

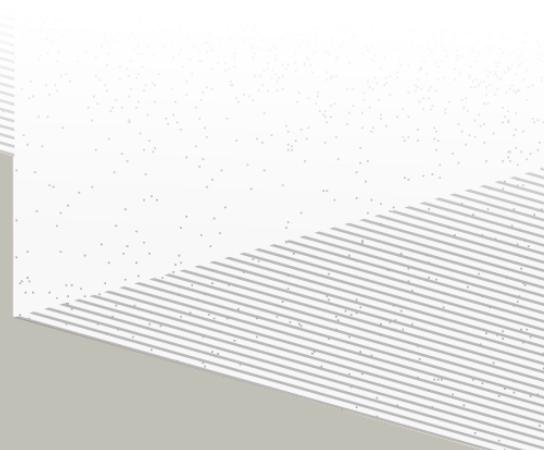
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Par

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**Precision measurement of solar neutrino oscillation parameters
with the JUNO small PMTs system and test of the unitarity of the
PMNS matrix**

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⁹⁰ **Remerciements**

⁹¹ Introduction

⁹² **Chapter 1**

⁹³ **Neutrino physics**

⁹⁴

The neutrino, or ν for the close friends, a fascinating and invisible particle. Some will say that dark matter also have those property but at least we are pretty confident that neutrinos exists.

⁹⁵ **1.1 Standard model**

⁹⁶ **1.1.1 Limits of the standard model**

⁹⁷ **1.2 Historic of the neutrino**

⁹⁸ **First theories**

⁹⁹ **Discovery**

¹⁰⁰ **Milestones and anomalies**

¹⁰¹ **1.3 Oscillation**

¹⁰² **1.3.1 Phenomologies**

¹⁰³ **1.4 Open questions**

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¹⁰⁴ **Chapter 2**

¹⁰⁵ **The JUNO experiment**

¹⁰⁶ "Ave Juno, rosae rosam, et spiritus rex". It means nothing but I found it in tone.

¹⁰⁷ The first idea of a medium baseline (~ 52 km) experiment, was explored in 2008 [1] where it was
¹⁰⁸ demonstrated that the Neutrino Mass Ordering (NMO) could be determined by a medium baseline
¹⁰⁹ experiment if $\sin^2(2\theta_{13}) > 0.005$ without the requirements of accurate knowledge of the reactor
¹¹⁰ antineutrino spectra and the value of Δm_{32}^2 . From this idea is born the Jiangmen Underground
¹¹¹ Neutrino Observatory (JUNO) experiment.

¹¹² JUNO is a neutrino detection experiment under construction located in China, in Guangdong prov-
¹¹³ ing, near the city of Kaiping. Its main objectives are the determination of the mass ordering at the
¹¹⁴ $3\text{-}4\sigma$ level in 6 years of data taking and the measurement at the sub-percent precision of the oscillation
¹¹⁵ parameters Δm_{21}^2 , $\sin^2 \theta_{12}$, Δm_{32}^2 and with less precision $\sin^2 \theta_{13}$ [2].



FIGURE 2.1 – On the left: Location of the JUNO experiment and its reactor sources in southern China. On the right: Aerial view of the experimental site

¹¹⁶ For this JUNO will measure the electronic anti-neutrinos ($\bar{\nu}_e$) flux coming from the nuclear reactors
¹¹⁷ of Taishan, Yangjiang, for a total power of 26.6 GW_{th} , and the Daya Bay power plant to a lesser
¹¹⁸ extent. All of those cores are the second-generation pressurized water reactors CPR1000, which is a
¹¹⁹ derivative of Framatome M310. Details about the power plants characteristics and their expected flux
¹²⁰ of $\bar{\nu}_e$ can be found in the table 2.1. The distance of 53 km has been specifically chosen to maximize
¹²¹ the disappearance probability of the $\bar{\nu}_e$. The data taking is scheduled to start early 2025.

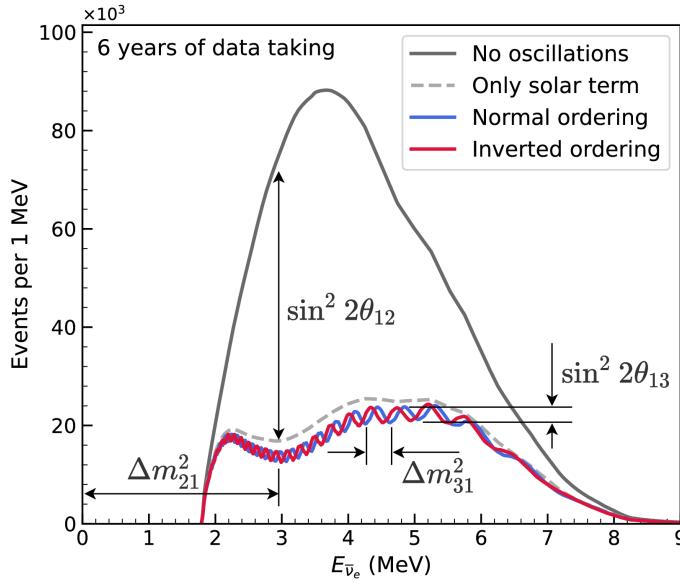


FIGURE 2.2 – Expected number of neutrinos event per MeV in JUNO after 6 years of data taking. The black curve shows the flux if there was no oscillation. The light gray curve shows the oscillation if only the solar terms are taken in account (θ_{12} , Δm_{21}^2). The blue and red curve shows the spectrum in the case of, respectively, NO and IO. The dependency of the oscillation to the different parameters are schematized by the double sided arrows. We can see the NMO sensitivity by looking at the fine phase shift between the red and blue curve.

¹²² 2.1 Neutrinos physics in JUNO

¹²³ Even if the JUNO design detailed in section 2.2 was optimized for the measurement of the NMO, its
¹²⁴ large detection volume, excellent energy resolution and background level and understanding make it
¹²⁵ also an excellent detector to measure the flux coming from other neutrino sources. Thus the scientific
¹²⁶ program of JUNO extends way over reactor antineutrinos. The following section is an overview of
¹²⁷ the different physics topic JUNO will contribute in the coming years.

¹²⁸ 2.1.1 Reactor neutrino oscillation for NMO and precise measurements

Previous works [1, 3] shows that oscillation parameters and the NMO can be observed by looking at the $\bar{\nu}_e$ disappearance energy spectrum coming from medium baseline nuclear reactor. This disappearance probability can be expressed as [2] :

$$P(\bar{\nu}_e \rightarrow \bar{\nu}_e) = 1 - \sin^2 2\theta_{12} c_{13}^4 \sin^2 \frac{\Delta m_{21}^2 L}{4E} - \sin^2 2\theta_{13} \left[c_{12}^2 \sin^2 \frac{\Delta m_{31}^2 L}{4E} + s_{12}^2 \sin^2 \frac{\Delta m_{32}^2 L}{4E} \right]$$

¹²⁹ Where $s_{ij} = \sin \theta_{ij}$, $c_{ij} = \cos \theta_{ij}$, E is the $\bar{\nu}_e$ energy and L is the baseline. We can see the sensitivity
¹³⁰ to the NMO in the dependency to Δm_{32}^2 and Δm_{31}^2 causing a phase shift of the spectrum as we can
¹³¹ see in the figure 2.2. By carefully adjusting a theoretical spectrum to the data, one can extract the
¹³² NMO and the oscillation parameters. The statistic procedure used to adjust the theoretical spectrum
¹³³ is reviewed in more details in the section 2.7. To reach the desired sensitivity, JUNO must meet
¹³⁴ multiple requirements but most notably:

- 135 1. An energy resolution of $3\%/\sqrt{E(\text{MeV})}$ to be able to distinguish the fine structure of the fast
 136 oscillation.
- 137 2. An energy precision of 1% in order to not err on the location of the oscillation pattern.
- 138 3. A baseline between 40 and 65 km to maximise the $\bar{\nu}_e$ oscillation probability. The optimal
 139 baseline would be 58 km and JUNO baseline is 53 km.
- 140 4. At least $\approx 100,000$ events to limit the spectrum distortion due to statistical uncertainties.

141 $\bar{\nu}_e$ flux coming from nuclear power plants

142 To get such high measurements precision, it is necessary to have a very good understanding of the
 143 sources characteristics. For its NMO and precise measurement studies, JUNO will observe the energy
 144 spectrum of neutrinos coming from the nuclear power plants Taishan and Yangjiang's cores, located
 145 at 53 km of the detector to maximise the disappearance probability of the $\bar{\nu}_e$.

Reactor	Power (GW _{th})	Baseline (km)	IBD Rate (day ⁻¹)	Relative Flux (%)
Taishan	9.2	52.71	15.1	32.1
Core 1	4.6	52.77	7.5	16.0
Core 2	4.6	52.64	7.6	16.1
Yangjiang	17.4	52.46	29.0	61.5
Core 1	2.9	52.74	4.8	10.1
Core 2	2.9	52.82	4.7	10.1
Core 3	2.9	52.41	4.8	10.3
Core 4	2.9	52.49	4.8	10.2
Core 5	2.9	52.11	4.9	10.4
Core 6	2.9	52.19	4.9	10.4
Daya Bay	17.4	215	3.0	6.4

TABLE 2.1 – Characteristics of the nuclear power plants observed by JUNO. The IBD rate are estimated from the baselines, the reactors full thermal power, selection efficiency and the current knowledge of the oscillation parameters

146 The $\bar{\nu}_e$ coming from reactors are emitted from β -decay of unstable fission fragments. The Taishan
 147 and Yangjiang reactors are Pressurised Water Reactor (PWR), the same type as Daya Bay. In those
 148 type of reactor more the 99.7 % and $\bar{\nu}_e$ are produced by the fissions of four fuel isotopes ^{235}U , ^{238}U ,
 149 ^{239}Pu and ^{241}Pu . The neutrino flux per fission of each isotope is determined by the inversion of the
 150 measured β spectra of fission product [4–8] or by calculation using the nuclear databases [9, 10].

151 The neutrino flux coming from a reactor at a time t can be predicted using

$$\phi(E_\nu, t)_r = \frac{W_{th}(t)}{\sum_i f_i(t) e_i} \sum_i f_i(t) S_i(E_\nu) \quad (2.1)$$

152 where $W_{th}(t)$ is the thermal power of the reactor, $f_i(t)$ is the fraction fission of the i th isotope, e_i its
 153 thermal energy released in each fission and $S_i(e_\nu)$ the neutrino flux per fission for this isotope. Using
 154 this method, the flux uncertainty is expected to be of an order of 2-3 % [11].

155 In addition to those prediction, a satellite experiment named TAO[12] will be setup near the reactor
 156 core Taishan-1 to measure with an energy resolution of 2% at 1 MeV the neutrino flux coming from
 157 the core, more details can be found in section 2.4.1. It will help identifying unknown fine structure
 158 and give more insight on the $\bar{\nu}_e$ flux coming from this reactor.

159 One the open issue about reactor anti-neutrinos flux is the so-called neutrino anomaly [13], an
 160 unexpected surplus of neutrino emission in the spectra around 5 MeV. Multiples scientists are trying

161 to explain this surplus by advanced recalculation of the nuclei model during beta decay [14, 15] but
 162 no consensus on this issue has been reached yet.

163 **Background in the neutrinos reactor spectrum**

164 Considering the close reactor neutrinos flux as the main signal, the signals that are considered as
 165 background are:

- 166 — The geoneutrinos producing background in the $0.511 \sim 2.7$ MeV region.
- 167 — The neutrinos coming from the other nuclear reactors around Earth.

168 In addition to all those physics signal, non-neutrinos signal that would mimic an IBD will also be
 169 present. It is composed of:

- 170 — The signal coming from radioactive decay (α , γ , β) from natural radioactive isotopes in the
 material of the detector.
- 172 — Cosmogenic event such as fast neutrons and activated isotopes induced by muons passing
 through the detector, most notably the spallation on ^{12}C .

174 All those events represent a non-negligable part of the spectrum as shown in figure 2.3.

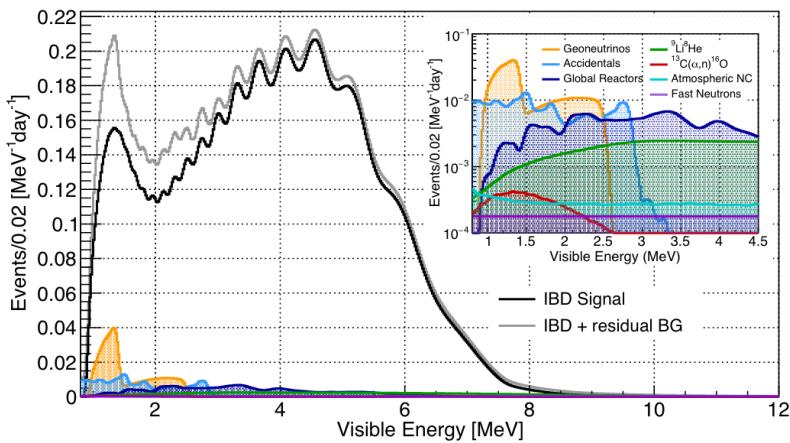


FIGURE 2.3 – Expected visible energy spectrum measured with the LPMT system with (grey) and without (black) backgrounds. The background amount for about 7% of the IBD candidate and are mostly localized below 3 MeV [11]

175 **Identification of the mass ordering**

176 To identify the mass ordering, we adjust the theoretical neutrino energy spectrum under the two
 177 hypothesis of NO and IO. Those give us two χ^2 , respectively χ^2_{NO} and χ^2_{IO} . By computing the
 178 difference $\Delta\chi^2 = \chi^2_{NO} - \chi^2_{IO}$ we can determine the most probable mass ordering and the confidence
 179 interval: NO if $\Delta\chi^2 > 0$ and IO if $\Delta\chi^2 < 0$. Current studies shows that the expected sensitivity
 180 the mass ordering would be of 3.4σ after 6 years of data taking in nominal setup[2]. More detailed
 181 explanations about the procedure can be found in the section 2.7.

182 **Precise measurement of the oscillations parameters**

183 The oscillations parameters θ_{12} , θ_{13} , Δm_{21}^2 , Δm_{31}^2 are free parameters in the fit of the oscillation
 184 spectrum. The precision on those parameters have been estimated and are shown in table 2.2. Wee
 185 see that for θ_{12} , Δm_{21}^2 , Δm_{31}^2 , precision at 6 years is better than the reference precision by an order of
 186 magnitude [11]

	Central Value	PDG 2020	100 days	6 years	20 years
$\Delta m_{31}^2 (\times 10^{-3} \text{ eV}^2)$	2.5283	± 0.034 (1.3%)	± 0.021 (0.8%)	± 0.0047 (0.2%)	± 0.0029 (0.1%)
$\Delta m_{21}^2 (\times 10^{-3} \text{ eV}^2)$	7.53	± 0.18 (2.4%)	± 0.074 (1.0%)	± 0.024 (0.3%)	± 0.017 (0.2%)
$\sin^2 \theta_{12}$	0.307	± 0.013 (4.2%)	± 0.0058 (1.9%)	± 0.0016 (0.5%)	± 0.0010 (0.3%)
$\sin^2 \theta_{13}$	0.0218	± 0.0007 (3.2%)	± 0.010 (47.9%)	± 0.0026 (12.1%)	± 0.0016 (7.3%)

TABLE 2.2 – A summary of precision levels for the oscillation parameters. The reference value (PDG 2020 [16]) is compared with 100 days, 6 years and 20 years of JUNO data taking.

2.1.2 Other physics

While the design of JUNO is tailored to measure $\bar{\nu}_e$ coming from nuclear reactor, JUNO will be able to detect neutrinos coming from other sources thus allowing for a wide range of physics studies as detailed in the table 2.3 and in the following sub-sections.

Research	Expected signal	Energy region	Major backgrounds
Reactor antineutrino	60 IBDs/day	0–12 MeV	Radioactivity, cosmic muon
Supernova burst	5000 IBDs at 10 kpc	0–80 MeV	Negligible
DSNB (w/o PSD)	2300 elastic scattering		
Solar neutrino	2–4 IBDs/year	10–40 MeV	Atmospheric ν
Atmospheric neutrino	hundreds per year for ${}^8\text{B}$	0–16 MeV	Radioactivity
Geoneutrino	hundreds per year	0.1–100 GeV	Negligible
	≈ 400 per year	0–3 MeV	Reactor ν

TABLE 2.3 – Detectable neutrino signal in JUNO and the expected signal rates and major background sources

Geoneutrinos

Geoneutrinos designate the antineutrinos coming from the decay of long-lived radioactive elements inside the Earth. The 1.8 MeV threshold necessary for the IBD makes it possible to measure geoneutrinos from ${}^{238}\text{U}$ and ${}^{232}\text{Th}$ decay chains. The studies of geoneutrinos can help refine the Earth crust models but is also necessary to characterise their signal, as they are a background to the mass ordering and oscillations parameters studies.

Atmospheric neutrinos

Atmospheric neutrinos are neutrinos originating from the decay of π and K particles that are produced in extensive air showers initiated by the interactions of cosmic rays with the Earth atmosphere. Earth is mostly transparent to neutrinos below the PeV energy, thus JUNO will be able to see neutrinos coming from all directions. Their baseline range is large (15km \sim 13000km), they can have energy between 0.1 GeV and 10 TeV and will contain all neutrino and antineutrinos flavour. Their studies is complementary to the reactor antineutrinos and can help refine the constraints on the NMO [2].

Supernovae burst neutrinos

Neutrinos are crucial component during all stages of stellar collapse and explosion. Detection of neutrinos coming for core collapse supernovae will provide us important informations on the mech-

208 anisms at play in those events. Thanks to its 20 kt sensible volume, JUNO has excellent capabilities
 209 to detect all flavour of the $\mathcal{O}(10 \text{ MeV})$ postshock neutrinos, and using neutrinos of the $\mathcal{O}(1 \text{ MeV})$
 210 will give informations about the pre-supernovae neutrinos. All those informations will allow to
 211 disentangle between the multiple hydro-dynamic models that are currently used to describe the
 212 different stage of core-collapse supernovae.

213 Diffuse supernovae neutrinos background

214 Core-collapse supernovae in our galaxy are rare events, but they frequently occur throughout the
 215 visible Universe sending burst of neutrinos in direction of the Earth. All those events contributes to
 216 a low background flux of low-energy neutrinos called the Diffuse Supernovae Neutrino Background
 217 (DSNB). Its flux and spectrum contains informations about the red-shift dependent supernovae rate,
 218 the average supernovae neutrino energy and the fraction of black-hole formation in core-collapse su-
 219 pernovae. Depending of the DSNB model, we can expect 2-4 IBD events per year in the energy range
 220 above the reactor $\bar{\nu}_e$ signal, which is competitive with the current Super-Kamiokande+Gadolinium
 221 phase [17].

222 Beyond standard model neutrinos interactions

223 JUNO will also be able to probe for beyond standard model neutrinos interactions. After the main
 224 physics topics have been accomplished, JUNO could be upgraded to probe for neutrinoless beta
 225 decay ($0\nu\beta\beta$). The detection of such event would give critical informations about the nature of
 226 neutrinos, is it a majorana or a dirac particle. JUNO will also be able to probe for neutrinos that
 227 would come for the decay or annihilation of Dark Matter inside the sun and neutrinos from putative
 228 primordial black hole. Through the unitary test of the mixing matrix, JUNO will be able to search for
 229 light sterile neutrinos. Thanks to JUNO sensitivity, multiple other exotic research can be performed
 230 on neutrino related beyond standard model interactions.

231 Proton decay

232 Proton decay is a potential unobserved event where the proton decay by violating the baryon num-
 233 ber. This violation is necessary to explain the baryon asymmetry in the universe and is predicted
 234 by multiple Grand Unified Theories which unify the strong, weak and electromagnetic interactions.
 235 Thanks to its large active volume, JUNO will be able to take measurement of the potential proton
 236 decay channel $p \rightarrow \bar{\nu}K^+$. Study [18] show that JUNO should be competitive with the current best
 237 limit at 5.9×10^{33} years from Super-K. This studies show that JUNO, considering no proton decay
 238 events observed, would be able to rules a limit of 9.6×10^{33} years at 90 % C.L.

239 2.2 The JUNO detector

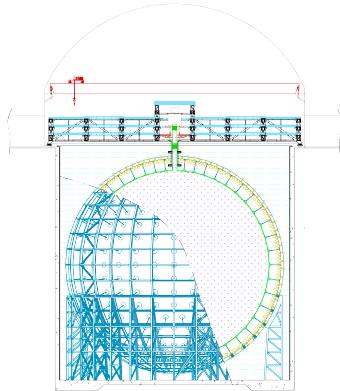
240 The JUNO detector is a scintillator detector buried 693.35 meters under the ground (1800 meters
 241 water equivalent). It consist of Central Detector (CD), a water pool and a Top Tracker (TT) as showed
 242 in figure 2.4a. The CD is an acrylic vessel containing the 20 ktons of Liquid Scintillator (LS). It is
 243 supported by a stainless steel structure and is immersed in that water pool that is used as shielding
 244 from external radiation and as a cherenkov detector for the background. The top of the experiment
 245 is partially covered by the Top Tracker (TT), a plastic scintillator detector which is use to detect the
 246 atmospheric muons background and is acting as a veto detector.

247 The top of the experiment also host the LS purification system, a water purification system, a ven-
 248 tilation system to get rid of the potential radon in the air. The CD is observed by two system of

249 Photo-Multipliers Tubes (PMT). They are attached to the steel structure and their electronic readout
 250 is submersed near them. A third system of PMT is also installed on the structure but are facing
 251 outward of the CD, instrumenting the water to be cherenkov detector. The CD and the cherenkov
 252 detector are optically separated by Tyvek sheet. A chimney for LS filling and purification and for
 253 calibration operations connects the CD to the experimental hall from the top.

254 The CD has been dimensioned to meet the requirements presented in section 2.1.1:

- 255 — Its 20 ktons monolithic LS provide a volume sizeable enough, in combination with the ex-
 256 pected $\bar{\nu}_e$ flux, to reach the desired statistic in 6 years. Its monolithic nature also allow for a
 257 full containment of most of the events, preventing the energy loss in non-instrumented parts
 258 that would arise from a segmented detector.
- 259 — Its large overburden shield it from most of the atmospheric background that would pollute
 260 the signal.
- 261 — The localization of the experiment, chosen to maximize the disappearance with a 53km base-
 262 line and in a region that allow two nuclear power plant to be used as sources.



(A) Schematics view of the JUNO detector.



(B) Top down view of the JUNO detector under construction

FIGURE 2.4

263 This section cover in details the different components of the detector and the detection systems.

264 2.2.1 Detection principle

The CD will detect the neutrino and measure their energy mainly via an Inverse Beta Decay (IBD) interaction with proton mainly from the ^{12}C and H nucleus in the LS:

$$\bar{\nu}_e + p \rightarrow n + e^+$$

265 Kinematics calculation shows that this interaction has an energy threshold for the $\bar{\nu}_e$ of $(m_n + m_e -$
 266 $m_p) \approx 1.806$ MeV [19]. This threshold make the experiment blind to very low energy neutrinos.
 267 The residual energy $E_\nu - 1.806$ MeV is be distributed as kinetic energy between the positron and the
 268 neutron. The energy of the emitted positron E_e is given by [19]

$$E_e = \frac{(E_\nu - \delta)(1 + \epsilon_\nu) + \epsilon_\nu \cos \theta \sqrt{(E_\nu - \delta)^2 + \kappa m_e^2}}{\kappa} \quad (2.2)$$

269 where $\kappa = (1 + \epsilon_\nu)^2 - \epsilon_\nu^2 \cos^2 \theta \approx 1$, $\epsilon_\nu = \frac{E_\nu}{m_p} \ll 1$ and $\delta = \frac{m_n^2 - m_p^2 - m_e^2}{2m_p} \ll 1$. We can see from this
 270 equation that the positron energy is strongly correlated to the neutrino energy.

271 The positron and the neutron will then propagate in the detection medium, the Liquid Scintillator
 272 (LS), loosing their kinetic energy by exciting the molecule of the LS (more details in section 2.2.2).
 273 Once stopped, the positron will annihilate with an electron from the medium producing two 511
 274 KeV gamma. Those gamma will themselves interact with the LS, exciting it before being absorbed
 275 by photoelectrical effect. The neutron will be captured by an hydrogen, emitting a 2.2 MeV gamma
 276 in the process. This gamma will also deposit its energy before being absorbed by the LS.

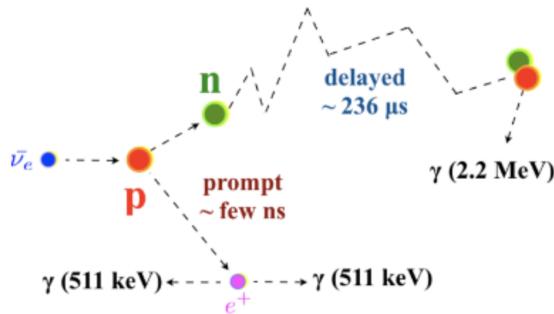


FIGURE 2.5 – Schematics of an IBD interaction in the central detector of JUNO

277 The scintillation photons have frequency in the UV and will propagate in the LS, being re-absorbed
 278 and re-emitted by compton effect before finally be captured by PMTs instrumenting the acrylic
 279 sphere. The analog signal of the PMTs digitized by the electronic is the signal of our experiment.
 280 The signal produced by the positron is subsequently called the prompt signal, and the signal coming
 281 from the neutron the delayed signal. This naming convention come from the fact that the positron
 282 will deposit its energy rather quickly (few ns) where the neutron will take a bit more time ($\sim 236 \mu s$).

283 2.2.2 Central Detector (CD)

284 The central detector, composed of 20 ktons of Liquid Scintillator (LS), is the main part of JUNO. The
 285 LS is contained in a spherical acrylic vessel supported by a stainless steel structure. The CD and
 286 its structural support are submerged in a cylindrical water pool of 43.5m diameter and 44m height.
 287 We're confident that the water pool provide sufficient buffer protection in every direction against the
 288 rock radioactivity.

289 Acrylic vessel

290 The acrylic vessel is a spherical vessel of inner diameter of 35.4 m and a thickness of 120 mm. It is
 291 assembled from 265 acrylic panels, thermo bonded together. The acrylic recipes has been carefully
 292 tuned with extensive R&D to ensure it does not include plasticizer and anti-UV material that would
 293 stop the scintillation photons. Those panels requires to be pure of radioactive materials to not
 294 cause background. Current setup where the acrylic panels are molded in cleanrooms of class 10000,
 295 let us reach a uranium and thorium contamination of <0.5 ppt. The molding and thermoforming
 296 processes is optimized to increase the assemblage transparency in water to >96%. The acrylic vessel
 297 is supported by a stainless steel structure via supporting node (fig 2.6). The structure and the nodes
 298 are designed to be resilient to natural catastrophic events such as earthquake and can support many
 299 times the effective load of the acrylic vessel.

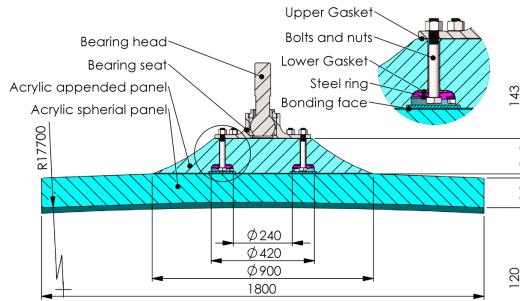


FIGURE 2.6 – Schematics of the supporting node for the acrylic vessel

300 **Liquid scintillator**

301 The Liquid Scintillator (LS) has a similar recipe as the one used in Daya Bay [20] but without gadolinium
 302 doping. It is made of three components, necessary to shift the wavelength of emitted photons to
 303 prevent their reabsorption and to shift their wavelength to the PMT sensitivity region as illustrated
 304 in figure 2.7:

- 305 1. The detection medium, the *linear alkylbenzene* (LAB). Selected because of its excellent trans-
 306 parency, high flash point, low chemical reactivity and good light yield. Accounting for \sim
 307 98% of the LS, it is the main component with which ionizing particles and gamma interact.
 308 Charged particles will collide with its electronic cloud transferring energy to the molecules,
 309 gamma will interact via compton effect with the electronic cloud before finally be absorbed
 310 via photoelectric effect.
- 311 2. The second component of the LS is the *2,5-diphenyloxazole* (PPO). A fraction of the excitation
 312 energy of the LAB is transferred to the PPO, mainly via non radiative process [21]. The
 313 PPO molecules de-excites in the same way, transferring their energy to the bis-MSB. The PPO
 314 makes for 1.5 % of the LS.
- 315 3. The last component is the *p-bis(o-methylstyryl)-benzene* (bis-MSB). Once excited by the PPO, it
 316 will emit photon with an average wavelength of \sim 430 nm (full spectrum in figure 2.7) that
 317 can thus be detected by our photo-multipliers systems. It amount for \sim 0.5% of the LS.

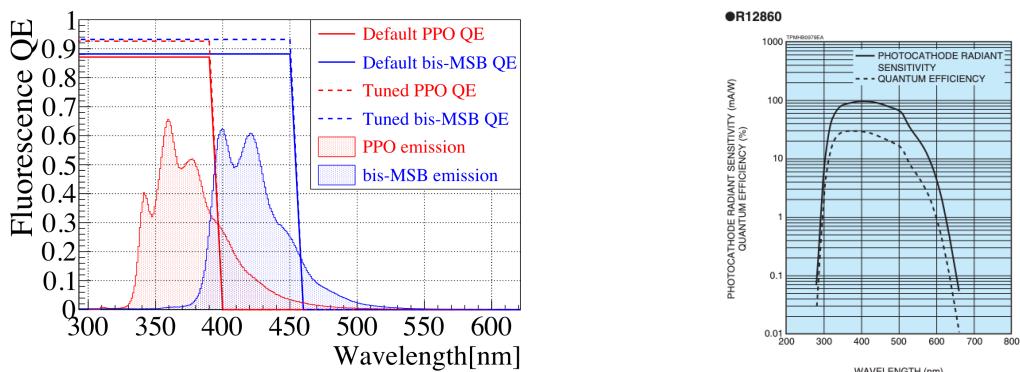


FIGURE 2.7 – On the left: Quantum efficiency (QE) and emission spectrum of the LAB and the bis-MSB [20]. On the right: Sensitivity of the Hamamatsu LPMT depending on the wavelength of the incident photons [22].

318 This formula has been optimized using dedicated studies with a Daya Bay detector [20, 23] to reach
 319 the requirements for the JUNO experiment:

- 320 — A light yield / MeV of the amount of 10^4 photons to maximize the statistic in the energy
 321 measurement.

- An attenuation length comparable to the size of the detector to prevent losing photons during their propagation in the LS. The final attenuation length is 25.8m [24] to compare with the CD diameter of 35.4m.
- Uranium/Thorium radiopurity to prevent background signal. The reactor neutrino program require a contamination fraction $F < 10^{-15}$ while the solar neutrino program require $F < 10^{-17}$.

The LS will frequently be purified and tested in the Online Scintillator Internal Radioactivity Investigation System (OSIRIS) [25] to ensure that the requirements are kept during the lifetime of the experiment, more details to be found in section 2.4.2.

331 Large Photo-Multipliers Tubes (LPMTs)

332 The scintillation light produced by the LS is then collected by Photo-Multipliers Tubes (PMT) that
 333 transform the incoming photon into an electric signal. As described in figure 2.8, the incident photons
 334 interact with the photocathode via photoelectric effect producing an electron called a Photo-Electron
 335 (PE). This PE is then focused on the dynodes where the high voltage will allow it to be multiplied.
 336 After multiple amplification the resulting charge - in coulomb [C] - is collected by the anode and
 337 the resulting electric signal can be digitalized by the readout electronics from which the charge and
 338 timing can be extracted.

