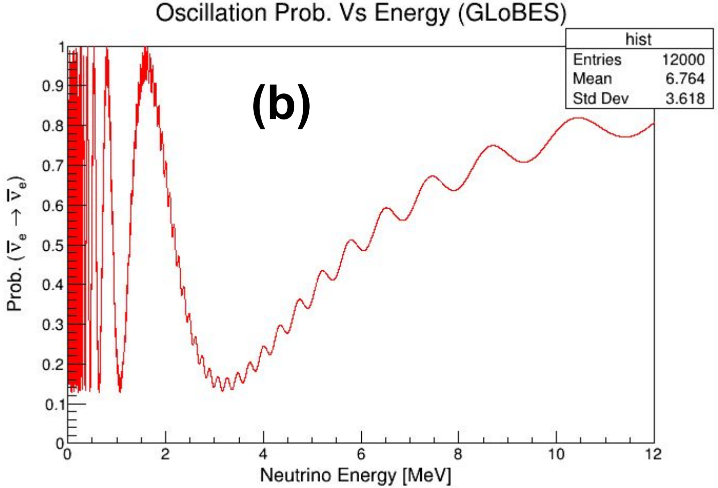
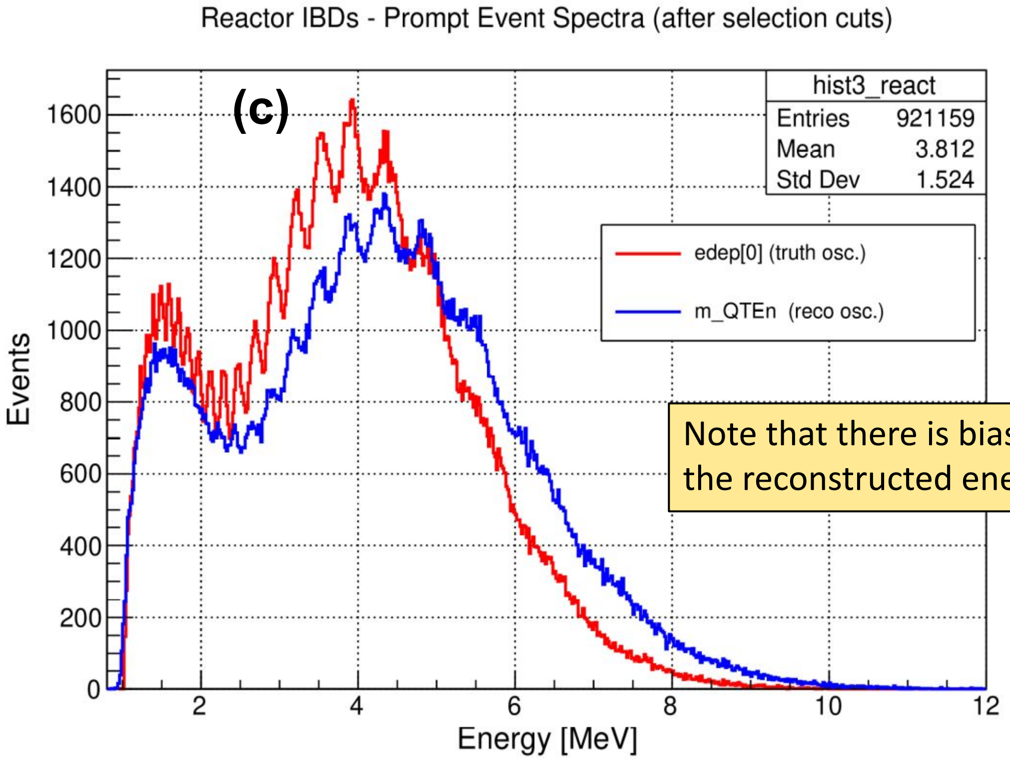
Incorporating Oscillations