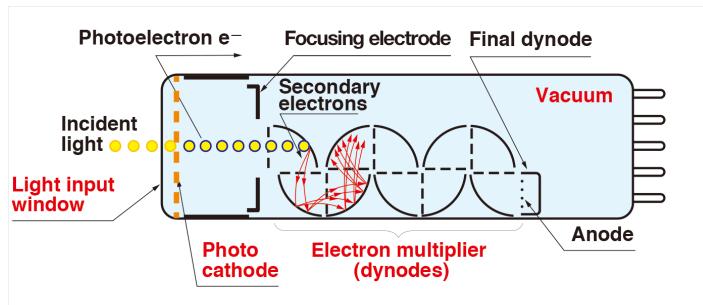


FIGURE 2.8 – Schematic of a PMT

339 The Large Photo-Multipliers Tubes (LPMT), used in the central detector and in the water pool, are
 340 20-inch (50.8 cm) radius PMTs. ~ 5000 dynode-PMTs [22] were produced by the Hamamatsu[®]
 341 company and ~ 15000 Micro-Channel Plate (MCP) [26] by the NNVT[®] company. This system is
 342 the one responsible for the energy measurement with a energy resolution of $3\%/\sqrt{E}$, resolution
 343 necessary for the mass ordering measurement. To reach this precision, the system is composed of
 344 17612 PMTs quasi uniformly distributed over the detector for a coverage of 75.2% reaching ~ 1800
 345 PE/MeV or $\sim 2.3\%$ resolution due to statistic, leaving $\sim 0.7\%$ for the systematic uncertainties. They
 346 are located outside the acrylic sphere in the water pool facing the center of the detector. To maintain
 347 the resolution over the lifetime of the experiment, JUNO require a failure rate $< 1\%$ over 6 years.

348 The LPMTs electronic are divided in two parts. One "near", located underwater, in proximity of the
 349 LPMT to reduce the cable length between the PMT and early electronic. A second one, outside of the
 350 detector that is responsible for higher level analysis before sending the data to the DAQ.

351 The light yield per MeV induce that a LPMT can collect between 1 and 1000 PE per event, a wide
 352 dynamic range, causing non linearity in the PMT response that need to be understood and calibrated,
 353 see section 2.3 for more details.

354 Before performing analysis, the analog readout of the LPMT need to be amplified, digitised and
 355 packaged by the readout electronics schematized in figure 2.9. This electronic is splitted in two parts:
 356 *wet* electronic that are located near the LPMTs, protected in an Underwater Box (UWB) and the *dry*
 357 electronics located in deicated rooms outside of the water pool.

358 The LPMTs are connected to the UWB by groups of three. Each UWB contains:

- 359 — Three high voltage units, each one powering a PMT.
 360 — A global control unit, responsible for the digitization of the waveform, composed of six analog-
 361 digital units that produce digitized waveform and a Field Programmable Gate Array (FPGA)
 362 that complete the waveform with metadatas such as the local timestamp trigger, etc... This
 363 FPGA also act as a data buffer when needed by the DAQ and trigger system.
 364 — Additional memory in order to temporally store the data in case of sudden burst of the input
 365 rate (such as in the case of nearby supernovae).

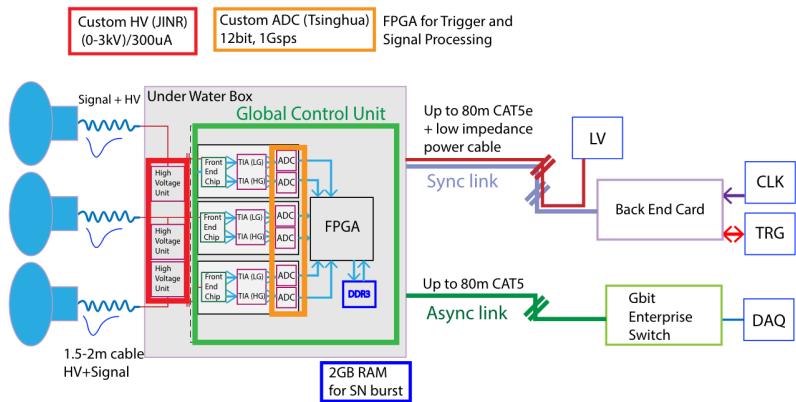


FIGURE 2.9 – The LPMT electronics scheme. It is composed of two part, the *wet* electronics on the left, located underwater and the *dry* electronics on the right. They are connected by Ethernet cable for data transmission and a dedicated low impedance cable for power distribution

366 The *dry* electronic synchronize the signals from the UWBs abd centralise the information of the CD
 367 LPMTs. It act as the Global Trigger by sending the UWB data to DAQ in the case if the LPMT
 368 multiplicity condition is fulfilled.

369 Small Photo-Multipliers Tubes (SPMTs)

370 The Small PMT (SPMTs) system is made of 3-inch (7.62 cm) PMTs. They will be used in the CD
 371 as a secondary detection system. Those 25600 SPMTs will observe the same events as the LPMTs,
 372 thus sharing the physics and detector systematics up until the photon conversion. With a detector
 373 coverage of 2.7%, this system will collect ~ 43 PE/MeV for a final energy resolution of $\sim 17\%$.
 374 This resolution is not enough to measure the NMO, θ_{13} , Δm^2_{31} but will be sufficient to independently
 375 measure θ_{12} and Δm^2_{21} .

376 The benefit of this second system is to be able to perform another, independent measure of the same
 377 events as the LPMTs, constituting the Dual Calorimetry. Due to the low PE rate, SPMTs will be
 378 running in photo-counting mode in the reactor range and thus will be insensitive to non-linearity
 379 effect. Using this property, the intrinsic charge non linearity of the LPMTs can be measured by
 380 comparing the PE count in the SPMTs and LPMTs [27]. Also, due to their smaller size and electronics,
 381 SPMTs have a better timing resolutions than the LPMTs. At higher energy range, like supernovae
 382 events, LPMTs will saturate where SPMTs due to their lower PE collection will to produce a reliable
 383 measure of the energy spectrum.

384 The SPMTs will be grouped by pack of 128 to an UWB hosting their electronics as illustrated in figure
 385 2.10. This underwater box host two high voltage splitter boards, each one supplying 64 SPMTs, an
 386 ASIC Battery Card (ABC) and a global control unit.

387 The ABC board will readout and digitize the charge and time of the 128 SPMTs signals and a FPGA
 388 will joint the different metadata. The global control unit will handle the powering and control of the
 389 board and will be in charge of the transmission of the data to the DAQ.

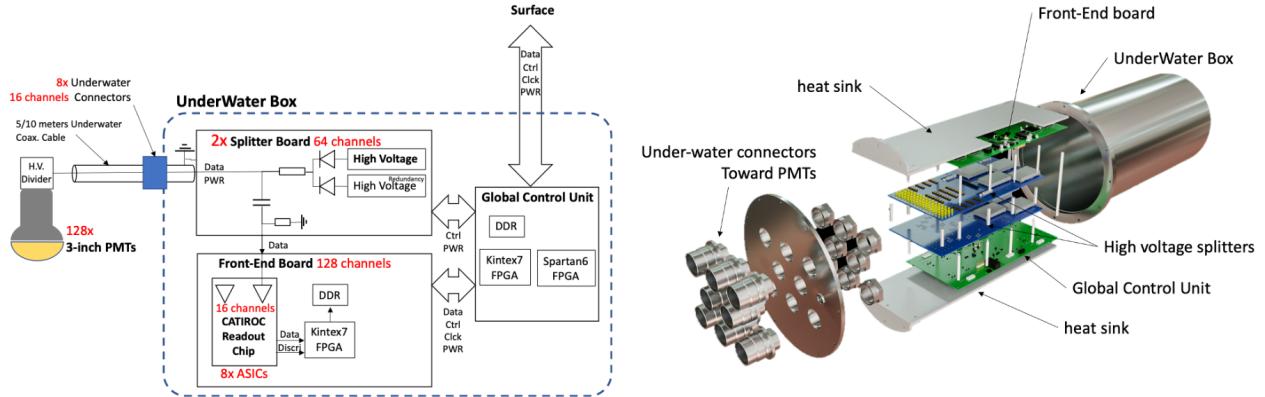


FIGURE 2.10 – Schematic of the JUNO SPMT electronic system (left), and exploded view of the main component of the UWB (right)

390 2.2.3 Veto detector

391 The CD will be bathed in constant background noise coming from numerous sources : the radioac-
 392 tivity from surrounding rock and its own components or from the flux of cosmic muons. This
 393 background needs to be rejected to ensure the purity of the IBD spectrum. To prevent a big part
 394 of them, JUNO use two veto detector that will tag events as background before CD analysis.

395 Cherenkov in water pool

396 The Water Cherenkov Detector (WCD) is the instrumentation of the water buffer around the CD.
 397 When high speed charged particles will pass through the water, they will produce cherenkov
 398 photons. The light will be collected by 2400 MCP LPMTs installed on the outer surface of the CD
 399 structure. The muons veto strategy is based on a PMT multiplicity condition. WCD PMTs are
 400 grouped in ten zones: 5 in the top, 5 in the bottom. A veto is raised either when more than 19
 401 PMTs are triggered in one zone or when two adjacent zones simultaneously trigger more than 13
 402 PMTs. Using this trigger, we expect to reach a muon detection efficiency of 99.5% while keeping the
 403 noise at reasonable level.

404 Top tracker

405 The JUNO Top Tracker (TT) is a plastic scintillator detector located on the top of the experiment (see
 406 figure 2.11). Made from plastic scintillator from OPERA [28] layered horizontally in 3 layers on the
 407 top of the detector, the TT will be able to detect incoming atmospheric muons. With its coverage,
 408 about 1/3 of the of all atmospheric muons that passing through the CD will also pass through the 3
 409 layer of the detector. While it does not cover the majority of the CD, the TT is particularly effective
 410 to detect muons coming through the filling chimney region which might present difficulties from the
 411 other subsystems in some classes of events.

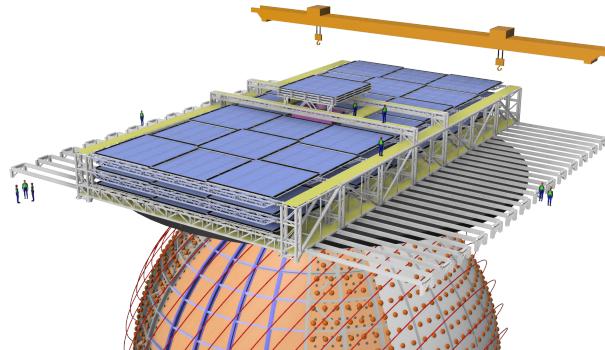


FIGURE 2.11 – The JUNO top tracker

412 2.3 Calibration strategy

413 The calibration is a crucial part of the JUNO experiment. The detector will continuously bath in
 414 neutrinos coming from the close nuclear power plant, from other sources such as geo neutrinos,
 415 the sun and will be exposed to background noise coming from atmospheric muons and natural
 416 radioactivity. Because of this continuous rate, low frequency signal event, we need high frequency,
 417 recognisable sources in the energy range of interest : [0-12] MeV for the positron signal and 2.2 MeV
 418 for the neutron capture. It is expected that the CD response will be different depending on the type
 419 of particle, due to the interaction with LS, the position on the event and the optical response of the
 420 acrylic sphere (see section 2.6). We also expect a non-linear energy response of the CD due to the LS
 421 properties [20] but also due to the saturation of the LPMTs system when collecting a large amount of
 422 PE [27].

423 2.3.1 Energy scale calibration

424 While electrons and positrons sources would be ideal, for a large LS detector thin-walled electrons
 425 or positrons sources could lead to leakage of radionucleides causing radioactive contamination.
 426 Instead, we consider gamma sources in the range of the prompt energy of IBDs. The sources are
 427 reported in table 2.4.

Sources / Processes	Type	Radiation
^{137}Cs	γ	0.0662 MeV
^{54}Mn	γ	0.835 MeV
^{60}Co	γ	1.173 + 1.333 MeV
^{40}K	γ	1.461 MeV
^{68}Ge	e^+	annihilation 0.511 + 0.511 MeV
$^{241}\text{Am-Be}$	n, γ	neutron + 4.43 MeV ($^{12}\text{C}^*$)
$^{241}\text{Am-}^{13}\text{C}$	n, γ	neutron + 6.13 MeV ($^{16}\text{O}^*$)
$(n, \gamma)p$	γ	2.22 MeV
$(n, \gamma)^{12}\text{C}$	γ	4.94 MeV or 3.68 + 1.26 MeV

TABLE 2.4 – List of sources and their process considered for the energy scale calibration

428 For the ^{68}Ge source, it will decay in ^{68}Ga via electron capture, which will itself β^+ decay into ^{68}Zn .
 429 The positrons will be absorbed by the enclosure so only the annihilation gamma will be released. In
 430 addition, (α, n) sources like $^{241}\text{Am-Be}$ and $^{241}\text{Am-}^{13}\text{C}$ are used to provide both high energy gamma
 431 and neutrons, which will later be captured in the LS producing the 2.2 MeV gamma.

432 From this calibration we call E_{vis} the "visible energy" that is reconstructed by our current algorithms
 433 and we compare it to the true energy deposited by the calibration source. The results shown in figure
 434 2.12 show the expected response of the detector from calibration sources. The non-linearity is clearly
 435 visible from the E_{vis} / E_{true} shape. See [29] for more details.

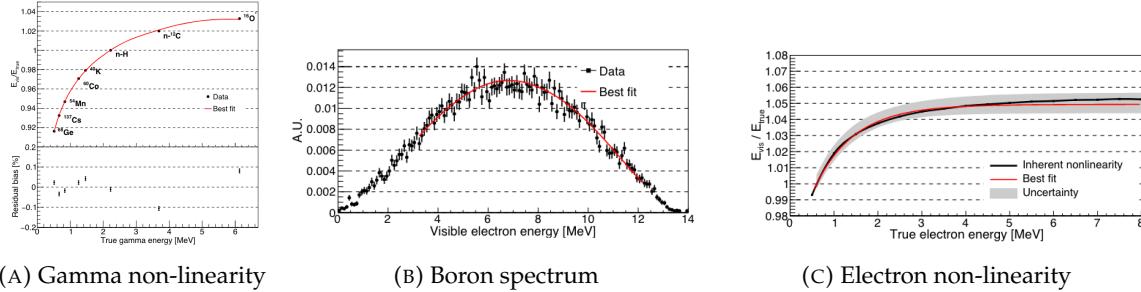


FIGURE 2.12 – Fitted and simulated non linearity of gamma, electron sources and from the ^{12}B spectrum. Black points are simulated data. Red curves are the best fits. Figures taken from [29].

436 2.3.2 Calibration system

437 The non-uniformity due to the event position in the detector (more details in section 2.6) will be
 438 studied using multiples systems that are schematized in figure 2.13. They allow to position sources
 439 at different location in the CD.

- 440 — For a one-dimension vertical calibration, the Automatic Calibration Unit (ACU) will be able
 441 to deploy multiple radioactive sources or a pulse laser diffuser ball along the central axis of
 442 the CD through the top chimney. The source position precision is less than 1cm.
- 443 — For off-axis calibration, a calibration source attached to a Cable Loop System (CLS) can be
 444 moved on a vertical half-plane by adjusting the length of two connection cable. Two set of
 445 CSL will be deployed to provide a 79% effective coverage of a vertical plane.
- 446 — A Guiding Tube (GT) will surround the CD to calibrate the non-uniformity of the response at
 447 the edge of the detector
- 448 — A Remotely Operated under-LS Vehicle (ROV) can be deployed to desired location inside LS
 449 for a more precise and comprehensive calibration. The ROV will also be equipped with a
 450 camera for inspection of the CD.

451 The preliminary calibration program is depicted in table 2.5.

452 2.3.3 Instrumental non-linearity calibration

453 As mentioned in the introduction of this section, we expect an instrumental non-linearity due to the
 454 LPMT system saturating. This results in the LPMT underestimating the number of collected photo-
 455 electrons. This non-linearity is illustrated in figure 2.14. This non-linearity would consequently
 456 convolve with the LS non-linearity. To correct this effect, the LPMT are first calibrated to the channel
 457 level using the dual calorimetry calibration technique which consist of comparing the LPMT and
 458 SPMT calorimetry calibration using a tunable light source covering the range of 0 to 100 PE per
 459 LPMT channel.

460 Within such range, the SPMT serve as an approximate linear reference since SPMT operate primarily
 461 operate in photo-counting mode in this range. Using this technique, the residual non-linearity in the
 462 LPMT response due to the saturation effect is under 0.3 %.

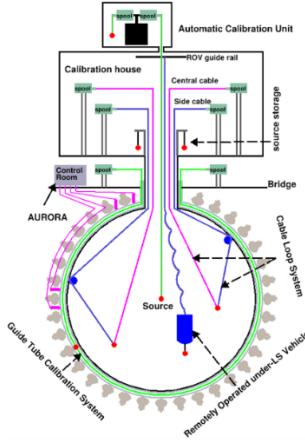


FIGURE 2.13 – Overview of the calibration system

Program	Purpose	System	Duration [min]
Weekly calibration	Neutron (Am-C)	ACU	63
	Laser	ACU	78
Monthly calibration	Neutron (Am-C)	ACU	120
	Laser	ACU	147
	Neutron (Am-C)	CLS	333
	Neutron (Am-C)	GT	73
Comprehensive calibration	Neutron (Am-C)	ACU, CLS and GT	1942
	Neutron (Am-Be)	ACU	75
	Laser	ACU	391
	^{68}Ge	ACU	75
	^{137}Cs	ACU	75
	^{54}Mn	ACU	75
	^{60}Co	ACU	75
	^{40}K	ACU	158

TABLE 2.5 – Calibration program of the JUNO experiment

463 2.4 Satellite detectors

464 As introduced in section 2.1.1 and section 2.2.2, the precise knowledge and understanding of the
 465 detector condition is crucial for the measurements of the NMO and oscillation parameters. Thus two
 466 satellite detectors will be setup to monitor the experiment condition. TAO to monitor and understand
 467 the $\bar{\nu}_e$ flux and spectrum coming from the nuclear reactor and OSIRIS to monitor the LS response.

468 2.4.1 TAO

469 The Taishan Antineutrino Observatory (TAO) [12, 30] is a ton-level gadolinium doped liquid scin-
 470 tillator detector that will be located near the Taishan-1 reactor. It aim to measure the $\bar{\nu}_e$ spectrum at
 471 very low distance (45m) from the reactor to measure a quasi-unoscillated spectrum. TAO also aim to
 472 provide a major contribution to the so-called reactor anomaly [13]. Its requirement are to the level of
 473 2 % energy resolution at 1 MeV.

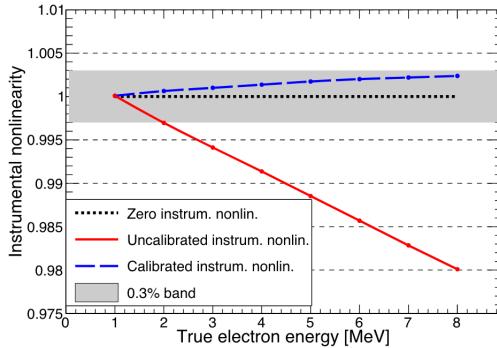


FIGURE 2.14 – Event-level instrumental non-linearity, defined as the ratio of the total measured LPMT charge to the true charge for events uniformly distributed in the detector. The solid red line represents event-level non-linearity without the channel-level correction, with position non-uniformity obtained at 1 MeV applied, in an extreme hypothetical scenario of 50% non-linearity over 100 PEs for the LPMTs. The dashed blue line represents that after the channel-level correction. The gray band shows the residual uncertainty of 0.3%, after the channel-level correction. Figure taken from [29].

474 Detector

475 The TAO detector is close, in concept, to the CD of JUNO. It is composed of an acrylic vessel
 476 containing 2.8 tons of gadolinium-loaded LS instrumented by an array of silicon photomultipliers
 477 (SiPM) reaching a 95% coverage. To efficiently reduce the dark count of those sensors, the detector
 478 is cooled to -50 °C. The $\bar{\nu}_e$ will interact with the LS via IBD, producing scintillation light, that will
 479 be detected by the SiPMs. From this signal the $\bar{\nu}_e$ energy and the full spectrum reconstructed. This
 480 spectrum will then be used by JUNO to calibrate the unoscillated spectrum, most notably the fission
 481 product fraction that impact the rate and shape of the spectrum. A schema of the detector is presented
 482 in figure 2.15a.
 483

2.4.2 OSIRIS

484 The Online Scintillator Internal Radioactivity Investigation System (OSIRIS) [25] is an ultralow back-
 485 ground, 20 m³ LS detector that will be located in JUNO cavern. It aim to monitor the radioactive
 486 contamination, purity and overall response of the LS before it is injected in JUNO. OSIRIS will
 487 be located at the end of the purification chain of JUNO, monitoring that the purified LS meet the
 488 JUNO requirements. The setup is optimized to detect the fast coincidences decay of $^{214}\text{Bi} - ^{214}\text{Po}$
 489 and $^{212}\text{Bi} - ^{212}\text{Po}$, indicators of the decay chains of U and Th respectively.

490 Detector

491 OSIRIS is composed of an acrylic vessel that will contains 17t of LS. The LS is instrumented by
 492 a PMT array of 64 20 inch PMTs on the top and the side of the vessel. To reach the necessary
 493 background level required by the LS purity measurements, in addition to being 700m underground
 494 in the experiment cavern, the acrylic vessel is immersed in a tank of ultra pure water. The water is
 495 itself instrumented by another array of 20 inch PMTs, acting as muon veto. A schema of the detector
 496 is presented in figure 2.15b.

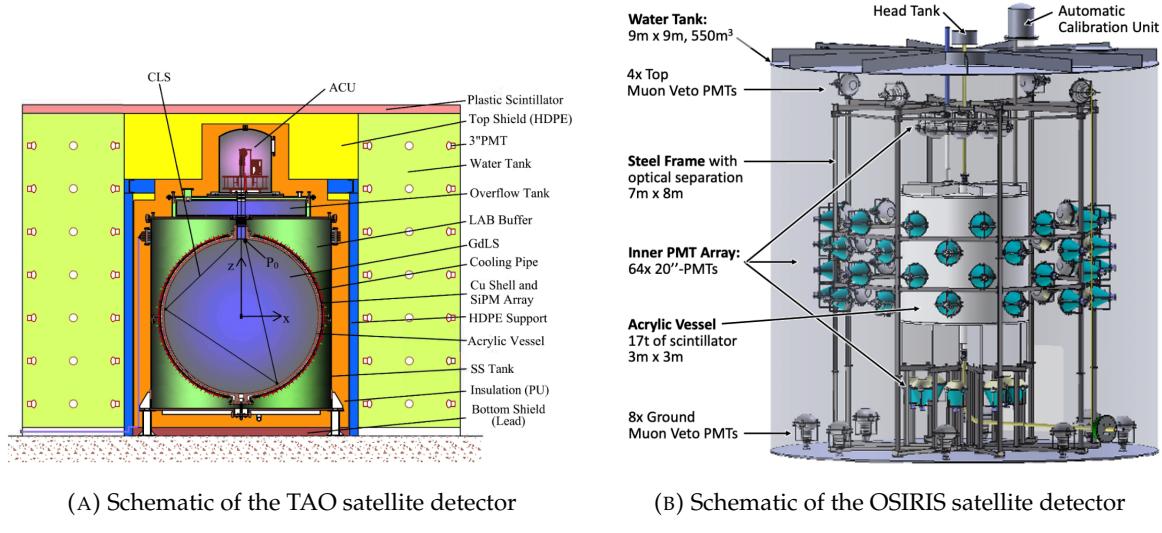


FIGURE 2.15

2.5 Software

498 The simulation, reconstruction and analysis algorithms are all packaged in the JUNO software,
 499 subsequently called the software. It is composed of multiple components integrated in the SNiPER
 500 [31] framework:

- 501 — Various primary particles simulators for the different kind of events, background and calibra-
 502 tion sources.
- 503 — A Geant4 [32–34] Monte Carlo (MC) simulation containing the detectors geometries, a custom
 504 optical model for the LS and the supporting structures of the detectors. The Geant4 simulation
 505 integrate all relevant physics process for JUNO, validated by the collaboration. This step of the
 506 simulation is commonly called *Detsim* and compute up to the production of photo-electrons
 507 in the PMTs. The optics properties of the different materials and detector components have
 508 been measured beforehand to be used to define the material and surfaces in the simulation.
- 509 — An electronic simulation, simulating the response waveform of the PMTs, tracking it through
 510 the digitization process, accounting for effects such as non-linearity, dark noise, Time Trans-
 511 it Spread (TTS), pre-pulsing, after-pulsing and ringing if the waveform. It's also the step
 512 handling the event triggers and mixing. This step is commonly referenced as *Elecsim*.
- 513 — A waveform reconstruction where the digitized waveform are filtered to remove high-frequency
 514 white noise and then deconvoluted to yield time and charge informations of the photons hits
 515 on the PMTs. This step is commonly referenced as *Calib*.
- 516 — The charge and time informations are used by reconstruction algorithms to reconstruct the
 517 interaction vertex and the deposited energy. This step is commonly reported as *Reco*. See
 518 section 2.6 for more details on the reconstruction.
- 519 — Once the singular events are reconstructed, they go through event pairing and classification
 520 to select IBD events. This step is named Event Classification.
- 521 — The purified signal is then analysed by the analysis framework which depend of the physics
 522 topic of interest.

523 The steps Reco and Event Classification are divided into two category of algorithm. Fast but less
 524 accurate algorithms that are running during the data taking designated as the *Online* algorithms.
 525 Those algorithm are used to take the decision to save the event on tape or to throw it away. More
 526 accurate algorithms that run on batch of events designated *Offline* algorithms. They are used for the
 527 physics analysis. The Offline Reco will be one of the main topic of interest for this thesis.

528 2.6 State of the art of the Offline IBD reconstruction in JUNO

529 The main reconstruction method currently run in JUNO is a data-driven method based on a like-
 530 lihood maximization [35, 36] using only the LPMTs. The first step is to reconstruct the interaction
 531 vertex from which the energy reconstruction is dependent. It is also necessary for event pairing and
 532 classification.

533 **2.6.1 Interaction vertex reconstruction**

534 To start the likelihood maximization, a rough estimation of the vertex and of the event timing is
 535 needed. We start by estimating the vertex position using a charge based algorithm.

536 **Charge based algorithm**

537 The charge-based algorithm is basically base on the charge-weighted average of the PMT position.

$$\vec{r}_{cb} = a \cdot \frac{\sum_i q_i \cdot \vec{r}_i}{\sum_i q_i} \quad (2.3)$$

538 Where q_i is the reconstructed charge of the pulse of the i th PMT and \vec{r}_i is its position. \vec{r}_0 is the
 539 reconstructed interaction position. a is a scale factor introduced because a weighted average over
 540 a 3D sphere is inherently biased. Using calibration we can estimate $a \approx 1.3$ [37]. The results in
 541 figure 2.16b shows that the reconstruction is biased from around 15m and further. This is due to the
 542 phenomena called “total reflection area” or TR Area.

543 As depicted in the figure 2.16a the optical photons, given that they have a sufficiently large incidence
 544 angle, can be deviated of their trajectories when passing through the interfaces LS-acrylic and water-
 545 acrylic due to the optical index difference. This cause photons to be lost or to be detected by PMT
 546 further than anticipated if we consider their rectilinear trajectories. This cause the charge barycenter
 547 the be located closer to the center than the event really is.

548 It is to be noted that charge based algorithm, in addition to be biased near the edge of the detector,
 549 does not provide any information about the timing of the event. Therefore, a time based algorithm
 550 needs to be introduced to provide initial values.

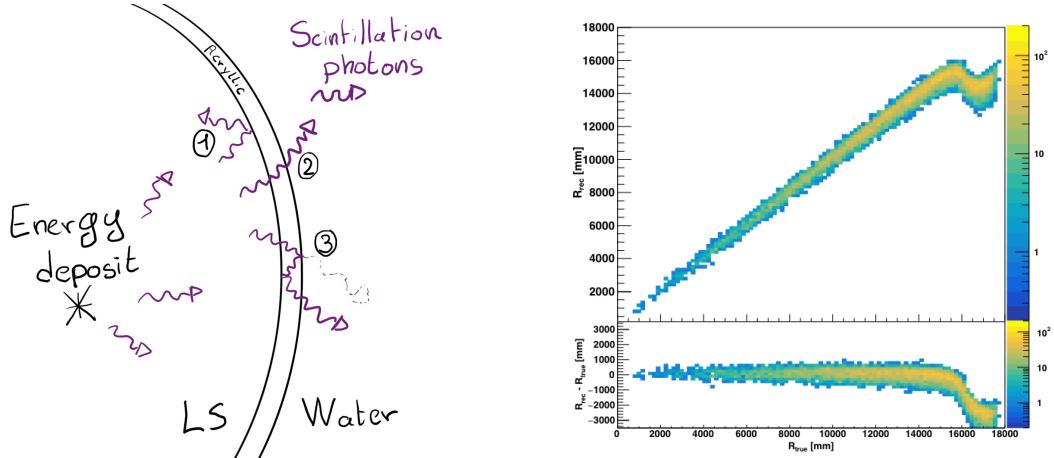
551 **Time based algorithm**

552 The time based algorithm use the distribution of the time of flight corrections Δt (Eq 2.4) of an event
 553 to reconstruct its vertex and t_0 . It follow the following iterations:

- 554 1. Use the charge based algorithm to get an initial vertex to start the iteration.
 555 2. Calculate the time of flight correction for the i th PMT using

$$\Delta t_i(j) = t_i - \text{tof}_i(j) \quad (2.4)$$

556 where j is the iteration step, t_i is the timing of the i th PMT, and tof_i is the time-of-flight of the
 557 photon considering an rectilinear trajectory and an effective velocity in the LS and water (see
 558 [37] for detailed description of this effective velocity). Plot the Δt distribution and label the
 559 peak position as Δt^{peak} (see fig 2.17a).



(A) Illustration of the different optical photons reflection scenarios. 1 is the reflection of the photon at the interface LS-acrylic or acrylic-water. 2 is the transmission of the photons through the interfaces. 3 is the conduction of the photon in the acrylic.

(B) Heatmap of R_{rec} and $R_{rec} - R_{true}$ as a function of R_{true} for 4MeV prompt signals uniformly distributed in the detector calculated by the charge based algorithm

FIGURE 2.16

560 3. Calculate a correction vector $\vec{\delta}[\vec{r}(j)]$ as

$$\vec{\delta}[\vec{r}(j)] = \frac{\sum_i \left(\frac{\Delta t(j) - \Delta t^{peak}(j)}{tof_i(j)} \right) \cdot (\vec{r}_0(j) - \vec{r}_i)}{N^{peak}(j)} \quad (2.5)$$

561 where \vec{r}_0 is the vertex position at the beginning of this iteration, \vec{r}_i is the position of the i th
562 PMT. To minimize the effect of scattering, dark noise and reflection, only the pulse happening
563 in a time window (-10 ns, +5 ns) around Δt^{peak} are considered. N^{peak} is the number of PE
564 collected in this time-window.

565 4. if $\vec{\delta}[\vec{r}(j)] < 1\text{mm}$ or $j \geq 100$, stop the iteration. Otherwise $\vec{r}_0(j+1) = \vec{r}_0(j) + \vec{\delta}[\vec{r}(j)]$ and go to
566 step 2.

567 However because the earliest arrival time is used, t_i is related to the number photoelectrons N_i^{pe}
568 detected by the PMT [38–40]. To reduce bias in the vertex reconstruction, the following equation is
569 used to correct t_i into t'_i :

$$t'_i = t_i - p_0 / \sqrt{N_i^{pe}} - p_1 - p_2 / N_i^{pe} \quad (2.6)$$

570 The parameters (p_0, p_1, p_2) were optimized to (9.42, 0.74, -4.60) for Hamamatsu PMTs and (41.31,
571 -12.04, -20.02) for NNVT PMTs [37]. The results presented in figure 2.17b shows that the time based
572 algorithm provide a more accurate vertex and is unbiased even in the TR area. This results (\vec{r}_0, t_0) is
573 used as initial value for the likelihood algorithm.

574 Time likelihood algorithm

575 The time likelihood algorithm use the residual time expressed as follow

$$t_{res}^i(\vec{r}_0, t_0) = t_i - tof_i - t_0 \quad (2.7)$$

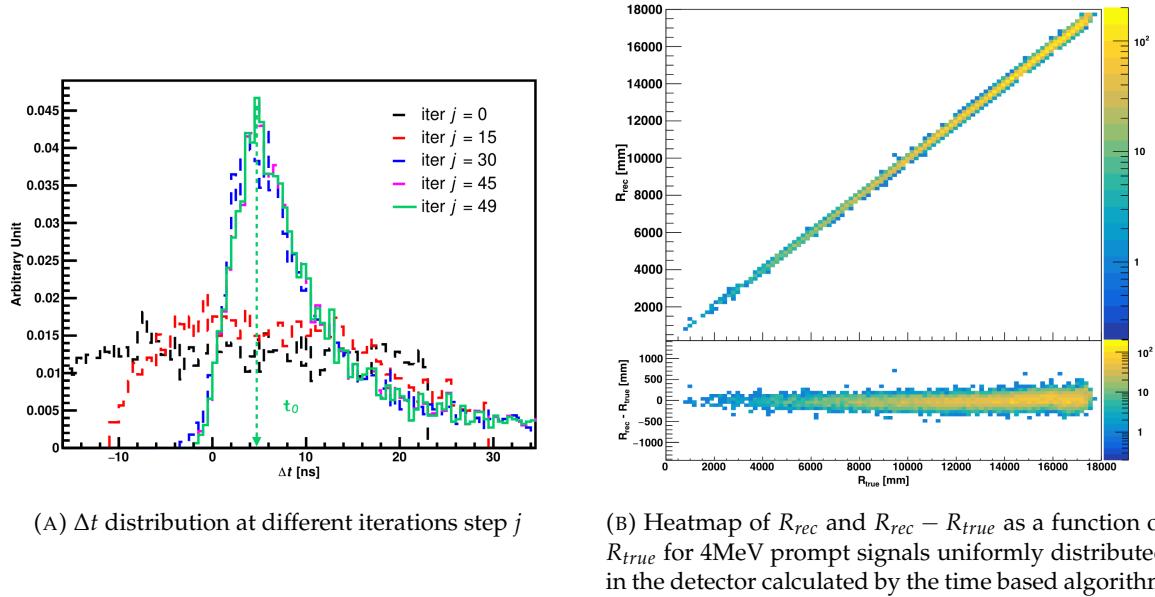


FIGURE 2.17

576 In a first order approximation, the scintillator time response Probability Density Function (PDF) can
 577 be described as the emission time profile of the scintillation photons, the Time Transit Spread (TTS)
 578 and the dark noise of the PMTs. The emission time profile $f(t_{res})$ is described like

$$f(t_{res}) = \sum_k \frac{\rho_k}{\tau_k} e^{-\frac{t_{res}}{\tau_k}}, \quad \sum_k \rho_k = 1 \quad (2.8)$$

579 as the sum of the k component that emit light in the LS each one characterised by it's decay time τ_k
 580 and intensity fraction ρ_k . The TTS component is expressed as a gaussian convolution

$$g(t_{res}) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(t_{res}-\nu)^2}{2\sigma^2}} \cdot f(t_{res}) \quad (2.9)$$

581 where σ is the TTS of PMTs and ν is the average transit time. The dark noise is not correlated with any
 582 physical events and considered as constant rate over the time window considered T . By normalizing
 583 the dark noise probability $\epsilon(t_{res})$ as $\int_T \epsilon(t_{res}) dt_{res} = \epsilon_{dn}$, it can be integrated in the PDF as

$$p(t_{res}) = (1 - \epsilon_{dn}) \cdot g(t_{res}) + \epsilon(t_{res}) \quad (2.10)$$

584 The distribution of the residual time t_{res} of an event can then be compared to $p(t_{res})$ and the best
 585 fitting vertex \vec{r}_0 and t_0 can be chosen by minimizing

$$\mathcal{L}(\vec{r}_0, t_0) = -\ln \left(\prod_i p(t_{res}^i) \right) \quad (2.11)$$

586 The parameter of Eq. 2.10 can be measured experimentally. The results shown in figure 2.18 used
 587 PDF from monte carlo simulation. The results shows that $R_{rec} - R_{true}$ is biased depending on the
 588 energy. While this could be corrected using calibration, another algorithm based on charge likelihood
 589 was developed to correct this problem.

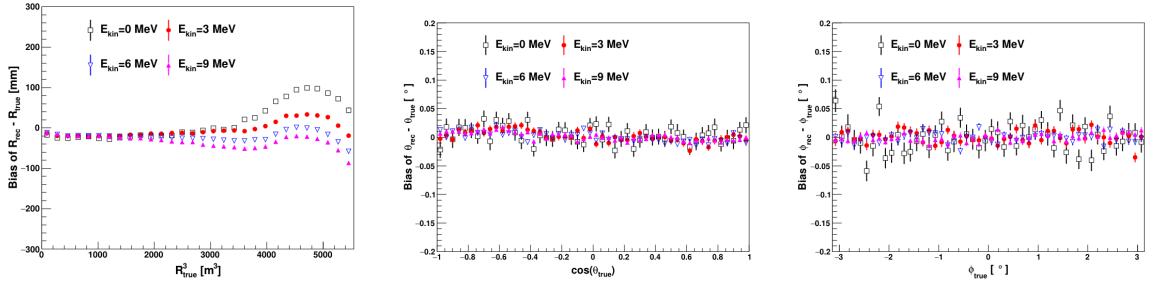


FIGURE 2.18 – Bias of the reconstructed radius R (left), θ (middle) and ϕ (right) for multiple energies by the time likelihood algorithm

590 Charge likelihood algorithm

591 Similarly to the time likelihood algorithms that use a timing PDF, the charge likelihood algorithm
 592 use a PE PDF for each PMT depending on the energy and position of the event. With $\mu(\vec{r}_0, E)$ the
 593 mean expected number of PE detected by each PMT, the probability to observe N_{pe} in a PMT follow
 594 a Poisson distribution. Thus

- 595 — The probability to observe no hit ($N_{pe} = 0$) in the j th PMT is $P_{nohit}^j(\vec{r}_0, E) = e^{-\mu_j}$
- 596 — The probability to observe $N_{pe} \neq 0$ in the i th PMT is $P_{hit}^i(\vec{r}_0, E) = \frac{\mu^{N_{pe}} e^{-\mu_i}}{N_{pe}^i!}$

597 Therefore, the probability to observe a specific hit pattern can be expressed as

$$P(\vec{r}_0, E) = \prod_j P_{nohit}^j(\vec{r}_0, E) \cdot \prod_i P_{hit}^i(\vec{r}_0, E) \quad (2.12)$$

598 The best fit values of \vec{R}_0 and E can then be calculated by minimizing the negative log-likelihood

$$\mathcal{L}(\vec{r}_0, E) = -\ln(P(\vec{r}_0, E)) \quad (2.13)$$

599 In principle, $\mu_i(\vec{r}_0, E)$ could be expressed

$$\mu_i(\vec{r}_0, E) = Y \cdot \frac{\Omega(\vec{r}_0, r_i)}{4\pi} \cdot \epsilon_i \cdot f(\theta_i) \cdot e^{-\sum_m \frac{d_m}{\zeta_m}} \cdot E + \delta_i \quad (2.14)$$

600 where Y is the energy scale factor, $\Omega(\vec{r}_0, r_i)$ is the solid angle of the i th PMT, ϵ_i is its detection
 601 efficiency, $f(\theta_i)$ its angular response, ζ_m is the attenuation length in the materials and δ_i the expected
 602 number of dark noise.

603 However Eq. 2.14 assume that the scintillation light yield is linear with energy and describe poorly
 604 the contribution of indirect light, shadow effect due to the supporting structure and the total reflec-
 605 tion effects. The solution is to use data driven methods to produce the pdf by using the calibra-
 606 tions sources and position described in section 2.3. In the results presented in figures 2.19, the PDF was
 607 produced using MC simulation and 29 specific calibrations position [37] along the Z-axis of the
 608 detector. We see that the charge likelihood algorithm show little bias in the TR area and a better
 609 resolution than the time likelihood. The figure 2.20 shows the radial resolution of the different
 610 algorithm presented for this section, we can see the refinement at each step and that the charge
 611 likelihood yield the best results.

612 The charge based likelihood algorithms already give use some information on the energy as Eq. 2.13
 613 is minimized but the energy can be further refined as shown in the next section.

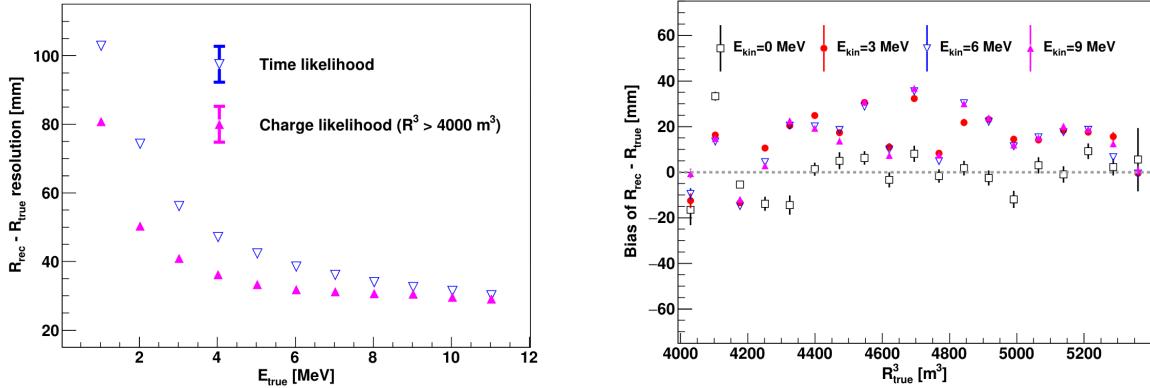


FIGURE 2.19 – On the left: Resolution of the reconstructed R as a function of the energy in the TR area ($R^3 > 4000 \text{ m}^3 \equiv R > 16 \text{ m}$) by the charge and time likelihood algorithms. On the right: Bias of the reconstructed R in the TR area for different energies by the charge likelihood algorithm

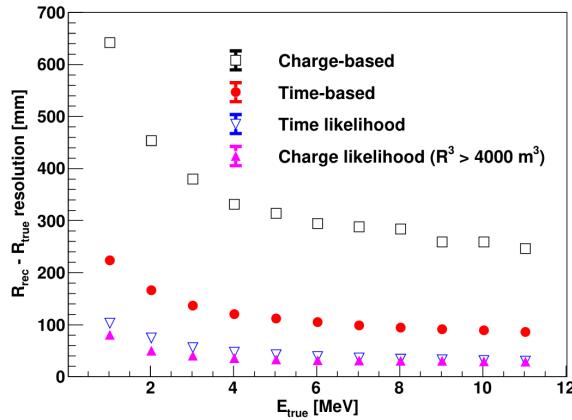


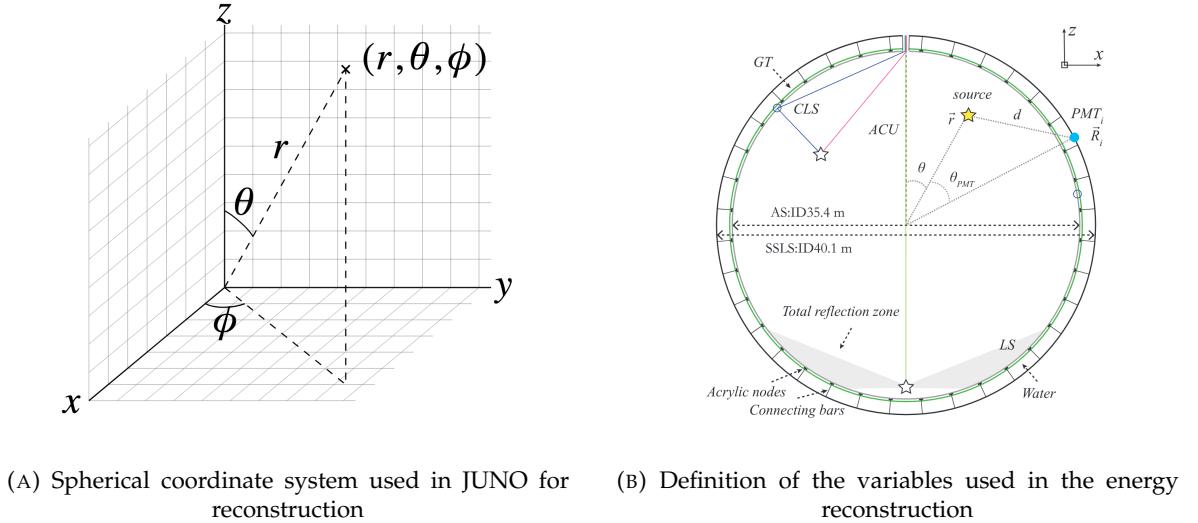
FIGURE 2.20 – Radial resolution of the different vertex reconstruction algorithms as a function of the energy

614 2.6.2 Energy reconstruction

615 As explained in section 2.1.1, energy resolution is crucial for the NMO and oscillation parameters
 616 measurements. Thus the energy reconstruction algorithm should take into consideration as much
 617 detector effect as possible. The following method is a data driven method based on calibration
 618 samples inspired by the charge likelihood algorithm described above [41].

619 Charge estimation

620 The most important element in the energy reconstruction is $\mu_i(\vec{r}_0, E)$ described in Eq. 2.14. For
 621 realistic cases, we also need to take into account the electronics effect that were omitted in the
 622 previous section. Those effect will cause a charge smearing due to the uncertainties in the N_{pe}
 623 reconstruction. Thus we define $\hat{\mu}^L(\vec{r}_0, E)$ which is the expected N_{pe}/E in the whole detector for an
 624 event with visible energy E_{vis} and position \vec{r}_0 . The position of the event and PMTs are now defined



(A) Spherical coordinate system used in JUNO for reconstruction

(B) Definition of the variables used in the energy reconstruction

FIGURE 2.21

625 using $(r, \theta, \theta_{pmt})$ as defined in figure 2.21b.

$$\hat{\mu}(r, \theta, \theta_{pmt}, E_{vis}) = \frac{1}{E_{vis}} \frac{1}{M} \sum_i^M \frac{\bar{q}_i - \mu_i^D}{\text{DE}_i}, \quad \mu_i^D = \text{DNR}_i \cdot L \quad (2.15)$$

626 where i runs over the PMTs with the same θ_{pmt} , DE_i is the detection efficiency of the i th PMT. μ_i^D
627 is the expected number of dark noise photoelectrons in the time window L . The time window have
628 been optimized to $L = 280$ ns [41]. \bar{q}_i is the average recorded photoelectrons in the time window
629 and \hat{Q}_i is the expected average charge for 1 photoelectron. The N_{pe} map is constructed following the
630 procedure described in [36].

631 Time estimation

632 The second important observable is the hit time of photons that was previously defined in Eq. 2.7. It
633 is here refined as

$$t_r = t_h - \text{tof} - t_0 = t_{LS} + t_{TT} \quad (2.16)$$

634 where t_h is the time of hit, t_{LS} is the scintillation time and t_{TT} the transit time of PMTs that is described
635 by a gaussian

$$t_{TT} = \mathcal{N}(\overline{\mu_{TT} + t_d}, \sigma_{TT}) \quad (2.17)$$

636 where μ_{TT} is the mean transit time in PMTs, σ_{TT} is the Transit Time Spread (TTS) of the PMTs and t_d
637 is the delay time in the electronics. The effective refraction index of the LS is also corrected to take
638 into account the propagation distance in the detector.

639 The timing PDF $P_T(t_r | r, d, \mu_l, \mu_d, k)$ can now be generated using calibration sources [41]. This PDF
640 describe the probability that the residual time of the first photon hit is in $[t_r, t_r + \delta]$ with r the radius
641 of the event vertex, $d = |\vec{r} - \vec{r}_{PMT}|$ the propagation distance, μ_l and μ_d the expected number of PE
642 and dark noise in the electronic reading window and k is the detected number of PE.

643 Now let denote $f(t, r, d)$ the probability density function of "photoelectron hit a time t" for an event

644 happening at r where the photons traveled the distance d in the LS

$$F(t, r, d) = \int_t^L f(t', r, d) dt' \quad (2.18)$$

645 Based on the PDF for one photon $k = 1$, one can define

$$P_T^l(t|k = n) = I_n^l [f_l(t) F_l^{n-1}(t)] \quad (2.19)$$

646 where the indicator l means that the photons comes from the LS and I_n^l a normalisation factor. To this
647 pdf we add the probability to have photons coming from the dark noise indicated by the indicator d
648 using

$$f_d(t) = 1/L, F_d(t) = 1 - \frac{t}{L} \quad (2.20)$$

649 and so for the case where only one photon is detected by the PMT ($k = 1$)

$$P_T(t|\mu_l, \mu_d, k = 1) = I_1[P(1, \mu_l)P(0, \mu_d)f_l(t) + P(0, \mu_l)P(1, \mu_d)f_d(t)] \quad (2.21)$$

650 where $P(k_\alpha, \mu_\alpha)$ is the Poisson probability to detect k_α PE from $\alpha \in \{l, d\}$ with the condition $k_l + k_d =$
651 k .

652 Now that we have the individual timing and charge probability we can construct the charge likeli-
653 hood referred as QMLE:

$$\mathcal{L}(q_1, q_2, \dots, q_N | \vec{r}, E_{vis}) = \prod_{j \in \text{unfired}} e^{-\mu_j} \prod_{i \in \text{fired}} \left(\sum_{k=1}^K P_Q(q_i|k) \cdot P(k, \mu_i) \right) \quad (2.22)$$

654 where $\mu_i = E_{vis}\hat{\mu}_i^L + \mu_i^D$ and $P(k, \mu_i)$ is the Poisson probability of observing k PE. $P_Q(q_i|k)$ is the
655 charge pdf for k PE. And we can also construct the time likelihood referred as TMLE:

$$\mathcal{L}(t_{1,r}, t_{2,r}, \dots, t_{N,r} | \vec{r}, t_0) = \prod_{i \in \text{hit}} \frac{\sum_{k=1}^K P_T(t_{i,r}|r, d, \mu_i^l, \mu_i^d, k) \cdot P(k, \mu_i^l + \mu_i^d)}{\sum_{k=1}^K P(k, \mu_i^l + \mu_i^d)} \quad (2.23)$$

656 where K is cut to 20 PE and hit is the set of hits satisfying $-100 < t_{i,r} < 500$ ns.

657 Merging those two likelihood give the charge-time likelihood QTMLE

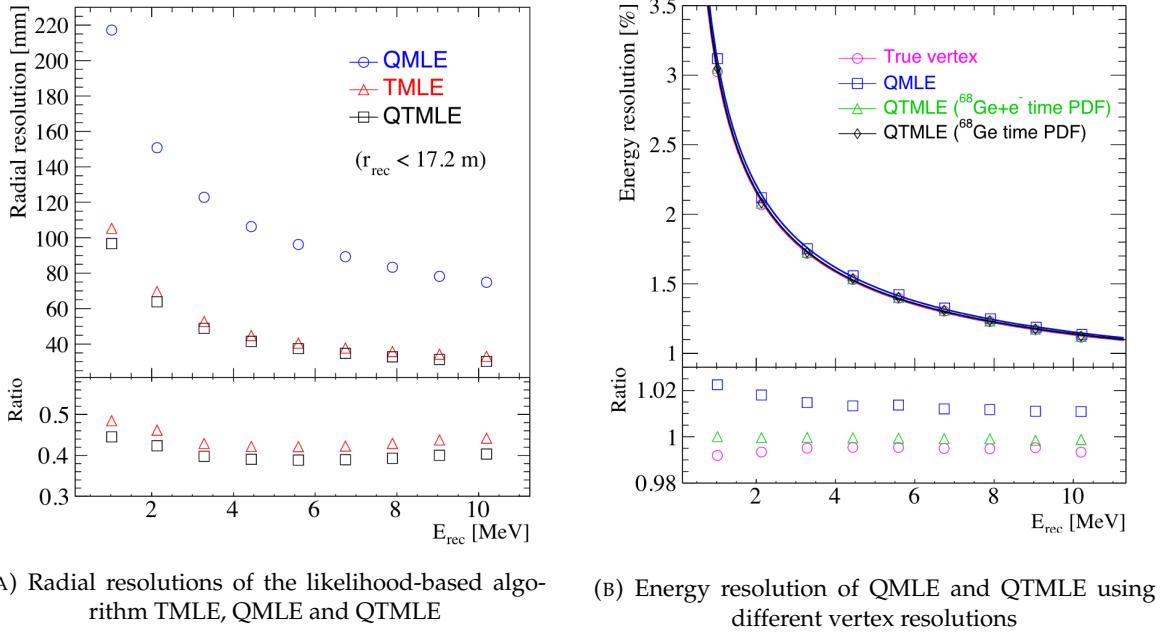
$$\mathcal{L}(q_1, q_2, \dots, q_N; t_{1,r}, t_{2,r}, \dots, t_{N,r} | \vec{r}, t_0, E_{vis}) = \mathcal{L}(q_1, q_2, \dots, q_N | \vec{r}, E_{vis}) \cdot \mathcal{L}(t_{1,r}, t_{2,r}, \dots, t_{N,r} | \vec{r}, t_0) \quad (2.24)$$

658 The radial and energy resolutions of the different likelihood are presented in figure 2.22 (from [41]).
659 We can see the improvement of adding the time information to the vertex reconstruction and that
660 an increase in vertex precision can bring improvement in the energy resolution, especially at low
661 energies.

662 Data driven methods prove to be performant in the energy and vertex reconstruction given that we
663 have enough calibrations sources to produce the PDF. In the next section, we'll see another type of
664 data-driven method based on machine learning.

665 2.6.3 Machine learning for reconstruction

666 Machine learning (ML) is family of data-driven algorithms that are inferring behavior and results
667 from a training dataset. A overview of methods and detailed explanation of the Neural Network
668 (NN) subfamily can be found in Chapter 3.



(A) Radial resolutions of the likelihood-based algorithm TMLE, QMLE and QTML

(B) Energy resolution of QMLE and QTML using different vertex resolutions

FIGURE 2.22

The power of ML is the ability to model complex response to a specific problem. In JUNO the reconstruction problematic can be expressed as follow: knowing that each PMT, large or small, detected a given number of PE Q at a given time t and their position is x, y, z where did the energy was deposited and how much energy was it, modeling a function that naively goes:

$$\mathbb{R}^{5 \times N_{\text{pmt}}} \mapsto \mathbb{R}^4 \quad (2.25)$$

It is worth pointing that while this is already a lot in informations, this is not the rawest representation of the experiment. We could indeed replace the charge and time by the waveform in the time window of the event but that would lead to an input representation size that would exceed our computational limits. Also, due to those computational limits, most of the ML algorithm reduce this input phase space either by structurally encoding the information (pictures, graph), by aggregating it (mean, variance, ...) or by exploiting invariance and equivariance of the experiment (rotational invariance due to the sphericity, ...).

For machine learning to converge to performant algorithm, a large dataset exploring all the phase space of interest is needed. For the following studies, data from the monte carlo simulation presented in section 2.5 are used for training. When the detector will be finished calibrations sources will be complementarily be used.

Boosted Decision Tree (BDT)

On of the most classic ML method used in physics in last years is the Boosted Decision Tree (see chapter 3.1). They have been explored for vertex reconstruction [42] et for energy reconstruction [42, 43].

For vertex and energy reconstruction a BDT was developed using the aggregated informations presented in 2.6.

Its reconstruction performances are presented in figure 2.24.

Parameter	description
$nHits$	Total number of hits
$x_{cc}, y_{cc}, z_{cc}, R_{cc}$	Coordinates of the center of charge
ht_{mean}, ht_{std}	Hit time mean and standard deviation

TABLE 2.6 – Features used by the BDT for vertex reconstruction

AccumCharge	$ht_{5\% - 2\%}$
R_{cht}	pe_{mean}
z_{cc}	J_{cht}
pe_{std}	ϕ_{cc}
nPMTs	$ht_{35\% - 30\%}$
$ht_{kurtosis}$	$ht_{20\% - 15\%}$
$ht_{25\% - 20\%}$	$pe_{35\%}$
R_{cc}	$ht_{30\% - 25\%}$

TABLE 2.7 – Features used by the BDTE algorithm. pe and ht reference the charge and hit-time distribution respectively and the percentages are the quantiles of those distributions. cht and cc reference the barycenters of hit time and charge respectively

691 A second and more advanced BDT, subsequently named BDTE, that only reconstruct energy use a
 692 different set of features [43]. They are presented in the table 2.7

693 Neural Network (NN)

694 The physics have shown a rising for Neural Network (NN) in the past years for event reconstruction,
 695 notably in the neutrino community [44–47]. Three type of neural networks have explored for event
 696 reconstruction in JUNO Deep Neural Network (DNN), Convolutional Neural Network (CNN) and
 697 Graph Network (GNN). More explanation about those neural network can be found in chapter 3.

700 The CNN are using 2D projection of the detector representing it as an image with two channel, one
 701 for the charge Q and one for the time t . The position of the PMTs is structurally encoded in the pixel
 702 containing the information of this PMT. In [42], the pixel is chosen based on a transformation of θ
 703 and ϕ coordinates to the 2D plane and rounded to the nearest pixel. A sufficiently large image has
 704 been chosen to prevent two PMT to be located in the same pixel. An example of this projection can
 705 be found in figure 2.23. The performances of the CNN can be found in figure 2.24.

706 Using 2D have the upside of encoding a large part of the informations structurally but loose the rotational
 707 invariance of the detector. It also give undefined information to the neural network (what is a
 708 pixel without PMT ? What should be its charge and time ?), cause deformation in the representation
 709 of the detector (sides of projection) and loose topological informations.

710 One of the way to present structurally the sphericity of JUNO to a NN is to use a graph: A collection
 711 of objects V called nodes and relations E called edges, each relation associated to a couple v_1, v_2
 712 forming the graph $G(E, V)$. Nodes and edges can hold informations or features. In [42] the nodes,
 713 are geometrical region of the detector as defined by the HealPix [48]. The features of the nodes are
 714 aggregated informations from the PMTs it contains. The edges contains geographic informations of
 715 the nodes relative positions.

716 This data representation has the advantages to keep the topology of the detector intact. It also permit
 717 the use of rotational invariant algorithms for the NN, thus taking advantage of the symmetries of the
 718 detector.

719 The neural network then process the graph using Chebyshev Convolutions [49]. The performances
 720 of the GNN are presented in figure 2.24.

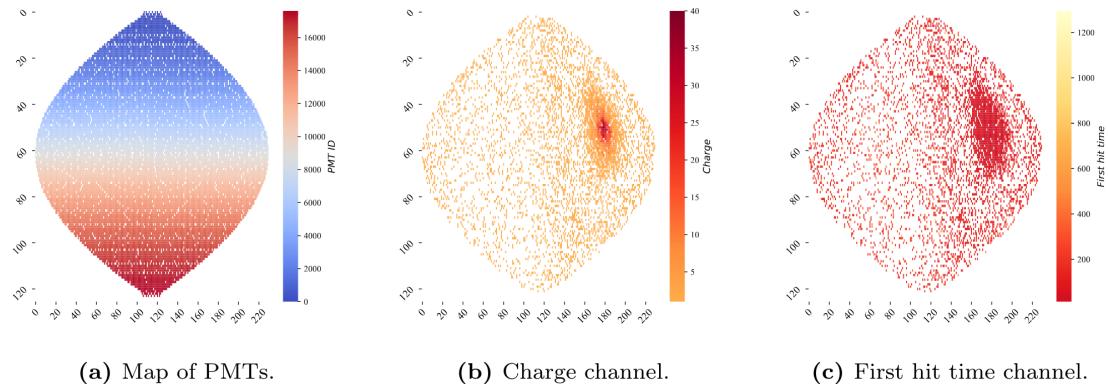


FIGURE 2.23 – Projection of the LPMTs in JUNO on a 2D plane. (a) Show the distribution of all PMTs and (b) and (c) are example of what the charge and time channel looks like respectively

Overall ML algorithms show similar performances as classical algorithms in term of energy reconstructions with the more complex structure CNN and GNN showing better performances than BDT and DNN. For vertex reconstruction, the BDT and DNN show poor performance while CNN are on the level of the classical algorithms.

2.7 JUNO sensitivity to NMO and precise measurements

Now that the event have been reconstructed, selected and that the non-IBD background have been rejected, we have access to the measured energy flux from JUNO. We consider two spectra, the one measured by the LPMT system and the one measured by the SPMT system. This give rise to three possible analysis: A LPMT only analysis, a SPMT only analysis and a joint analysis. This joint analysis is the subject of the chapter 7 of this thesis.

The following details about JUNO measurement is common to the three analysis. The details and specific of the joint analysis are detailed in chapter 7.

2.7.1 Theoretical spectrum

To extract the oscillation parameters and the NMO from the measured spectrum, it is compared to a theoretical spectrum. This theoretical spectrum is produced based on the theory of the three flavour oscillation (see section 1.3), the measurements produced by the calibration, the input from TAO and adjusted Monte Carlo simulations:

- The absolute flux and the fission product fraction yield calibrated by TAO.
 - The estimation of the neutrinos flux from other sources, such as the geoneutrinos, by theoretical model.
 - The computed cross-section of $\bar{\nu}_e$ and the LS.
 - The estimation of mislabelled event, such as fast neutron events from cosmic muons, using Monte Carlo simulation.
 - The measured bias and resolution of the LPMT and SPMT system by the calibration.
 - The time dependent reactor parameters (age of fuel, instantaneous power of the reactors, etc...)
- These systematics parameters come with their uncertainties that need to be taken into account by the fitting framework. This theoretical spectrum will, in the end, depend of the oscillation parameters of

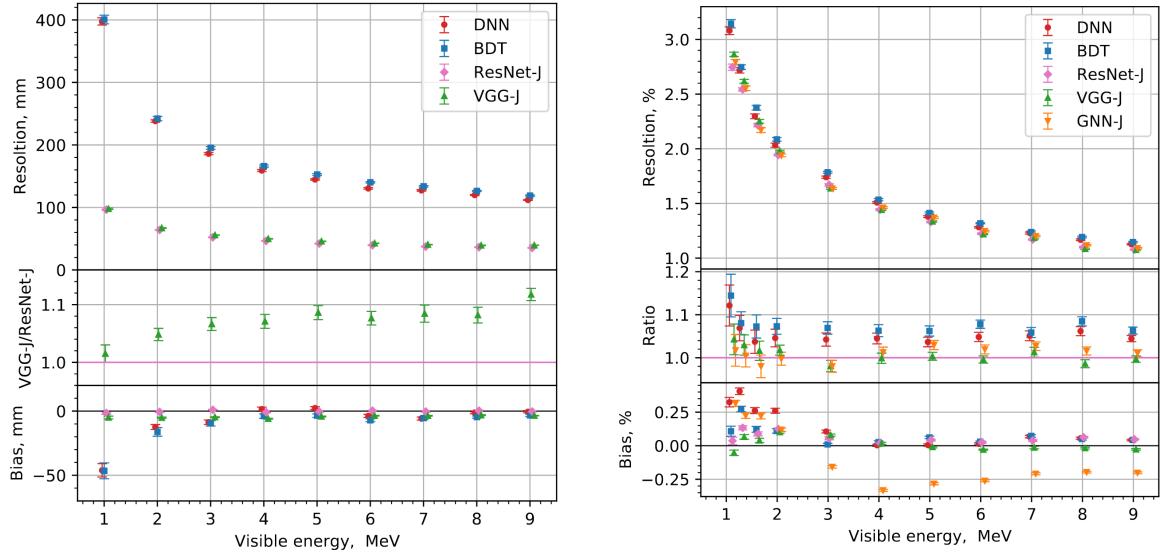


FIGURE 2.24 – Radial (left) and energy (right) resolutions of different ML algorithms. The results presented here are from [42]. DNN is a deep neural network, BDT is a BDT, ResNet-J and VGG-J are CNN and GNN-J is a GNN.

interest $\theta_{13}, \theta_{12}, \Delta m_{21}^2, \Delta m_{31}^2$. Noise parameters can be included in the parameters spectrum such as the earth density ρ between the power plants and JUNO.