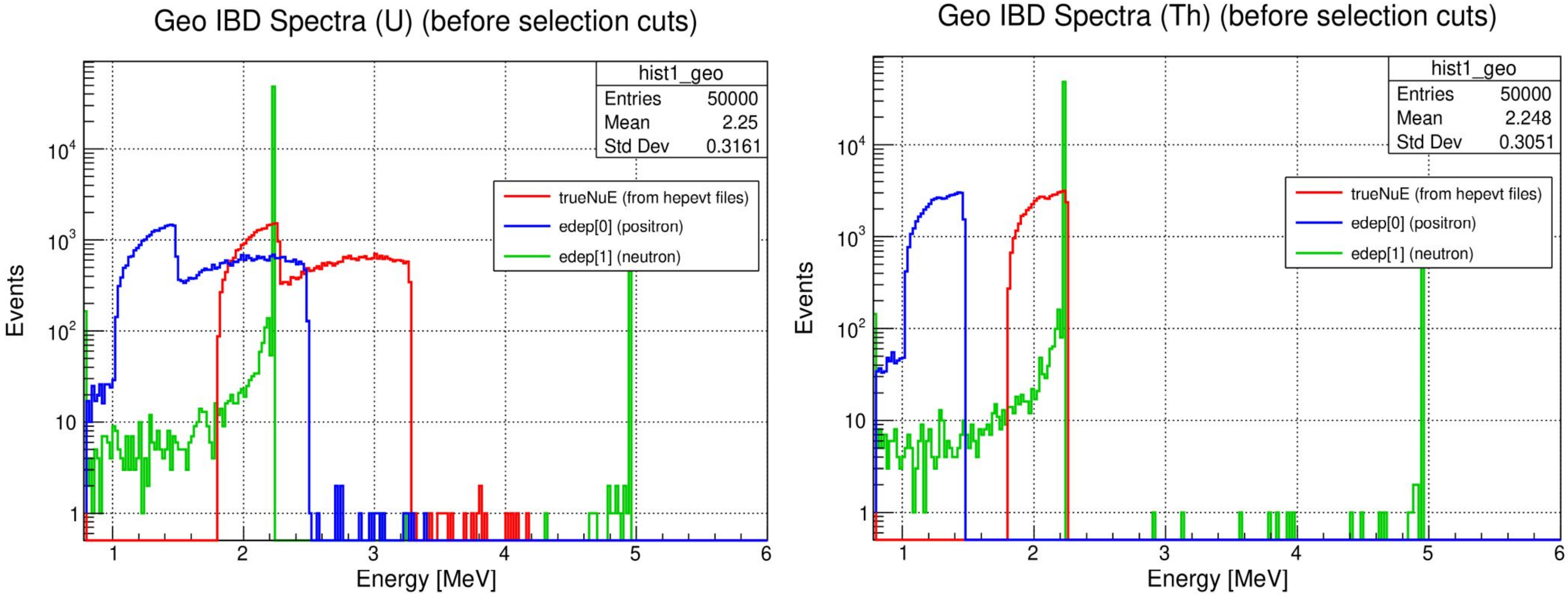


Note that there is bias for the reconstructed energy

The oscillated spectra **(c)** is obtained by weighing the unoscillated event spectra **(a)** with Pee calculated using GLoBES[2] **(b)**.