2.7.2 Fitting procedure

The theoretical and measured spectra are represented as two histograms depending on the energy. The theoretical spectrum is adjusted with the data using a χ^2 minimization where χ^2 is naively defined as

$$\chi^2 = \sum_i \frac{(N_{th}^i - N_{data}^i)^2}{\sigma_i^2} \quad (2.26)$$

where N_{th}^i is the number event in the i th bin of the theoretical spectrum, N_{data}^i is the number of event in the i th bin of the measured spectrum and σ_i is the uncertainty of this bin. Two classic statistic test exist Pearson and Neyman where the difference is the estimation of σ_i parameters.

This σ_i is composed of the systematics uncertainties discussed above but also from the statistic uncertainty of the spectrum. Considering a Poisson process, the statistic uncertainty is estimated as $\sigma_{stat}^i = \sqrt{N^i}$. In a Pearson test, $N^i \equiv N_{th}^i$ whereas in a Neyman test $N^i \equiv N_{data}^i$. Under the assumption that the content of each bin follow a Gaussian distribution (a Poisson with high enough statistic), the two test are equivalent. But studies on Monte Carlo spectrum showed that the Pearson and Neyman statistic are biased in opposite direction. It is easily visible where, for the same data, Pearson will prefer a higher N_{th}^i to reduce the ration $\frac{1}{N_{th}^i}$ whereas Neyman will prefer a lower N_{th}^i to reduce the $(N_{th}^i - N_{data}^i)$ term.

This problematic can be circumvented by summing the two test, yielding the CNP statistic test and/or by adding a term

$$\chi^2 = \sum_i \frac{(N_{th}^i - N_{data}^i)^2}{\sigma_i^2} - \ln |V| \quad (2.27)$$

where V is the covariance matrix of the theoretical spectrum yielding the PearsonV and CNPV

⁷⁶⁶ statistic test.

⁷⁶⁷ The χ^2 is minimized by exploring the parameter phase space via gradient descent.

⁷⁶⁸ 2.7.3 Physics results

⁷⁶⁹ The oscillation parameters are directly extracted from the minimization procedure and the error can
⁷⁷⁰ be estimated directly from the procedure. For the NMO, the data are fitted under the two assumption
⁷⁷¹ of NO and IO. The difference in χ^2 give us the preferred ordering and the significance of our test.
⁷⁷² Latest studies show that the precision on oscillation parameters after six year of data taking will be
⁷⁷³ of 0.2%, 0.3%, 0.5% and 12.1% for Δm_{31}^2 , Δm_{21}^2 , $\sin^2 \theta_{12}$ and $\sin^2 \theta_{13}$ respectively [11]. The expected
⁷⁷⁴ sensitivity to mass ordering is 3σ after 6 years [50].

⁷⁷⁵ 2.8 Summary

⁷⁷⁶ JUNO is one the biggest new generation neutrino experiment. Its goal, the measurements of oscil-
⁷⁷⁷ lation parameters with unprecedented precision and an NMO preference at the 3 sigma confidence
⁷⁷⁸ level, needs an in depth knowledge and understanding of the detector and the physics at hand. The
⁷⁷⁹ characterisation and calibration of the detector are of the utmost importance and the understanding
⁷⁸⁰ of the detector response in its resolution and bias is capital to be able to correctly carry the high
⁷⁸¹ precision physics analysis of the neutrino oscillation.

⁷⁸² In this thesis, I explore the usage of data-driven reconstruction methods to validate and optimize the
⁷⁸³ reconstruction of IBD events in JUNO in the chapters 4, 5 and 6 and the usage of the dual calorimetry
⁷⁸⁴ in the detection of possible mis-modelisation in the theoretical spectrum 7.

⁷⁸⁵ **Chapter 3**

⁷⁸⁶ **Machine learning and Artificial
Neural Network**

⁷⁸⁸ *"I have the shape of a human being and organs equivalent to those of a
human being. My organs, in fact, are identical to some of those in a
prostheticized human being. I have contributed artistically, literally, and
scientifically to human culture as much as any human being now
alive. What more can one ask?"*

Isaac Asimov, The Complete Robot

⁷⁸⁹ Machine Learning (ML) and more specifically Neural Network (NN) are families of data-driven
⁷⁹⁰ algorithm. They are used to model complex distributions from a finite dataset to extract a generalist
⁷⁹¹ behavior. They learn, adapt their intrinsic parameters, interactively by computing its performance
⁷⁹² or *loss* on those dataset. They take advantage of simple microscopic operation such as *if condition* or
⁷⁹³ non-continuous but differentiable function like *ReLU*. Through optimizers and the combination of a
⁷⁹⁴ lot of those microscopic operations, they can obtain complex and precise behaviours.

⁷⁹⁵ They are now widely used in a wide variety of domain including natural language processing,
⁷⁹⁶ computer vision, speech recognition and, the subject of this thesis, scientific studies.

⁷⁹⁷ We found them in particle physics, either as the main algorithm or as secondary algorithm, for event
⁷⁹⁸ reconstruction, event classification, waveform reconstruction, etc..., domains where the underlying
⁷⁹⁹ physic and detector process is complex and highly dimensional. Physicists have traditionally been
⁸⁰⁰ forced to use simplifications or assumptions to ease the development of algorithms or equations
⁸⁰¹ (a good example is the algorithm presented in section 2.6) where machine learning could refine and
⁸⁰² take into account those effects, provided that they have enough data and computing power.

⁸⁰³ This chapter present an overview of the different kind of machine learning methods and neural
⁸⁰⁴ networks that will be discussed in this thesis.

⁸⁰⁵ **3.1 Boosted Decision Tree (BDT)**

⁸⁰⁶ One of the most classic machine learning algorithm used in particle physics is Boosted Decision Tree
⁸⁰⁷ (BDT) [51] (or more recently Gradient Boosting Machine [52]). The principle of a BDT is fairly simple
⁸⁰⁸ : based on a set of observables, a serie of decisions, represented as node in a tree, are taken by the
⁸⁰⁹ algorithm. Each decision point, or node, takes its decision based on a set of trainable parameters
⁸¹⁰ leading to a subtree of decision. The process is repeated until it reach the final node, yielding the
⁸¹¹ prediction. A simplistic example is given in figure 3.1.

⁸¹² The training procedure follow a simple score reward procedure. During the training phase the
⁸¹³ prediction of the BDT is compared to a known truth about the data. The score is then used to

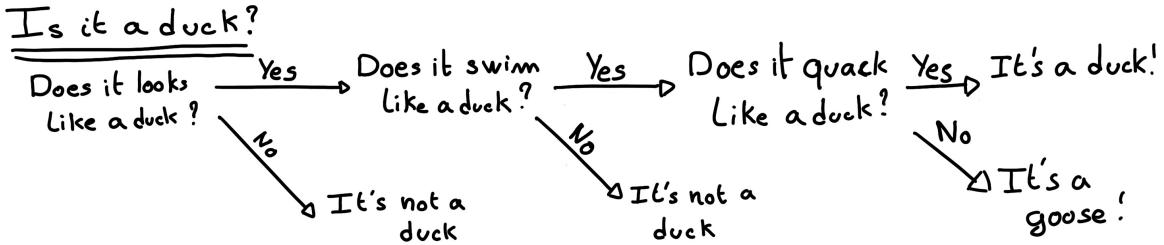


FIGURE 3.1 – Example of a BDT that determine if the given object is a duck

814 backpropagate corrections to the parameters of the tree. Modern BDT use gradient boosting where
 815 the gradient of the loss is calculated for each of the BDT parameters. Following the gradient descent,
 816 we can reach the, hopefully, global minima of the loss for our set of parameters.

817 3.2 Artificial Neural Network (NN)

818 One other big family of machine learning algorithm is the artificial Neural Networks (NN). The idea
 819 of developing automates which component mimic, in a simplistic way, the behavior of biological
 820 neurons emerge in 1959 with the paper “*What the Frog’s Eye Tells the Frog’s Brain*” [53]. They develop
 821 an automate where each component possess an *activation function*. Each one of those component then
 822 transmit its information to the other following a certain efficiency or *weight*. Those works influenced
 823 scientist and notably Frank Rosenblatt who published in 1958 what is considered the first neural
 824 network model the Perceptron [54].

825 Modern neural network still nowadays use the neuron metaphor to represent neural network, but
 826 approach them as a graph where the nodes are neurons possessing an activation function and edges
 827 holding the weights, or *parameters* in modern literature, between those nodes. Most of the modern
 828 neural network work with the principle of neurons layers. Each neurons belong to a layer and takes
 829 input from the preceding layer and forward it result to next layer. For example the most basic set
 830 layer is the fully connected layer where each of its neurons is connected to every other neurons of
 831 the precessing layer. All the neurons posses the same activation function F . The connection between
 832 two the two layers is expressed as a tensor T_j^i where i is the index of the precedent layer and j the
 833 index of the current layer. The propagation from the layer I to J is then described as

$$J_j = F_j(T_j^i I_i + B_j) \quad (3.1)$$

834 where the learning parameters are the tensor T_j^i and the bias tensor B_j . This is the fundamental
 835 component of the Fully Connected Deep NN (FCDNN) family presented in section 3.2.1. Most of the
 836 modern neural networks use gradient descent to optimize their parameters, i.e. the gradient of the
 837 parameter θ in respect of the loss function \mathcal{L} is subtracted to it

$$\theta_{i+1} = \theta_i - \frac{\partial \mathcal{L}}{\partial \theta} \quad (3.2)$$

838 i being the training iteration index. This needs the expression of \mathcal{L} dependent of θ to be differentiable,
 839 thus the layer and their activation function also need to be differentiable. This simple gradient
 840 descent, designated as Stochastic Gradient Descent (SGD), can be completed with first and second
 841 order momentum like with the Adam optimizer [55] (more details in section 3.2.5).

842 This description of neural networks as layer introduced the principle of *depth* and *width*, the number
 843 of layers in the NN and the number of neurons in each layer respectively. Those quantities that not

844 directly used for the computation of the results but describe the NN or its training are designated as
 845 *hyperparameters*.

846 The loss \mathcal{L} described above is a score representing how well the NN is doing. As seen above, it
 847 needs to be differentiable with respect to the parameter of the NN. Depending if we try to minimize
 848 or maximize it, it need to posses a minima or a maxima. For example when doing *regression*, i.e.
 849 produce a scalar result, a common loss is the Mean Square Error (MSE). Let i be our dataset, y_i be the
 850 target scalar, x_i the input data and $f(x_i, \theta)$ the result of the network. The network here is modelled by
 851 f , and its parameter by the set

$$\mathcal{L} := MSE = \frac{1}{N} \sum_i^N (y_i - f(x_i))^2 \quad (3.3)$$

852 Another common loss function is the Mean Absolute Error (MAE)

$$\mathcal{L} := MAE = \frac{1}{N} \sum_i^N |y_i - f(x_i)| \quad (3.4)$$

853 3.2.1 Fully Connected Deep Neural Network (FCDNN)

854 Fully Connected Deep Neural Network (FCDNN) architecture is the natural evolution of the Perceptron.
 855 The input data is represented as a first order tensor I_j and then fed forward to multiple fully
 856 connected layers (Eq 3.1) as presented in the figure 3.2a. Most of the time, the classic ReLU function

$$\text{ReLU}(x) = \begin{cases} x & \text{if } x \geq 0 \\ 0 & \text{otherwise} \end{cases} \quad (3.5)$$

857 is used as activation function. Prelu and Sigmoid are also popular choices:

$$\text{Sigmoid}(x) = \frac{1}{1 + e^{-x}} \quad (3.6) \quad \text{PReLU}(x) = \begin{cases} x & \text{if } x \geq 0 \\ \alpha x & \text{otherwise} \end{cases} \quad (3.7)$$

858 The reasoning behind ReLU and PReLU is that with enough of them, you can mimic any continuous
 859 function as illustrated in figure 3.2b. Sigmoid is more used in case of classification, its behavior going
 860 hand in hand with the Cross Entropy loss function used in classification problems.

861 Due to its simplicity, FCDNN are also used as basic pieces for more complex architectures such as
 862 the CNN and GNN that will be presented in the next section.

864 3.2.2 Convolutional Neural Network (CNN)

865 Convolutional Neural Networks are a family of neural networks that use discrete convolution filters,
 866 as illustrated in an example in figure 3.3, to process the input data, often images. They have the
 867 advantage to be translation invariant by construction, this mean that they are capable of detecting
 868 oriented features independently of their location on the image. The learning parameters are located
 869 in the filters, the network thus learn the optimal filters to extract the desired features. 2D CNN,
 870 where the filters are second order tensors that span over third order tensors, are commonly used in
 871 image recognition [56] for classification or regression problematics.

872 The convolution layers are commonly chained [57], reducing the input dimension while increasing
 873 the number of filters. The idea behind is that the first layers will process local informations and the
 874 latest layers will process more global informations. To try to preserve the amount of information, we
 875 tend to double the numbers of filters for each division of the input data. The results of the convolution

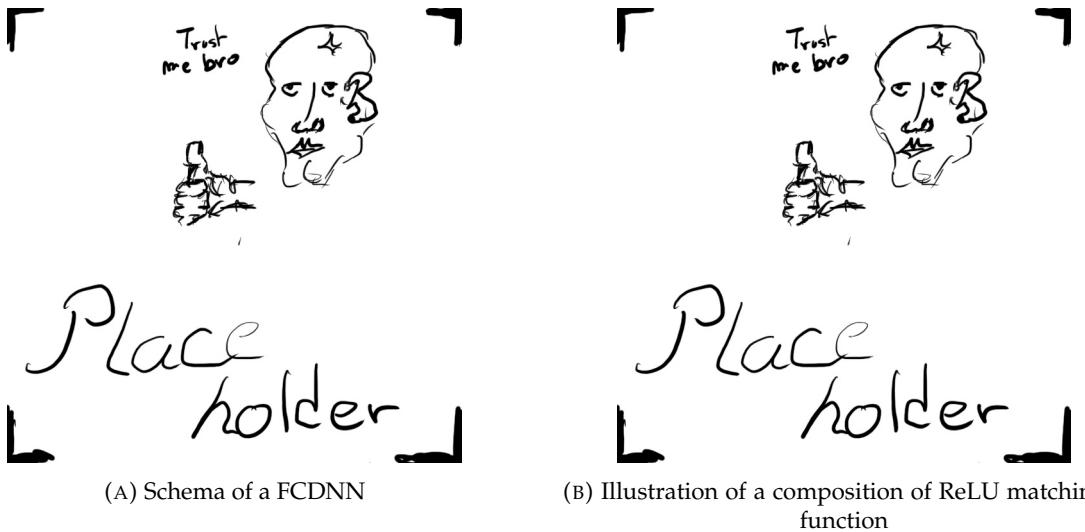


FIGURE 3.2

⁸⁷⁶ filters is commonly then flattened and feed to a smaller FCDNN which will process the filters results
⁸⁷⁷ to yield the desired output.

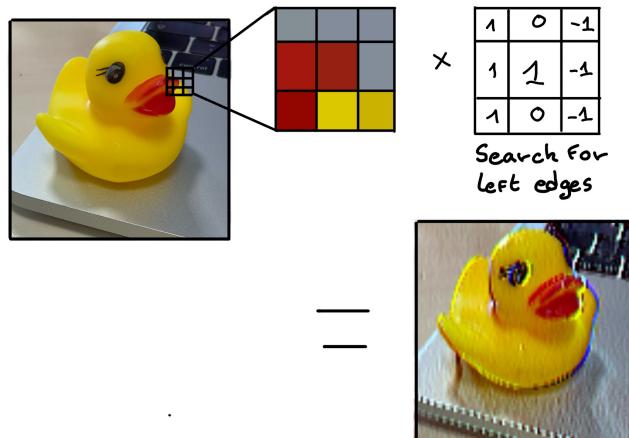


FIGURE 3.3 – Illustration of the effect of a convolution filter. Here we apply a filter with the aim do detect left edges. We see in the resulting image that the left edges of the duck are bright yellow where the right edges are dark blue indicating the contour of the object. The convolution was calculated using [58].

⁸⁷⁸ As an example, let's take the Pytorch [59] example for the MNIST [60], a dataset of black and white
⁸⁷⁹ images of handwritten digits. Those images are 28×28 pixels with only one channel corresponding
⁸⁸⁰ to the grey level of the pixel. Example of images from this dataset are presented in figure 3.4a

⁸⁸¹ A schema of the CNN used in the Pytorch example is presented in figure 3.4b. Using this schema as
⁸⁸² a reference, the trained network is made of:

- ⁸⁸³ 1. A convolutional layer of (3×3) filters yielding 32 channels. A bias parameter is applied
⁸⁸⁴ to each channel for a total of $(32 \cdot (3 \times 3) + 32) = 320$ parameters. The resulting image is
⁸⁸⁵ $(26 \times 26 \times 32)$ (26 per 26 pixels with 32 channels). The ReLU activation function is applied to
⁸⁸⁶ each pixel.
- ⁸⁸⁷ 2. A second convolutional layer of (3×3) filters yielding 64 channels. This channel also posses

888 a bias parameter for a total of $(64 \cdot (3 \times 3) + 64) = 640$ parameters. Resulting image is $(24 \times$
 889 $24 \times 64)$. Also with with a ReLU activation function.

890 3. Then comes a (2×2) max pool layer with a stride of 1 meaning that for each channel the max
 891 value of pixels in a (2×2) block is condensed in a single resulting pixel. The resulting image
 892 is $(12 \times 12 \times 64)$.

893 4. This image goes through a dropout layer which will set the pixel to 0 with a probability of
 894 0.25. This help prevent overtraining of the neural network (see section 3.2.6 for more details).

895 5. The data is the flattened i.e. condensed into a vector of $(12 \times 12 \times 64) = 9216$ values.

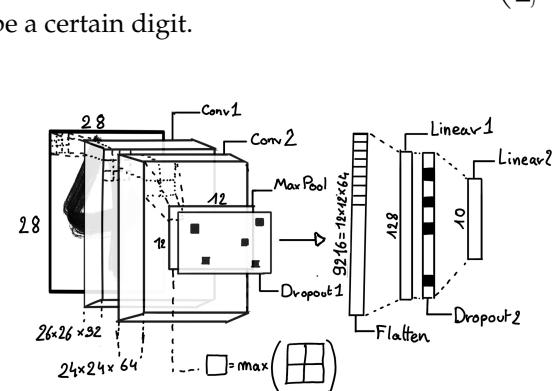
896 6. Then comes a fully connected linear layer (Eq. 3.1) with a ReLU activation that output 128
 897 feature. It needs $(9216 \cdot 128) + 128 = 1'179'776$ parameters.

898 7. This 128 item vector goes through another dropout layer with a probability of 0.5

899 8. The vector is then transformed through a linear layer with ReLU activation. It output 10
 900 values, one for each digit class $(0, 1, 2, \dots, 9)$. It need $(128 \cdot 10) + 128 = 1408$ parameters.

901 9. Finally the 10 values are normalized using a log softmax function $\text{LogSoftmax}(x_i) = \log \left(\frac{\exp(x_i)}{\sum_j \exp(x_j)} \right)$
 902 to give the probability of the input image to be a certain digit.

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4
 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5
 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6
 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7
 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8
 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9



(A) Example of images in the MNIST dataset

(B) Schema of the CNN used in Pytorch example to process the MNIST dataset

FIGURE 3.4

903 The final network needs 1'182'144 parameters or, if we consider each parameters to be a double
 904 precision floating point, 9.45 MB of data. To gives a order of magnitude, such neural network is
 905 considered "simple", train in a matter of minutes on T4 GPU [61] (14 epochs) and reach an accuracy
 906 in its prediction of 99%.

907 3.2.3 Graph Neural Network (GNN)

908 Graph neural network is a family of neural network where the data is represented as a graph $G(\mathcal{N}, \mathcal{E})$
 909 composed of vertex or node $n \in \mathcal{N}$ and edges $e \in \mathcal{E}$. The edges are associated to two nodes $(u, v) \in$
 910 \mathcal{N}^2 , "connecting" them. The node and the edges can hold features, commonly represented as vector
 911 $n \in \mathbb{R}^{k_n}$, $e \in \mathbb{R}^{k_e}$. We can thus define a graph using two tensors A_e^{ij} the adjacency tensors that hold
 912 the features e of the edge connecting the node i and j and the tensor N_v^i that hold the features v of a
 913 node i .

914 To efficiently manipulate such object we need to structurally encode their property in the neural
 915 network architecture: each node is equivalent (as opposite to ordered data in a vector), each node has
 916 a set of neighbours, ... One of this method is the message passing algorithm presented historically

917 in “Neural Message Passing for Quantum Chemistry” [62]. In this algorithm, with each layer of
 918 message passing a new set of features is computed for each node following

$$n_i^{k+1} = \phi_u(n_i^k, \square_j \phi_m(n_i^k, n_j^k, e_{ij}^k)); n_j \in \mathcal{N}'_i \quad (3.8)$$

919 where ϕ_u is a differentiable update function, \square_j is a differentiable aggregation function and ϕ_m is a
 920 differentiable message function. $\mathcal{N}'_i = \{n_j \in \mathcal{N} | (n_i, n_j) \in \mathcal{E}\}$ is the set of neighbours of n_i , i.e. the
 921 nodes n_j from which it exist an edge $e_{ij} \rightarrow (n_i, n_j)$. k is the layer on which the message passing
 922 algorithm is applied. \square need also a few other property if we want to keep the graph property, most
 923 notably the permutational invariance of its parameters (example: mean, std, sum, ...).

924 The edges features can also be updated, either by directly taking the results of ϕ_m or by using another
 925 message function ϕ_e .

926 Message passing is a very generic way of describing the process of GNN and it can be specialized
 927 for convolutional filtering [49], diffusion [63] and many other specific operation. GNN are used in a
 928 wide variety of application such as regression problematics, node classification, edge classification,
 929 node and edge prediction, ...

930 It is a very versatile but complex tool.

931 3.2.4 Adversarial Neural Network (ANN)

932 The adversarial machine learning, Adversarial Neural Networks (ANN) in the case of neural net-
 933 work, is a family of unsupervised machine learning algorithms where the learning algorithm (gen-
 934 erator) is competing against another algorithm (discriminator). Taking the example of Generative
 935 Adversarial Networks, concept initially developed by Goodfellow et al. [64], the discriminator goal
 936 is to discriminate between data coming from a reference dataset and data produced by the generator.
 937 The generator goal, on the other hand, is to produce data that the discriminator would not be able to
 938 differentiate from data from the reference dataset. The expression of duality between the two models
 939 is represented in the loss where, at least a part of it, is driven by the results of the discriminator.

940 3.2.5 Training procedure

941 A neural network without the adequate training is like an empty shell. If the parameters are not
 942 optimized they are, most of the time, initialized to random number and so the output will just be
 943 random. The training is a key step in the production of a solid and reliable NN. This section aim to
 944 give an overview of the different concept and tools used in the training of our neural networks.

945 Training lifecycle

946 The training of NN does not follow strict rules, you could imagine totally different lifecycle but I will
 947 describe here the one used in this thesis, the most common one.

948 The training is split into *epochs* during which the NN will train on a set of subsamples called *batch*.
 949 The size of those batch is called *batch size*, a.k.a. the number of data it contains (how many images,
 950 how many events,...). Each process of a batch is called a *step*. At the end of each epochs, the neural
 951 network is evaluated over a validation dataset. This validation dataset is not used for training (no
 952 gradient of the loss is computed) and is used as reference for the network performance and monitor
 953 overtraining (see section 3.2.6). Most of the time, the parameters are updated at each step using the
 954 mean loss over the batch and the optimizer hyperparameters are updated at each epochs.

955 **The optimizer**

956 As briefly introduced section 3.2, the parameters of the neural network are optimized using the
 957 gradient descent method. We calculate the gradient of the mean loss over the batch with respect
 958 of each parameters and we update the parameters in accord to minimize the loss. The gradient is
 959 computed backward from the loss up to the first layer parameters using the chain rule:

$$\frac{\partial \mathcal{L}}{\partial \theta_1} = \frac{\partial \theta_2}{\partial \theta_1} \frac{\partial \mathcal{L}}{\partial \theta_2} = \frac{\partial \theta_2}{\partial \theta_1} \frac{\partial \theta_3}{\partial \theta_2} \frac{\partial \mathcal{L}}{\partial \theta_3} = \frac{\partial \theta_2}{\partial \theta_1} \prod_{i=2}^{N-1} \frac{\partial \theta_{i+1}}{\partial \theta_i} \frac{\partial \mathcal{L}}{\partial \theta_N} \quad (3.9)$$

960 where θ is a parameter, i is the layer index. We see here that the gradient of the first layer is dependent
 961 of the gradient of all the following layers. We thus need to compute the gradient closest to loss first
 962 before computing the gradient of the earlier layers. This is called the *backward propagation*.

963 This update of the parameters is done following an optimizer policy. Those optimizers depends on
 964 hyperparameters. The ones used in this thesis are:

- 965 1. SGD (Stochastic Gradient Descent). This is the simplest optimizer, it depend on only one
 966 hyperparameter, the learning rate λ (LR) and update the parameters θ following

$$\theta_{t+1} = \theta_t - \lambda \frac{\partial \mathcal{L}}{\partial \theta} \Big|_{\theta_t} \quad (3.10)$$

967 where t is the step index. It is a powerful optimizer but is very sensible to local minima of the
 968 loss in the parameters phase space as illustrated in figure 3.5a.

- 969 2. Adam [55]. The concept is, in short, to have and SGD but with momentum. Adam possess
 970 two momentum $m(\beta_1)$ and $v(\beta_2)$ which are respectively proportional to $\frac{\partial \mathcal{L}}{\partial \theta}$ and $(\frac{\partial \mathcal{L}}{\partial \theta})^2$. β_1
 971 and β_2 are hyperparameters that dictate the moment update at each optimization step. The
 972 parameters are then upgraded following

$$m_{t+1} = \beta_1 m_t + (1 - \beta_1) \frac{\partial \mathcal{L}}{\partial \theta} \quad (3.11)$$

$$v_{t+1} = \beta_2 v_t + (1 - \beta_2) \left(\frac{\partial \mathcal{L}}{\partial \theta} \right)^2 \quad (3.12)$$

$$\theta_{t+1} = \theta_t - \lambda \frac{m_{t+1}}{\sqrt{v_{t+1}} + \epsilon} \quad (3.13)$$

969 where ϵ is a small number to prevent divergence when v is close to 0. These momentums
 970 allow to overcome small local minima in the parameters phase space as illustrated in figure
 971 3.5a.

972 The LR is a crucial parameter in the training of NN, as illustrated in figure 3.6. To prevent possible
 973 issues, we setup scheduler policies.

974 **Scheduler policies**

975 Sometimes we want to update our hyperparameters or take a set of action during the training
 976 procedure. We use for this scheduler policies, for example a common policy is a decrease of the
 977 learning rate after each epochs. The reasoning is that if the learning rate is too high, the optimizer
 978 will continuously miss the minimum and oscillate around it (figure 3.6a). By reducing the learning
 979 rate, we allow it to make more fine steps in the parameters phase space, hopefully converging to the
 980 true minima.

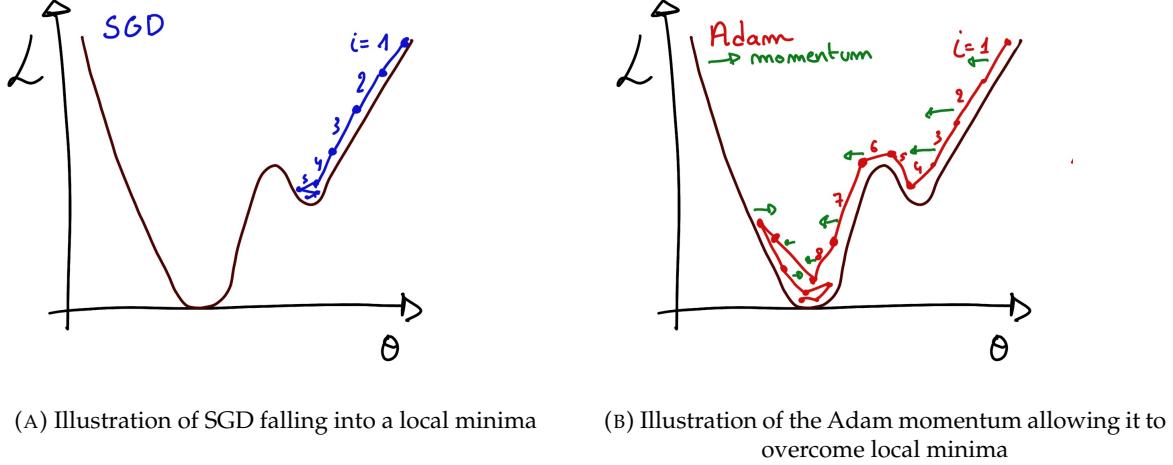


FIGURE 3.5

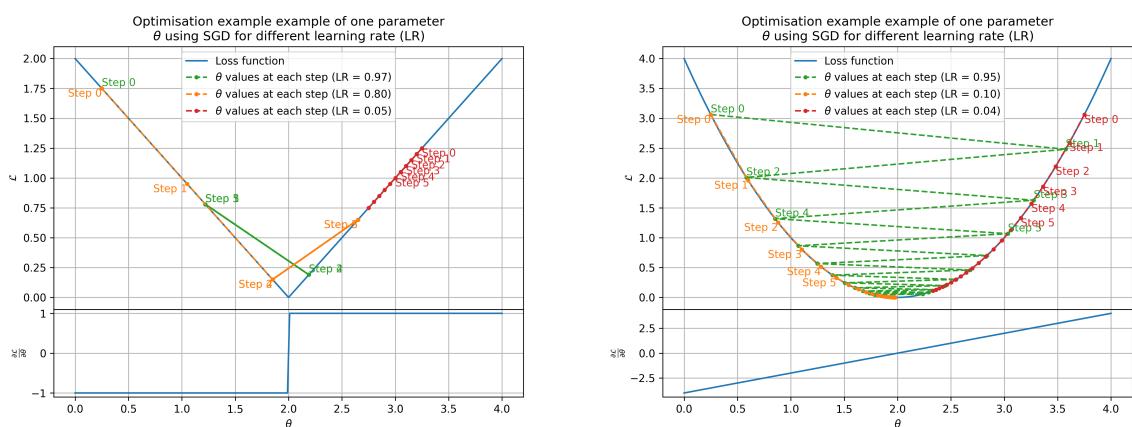
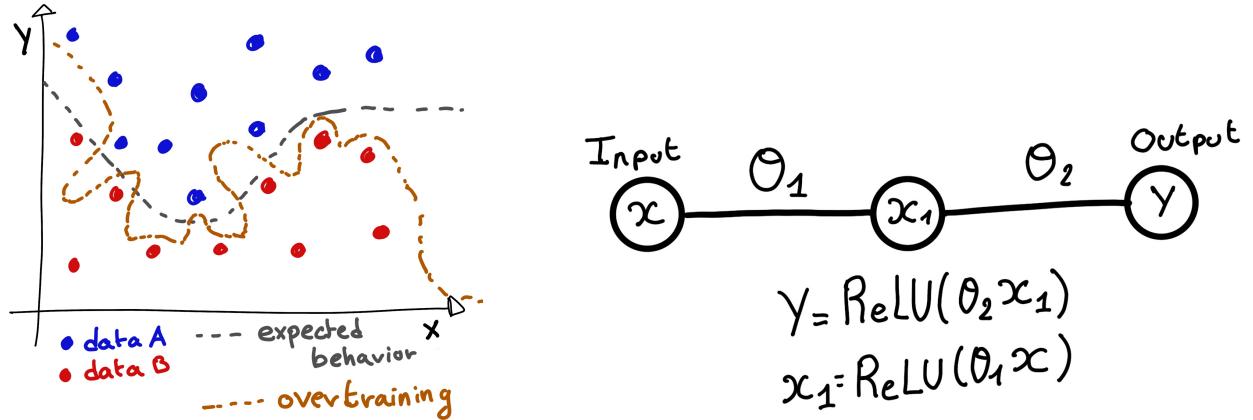


FIGURE 3.6 – Illustration of the SGD optimizer. In blue is the value of the loss function, orange, green and red are the path taken by the optimized parameter during the training for different LR.



(A) Illustration of overtraining. The task at hand is to determine depending on two input variable x and y if the data belong to the dataset A or the dataset B . The expected boundary between the two dataset is represented in grey. A possible boundary learnt by overtraining is represented in brown.

(B) Illustration of a very simple NN

FIGURE 3.7

981 Another policy that is often used is the save of the best model. In some situations, the loss value after
 982 each epoch will strongly oscillate or even worsen. This policy allows us to keep the best version
 983 of the model attained during the training phase.

984 3.2.6 Potential pitfalls

985 Apart from being stuck in local minima, there are also other behaviors and effects we want to prevent
 986 during training.

987 Overtraining

988 This happens when the network learns the specificities of the training dataset instead of a more general
 989 representation of the underlying data distribution. This can happen if there is not enough data
 990 in comparison to the number of learning parameters, if the data contains some specific signatures
 991 specific to the training dataset or if it trains for too long on the same dataset. This behavior is illustrated
 992 in figure 3.7a. Overtraining can be fought in multiple ways, for example:

- 993 — **More data.** By having more data in the training dataset, the network will not be able to learn the
 994 specificities of every data.
- 995 — **Less parameters.** By reducing the number of parameters, we reduce the computing and
 996 learning capacities of the network. This will force it to fallback to generalist behaviors.
- 997 — **Dropout.** This technique implies to randomly set part of the neural network to 0. By doing
 998 this, we force the redundancy in its computing capability and, in a way, modify the data
 999 decreasing the possibility for specific learning.
- 1000 — **Early stopping.** During the training we monitor the network performance over a validation
 1001 dataset. The network does not train on this dataset and thus cannot learn its specificities. If
 1002 the loss on the training dataset diverges too much from the loss on the validation dataset, we
 1003 can stop the training earlier to prevent it from overtraining.

1004 **Gradient vanishing**

1005 Gradient vanishing is the effect of the gradient being so small for the upper layer that the parameters
 1006 are barely updated after each step. This cause the network to be unable to converge to the minima.

1007 This comes from the way the gradient descent is calculated. Imagine a simple network composed of
 1008 three fully connected layers: the input layer, a intermediate layer and the output layer. Let L be the
 1009 loss, θ_1 the parameter between the input and the intermediate layer and θ_2 the parameter between
 1010 the intermediate and output layer. This network is schematized in figure 3.7b.

1011 The gradient for θ_1 will be computed using the chain rule presented in equation 3.9. Because θ_1
 1012 depends on θ_2 , if the gradient of θ_2 is small, so will be the gradient of θ_1 . Now if we would have
 1013 much more layer, we can see how the subsequent multiplication of small gradients would lead to
 1014 very small update of the parameters thus "vanishing gradient".

1015 Multiple actions can be taken to prevent this effect such as:

- 1016 — **Batch normalization:** In this case we apply a normalization layer that will normalize the data
 1017 so that, let D be the data, $\langle D \rangle = 0$ and $\sigma_D = 1$. This help the weight of the network to
 1018 maintain an appropriate scale.
- 1019 — **Residual Network (ResNet) [65]:** Residual network is a technique for neural network in
 1020 which, instead of just sequentially feeding the results of each layer to the next one, you ask
 1021 each layer to calculate the residual of the input data. This technique is illustrated in figure 3.8.

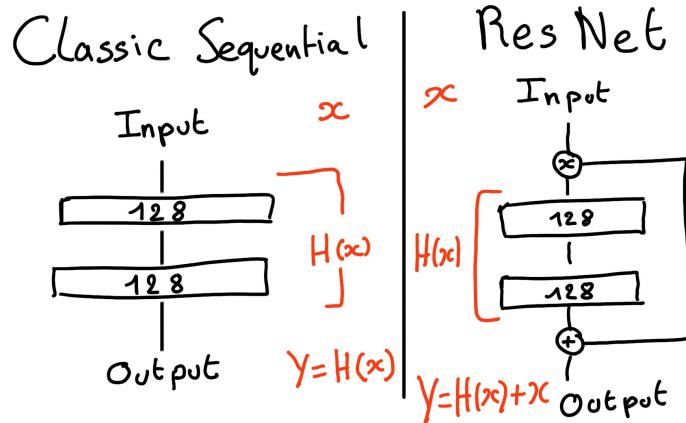


FIGURE 3.8 – Illustration of the ResNet framework

1022 **Gradient explosion**

Gradient explosion happens when the consecutive multiplication of gradient cause exponential grow in the parameter value or if the training lead the network in part of the parameter space where the gradient is significantly higher than usual. For illustration, consider that the loss dependency in θ follow

$$\mathcal{L}(\theta) = \frac{\theta^2}{2} + e^{4\theta}$$

$$\frac{\partial \mathcal{L}}{\partial \theta} = \theta + 4e^{4\theta}$$

1023 The explosion is illustrated in figure 3.9 where we can see that the loss degrade with each step of
 1024 optimization. In this illustration it is clear that reducing the learning rate suffice but this behaviour
 1025 can happens in the middle of the training where the learning rate schedule does not permit reactivity.

1026 There exist solutions to prevent this explosions:

- 1027 — **Gradient clipping:** In this case we work on the gradient so that the norm of gradient vector
 1028 does not exceed a certain threshold. In our illustration in figure 3.9 the gradient for $\theta > 0$
 1029 could be clipped at 3 for example.
- 1030 — **Batch normalization:** For the same reasons as for gradient vanishing, normalizing the input
 1031 data help reduce erratic behaviour.

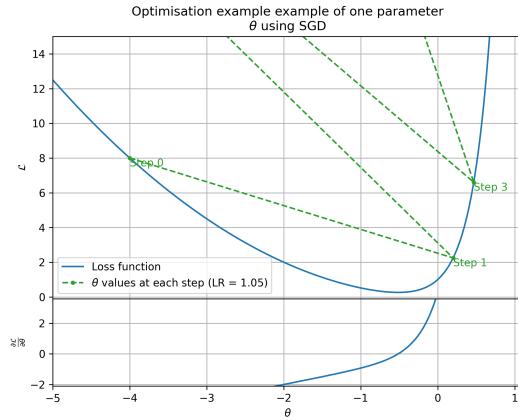


FIGURE 3.9 – Illustration of the gradient explosion. Here it can be solved with a lower learning rate but its not always the case.

1032 **Chapter 4**

1033 **Image recognition for IBD
reconstruction with the SPMT system**

1034 *Dave - Give me the position and momentum, HAL.*

HAL - I'm afraid I can't do that Dave.

Dave - What's the problem ?

HAL - I think you know what the problem is just as well as I do.

Dave - What are you talking about, HAL?

HAL - $\sigma_x \sigma_p \geq \frac{\hbar}{2}$

1035 As explained in chapter 2, JUNO is an experiment composed of two systems, the Large Photomultiplier (LPMT) system and the Small Photomultiplier (SPMT) system. Both of them observe the same physics events inside of the same medium but they differ in their photo-coverage, respectively 75.2% and 2.7%, their dynamic range (see section 2.2.2), a thousands versus a few dozen, and their front-end electronics (see section 2.2.2).

1041 They are complementary in their strengths and weaknesses and support each other, this is what we call *Dual Calorimetry*. One important point is their differences in expected resolution, the LPMT 1042 system outperform largely the SPMT system but is subject to effects such as charge non linearity [29] 1043 that could bias the reconstruction. Effects that the SPMT system is impervious to. This topic will 1044 be studied in more detail in chapter 7. Also, due to the dynamic range of the LPMT, in case of high 1045 energy and high density event such as core-collapse supernova, the LPMT system could saturate and 1046 the lower photo-coverage become a benefit.

1048 Thus, although event reconstruction algorithm and physics analysis combines both LPMT and SPMT 1049 systems, individual approach are key studies to understand the detector and ensure their reliability. 1050 This topic will also be studied in more details in chapter 7. The subject of this chapter is to propose 1051 a machine learning algorithm for the SPMT reconstruction based on Convolutional Neural Network 1052 (CNN).

1053 **4.1 Motivations**

1054 As explained in chapter 3, Machine Learning (ML) algorithms shine when modeling highly dimensional 1055 data from a given dataset. In our case, we have access to complete monte-carlo simulation of 1056 our detector to produce arbitrary large datasets that could represent multiple years of data taking. 1057 Ideally ML algorithms would be able to consider the entirety of the information in the detector and 1058 converge on the best parameters to yield optimal results, while classical methods could be biased by 1059 the prior knowledge of the detector and physics processes. To study this potential phenomena, we

1060 will compare our machine algorithm to a classical reconstruction method developed for energy and
 1061 vertex reconstruction [66].

1062 We have access to a very detailed simulation of the detector (section 2.5) that will allow us to simulate
 1063 arbitrary large dataset while giving access to all the physics parameters of the event. Those
 1064 parameters include the target of our reconstruction algorithms: the vertex and energy of our event.
 1065 As introduced above, we hope that the ML algorithm will be able to use all the informations in the
 1066 event, but that could lead that potential mismodelings in our simulation could be exploited by the
 1067 algorithm. This specific subject will be studied in chapter 6.

1068 4.2 Method and model

1069 One of simplest way to look at JUNO data is to consider the detector as an array of geometrically
 1070 distributed sensors on a sphere. Their repartition is almost homogeneous, on this sphere surface
 1071 providing an almost equal amount of information per unit surface on this sphere. It is then tempting
 1072 to represent the detector as a spherical image with the PMTs in place of pixels. Two events with two
 1073 different energy or position would produce two different images.

1074 The most common approach in machine learning for image processing and image recognition is the
 1075 Convolutional Neural Network (CNN). It is widely used in research and industry [57, 67–69] due to
 1076 its strengths (see section 3.2.2) and has proven its relevance in image processing.

1077 Some CNN are developed to process spherical images [70] but for the sake of simplicity and as a
 1078 first approach we decided to go with a planar projection of the detector, approach that has proven its
 1079 efficiency using the LPMT system (see section 2.6.3). The details about this planar projection will be
 1080 discussed in section 4.2.2.

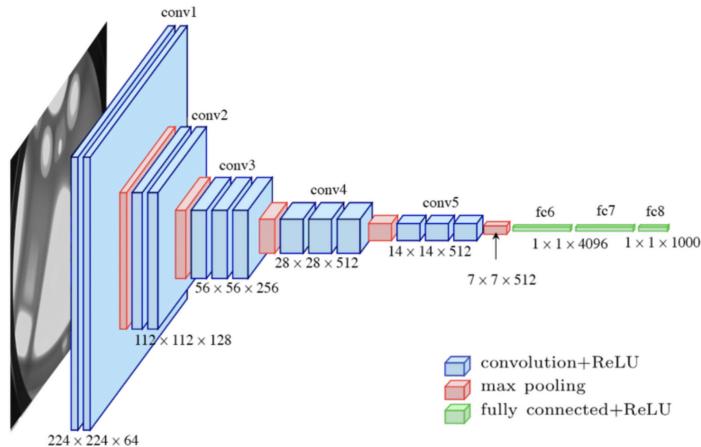


FIGURE 4.1 – Graphic representation of the VGG-16 architecture, presenting the different kind of layer composing the architecture.

1081 4.2.1 Model

1082 The architecture we use is derived from the VGG-16 architecture [57] illustrated in figure 4.1. We
 1083 define a set of hyperparameters that will define the size, complexity and computational power of the
 1084 NN. The chose hyperparameters are detailed below and their values are presented in table 4.1.

- 1085 — **N_{blocks}**: the number of convolution blocks, a block being composed of two convolutional
1086 layers with 3×3 filters using ReLU activation function, a 3×3 max-pooling layer (except for
1087 the last block).
- 1088 — **N_{channels}**: The number of channels in the first block. The number of channels in the subse-
1089 quent blocks is computed using $N_{\text{channels}}^i = i * N_{\text{channels}}$, $i \in [1..N_{\text{blocks}}]$.
- 1090 — **FCDNN configuration**: The result of the last convolution layer is flattened then fed to a
1091 FCDNN. Its configuration is expressed as a sequence of fully connected linear layer using
1092 the PReLU activation function. For example $2 * 1024 + 2 * 512$ is the sequence of 2 layers
1093 with a width of 1024 followed by 2 other layers with a width of 512. Finally the last layer
1094 is a 4 neurons wide linear layers without activation function. Each neurons of the last layer
1095 represent a component of the interaction vertex: Energy, X, Y, Z.
- 1096 — **Loss**: The loss function. In this work we study two different loss function ($E + V$) and ($E_r +$
1097 V_r) detailed below.

$$(E + V)(E, x, y, z) = \left\langle (E - E_{\text{true}})^2 + 0.85 \sum_{\lambda \in [x, y, z]} (\lambda - \lambda_{\text{true}})^2 \right\rangle \quad (4.1)$$

$$(E_r + V_r)(E, x, y, z) = \left\langle \frac{(E - E_{\text{true}})^2}{E_{\text{true}}} + \frac{10}{R} \sum_{\lambda \in [x, y, z]} (\lambda - \lambda_{\text{true}})^2 \right\rangle \quad (4.2)$$

1098 where R is the radius of the CD. With the energy in MeV and the distance in meters, we use the factor
1099 0.85 and 10 to equilibrate the two term of the loss function so they have the same magnitude.

- 1100 — The loss function ($E + V$) is close to a simple Mean Squared Error (MSE). MSE is one of the
1101 most basic loss function, the derivative is simple and continuous in every point. It is a strong
1102 starting point to explore the possibility of CNNs.
- 1103 — $(E_r + V_r)$ can be seen as a relative MSE.

1104 The idea is that: due to the inherent statistic uncertainty over the number of collected Number of
1105 Photo Electrons (NPE), the absolute resolution $\sigma(E - E_{\text{true}})$ will be larger at higher energy than at
1106 low energy. But we expect the *relative* energy resolution $\frac{\sigma(E - E_{\text{true}})}{E_{\text{true}}}$ to be smaller at high energy than
1107 lower energy as illustrated in figure 2.22. Because of this, by using simple MSE the most important
1108 part in the loss come from the high energy part of the dataset whereas with a relative MSE, the
1109 most important part become the low energy events in the dataset. We hope that by using a relative
1110 MSE, the neural network will focus on low energy events where the reconstruction is considered the
1111 hardest.

1112 Each combination of those hyperparameters (for example ($N_{\text{blocks}} = 2, N_{\text{channels}} = 32$, FCDNN =
1113 $(2 * 1024)$, Loss = $(E + V)$)), subsequently designated as configurations, is then tested and compared
1114 to each other over an analysis sample.

1115 On top those generated models, we define 4 hand tailored models:

- 1116 — “gen_0”: $N_{\text{blocks}} = 4, N_{\text{channels}} = 64$, FCDNN configuration: $1024 * 2 + 512 * 2$, Loss := $E + V$
- 1117 — “gen_1”: $N_{\text{blocks}} = 4, N_{\text{channels}} = 64$, FCDNN configuration: $1024 * 2 + 512 * 2$, Loss := $E_r + V_r$
- 1118 — “gen_2”: $N_{\text{blocks}} = 5, N_{\text{channels}} = 64$, FCDNN configuration: $4096 * 2 + 1024 * 2$, Loss := $E + V$
- 1119 — “gen_3”: $N_{\text{blocks}} = 5, N_{\text{channels}} = 64$, FCDNN configuration: $4096 * 2 + 1024 * 2$, Loss := $E_r + V_r$

1120 We cannot use the mean loss because we consider multiple loss functions, there is no guarantee that
1121 comparison of their numerical value will be meaningful. We use multiple observables to rank the
1122 performances of each configuration:

- 1123 — The mean absolute energy error $\langle E \rangle = \langle |E - E_{\text{true}}| \rangle$. It is an indicator of the energy bias of our
1124 reconstruction.
- 1125 — The standard deviation of the energy error $\sigma E = \sigma(E - E_{\text{true}})$. This the indicator on our
1126 precision in energy reconstruction.
- 1127 — The mean distance between the reconstructed vertex and the true vertex $\langle V \rangle = \langle |\vec{V} - \vec{V}_{\text{true}}| \rangle$.
1128 This an indicator of the bias and precision of our vertex reconstruction.

N_{blocks}	{2, 3, 4}
$N_{channels}$	{32, 64, 128}
FCDNN configurations	2 * 1024 2 * 2048 + 2 * 1024 3 * 2048 + 3 * 512 2 * 4096
Loss	{ $E + V, E_r + V_r$ }

TABLE 4.1 – Sets of hyperparameters values considered in this study

— The standard deviation of the distance between the true and reconstructed vertex $\sigma V = \sigma |\vec{V} - \vec{V}_{true}|$. This is an indicator if the precision in our vertex reconstruction.

The models were developped in Python using the pytorch framework [59] using NVIDIA A100 [71] and NVIDIA V100 [72] gpus. The A100 was split in two, thus the accessible gpu memory was 20 Gb making it impossible to train some of the architectures due to memory consumption.

The training was monitored in realtime by a custom tooling that was developed during this thesis, DataMo [73].

The training of one model takes between 4h and 15h depending of its size, overall training the full 72 model takes around 500 GPU hours. Even with parallel training, this random search hyper-optimisation was time consuming.

4.2.2 Data representation

This data is represented as 240×240 images with a charge Q channel and a time t channel. The SPMTs are then projected on the plane as illustrated in figure 4.2. The x position is proportional to θ and the y position is defined by $\phi \sin \theta$ in spherical coordinates. $\theta = 0$ is defined as being the top of the detector and $\phi = 0$ is defined as an arbitrary direction in the detector. In practice, $\phi = 0$ is given by the MC simulation.

$$x = \left\lfloor \frac{\theta \cdot H}{\pi} \right\rfloor, \theta \in [0, \pi] \quad (4.3)$$

$$y = \left\lfloor \frac{(\phi + \pi) \sin \theta \cdot W}{2\pi} \right\rfloor, \phi \in [-\pi, \pi], \theta \in [0, \pi] \quad (4.4)$$

where H is the height of the image, W the width of the image and $(0, 0)$ the top left corner of the image.

When two SPMTs are in the same pixel, the charges are summed and the lowest of the hit-time is chosen. The SPMTs being located close to each other, we expect the time difference between two successive physics signals, two photons being collected, to be small. The first hit time is chosen because it can be considered as the relative propagation time of the photons that went the "straightest", i.e. that went under the less perturbation of the two. The only potential problem in using this first time come from the Dark Noise (DN). Its time distribution is uniform over the signal and could come before a physics signal on the other SPMT in the pixel. In that case, the time information in the pixel become irrelevant and we lose the timing information for this part of the detector. As illustrated in figure 4.2 the image dimension have been optimized so that at most two SPMTs are in the same pixel while keeping the number of empty pixels relatively low to prevent this kind of issue.

While it could be possible to use larger images (more pixel) to prevent overlapping, keeping image small images gives multiple advantages:

- 1159 — As presented in section 4.2.1, the convolution filter we use are 3×3 convolution filter, meaning
1160 that if SPMTs would be separated by more than one pixel, the first filter would only see one
1161 SPMT per filter. This behavior would be kind of counterproductive as the first convolution
1162 block would basically be a transmission layer and would just induce noise in the data.
- 1163 — It keep the network relatively small, while this do not impact the convolution layers, the
1164 flatten operation just before the FCDNN make the number parameters in the first layer of
1165 it dependent on the size of the image.
- 1166 — It reduce the number of empty pixel in the image.

1167 The question of empty pixel is an important question in this data representation. There is two kind
1168 of empty pixels in the data.

1169 The first kind is pixel that contain a SPMT but the SPMT did not get hit nor registered any dark noise
1170 during the event. In this case, the charge channel is zero, which have a physical meaning but then
1171 come the question of the time layer. One could argue that the correct time would be infinity (or the
1172 largest number our memory allows us) because the hit “never” happened, so extremely far from the
1173 time of the event. This cause numerical problem as large number, in the linear operation that are
1174 happening in the convolution layers, are more significant than smaller value. We could try to encode
1175 this feature in another way but no number have any significance due to our time being relative to
1176 the trigger of the experiment so -1 for example is out of question. Float and Double gives us access
1177 to special value such as NaN (Not a Number) [74] but the behavior is to propagate the NaN which
1178 leaves us with NaN for energy and position. We choose to keep the value 0 because it’s the absorbing
1179 element of multiplication, absorbing the “information” of the parameter it would be multiplied by.
1180 It also can be though as no activation in the ReLU activation function.

1181 The second kind of pixel is pixel that do not represent parts of the detector such as the corners of
1182 the image. The question is basically the same, what to put in the charge and the time channel. The
1183 decision is to set the charge and time to 0 following the above reasoning. It’s important to keep in
1184 mind the fact that a part of the detector that has not been hit is also an information: There is no signal
1185 in this part of the detector. This problematic will be explored in more details in chapter 5.

1186 Another problematic that happens with this representation, and this is not dependent of the chosen
1187 projection, is the deformation in the edges of the image and the loss of the neighbouring information
1188 in the for the SPMTs at the edge of the image $\phi \sim 180^\circ$. This deformation and neighbouring loss
1189 could be partially circumvented as explained in section 4.5

1190 4.2.3 Dataset

1191 In this study we will discuss two datasets of one millions events:

- 1192 — **J21:** The first one comes from the JUNO official mc simulation J21v1r0-Pre2 (released the 18th
1193 August 2021). This historical version is the one on which the classical algorithm presented in
1194 [66] was developed. This dataset is used as a reference for comparison to classical algorithm.
1195 The data in this dataset is *detsim* level (see section 2.5), where only the physic is simulated.
1196 The charge and time biases and uncertainties are implemented using toy MC adjusted using
1197 [26, 75]. The time window is not based on a selection algorithm but $t_0 := t = 0$ is defined as
1198 the first PMT hit. The window goes up to $t_0 + 1000$ ns.
- 1199 — **J23:** The second comes from the JUNO official monte-carlo simulations J23.0.1-rc8.dc1 (re-
1200 leased the 7th January 2024). The data is *calib* level (see section 2.5). Here the charge comes
1201 from the waveform integration, the time window resolution and trigger decision are all simu-
1202 lated inside the software. This dataset is more realistic and is used to confirm the performance
1203 of our algorithm.

1204 To put in perspective this amount of data, the expected IBD rate in JUNO is 47 / days. Taking into
1205 account the calibration time, and the source reactor shutdown, it amount to $\sim 94'000$ IBD events
1206 in 6 years. With this million of event, we are training the equivalent of ~ 10 years of data. With

1207 this amount we reach a density of $4783 \frac{\text{event}}{\text{m}^3 \cdot \text{MeV}}$, meaning our dataset is representative of the multiple
 1208 event scenarios that could be happening in the detector.

1209 While we expect and hope the monte-carlo simulation to give use a realistic representation of the detector,
 1210 there could be effect, even after the fine-tuning on calibration data, that the simulation
 1211 cannot handle. Thus, once the calibration will be available, we will need to evaluate, and if needed
 1212 retrain, the network on calibration data to establish definitive performances.

1213 The simulated data is composed of positron events, uniformly distributed in the CD volume and in
 1214 kinetic energy over $E_k \in [0; 9]$ MeV producing a deposited energy $E_{dep} \in [1.022; 10.022]$ MeV. This is
 1215 done to mimic the signal produced by the IBD prompt signal. Uniform distributions are used so that
 1216 the CNN does not learn a potential energy distribution, favoring some part of the energy spectrum
 1217 instead of other.

1218 Those events can be considered as “optimistic” as there is no pile-up with potential background or
 1219 other IBD.

1220 4.2.4 Data characteristics

1221 To delve a bit into the kind of data we will use, you can find in figure 4.2 the repartition of the SPMTs
 1222 in the image. The color represent the number of SPMTs per pixel.

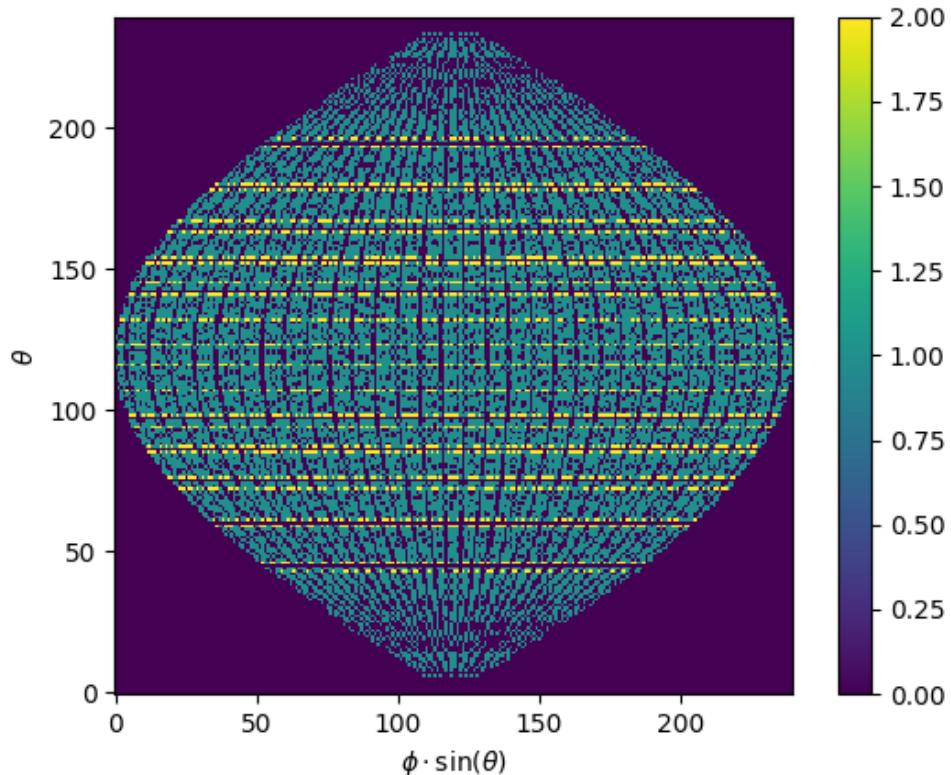


FIGURE 4.2 – Repartition of SPMTs in the image projection. The color scale is the
 number of SPMTs per pixel

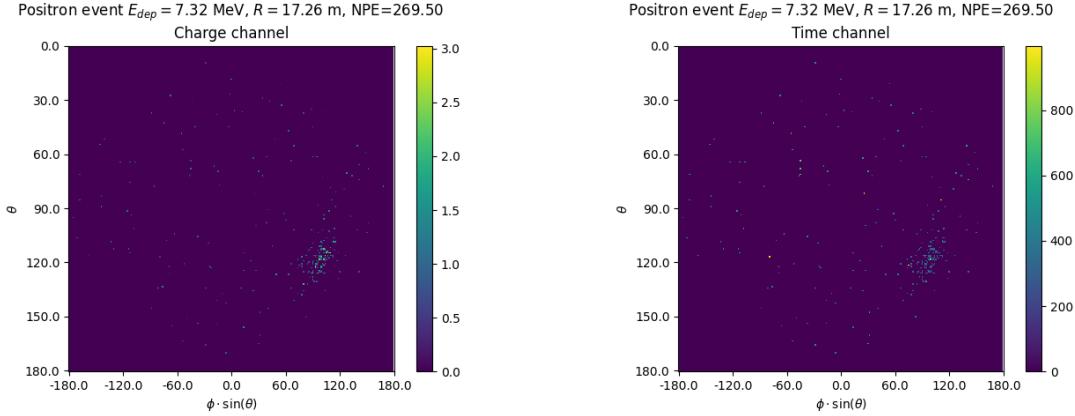


FIGURE 4.3 – Example of a high energy, radial event. We see a concentration of the charge on the bottom right of the image, clear indication of a high radius event. **On the left:** the charge channel. The color is the charge in each pixel in NPE equivalent. **On the right:** The time channel in nanoseconds.

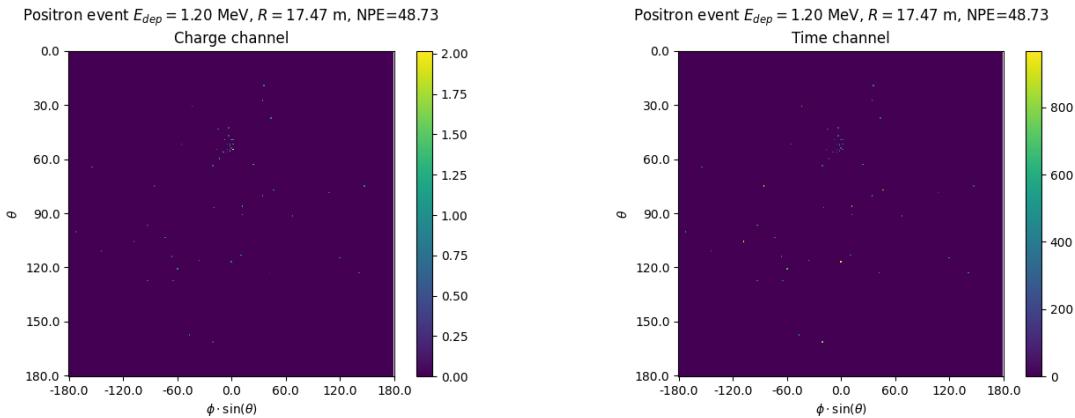


FIGURE 4.4 – Example of a low energy, radial event. The signal here is way less explicit, we can kind of guess that the event is located in the top middle of the image. **On the left:** the charge channel. The color is the charge in each pixel in NPE equivalent. **On the right:** The time channel in nanoseconds.

1223 In figures 4.3, 4.4, 4.5 and 4.6 are presented events from J23 for different positions and energies.
1224 We see some characteristics and we can instinctively understand how the CNN could discriminate
1225 different situations.

To give an idea of the strength of the signal in comparison to the dark noise background, figure 4.7a present the distribution of the ratio of NPE per deposited energy. Assuming a linear response of the LS we can model:

$$NPE_{tot} = E_{dep} \cdot P_{mev} + D_N \quad (4.5)$$

$$\frac{NPE_{tot}}{E_{dep}} = P_{mev} + \frac{D_N}{E_{dep}} \quad (4.6)$$

1226 where NPE_{tot} is the total number of PE detected by the event, P_{mev} is the mean number of PE detected
1227 per MeV and D_N is the dark noise contribution that is considered energy independent. In the case
1228 where the readout time window is dependent of the energy the dark noise contribution become

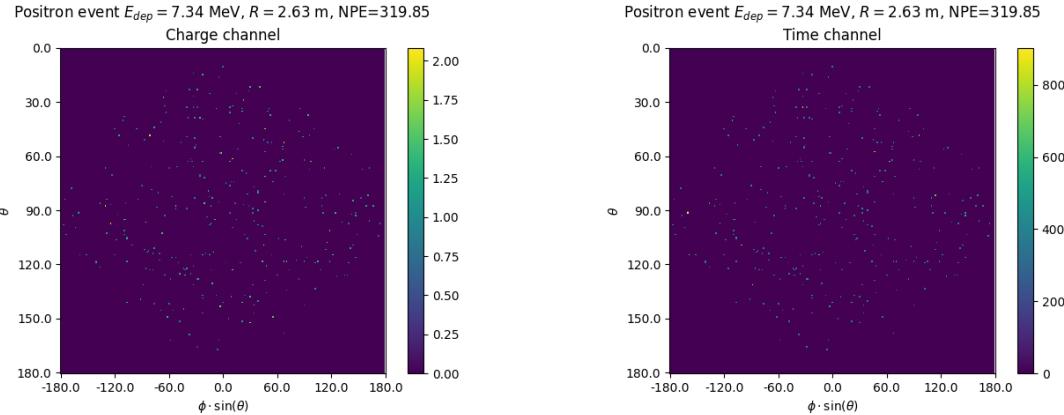


FIGURE 4.5 – Example of a high energy, central event. In this image we can see a lot of signal but uniformly spread, this is indicative of a central event. **On the left:** the charge channel. The color is the charge in each pixel in NPE equivalent. **On the right:** The time channel in nanoseconds.