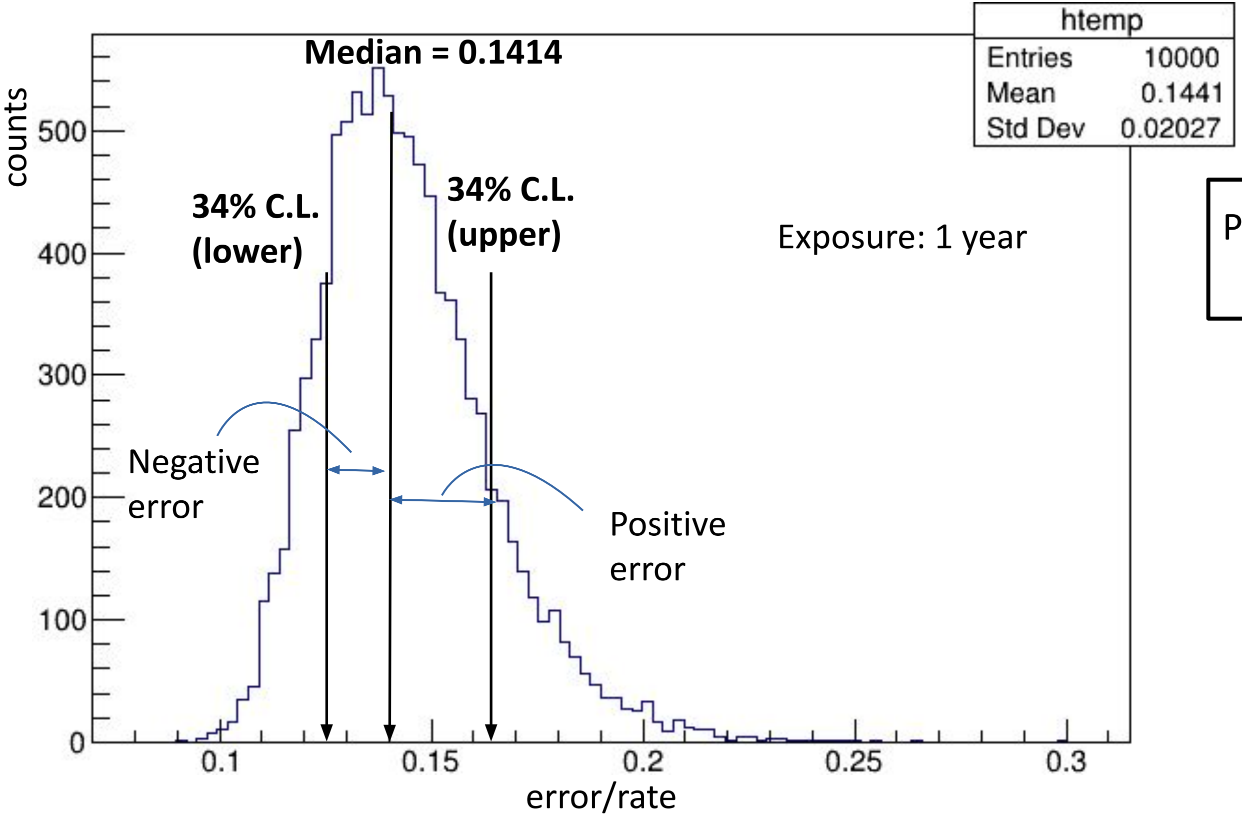
[2] Comput.Phys.Commun. 167 (2005) 195

Geoneutrino IBD MC Simulation Spectra



Calculation of precision

The ratio of the fitted errors and the fitted rates for Geo-neutrinos are histogrammed for a definite binning.



Precision = median of error / rate distribution

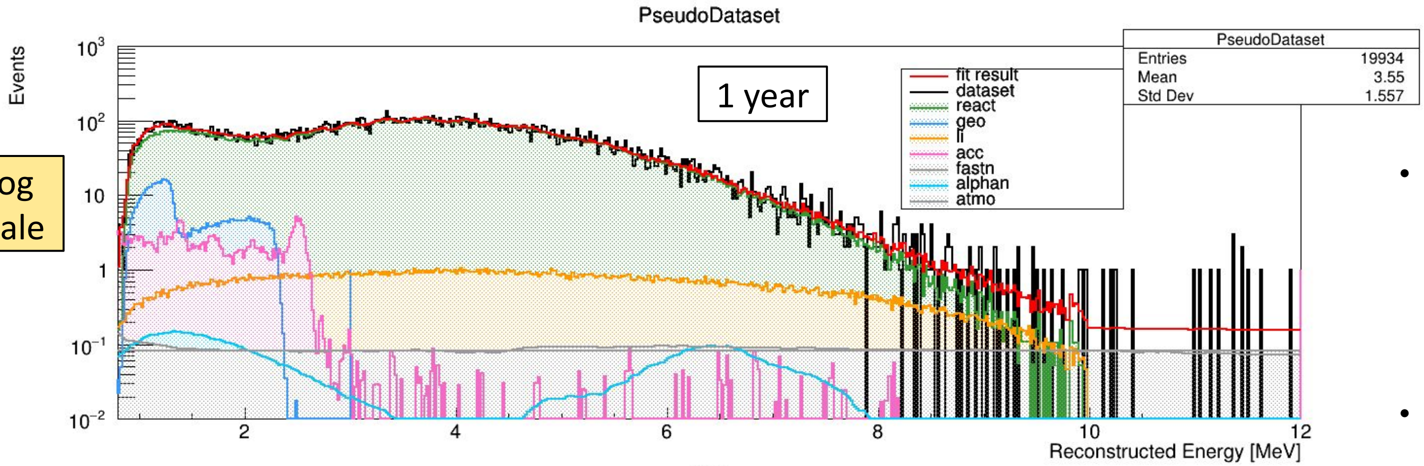
Calculation of Errors:

Negative error = |Median – 34% C.L. (lower)|

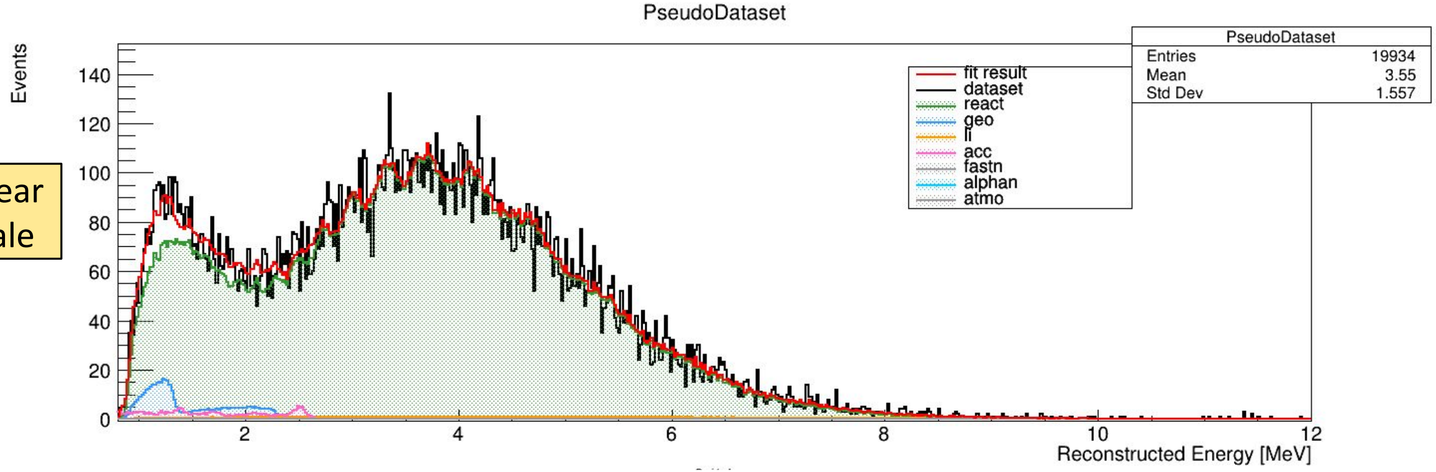
Positive error = |Median – 34% C.L. (upper)|

Case (5): Latest full MC PDFs of Reactor, Geo-neutrinos, Li-He & Accidentals

Log scale



Linear scale



- Fitted spectrum at the best fit point for one of the 10k fits for 1 year of exposure.
- The fit matches well with the MC expectation.

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Step 1: the pre-mixed radioactivity dataset

What we found:

- For each radioactive isotope, the time simulated is actually different. For example;
    - U238@LS: ~89 hours
    - C14@LS: ~8.4 hours
    - K40@LS: ~524 hours
- The external bkg **number of events** actually simulated is larger because at least 1 hour needed to be generated for the pre-mixing.

Step 1: the pre-mixed radioactivity dataset

The “bucket theory”

- Starting from the **single detsim files** of each isotope, some of them are merged.
- How many of them are **merged**? The minimum amount of number such to create a file corresponding to at least 1 hour
- Finally, the **pre-mixed dataset** is built (at the detsim level), by extracting for each isotope in the merge folder a number of events corresponding to **1 hour of data-taking**

After having understood the structure, we run all the 3600 pre-mixed detsim files until the reco stage

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