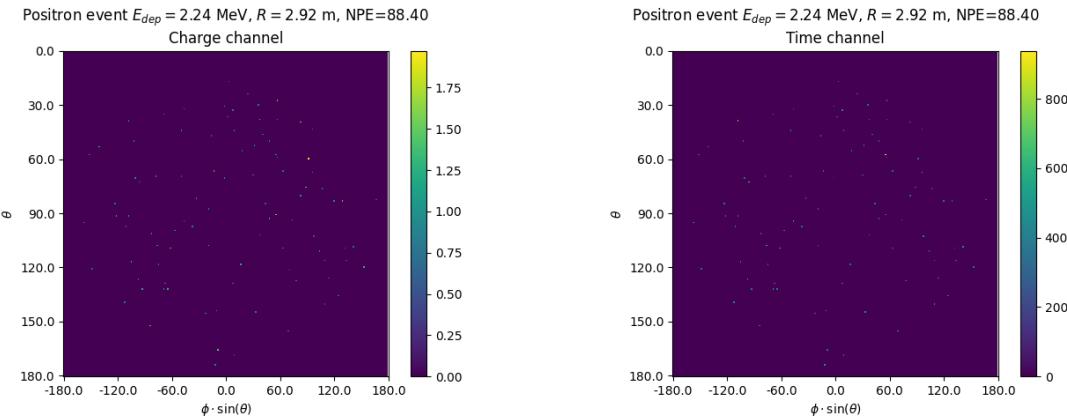


FIGURE 4.6 – Example of a low energy, central event. Here there is no clear signal, the uniformity of the distribution should make it central. **On the left:** the charge channel. The color is the charge in each pixel in NPE equivalent. **On the right:** The time channel in nanoseconds.

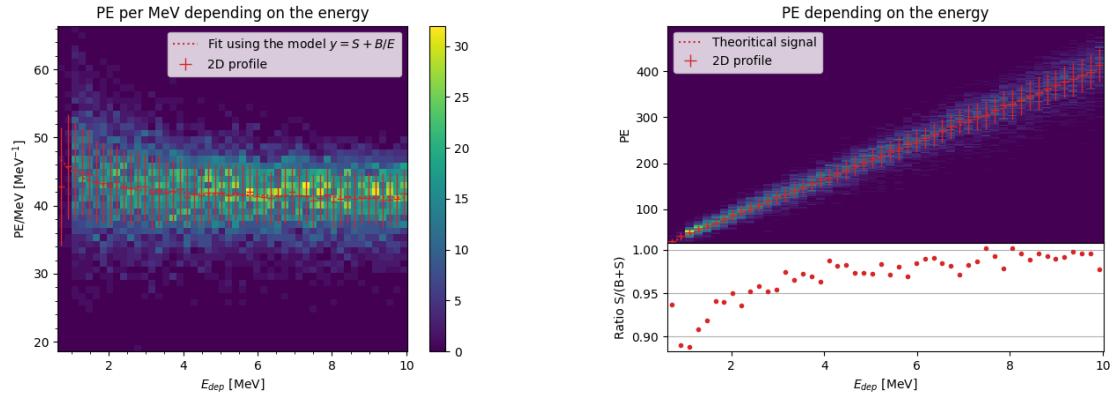
1229 energy dependant, also the LS response is realistically energy dependant but figure 4.7a shows that
1230 we have heavily dominated by statistical uncertainties which is why we are using this simple model.

1231 The fit shows a light yield of 40.78 PE/MeV and a dark noise contribution of 4.29 NPE. As shown in
1232 figure 4.7b, the physics makes for 90% of the signal at low energy.

1233 4.3 Training

1234 The optimizer used for the training is the Adam [55] optimizer, with a learning rate λ of 1e-3. The
1235 other hyperparameters were left to their default value ($\beta_1 = 0.9$, $\beta_2 = 0.999$ and $\epsilon = 1e - 8$). The
1236 learning rate was reduced exponentially during the training at a rate of $\gamma = 0.95$, thus $\lambda_{i+1} = 0.95\lambda_i$
1237 where i is the epoch.

1238 The training was composed of 30 epochs, each epoch constituted of 10k steps using a batch size of 64



(A) Distribution of PE/MeV in the J23 Dataset. This distribution is profiled and fitted using equation 4.6

(B) On top: Distribution of PE vs Energy. On bottom: Using the values extracted in 4.7a, we calculate the ration signal over background + signal

FIGURE 4.7

1239 events. The validation was computed over a 100 steps on the validation dataset.

1240 4.4 Results

1241 Before presenting the results, lets discuss the different observables.

1242 The event are considered point like in this study. The target truth position, or vertex, is the mean po-
 1243 sition of the energy deposits of the positron and the two annihilation gammas. Due to the symmetries
 1244 of the detector, we mainly consider and discuss the bias and precision evolution depending of the
 1245 radius R but we will still monitor the performances depending of the spheric angle θ and ϕ . From the
 1246 detector construction and effect we expect dependency in radius due to the TR area effect presented
 1247 in section 2.6 and the possibility for the positron or the gammas to escape from the CD for near the
 1248 edge events. We also expect dependency in θ , the top of the experiment being non-instrumented due
 1249 to the filling chimney. It is also to be noted that the events in the dataset are uniformly distributed in
 1250 the CD, and so are uniformly distributed in R^3 and ϕ . The θ distribution is not uniform and we will
 1251 have more event for $\theta \sim 90^\circ$ than $\theta \sim 0^\circ$ or $\theta \sim 180^\circ$.

1252 We define multiple energy in JUNO:

- 1253 — E_ν : The energy of the neutrino.
- 1254 — E_k : The kinetic energy of the resulting positron from the IBD.
- 1255 — E_{dep} : The deposited energy of the positron and the two annihilation gammas.
- 1256 — E_{vis} : The equivalent visible energy, so E_{dep} after the detector effect such as the absorption of
 scintillation photons by the LS and the LS response non-linearity.
- 1257 — E_{rec} : The reconstructed energy by the reconstruction algorithm. The expected value depend
 on the algorithm we discuss about. For example the algorithm presented in section 2.6 is
 reconstructing E_{vis} while the ones presented in section 2.6.3 reconstruct E_{dep} .

1258 In this study, we will set E_{dep} as our target for energy reconstruction. This choice is motivated by the
 1259 ease with which we can retrieve this information in the monte-carlo data while E_{vis} is less trivial to
 1260 retrieve.

1264 4.4.1 J21 results

1265 Those results comes from the “gen_30” model, meaning then 30th model generated using the table

1266 4.1 or

1267 — “gen_30”: $N_{blocks} = 3$, $N_{channels} = 32$, FCDNN configuration: $2048 * 2 + 1024 * 2$, Loss := $E + V$

1268 The performances of its reconstruction are presented in blue in figure 4.8. Superimposed in black is

1269 the performances of the classical algorithm from [66].

1270 Energy reconstruction

1271 By looking at the figure 4.8a and 4.8b, the CNN has similar performances in its energy resolution.

1272 Only at the end of the energy range does the resolution get a little better.

1273 This is explained by looking at the true and reconstructed energy distributions in figure 4.10a. We

1274 see that the distributions are similar for energies before 8 MeV but there is an excess of event recon-

1275 structed with energies around 9 MeV while a lack of them for 10 MeV. The neural network seems to

1276 learn the energy distribution and learn that it exist almost no event with an energy inferior to 1.022

1277 MeV and not event with an energy superior to 10 MeV.

1278 The first observation is a physics phenomena: for a positron, its minimum deposited energy is the
1279 mass energy coming from its annihilation with an electron 1.022 MeV. There is a few event with
1280 energies inferior to 1.022 MeV, in those case the annihilation gammas or even the positron escape the
1281 detector. The deposited energy in the LS is thus only a fraction of the energy of the event.

1282 The second observation is indeed true in this dataset but has no physical meaning, it is an arbitrary
1283 limit because the physics region of interest is mainly between 1 and 9 MeV of deposited energy
1284 (figure 2.2). By learning the energy distribution, the CNN pull event from the border of it to more
1285 central value. That’s why the energy resolution is better: the events are pulled in a small energy
1286 region , thus a small variance but the bias become very high (figure 4.8a).

1287 This behavior also explain the heavy bias at low energy in figure 4.8a. The energy bias of the CNN if
1288 fairly constant over the energy range, it is interesting to note that the energy bias depending on the
1289 radius is a bit worse than the classical method.

1290 Vertex reconstruction

1291 For the vertex reconstruction we do not study x , y and z independently but we use R as a proxy
1292 observable. Figure 4.9 shows the error distribution of the different vertex coordinates. We see that
1293 R errors and biases are slightly superior to the cartesian coordinates, thus R is a conservative proxy
1294 observable to discuss the subject of vertex reconstruction.

1295 The comparison of radius reconstruction between the classical algorithm and “gen_30” are presented
1296 in the figures 4.8c, 4.8d, 4.8e and 4.8f.

1297 Radius reconstruction is worse than the classical algorithms in all configuration. In energy, figure
1298 4.8c, where we see a degradation of almost 20cm over the energy range.

1299 When looking over the true event radius, figure 4.8d, we lose between 30 and 45cm of resolution.
1300 The performances are the best for central and radial event.

1301 The precision also worsen when looking at the edge of the image $\theta \approx 0$, $\theta \approx 2\pi$ respectively the
1302 top and bottom of the image, and when $\phi \approx -\pi$ and $\phi \approx \pi$ respectively the left and right side of
1303 the image. This is the confirmation that the deformation of the image is problematic for the event
1304 reconstruction.

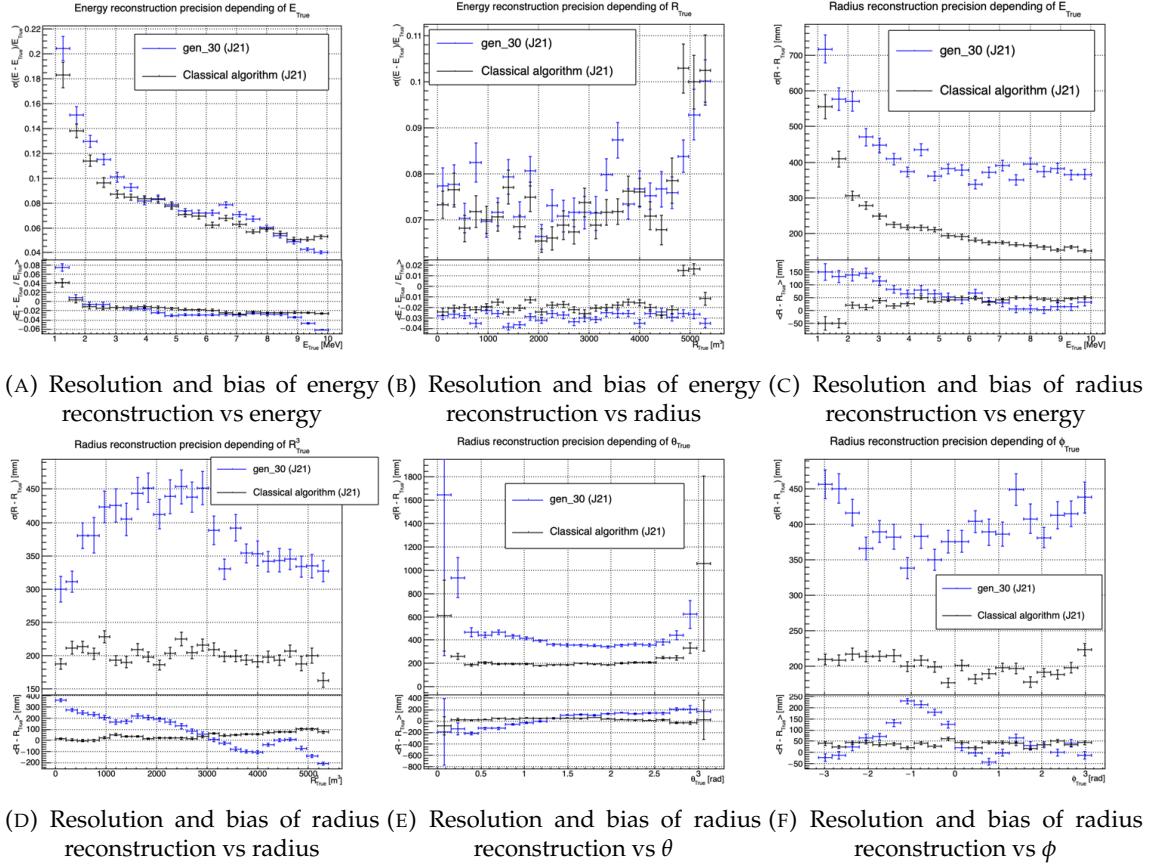


FIGURE 4.8 – Reconstruction performance of the “gen_30” model on J21 data and its comparison to the performances of the classic algorithm “Classical algorithm” from [66]. The top part of each plot is the resolution and the bottom part is the bias.

The bias in radius reconstruction is about the same order of magnitude depending of the energy but is of opposite sign. As for the energy, this behavior is studied in more details in section 4.4.2. Over radius, θ and ϕ the bias is inconsistent, sometimes event better than the classical reconstruction but can also be much worse than the classical method. This could come from the specialisation of some filters in the convolutional layers for specific part of the detector that would still work “correctly” for other parts but with much less precision.

4.4.2 J21 Combination of classic and ML estimator

As it has been presented in previous section, there is instances where the reconstructed energy and vertex behaves differently between the neural network and the classic algorithm. For instance, if we look at figure 4.8c, we see that while the CNN tend to overestimate the radius at low energy while the classical algorithm seems to underestimate it. Let’s designate the two reconstruction algorithms as estimator of X , the truth about the event in the phase space (E, x, y, z) . The CNN and the classical algorithm are respectively designated as $\theta_N(X)$ and $\theta_C(X)$.

$$E[\theta_N] = \mu_N + X; \text{Var}[\theta_N] = \sigma_N^2 \quad (4.7)$$

$$E[\theta_C] = \mu_C + X; \text{Var}[\theta_C] = \sigma_C^2 \quad (4.8)$$

where μ is the bias of the estimator and σ^2 its variance.

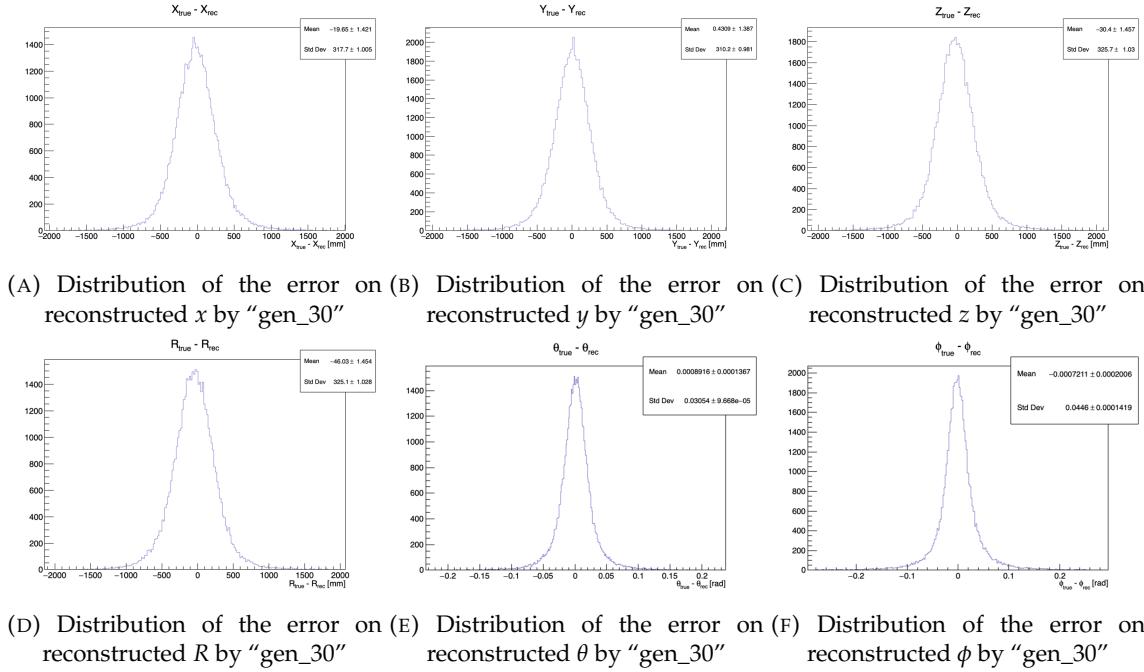


FIGURE 4.9 – Error distribution of the different component of the vertex by "gen_30". The reconstructed component are x , y and z but we see similar behavior in the error of R , θ and ϕ .

¹³¹³ Now if we were to combine the two estimators using a simple mean

$$\hat{\theta}(X) = \frac{1}{2}(\theta_N(X) + \theta_C(X)) \quad (4.9)$$

then the variance and mean would follow

$$E[\hat{\theta}] = \frac{1}{2}E[\theta_N] + \frac{1}{2}E[\theta_C] \quad (4.10)$$

$$= \frac{1}{2}(\mu_N + X + \mu_C + X) \quad (4.11)$$

$$= \frac{1}{2}(\mu_N + \mu_C) + X \quad (4.12)$$

$$\text{Var}[\hat{\theta}] = \frac{1}{4}\sigma_N^2 + \frac{1}{4}\sigma_C^2 + 2 \cdot \frac{1}{4} \cdot \sigma_{NC} \quad (4.13)$$

$$= \frac{1}{4}\sigma_N^2 + \frac{1}{4}\sigma_C^2 + \frac{1}{2} \cdot \sigma_{NC} \quad (4.14)$$

$$= \frac{1}{4}\sigma_N^2 + \frac{1}{4}\sigma_C^2 + \frac{1}{2} \cdot \sigma_N \sigma_C \rho_{NC} \quad (4.15)$$

¹³¹⁴ Where σ_{NC} is the covariance between θ_N and θ_C and ρ_{NC} their correlation.

¹³¹⁵ We see immediately that if the two estimators are of opposite bias, the bias of the resulting estimator
¹³¹⁶ is reduced. For the variance, it depends of ρ_{NC} but in this case if σ_C^2 is close to σ_N^2 then even for
¹³¹⁷ $\rho_{NC} \lesssim 1$ then we can gain in resolution.

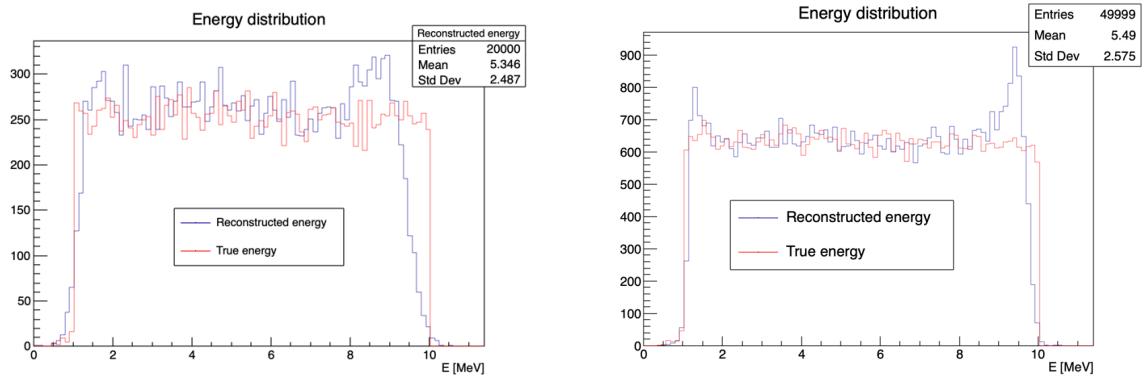
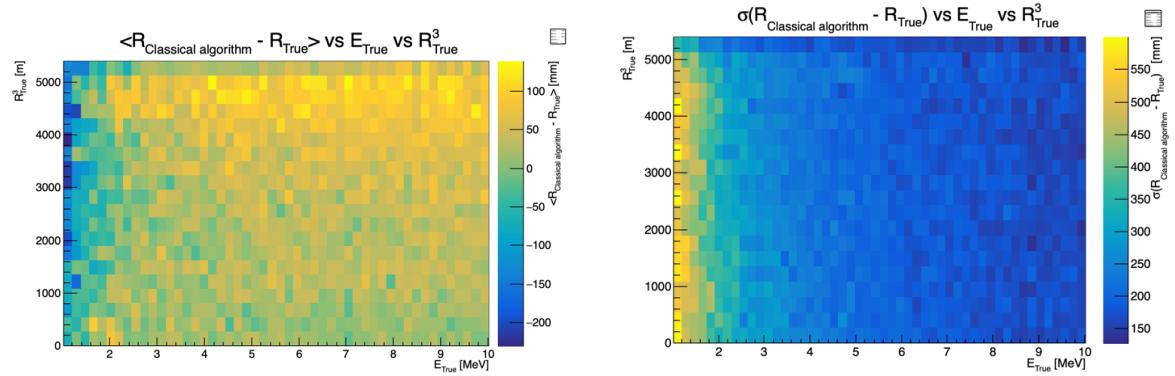


FIGURE 4.10

FIGURE 4.11 – Radius bias (on the left) and resolution (on the right) of the classical algorithm in a E, R^3 grid

1318 By generalising the equation 4.9 to

$$\hat{\theta}(X) = \alpha\theta_N + (1 - \alpha)\theta_C; \alpha \in [0, 1] \quad (4.16)$$

1319 we can determine an optimal α for two combined estimators. The estimators with the smallest
1320 variance

$$\alpha = \frac{\sigma_C^2 - \sigma_N\sigma_C\rho_C N}{\sigma_N^2 + \sigma_C^2 - 2\sigma_N\sigma_C\rho_N C} \quad (4.17)$$

1321 and the estimator without bias

$$\alpha = \frac{\mu_C}{\mu_C - \mu_N} \quad (4.18)$$

1322 See annex A for demonstration.

1323 Its pretty clear from the results shown in figure 4.8 that the bias, variances and correlation are not
1324 constant across the (E, R^3) phase space. We thus compute those parameters in a grid in E and R^3 for
1325 the following results as illustrated in 4.11.

1326 The map we are using are composed of 20 bins for R^3 going from 0 to 5400 m^3 (17.54 m) and 50 bins
1327 in energy ranging from 1.022 to 10.022 MeV. In the case where we are outside the grid, we use the
1328 closest cell.

1329 The performance of this weighted mean is presented in figure 4.12. We can see that even when the
 1330 CNN resolution is much worse than the classical algorithm, it can still bring some information thus
 1331 improving the resolution. This comes from the correlation of the reconstruction error to be smaller
 1332 than 1 as presented in figure 4.13. We even see some anticorrelation in the radius reconstruction for
 1333 High radius, high energy, event.

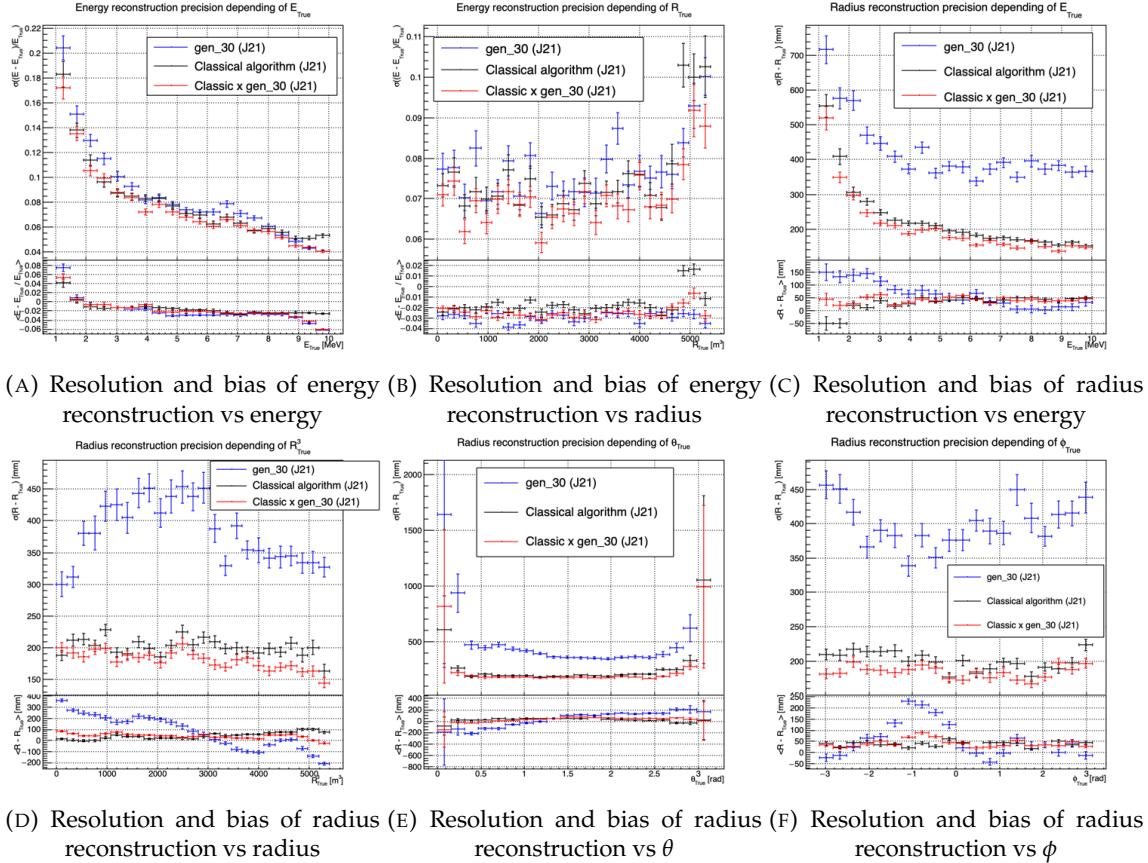


FIGURE 4.12 – Reconstruction performance of the “gen_30” model on J21, the classic algorithm “Classical algorithm” from [66] and the combination of both using weighted mean. The top part of each plot is the resolution and the bottom part is the bias.

1334 This technique is not suited for realistic reconstruction, we rely too much on the knowledge of
 1335 the resolution, bias and correlation between the two methods. While this is possible to determine
 1336 using simulated data or calibration sources, the real data might differ from our model and we
 1337 would need to really well understand the behavior of the two system. But this is an excellent tool
 1338 to indicate potential improvements to algorithms and reconstruction methods, showing with this
 1339 results a potential upper limit to the reconstruction performances.

1340 4.4.3 J23 results

1341 The J21 simulation is fairly old and newer version, such as J23, include refined measurements of the
 1342 light yield, reflection indices of materials of the detector, structural elements such as the connecting
 1343 structure and more realistic dark noise. Additionally, the trigger, waveform integration and time
 1344 window are defined using the algorithms that will ultimately be used by the collaboration to process
 1345 real physics events.

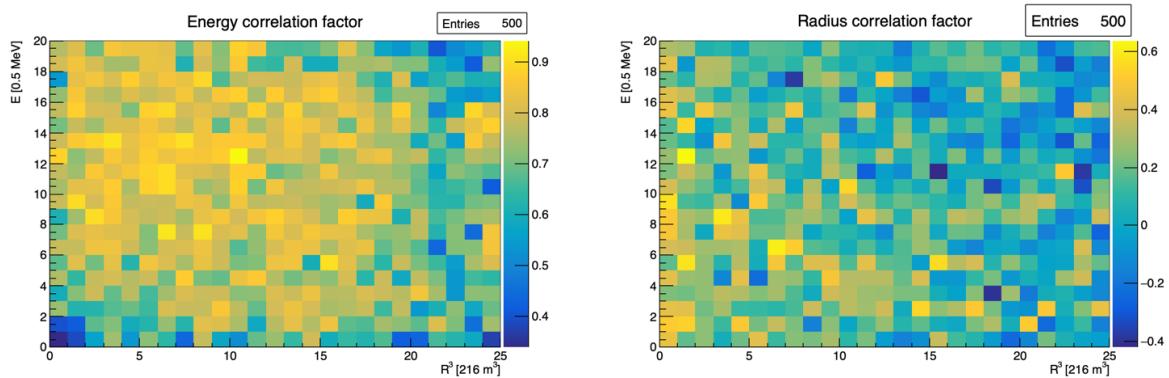


FIGURE 4.13 – Correlation between CNN and classical method reconstruction (on the left) for energy and (on the right) for radius in a E, R^3 grid

We retrained the models defined in 4.2.1 on the J23 data and used the same selection procedure. The results from the best architecture, “gen_42”, are presented in figure 4.14. Following the table 4.1, “gen_42” is defined as:

— “gen_42”: $N_{blocks} = 3$, $N_{channels} = 64$, FCDNN configuration: $4096 * 2$, Loss := $E + V$

1350 Energy reconstruction

The results of the energy reconstruction are presented in figures 4.14a and 4.14b. Similarly to what we seen for J21, the resolution is close to the one of the classical algorithm with the exception of the start and end of the spectrum. This come from “gen_42” learning the shape of the distribution and pulling events from the extreme energies, like 1 and 10 MeV, to more common seen energy, like 2 and 9 MeV as illustrated in figure 4.10b. The bias disappear with the exception of low and high energy events.

1357 Vertex reconstruction

The vertex reconstruction, presented in figures 4.14c, 4.14d, 4.14e and 4.14f is not yet to the level of the classical reconstruction but the degradation is smaller than for “gen_32” being at most a difference of 15cm of resolution and closing to the performance of the classical algorithm in the most favourable condition. “gen_42” has also very little bias in comparison with the classical method with the exception of the transition to the TR area and at the very edge of the detector.

Unfortunately could not rerun the classical algorithms over the J23 data, as the algorithm was optimised for J21 and was not included and maintained over J23. The combination method need for the two estimators to be run on the same set of event, which was impossible without the classical algorithm being maintained for J23.

Overall the resolution improved over the transition from J21 to J23, effect probably coming from a more complete and rigorous simulation.

1369 4.5 Conclusion and prospect

The CNN is a fine tool for event reconstruction in JUNO, and while the reconstruction performances are satisfactory, it show its limitation, the main one concerning the data representation. A lot of

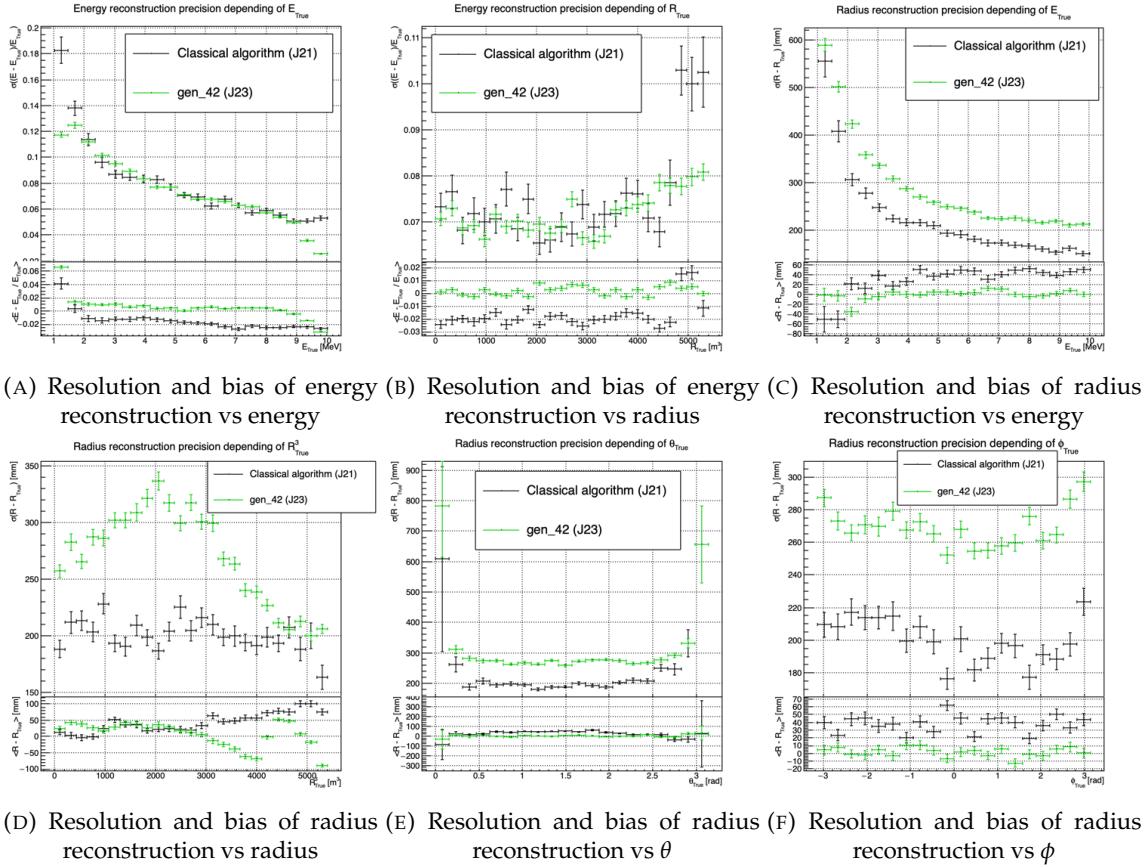


FIGURE 4.14 – Reconstruction performance of the “gen_42” model on J23 data and its comparison to the performances of the classic algorithm “Classical algorithm” from [66]. The top part of each plot is the resolution and the bottom part is the bias.

1372 training time and resources is consumed going and optimizing over pixel with no physical meaning,
 1373 the NN needs to optimized itself to take into account edges cases such as event at the edge of the
 1374 image and deformation of the charge distribution.

1375 Those problems could be circumvented, we could imagine a two part CNN where the first part
 1376 reconstruct the θ and ϕ spherical coordinates and then rotate the image to locate the event in the
 1377 center of the image. The second part, from this rotated image, would reconstruct the radius and
 1378 energy of the event.

1379 To overcome the problematic of the aggregation of PMT time information and the meaning of the
 1380 time channel in case of no hit, we could transform this channel into a dimension. This would results
 1381 in an image with multiple charge channels, each one representing the charge sum in a time interval.

1382 In this thesis, we decided to solve those problem by moving away from the 2D image representation,
 1383 looking into the graph representation and the Graph Neural Network (GNN). This is be the subject
 1384 of the next chapter.

1385 **Chapter 5**

1386 **Graph representation of JUNO for
IBD reconstruction**

1388

*"The Answer to the Great Question of Life, the Universe and
Everything is Forty-two"*

Douglas Adams, The Hitchhiker's Guide to the Galaxy

1389 We previously showed, in chapter 4, that neural networks are relevant as reconstruction tools in
1390 JUNO. Even if they show worse performances, the combination with classical estimators could still
1391 bring improvements. We discussed the use of Convolutional Neural Network (CNN) in the previous
1392 chapter and their limitations, more specifically the limitation of the image as data representation for
1393 the experiment.

1394 In this chapter we propose to use a Graph Neural Network (GNN), a Neural Network specialized to
1395 process graph as presented in section 3.2.3, to overcome those limitations.

1396 **5.1 Motivation**

1397 As explained in chapter 2 the JUNO sensors, the Large Photomultipliers (LPMT) and Small Photo-
1398 tomtmultipliers (SPMT), are arranged on a spherical plane. When trying to represent this plane as a
1399 2D image, due to the inherent problem of the projection, some part of the image are distorted and
1400 part of the image do not have any physical meaning (see section 4.2.2). A way to represent the data
1401 without inducing deformation is the graph, an object composed of a collection of nodes and edges
1402 representing the relation between the nodes.

1403 From this graph representation, we can construct a neural network that will process the data while
1404 keeping some interesting properties. For example the rotational invariance, i.e. the energy and
1405 radius of the event do change by rotation our referential. For more details see section 3.2.3. Graph
1406 representation also has the advantage to be able to encode global and higher order informations.

1407 An approach was already proposed in JUNO by Qian et al. [42] where each nodes of the graph are
1408 like pixels, they represent geometric region of the detector and are connected with their neighbours.
1409 The LPMT informations are then aggregated on those nodes. The network then process the data
1410 using the equivalent of convolution but on graph [49].

1411 In this work we want to take a step further in the graph representation by including the SPMT and
1412 including a maximum of raw informations.

5.2 Data representation

In an ideal world we would like to have every PMTs represented as node in the graph, each PMT being hit is an informations but the fact that PMTs were not hit is also an important information. It's by being aware of the whole of the system that we are able to give meaning to a subpart. As a reminder, in the Central Detector (CD), JUNO will posses 17612 LPMTs and 25600 SPMTs for a total of 43212 PMTs. This amount of information in itself is still manageable by modern computer if it were to be used in a neural network but when defining the relations between the nodes, it become a bit more tricky.

Excluding self relation and considering the relation to be undirected, the edge from A to B is the same from B to A , the amount of necessary edges is given by $\frac{n(n-1)}{2}$ which for 43212 PMTs amount for 933'616'866 edges. If we encode an information with double precision (64 bits) in what we call an adjacency matrix, each information we want to encode in the relation would consume 4 GB of data. When adding the overhead due to gradient computation during training, this would put us over the memory capacity of a single V100 gpu card (20 GB of memory). We could use parallel training to distribute the training over multiple GPU but we considered that the technical challenge to deploy this solution was not worth the trouble.

The option of connecting PMTs node only to their neighbours could be tempting to reduce the number of edge, but this solution does not translate well in term of internal representation in memory. Edges of sparsely connected nodes can be stored in efficient manner in a sparse matrix but the calculation in itself would often results in the concretization of the full matrix in memory, resulting in no memory gain during training.

We finally decided of a middle ground where we define three *families* of nodes:

- The core of the graph is composed of nodes representing geometric regions of the detector. We call those nodes **mesh** nodes. Those mesh nodes are densely connected to each other. We keep their number low to gain in memory consumption.
- All the fired PMTs, that have been hit, will be represented as nodes. We call those node **fire**. Fired nodes are connected to the mesh they geometrically belong.
- A final node which will hold global information about the detector and on which we will read the interaction vertex and energy. It's designated as the **I/O** node for input/output. This node will be connected to every mesh nodes.

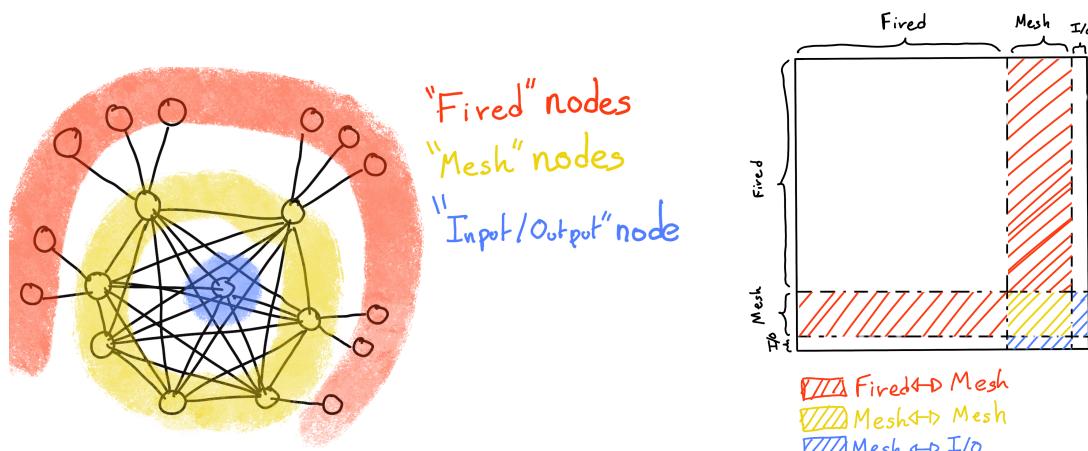
Those nodes and their relations are illustrated in figure 5.1a. From this representation, we end up with three distinct adjacency adjacency matrix

- A $N_{\text{fire}} \times N_{\text{mesh}}$ adjacency matrix, representing the relations between fired and mesh. Those relations are undirected.
- A $N_{\text{mesh}} \times N_{\text{mesh}}$ adjacency matrix, representing the relation between meshes. Those relation are directed.
- A $N_{\text{mesh}} \times 1$ adjacency between the mesh and I/O nodes. Those relations are undirected.

The adjacency matrix representing those relation is illustrated in figure 5.1b.

The mesh segmentation is following the Healpix segmentation [76]. This segmentation offer the advantage that almost each mesh have the same number of direct neighbours and it guarantee that each mesh represent the same extent of the detector surface. The segmentation can be infinitely subdivided to provide smaller and smaller pixels. The number of pixel follow the order n with $N_{\text{pix}} = 12 \cdot 4^n$. This segmentation is illustrated in figure 5.2. To keep the number of mesh small, we use the segmentation of order 3, $N_{\text{pix}} = 12 \cdot 4^3 = 768$.

We decided on having the different kind of nodes **mesh (M)**, **fire (F)** and **I/O** have different set of features. The features used in the graph are presented in figure 5.3. Most of the features are low level informations such as the charge or time information but we include some high order features such as



(A) Illustration of the different nodes in our graphs and their relations.

(B) Illustration of what a dense adjacency matrix would look like and the part we are really interested in. Because Fired → Mesh and Mesh → I/O relations are undirected, we only consider in practice the top right part of the matrix for those relations.

FIGURE 5.1

FIGURE 5.2 – Illustration of the healpix segmentation. **On the left:** A segmentation of order 0. **On the right:** A segmentation of order 1

- 1461 1. P_l^h : Is the normalized power of the l th spherical harmonic. For more details about spherical
1462 harmonics in JUNO, see annex B.
2. \mathbb{A} and \mathbb{B} are informations that represent the likeliness of the interaction vertex to be on the segment between the center of two meshes.

$$\mathbb{A}_{ij} = (\vec{j} - \vec{i}) \cdot \frac{\vec{l}_1}{D_{ij}} + \vec{i} \quad (5.1)$$

$$\mathbb{B}_{ij} = \frac{Q_i}{Q_2} \left(\frac{\vec{l}_2}{\vec{l}_1} \right)^2 \quad (5.2)$$

$$l_1 = \frac{1}{2}(D_{ij} - \Delta t \frac{c}{n}) \quad (5.3)$$

$$l_2 = \frac{1}{2}(D_{ij} + \Delta t \frac{c}{n}) \quad (5.4)$$

1463 where \vec{i} is the position vector of the mesh i , D_{ij} is the distance between the center of the meshes
1464 i and j , Q_i the sum of charges on the mesh i , $\Delta t = t_i - t_j$ where t_i the earliest time on the mesh
1465 i and n the optical index of the LS. \mathbb{A} is the vertex between center of meshes distance ratio
1466 between i and j based on the time information. For \mathbb{B} , the charge ratio evolve with the square
1467 of the distance, so the mesh couple with the smallest \mathbb{B} should be the one with the interaction
1468 vertex between its two center.

Nodes			Edges		
Fixed	Mesh	I/O	Fixed \rightarrow Mesh	Mesh \rightarrow Mesh (1)	Mesh \rightarrow I/O
Q	$\langle Q_m \rangle$	$\langle x \rangle$	$X - X_m$	$X_{m1} - X_{m2}$	$\langle x \rangle - x_m$
t	$6Q_m$	$\langle y \rangle$	$Y - Y_m$	$Y_{m1} - Y_{m2}$	$\langle y \rangle - y_m$
X	$\min(t_m)$	$\langle z \rangle$	$Z - Z_m$	$Z_{m1} - Z_{m2}$	$\langle z \rangle - z_m$
Y	$\max(t_m)$	ΣQ	$t - \min(t)$	$\min(t_1) - \min(t_2)$	$\Sigma Q_m / \Sigma Q$
Z	$6t_m$	$P_l^h; l \in [0, 8]$	$Q / \Sigma Q_m$	$\langle Q_{m1} \rangle - \langle Q_{m2} \rangle$ $\langle Q_{m1} \rangle + \langle Q_{m2} \rangle$	$\langle t_m \rangle$
LPMT: 1 SPMT: -1	X_m Y_m Z_m			$D_{m1 \rightarrow m2}^{-1}$ \mathbb{A} \mathbb{B}	

Q is the charge [nPE]
 t is the time [ns]
 X, Y, Z are the coordinates [m]
 Q_m, t_m are the set of charge and time in a mesh
 X_m, Y_m, Z_m the coordinates of the center of the mesh
 $\langle x \rangle, \langle y \rangle, \langle z \rangle$ the position of the charge barycenter.

FIGURE 5.3 – Features held by the nodes and edges in the graph. $D_{m1 \rightarrow m2}^{-1}$ is the inverse of the distance between two mesh center. The features P_l^h , \mathbb{A} and \mathbb{B} are detailed in section 5.2

1469 Because our different nodes do not have the same number of features, they live in different spaces.
1470 Most library and public algorithms available are designed with node living in the same space in
1471 mind, we thus had to develop a custom message passing algorithm.

5.3 Message passing algorithm

1473 As introduced in previous section and in figure 5.3, our graphs nodes and edges will have different
1474 number of features depending on their nature, meaning that we cannot have a single message passing
1475 function. We thus need to define a message passing function for each transition inside or outside

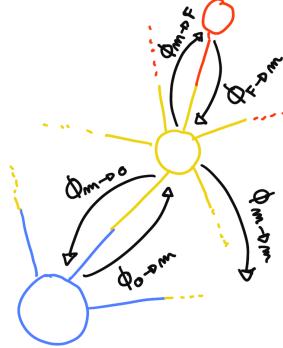


FIGURE 5.4 – Illustration of the different update function needed by our GNN

¹⁴⁷⁶ a family. Using the notation presented in section 3.2.3

$$n_i^{k+1} = \phi_u(n_i^k, \square_j \phi_m(n_i^k, n_j^k, e_{ij}^k)); n_j \in \mathcal{N}_i' \quad (5.5)$$

we need to define

$$\phi_{u;f \rightarrow m} \phi_{m;f \rightarrow m} \quad (5.6)$$

$$\phi_{u;m \rightarrow f} \phi_{m;m \rightarrow f} \quad (5.7)$$

$$\phi_{u;m \rightarrow m} \phi_{m;m \rightarrow m} \quad (5.8)$$

$$\phi_{u;m \rightarrow io} \phi_{m;m \rightarrow io} \quad (5.9)$$

$$\phi_{u;io \rightarrow m} \phi_{m;io \rightarrow m} \quad (5.10)$$

¹⁴⁷⁷ to update the nodes after each layers as illustrated in figure 5.4. We would also need update function
¹⁴⁷⁸ for the edges but for the sake of technical simplicity in this work, we will limit ourself to the nodes
¹⁴⁷⁹ update. A wide variety of message passing algorithm exists, with different use cases and goal behind
¹⁴⁸⁰ them. To stay generalist and to match to the best the specificity of our architecture, we implement
¹⁴⁸¹ the following algorithm:

$$\phi_u := I_{i'}^{n'} = I_i^n A_{i',e}^i W_n^{e,n'} + I_i^n S_n^{n'} + B^{n'} \quad (5.11)$$

¹⁴⁸² using the Einstein summation notation. I_i^n is the tensor holding the nodes informations with i
¹⁴⁸³ the node index and n the feature index. n represent the features of the previous layer and n' the
¹⁴⁸⁴ features of this layer. $A_{n,e}^i$ is the adjacency tensor, discussed in the previous section, representing the
¹⁴⁸⁵ connection between the node i' and the node i , each connections holding the features indexed by e .
¹⁴⁸⁶ The learnable weights are composed of:

- ¹⁴⁸⁷ — The tensor $W_n^{e,n'}$ which represent the passage from the previous feature domain n , the previous
¹⁴⁸⁸ layer, to the current domain n' , this layer knowing the relation e .
- ¹⁴⁸⁹ — $B^{n'}$ which is a learnable bias tensor on the new features n' .
- ¹⁴⁹⁰ — $S_n^{n'}$ which can be viewed as a self loop relation where the node update itself based on the
¹⁴⁹¹ previous layer informations.

¹⁴⁹² If a node have neighbours in different families, the different $I_{i'}^{n'}$ coming from the different ϕ_u are
¹⁴⁹³ summed.

$$I_{i'}^{n'} = \sum_{\mathcal{N}} \phi_{u,\mathcal{N}} \quad (5.12)$$

¹⁴⁹⁴ where \mathcal{N} are the neighbouring family and $\phi_{u,\mathcal{N}}$ the update function between the target node family
¹⁴⁹⁵ and the neighbour \mathcal{N} family.

¹⁴⁹⁶ We thus have a S , W and B for each of the ϕ_u function we defined above. The IAW sum can be seen

as the ϕ_m function and $IS + B$ as the second part of the phi_u function. Interestingly, the number on learnable weight in those layer is independent of the number of nodes in each family and depends solely on the number of features on the nodes and the edges.

The expression above only update the node features. We could update the edges, using the results of ϕ_m for example, but for technical simplicity we only update the nodes and keep the edges constant.

This operation of message passing is the constituent of our message passing layer, designed in this work as *JWGLayer*. To this layer, we can adjoin an activation function such as *PReLU*

$$I_i^{n'} = PReLU \left(\sum_{\mathcal{N}} I_i^n A_{i',e}^i W_n^{e,n'} + I_i^n S_n^{n'} + B^{n'} \right) \quad (5.13)$$

5.4 Data

For this study we will be using a 1M positrons event dataset, uniformly distributed in energy with $E_k \in [0, 9]$ MeV and uniformly distributed in the detector. Those events come from the JUNO official simulation version J23.0.1-rc8.dc1 (released the 7th January 2024). All the event are *calib* level, with simulation of the physics, electronics, digitizations and triggers. 900k events will be used for the training, 50k for validation and loss monitoring and 50k for the results analysis in section 5.8. Each events is between 2k and 12k fired PMTS, resulting in fired nodes being the largest family in our graphs in all circumstances as illustrated in figure 5.5c.

As expected, by comparing the scale between the figure 5.5a and 5.5b we see that the LPMT system is predominant in term of informations in our data. The number of PMT hits grow with energy but do not reach 0 for low energy event due to the dark noise contribution which seems to be around 1000 hits per event for the LPMT system (left limit of figure 5.5a) and around 15 hits per event for the SPMT system (left limit of figure 5.5b) which is consistent with the results show in section 4.2.2.

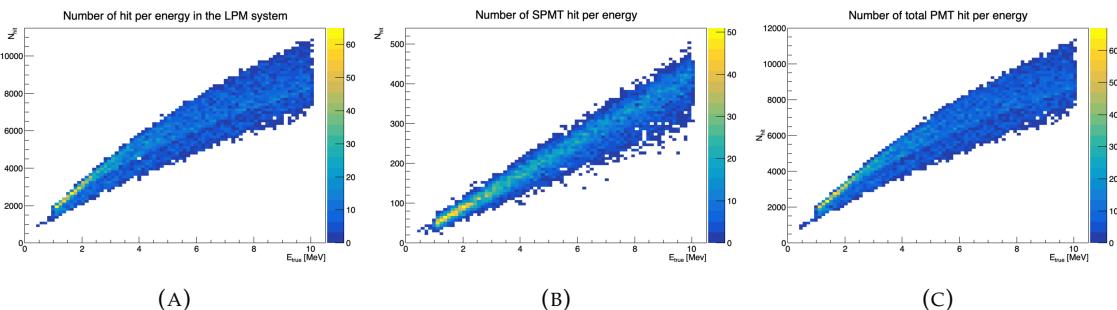


FIGURE 5.5 – Distribution of the number of hits depending on the energy. **On the right:** for the LPMT system. **In the middle :** for the SPMT system. **On the left:** For both system.

The structure seen in the distribution in figure 5.5a comes from the shape of the number of hits depending on the radius as shown in figures 5.6a and 5.6b where the number of hit decrease with radius. It is important to understand that this is not representative of the number of PE per event and the decrease in hits over the radius means that the PE are just more concentrated in a smaller number of PMTs.

No quality cut is applied here, we rely only on the trigger system. It means that event that would not trigger are not present in the dataset but for events that triggered twice, it happens rarely, the two trigger are considered as two separate event.

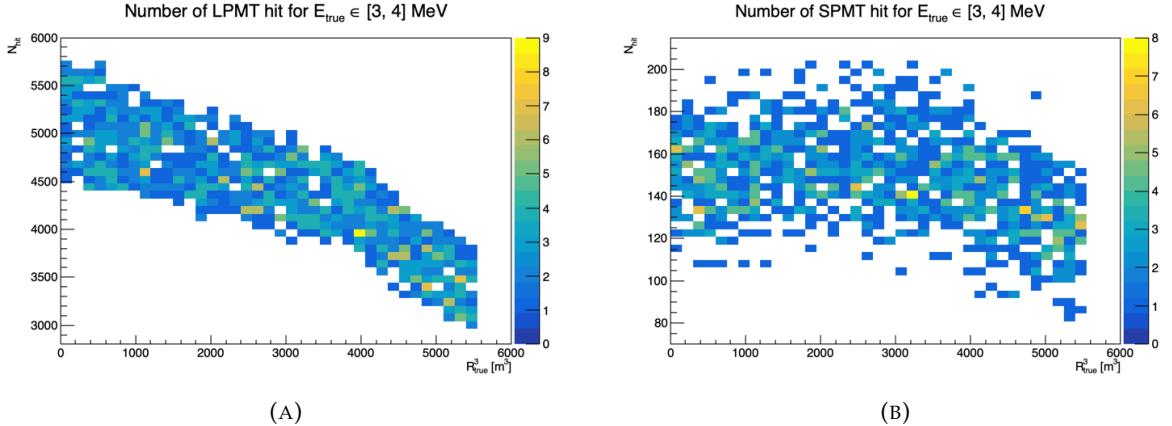


FIGURE 5.6 – Distribution of the number of hits depending on the radius. **On the right:** for the LPMT system. **On the right :** for the SPMT system. To prevent the superposition of structure of different scales we limit ourselves to the energy range $E_{\text{true}} \in [0, 9]$.

1525 5.5 Model

1526 In this section we'll discuss the different layer composing the final version of the model. As intro-
 1527 duced above, each JWGLayer is defined by the number of features on the nodes and edges of the
 1528 output graph, assuming it takes as input the graph from the precedent layer. For simplicity, when
 1529 discussing a graph configuration, it will be presented as follow: { N_f , N_m , N_{IO} , $N_{f \rightarrow m}$, $N_{m \rightarrow m}$, $N_{m \rightarrow f}$
 1530 } where

- 1531 — N_f is the number of feature on the fired nodes.
 - 1532 — N_m is the number of features on the mesh nodes.
 - 1533 — N_{IO} is the number of features on the I/O node.
 - 1534 — $N_{f \rightarrow m}$ is the number of features on the edges between the fired and mesh nodes.
 - 1535 — $N_{m \rightarrow m}$ is the number of features on the edges between two mesh nodes.
 - 1536 — $N_{m \rightarrow f}$ is the number of features on the edges between the mesh nodes and the I/O node.
- Because we do not change the number of features on the edges, we can simplify the notation to { N_f , N_m , N_{IO} }. As an example, the input graph configuration, following the figure 5.3, is { 6, 8, 13, 5, 8, 5 } or, without the edge features, { 6, 8, 13 }.

1540 The final version of the model, called JWGV7.3.0 is composed of

- 1541 — An JWGLayer, converting the input graph to { 32, 32, 32 } with a PReLU activation function.
- 1542 — 6 hidden JWGLayer, processing the data to { 32, 32, 32 } graphs with a PReLU activation
- 1543 function.
- 1544 — A flatten layer that flatten the features of the I/O and mesh nodes to a $(32 * 768 + 32) = 24608$
- 1545 dimensions vector.
- 1546 — 2 fully connected layers of 2048 neurons with a PReLU activation function.
- 1547 — 2 fully connected layers of 512 neurons with a PReLU activation function.
- 1548 — A final, fully connected layer of 4 neurons acting as the output of the network.

1549 5.6 Training

1550 The optimizer used for training is the Adam optimizer and default hyperparameters ($\beta_1 = 0.9$,
 1551 $\beta_2 = 0.999$ and $\epsilon = 1e - 8$) with a learning rate $\lambda = 1e - 8$. The training last 200 epochs of 800 steps.
 1552 We use a batch size of 8. The learning rate is constant during the first 20 epochs then exponentially

1553 decrease with a rate of 0.99. The model saved is the model with the best validation loss during the
 1554 training. The validation is computed over a single batch.

1555 5.7 Optimization

1556 Due to the extensive training time, up to 90h per training on the more complex architectures, and
 1557 the heavy memory consumption of the models that would often exceed the 20GB limit of the V100,
 1558 random search was not a realistic approach to the hyper optimisation. We were able to extend the
 1559 memory limit to 40GB thanks to a local A100 GPU card available at the lab.

1560 The hyperparameters optimization was thus done “by hand”, by looking at the results of the previous
 1561 training and tinker hyperparameters that seems to play a role in the training. During this process,
 1562 the model went into some heavy refactoring. At the start, the message passing algorithm was not
 1563 the one presented above but each ϕ_u and ϕ_m function were FCDNN. The memory consumption and
 1564 gradient vanishing caused is what made us pivot to the final message passing algorithm presented
 1565 above.

1566 Even the features on the graph went under investigation. With the addition of high level observables
 1567 to the mesh and I/O nodes and edge, there was too much possibility to test everything. We went
 1568 with the decision to keep the raw observables in the fired and for the higher order observables
 1569 we tried to take the one that would be difficult for the NN to reconstruct or at least would need
 1570 multiple layer to reproduce. Basically, because the operation in the JWGLayer are linear operation,
 1571 any variables dependent on order > 1 of the input would be candidates. This is why we introduce
 1572 standard deviation, \mathbb{A} , \mathbb{B} and P_l^h for example.

1573 Substantial effort went to the data processing process before the training. Due to the volatile nature
 1574 of the graph features during the optimization, the current code do not take preprocessed data and
 1575 compute the observables, adjacency matrix, etc... on the fly. This data processing is carried out on
 1576 the CPU, using a worker pool to allow for multiprocessing the data. The raw data are coming from
 1577 root file produced by the collaboration software, the Event Data Model (EDM) used internally by the
 1578 collaboration [77] had to be interfaced to our code, interface maintained through the evolution of the
 1579 collaboration software. For the harmonic power calculation, we migrated from the Healpix library
 1580 to Ducc0 [78] for a more fine control of the multithreading.

1581 Over the course of the project, the model went over more than 60 different configurations to end on
 1582 the one presented in this chapter.

1583 5.8 Results

1584 Present the results

1585 5.9 Conclusion

- 1586 — For now:
- 1587 — Not competitive
- 1588 — Aggregation on mesh nodes seems to loose informations
- 1589 — Maybe too complex ?
- 1590 — Next step would be to have the waveform directly included

¹⁵⁹¹ **Chapter 6**

¹⁵⁹² **Reliability of machine learning
methods**

¹⁵⁹³

"Psychohistory was the quintessence of sociology; it was the science of human behavior reduced to mathematical equations. The individual human being is unpredictable, but the reactions of human mobs, Seldon found, could be treated statistically"

Isaac Asimov, Second Foundation

¹⁵⁹⁴

¹⁵⁹⁵ **Chapter 7**

¹⁵⁹⁶ **Joint fit between the SPMT and LPMT
spectra**

¹⁵⁹⁸ “We demand rigidly defined areas of doubt and uncertainty!”

Douglas Adams, *The Hitchhiker’s Guide to the Galaxy*

¹⁵⁹⁹ JUNO is an experiment of precise measurements, where we try to observe small fluctuation in the en-
¹⁶⁰⁰ ergy spectrum and have the ambition to achieve sub-percent precision on the oscillation parameters
¹⁶⁰¹ measurement. It is crucial to understand extremely well the reconstruction and the effect we are deal-
¹⁶⁰² ing with. The challenge reside in the standard technology used in the detector, scintillator observed
¹⁶⁰³ by PMT, but in a scale never seen before, for scintillator volume as for its PMT. Understanding every
¹⁶⁰⁴ effect that goes in the detector can become extremely complicated. Being able to compare the results
¹⁶⁰⁵ of the same experiment with two systems is thus precious, this is the origin the dual calorimetry with
¹⁶⁰⁶ the LPMT and SPMT system.

¹⁶⁰⁷ The resolution and bias of the reconstruction needs to be extremely well characterized: the target
¹⁶⁰⁸ resolution of 3% [50] is unprecedented as is required to be able to distinguished between Normal
¹⁶⁰⁹ Ordering (NO) and Inverse Ordering (IO). The non-linearity uncertainty needs to be contained under
¹⁶¹⁰ 1% or the risk appear to measure the wrong ordering [27].

¹⁶¹¹ One of the possible non-linearity source, that will be used as a reference source in this chapter, is the
¹⁶¹² charge non-linearity (QNL) that will be detailed in next section. The dual calorimetry will be able to
¹⁶¹³ solve this problem, using calibrations method and measurements that will be used to correct it [27].

¹⁶¹⁴ More generally, comparing the results of the two system will allow to detect potential issues on
¹⁶¹⁵ the calibration or reconstruction. This is done in this thesis by comparing directly the spectra and
¹⁶¹⁶ oscillation parameters measurements of the two system.

¹⁶¹⁷ The study of the independents results of the two system can bring some informations [79] but this is
¹⁶¹⁸ missing the important correlation that should be present between the two system: they see the same
¹⁶¹⁹ events, in the same scintillator, their bound to be correlated. We explore in this chapter a preliminary
¹⁶²⁰ study of the impact of those correlation via multiple methods and the impact of QNL at various
¹⁶²¹ degree.

¹⁶²² In the next section will discuss the motivations behind this study. In section 7.2, I present the ap-
¹⁶²³ proaches and assumptions in this study. In section 7.3 I present the fit framework used and following
¹⁶²⁴ in section 7.4 the technical improvement brought and the difficulties faced during the development.
¹⁶²⁵ To end this chapter I present the results in 7.5 and discuss the conclusion and perspectives in 7.6.

1626 7.1 Motivations

1627 7.1.1 Discrepancies between the SPMT and LPMT results

1628 As discussed in the introduction of this chapter, the SPMT system and the LPMT system will observe
 1629 the same events. This mean that, after calibration, if the two system show significant differences
 1630 in their results this is the signal of potential overlook of an effect or problem. Being able to detect
 1631 such differences is thus crucial as, as discussed above, even the smallest deviation from our model
 1632 could lead to the impossibility to measure the Mass Ordering (MO) or even worse, wrong our
 1633 measurement.

1634 The two system are expected to have the same sensitivity to the oscillation parameters θ_{12} and Δm_{21}^2
 1635 [11]. We will thus rely on the measurement of those two parameters to detect potential discrepancies.

1636 We could just look at the value and compare them to the estimated independent error of the two
 1637 system, but we believe and will demonstrate in this chapter that the independent study of the two
 1638 system is missing a lot of informations, and that, by taking into account the statistic and systematic
 1639 correlations between the two systems, we can produce much more powerful statistical test.

1640 Our work in this chapter is to develop such tools. The first step is, of course, to verify that in the
 1641 case of no discrepancies, the results are coherent with the independent analysis. This will give us
 1642 the distribution of those statistical test in absence of discrepancies. When we will have real data, we
 1643 will be able to compare it to those distribution to obtain a p-value characterizing the absence of those
 1644 potential discrepancies.

1645 To evaluate the power of our methods, we need to simulate a concrete discrepancy. We decide to
 1646 study a plausible effect, the Charge Non-Linearity (QNL) that is detailed next section, but the goal of
 1647 those tools is to be discrepancy agnostic, as those discrepancies could come from a variety of source
 1648 (calibration issue, insufficient simulation tuning, etc...)

1649 7.1.2 Charge Non-Linearity (QNL)

1650 The CD energy response is subject of two kind on non-linearity, the first one is the LS response
 1651 non-linearity where the LS photo-production not linear with the deposited energy as illustrated in
 1652 figure 2.12a. The second one is the LPMT response non-linearity where the charge read from the
 1653 LPMT is not linear in respect to the number of collected Photo-Electron (PE) (see section 2.3).

1654 The LS non-linearity comes from physics sources. Particles interaction in the LS will produce mainly
 1655 scintillation light as discussed in section 2.2.2 but will also produce some cherenkov light (< 10% of
 1656 the collected light). Both mechanisms posses intrinsic non-linearity, for the Cherenkov emission it's
 1657 dependent on the velocity of charged particle velocity while the scintillation photon-yield follow a
 1658 so-called Birk's law with a "quenching" effect depending on the energy and type of particle [16]. This
 1659 results in a channel wise QNL.

1660 The LPMT response non-linearity can come from sheer saturation when subject to a high rate of
 1661 photon inducing a gain non-linearity or come from readout effects such as the electronic noise, the
 1662 overshoot, the integration time window and even the waveform algorithm. All of those effects results
 1663 in a channel wise QNL.

1664 Precedent studies [27] suggest a model to emulate this non-linearity response that will be used in this
 1665 work. We thus define to effect, the channel wise non-linearity that would be applied to each LPMT
 1666 readout

$$\frac{Q_{rec}}{Q_{true}} = \frac{-\gamma_{qnl}}{9} Q_{true} + \frac{\gamma_{qnl} + 9}{9} \quad (7.1)$$

¹⁶⁶⁷ where Q_{rec} is the reconstructed number of PE by the PMT, Q_{true} is true number of PE that hit the
¹⁶⁶⁸ PMT, and γ_{qnl} is a factor representing the amplitude of the non-linearity.

¹⁶⁶⁹ We also define an event-wise non-linearity characterized by

$$\frac{E_{vis}}{E_{true}} = \frac{-\alpha_{qnl}}{9} E_{true} + \frac{\alpha_{qnl} + 9}{9} \quad (7.2)$$

¹⁶⁷⁰ where E_{vis} is the visible energy that can be collected by the detector and E_{true} is the true deposited
¹⁶⁷¹ energy.

¹⁶⁷² 7.2 Approach

¹⁶⁷³ 7.3 Fit framework

¹⁶⁷⁴ 7.4 Technical challenges

¹⁶⁷⁵ 7.5 Results

¹⁶⁷⁶ 7.6 Conclusion and perspectives

¹⁶⁷⁷ Chapter 8

¹⁶⁷⁸ Conclusion

¹⁶⁷⁹ **Appendix A**

¹⁶⁸⁰ **Calculation of optimal α for estimator
combination**

¹⁶⁸² This annex the details of the determination of the optimal α for estimator combination presented in
¹⁶⁸³ section 4.4.2.

¹⁶⁸⁴ As a reminder, the combine estimator $\hat{\theta}$ of X is defined as

$$\hat{\theta}(X) = \alpha\theta_N + (1 - \alpha)\theta_C; \alpha \in [0; 1] \quad (\text{A.1})$$

¹⁶⁸⁵ where θ_N and θ_C are both estimator of X .

¹⁶⁸⁶ **A.1 Unbiased estimator**

For the unbiased estimator, it is straight-forward. We search α such as $E[\hat{\theta}] = X$

$$E[\hat{\theta}] = E[\alpha\theta_N + (1 - \alpha)\theta_C] \quad (\text{A.2})$$

$$= E[\alpha\theta_N] + E[(1 - \alpha)\theta_C] \quad (\text{A.3})$$

$$= \alpha E[\theta_N] + (1 - \alpha)E[\theta_C] \quad (\text{A.4})$$

$$= \alpha(\mu_N + X) + (1 - \alpha)(\mu_C + X) \quad (\text{A.5})$$

$$X = \alpha\mu_N + \mu_C - \alpha\mu_C + X \quad (\text{A.6})$$

$$0 = \alpha(\mu_N - \mu_C) + \mu_C \quad (\text{A.7})$$

$$(A.8)$$

$$\Rightarrow \alpha = \frac{\mu_C}{\mu_C - \mu_N} \quad (\text{A.9})$$

¹⁶⁸⁷ **A.2 Optimal variance estimator**

The α for this estimator is a bit more tricky. By expanding the variance we get

$$\text{Var}[\hat{\theta}] = \text{Var}[\alpha\theta_N + (1 - \alpha)\theta_C] \quad (\text{A.10})$$

$$= \text{Var}[\alpha\theta_N] + \text{Var}[(1 - \alpha)\theta_C] + \text{Cov}[\alpha(1 - \alpha)\theta_N\theta_C] \quad (\text{A.11})$$

$$= \alpha^2\sigma_N^2 + (1 - \alpha)^2\sigma_C^2 + 2\alpha(1 - \alpha)\sigma_N\sigma_C\rho_{NC} \quad (\text{A.12})$$

¹⁶⁸⁸ where, as a reminder, ρ_{NC} is the correlation factor between θ_C and θ_N .

Now we try to find the minima of $\text{Var}[\hat{\theta}]$ with respect to α . For this we evaluate the derivative

$$\frac{d}{d\alpha} \text{Var}[\hat{\theta}] = 2\alpha\sigma_N^2 - 2(1-\alpha)\sigma_C^2 + 2\sigma_N\sigma_C\rho_{NC}(1-2\alpha) \quad (\text{A.13})$$

$$= 2\alpha(\sigma_N^2 + \sigma_C^2 - 2\sigma_N\sigma_C\rho_{NC}) - 2\sigma_C^2 + 2\sigma_N\sigma_C\rho_{NC} \quad (\text{A.14})$$

then find the minima and maxima of this derivative by evaluating

$$\frac{d}{d\alpha} \text{Var}[\hat{\theta}] = 0 \quad (\text{A.15})$$

$$2\alpha(\sigma_N^2 + \sigma_C^2 - 2\sigma_N\sigma_C\rho_{NC}) - 2\sigma_C^2 + 2\sigma_N\sigma_C\rho_{NC} = 0 \quad (\text{A.16})$$

$$2\alpha(\sigma_N^2 + \sigma_C^2 - 2\sigma_N\sigma_C\rho_{NC}) = 2\sigma_C^2 - 2\sigma_N\sigma_C\rho_{NC} \quad (\text{A.17})$$

$$\alpha = \frac{\sigma_C^2 - \sigma_N\sigma_C\rho_{NC}}{\sigma_N^2 + \sigma_C^2 - 2\sigma_N\sigma_C\rho_{NC}} \quad (\text{A.18})$$

1689 This equation shows only one solution which is a minima. From Eq. A.18 arise two singularities:

- 1690 — $\sigma_N = \sigma_C = 0$. This is not a problem because as physicists we never measure with an absolute precision, neither us or our detectors are perfect.
- 1691 — $\sigma_N = \sigma_C$ and $\rho_{CN} = 1$. In this case θ_C and θ_N are the same estimator in term of variance thus any value for α yield the same result: an estimator with the same variance as the original ones.

1692

1693

¹⁶⁹⁴ **Appendix B**

¹⁶⁹⁵ Charge spherical harmonics analysis

¹⁶⁹⁶ When looking at JUNO events we can clearly see some pattern in the charge repartition based on
¹⁶⁹⁷ the event radius as illustrated in figure B.4. When dealing with identifying features and pattern on a
¹⁶⁹⁸ spherical plane, the astrophysics community have been using, with success, the spherical harmonic
¹⁶⁹⁹ decomposition. The principle is similar to a frequency analysis via Fourier transform. It comes to
¹⁷⁰⁰ saying that a function $f(r, \theta, \phi)$, here our charge repartition of the spherical plane constructed by our
¹⁷⁰¹ PMTs, can be expressed

$$f(r, \theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^l a_l^m r^l Y_l^m(\theta, \phi) \quad (\text{B.1})$$

¹⁷⁰² where a_l^m are constants complex factor, $Y_l^m(\theta, \phi) = Ne^{im\phi} P_l^m(\cos \theta)$ are the spherical harmonics of
¹⁷⁰³ degree l and order m and P_l^m their associated Legendre Polynomials. Those harmonics are illustrated
¹⁷⁰⁴ in figure B.1. By reducing the problem to the unit sphere $r = 1$, we get rid of the term r^l . The Healpix
¹⁷⁰⁵ library [76] offer function to efficiently find the a_l^m factor from a given Healpix map.

¹⁷⁰⁶ For the above decomposition, we will define the *Power* of an harmonic as

$$S_{ff}(l) = \frac{1}{2l+1} \sum_{m=-l}^l |a_l^m|^2 \quad (\text{B.2})$$

¹⁷⁰⁷ and the *Relative Power* as:

$$P_l^h = \frac{S_{ff}(l)}{\sum_l S_{ff}(l)} \quad (\text{B.3})$$

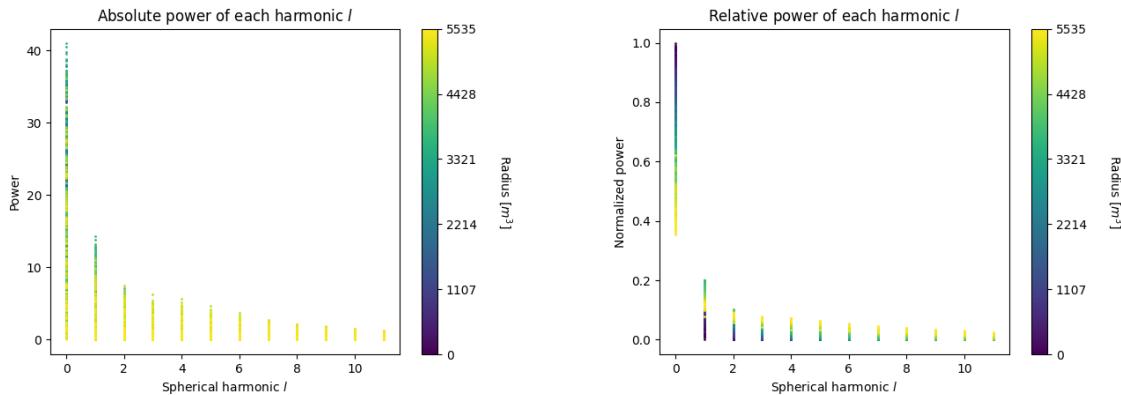
¹⁷⁰⁸ For this study we will use 10k positron events with $E_{kin} \in [0; 9]$ MeV uniformly distributed in the
¹⁷⁰⁹ CD from the JUNO official simulation version J23.0.1-rc8.dc1 (released the 7th January 2024). All the
¹⁷¹⁰ event are *calib* level, with simulation of the physics, electronics, digitizations and triggers. We first
¹⁷¹¹ take a sub-set of 1k events and look at the power and relative power distribution depending on the
¹⁷¹² radius and harmonic degree l . The results are shown in figure B.2. While don't see any pattern in
¹⁷¹³ absolute power, it is pretty clear that there is a correlation between the relative power of $l = 0$ and
¹⁷¹⁴ the radius of the event.

¹⁷¹⁵ When applying the same study but dependent on the energy, no clear correlation appear. The results
¹⁷¹⁶ for the $l = 0$ harmonic are presented in the figure B.5. Thus, in this study we will focus on the radial
¹⁷¹⁷ dependency of the relative power of each harmonic.

¹⁷¹⁸ In figures B.6 and B.7 are presented the distribution of the relative power of each harmonic for $l \in$
¹⁷¹⁹ $[0, 11]$. The relation between the radius and the relative power become even more clear, especially
¹⁷²⁰ for the first harmonics $l \in [0, 4]$. After that for $l > 4$ their relative power is close to 0 for central event,
¹⁷²¹ thus loosing power. It also interesting to note the change of behavior in the TR area, clearly visible
¹⁷²² for $l = 1$ and $l = 2$.

$l:$	$P_\ell^m(\cos \theta) \cos(m\varphi)$	$P_\ell^{ m }(\cos \theta) \sin(m \varphi)$
0 s		
1 p		
2 d		
3 f		
4 g		
5 h		
6 i		
$m:$	6 5 4 3 2 1 0	-1 -2 -3 -4 -5 -6

FIGURE B.1 – Illustration of the real part of the spherical harmonics

FIGURE B.2 – Scatter plot of the absolute and relative power, respectively on the left and right plot, of each harmonic degree l . The color indicate the radius of the event.

1723 As an erzats of reconstruction algorithm, we fit each of those distribution with a 9th degree polynomial
 1724 which give us the relation

$$F(R^3) \longmapsto P_l^h \quad (\text{B.4})$$

1725 We do it this way because some of the distribution have multiple solution for a given relative power,
 1726 for example $l = 1$, while each radius give only one power. We now just need to find

$$F^{-1}(P_l^h) \longmapsto R^3 \quad (\text{B.5})$$

1727 Inverting a 9th degree polynomial is hard, if not impossible. The presence of multiple roots for the
 1728 same power complexify the task even more. To circumvent this problem, we reconstruct the radius
 1729 by locating the minima of $(F(R^3) - \hat{P}_l^h)^2$ where \hat{P}_l^h is the measured power fraction.

1730 To distinguish between multiple possible minima, we use as a starting point the radius given by the
 1731 procedure on $l = 0$ that, by looking at the fit in figure B.6, should only present one minima. For $l > 0$
 1732 we also impose bound on the possible reconstructed R^3 as $R^3 \in [R_0^3 - 100, R_0^3 + 100]$ where R_0^3 is the
 1733 reconstructed R^3 by the harmonic $l = 0$.

1734 The minimization algorithm used are the Bent algorithm for $l = 0$ and the Bounded algorithm for
 1735 $l > 0$ provided by the Scipy library [80]. We then do the mean of the reconstructed radius from
 1736 the different harmonics. The reconstruction results are shown in figure B.3. The performance seems
 1737 correct but we see heavy fluctuation in the bias. To really be used as a reconstruction algorithm, the
 1738 method needs to be refined as discussed in the next section.

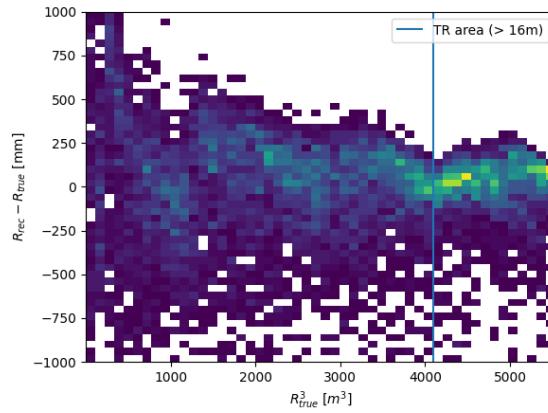


FIGURE B.3 – Error on the reconstructed radius vs the true radius by the harmonic method

1739 Conclusion

1740 We have clearly shown in this analysis the relevance the of relative harmonic power for radius
 1741 reconstruction, and provided an erzats of a reconstruction algorithm. We will not delve further in
 1742 this thesis but if we wanted to refine this algorithm multiple paths can be explored:

- 1743 — No energy signature in the harmonics: This is surprising that there is no correlation between
 1744 the energy and the amplitude of the harmonics. We know that the energy is heavily correlated
 1745 with the total number of photoelectrons collected, it would be unintuitive that we see no
 1746 relation.
- 1747 — Localization of the event: We shown here the relation between the relative power of the har-
 1748 monic and the radius but don't get any information about the θ and ϕ spherical coordinates.
 1749 This information is probably hidden in the individual power of each order m of the degree l .
 1750 This intuition comes from the figure B.1 where in the higher degree l we see that the order m
 1751 are oriented. Intuitively, the order should be able to indicate a direction where the signal is
 1752 more powerful.
- 1753 — Combination of the degree power: Here we combined the radius reconstructed by the dif-
 1754 ferent degree via a simple mean but we shown in section 4.4.2 and annex A that this is note
 1755 the optimal way to combine estimator. A more refined algorithm probably exist to take into
 1756 account the predicting power of each order.

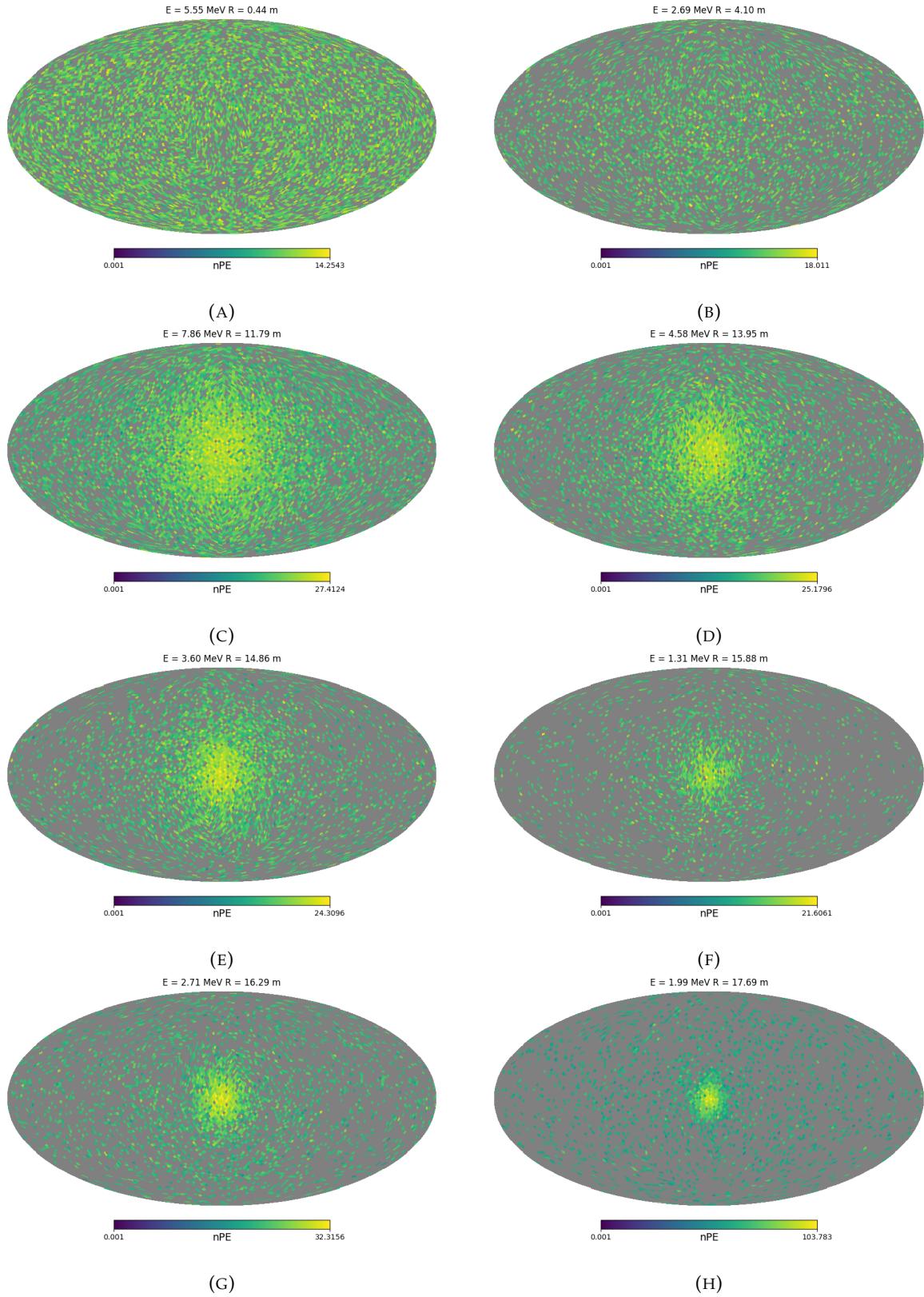


FIGURE B.4 – Charge repartition in JUNO as seen by the Healpix segmentation. Those are Healpix map of order 5 (i.e. 12288 pixels). The color represent the summed charge of the PMTs in each pixels. The color scale is logarithmic. The view have been centered to prevent event deformations.

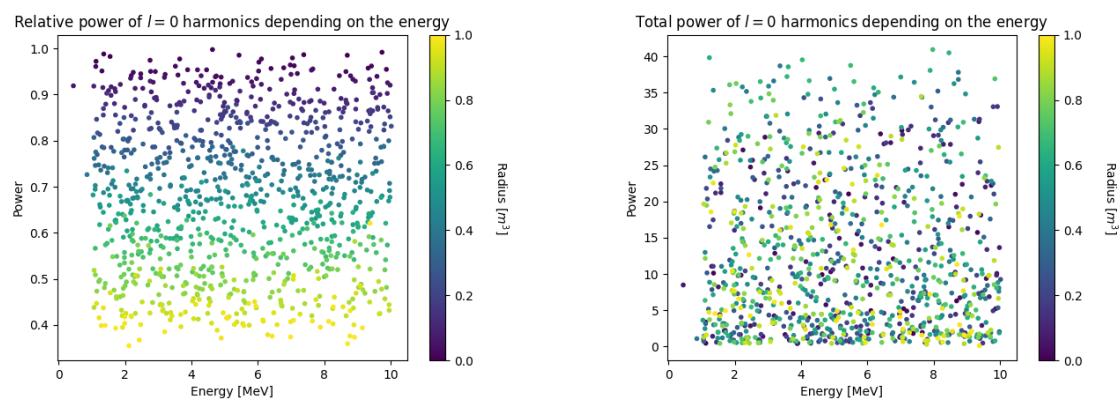


FIGURE B.5 – Scatter plot of the absolute and relative power, respectively on the left and right plot, of the $l = 0$ harmonic. The color indicate the radius of the event.

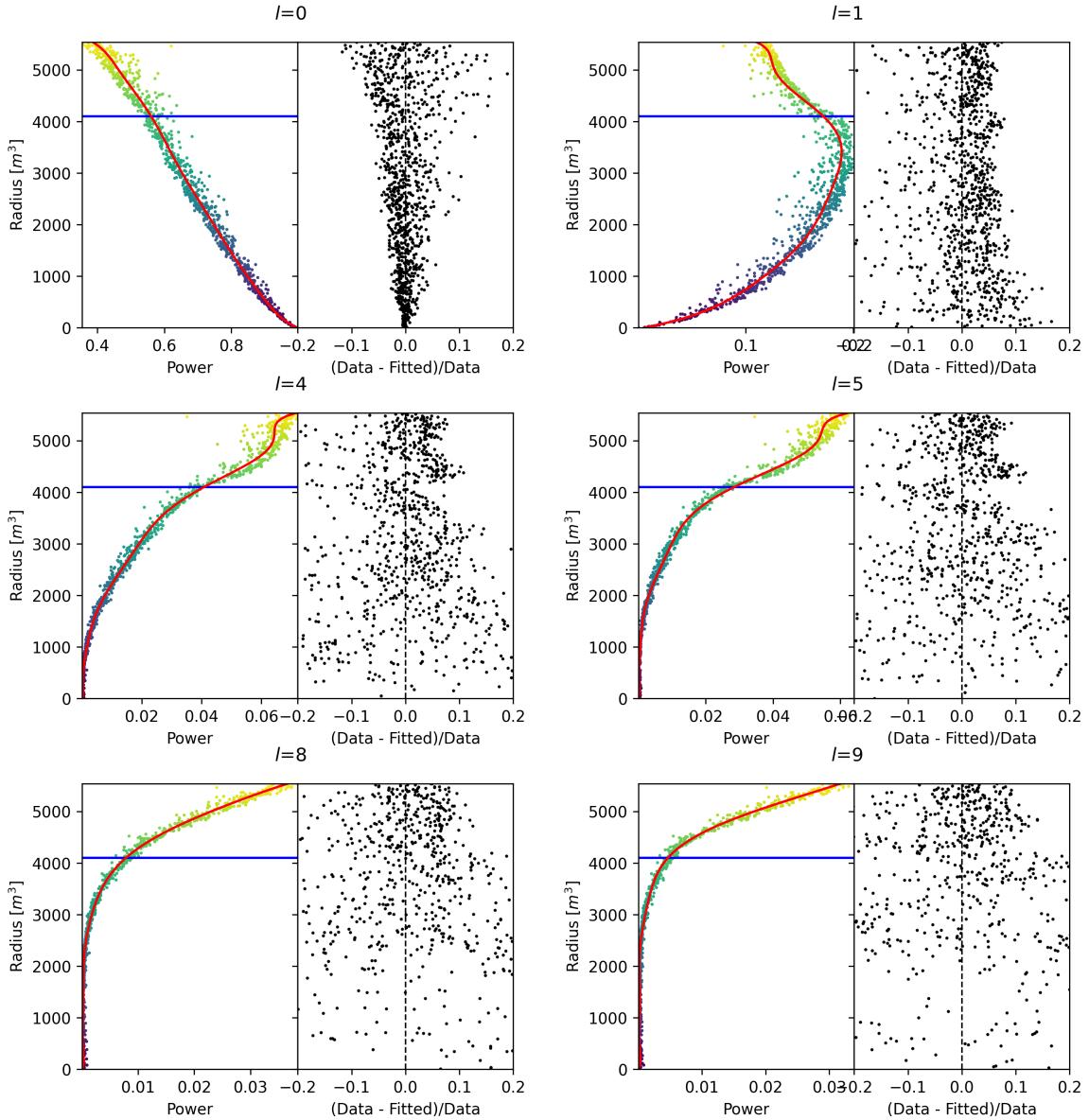


FIGURE B.6 – Plot of the distribution of the relative power of each harmonic dependent on R^3 (on the left). The Total Reflection (TR) area is represented by the horizontal blue line. The distribution are fitted using a 9th degree polynomial (red curve). The relative power error between the distribution and the fit is represented on the left. **Part 1**

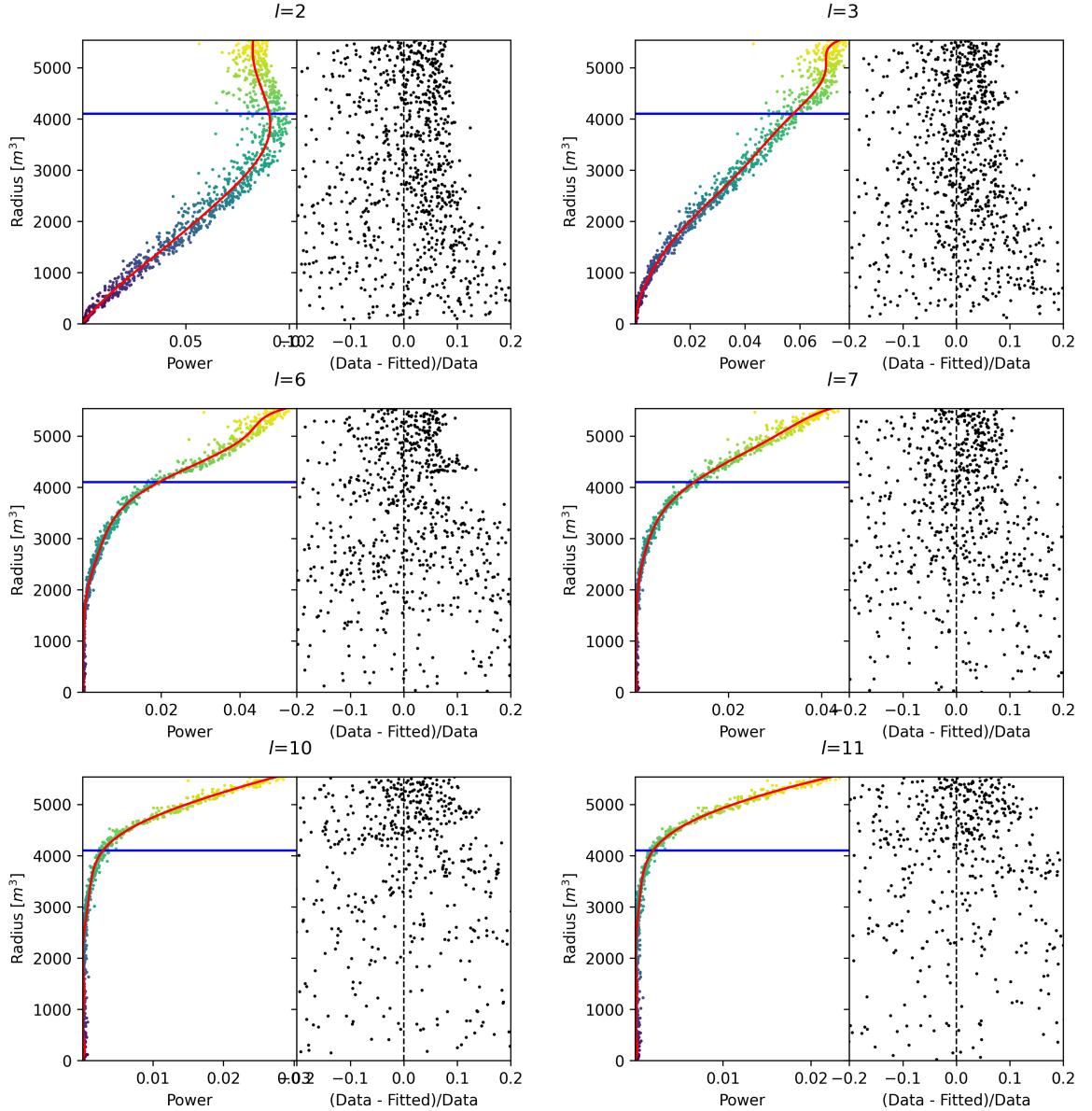


FIGURE B.7 – Plot of the distribution of the relative power of each harmonic dependent on R^3 (on the left). The Total Reflection (TR) area is represented by the horizontal blue line. The distribution are fitted using a 9th degree polynomial (red curve). The relative power error between the distribution and the fit is represented on the left. **Part 2**

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¹⁹⁹⁶ List of Abbreviations

ACU	Automatic Calibration Unit
BDT	Boosted Decision Tree
CD	Central Detector
CLS	Cable Loop System
CNN	Convolutional NN
DNN	Deep NN
DN	Dark Noise
EDM	Event Data Model
FCDNN	Fully Connected Deep NN
GNN	Graph NN
GT	Guiding Tube
IBD	Inverse Beta Decay
IO	Inverse Ordering
JUNO	Jiangmen Underground Neutrino Observatory
LPMT	Large PMT
LR	Learning Rate
LS	Liquid Scintillator
MC	Monte Carlo simulation
ML	Machine Learning
MSE	Mean Squared Error
NMO	Neutrino Mass Ordering
NN	Neural Network
NO	Normal Ordering
NPE	Number of Photo Electron
OSIRIS	Online Scintillator Internal Radioactivity Investigation System
PE	Photo Electron
PMT	Photo-Multipliers Tubes
PRelu	Parametrized Rectified Linear Unit
QNL	Charge (Q) Non Linearity
ROV	Remotely Operated under-LS Vehicle
ReLU	Rectified Linear Unit
ResNet	Residual Network
SGD	Stochastic Gradient Descent
SPMT	Small PMT
TAO	Taishan Antineutrino Oservatory
TR Area	Total Reflexion Area
TTS	Time Transit Spread
TT	Top Tracker
UWB	Under Water Boxes
WCD	Water Cherenkov Detector

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