Search for Heavy Neutral Leptons with IceCube DeepCore

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Colophon
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The source code of this thesis is available at:
https://github.com/LeanderFischer/phd_thesis

Zusammenfassung

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Abstract

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1.2 Model Specific Simulation

Re-write/re-formulate this section (copied from HNL technote).

1.2.1 Custom LeptonInjector

Signal events are simulated using a custom LeptonInjector (LI) tool [1], modified from its standard version to include the HNL particle and the description of the HNL decays needed to produce the double cascade signature (currently only ν_τ related). In its SM work mode, LI injects a lepton and a cascade (under the general name *Hadrons*) at the interaction vertex of the neutrino. Both objects have the same (x,y,z,t) coordinates. In the modified version, the lepton at the interaction vertex is replaced by the HNL. After a chosen distance the HNL is forced to decay. The decay is sampled from the kinematically accessible decay modes shown in Figure 1.2.

[1]: Abbasi et al. (2021), "LeptonInjector and LeptonWeighter: A neutrino event generator and weighter for neutrino observatories"

A big addition to the standard LI is that the decay products of the HNL are added to the list of particles in the I3MCTree with a displaced position and delayed time from the interaction vertex. These daughter particles form a second cascade, not in the form of a *Hadrons* object, but as the explicit particles forming the shower. The kinematics of the two-body decays are computed analytically, while the three-body decays are dealt with using MadGraph5. To do so, we randomly pick an event from a list that we generated for each three-body decay mode. Independent of the number of particles in the final state of the HNL decay, the kinematics are calculated/simulated at rest and then boosted along the HNL momentum. The decay mode is randomly chosen based on the mass dependent branching ratios shown in Figure 1.2.

Each file is produced by running the generation level processing script using the filenumber as random seed and the above settings for the sampling distributions. The main part is calling the *MultiLeptonInjector* module in *volume mode* adding two generators (for ν_τ and $\bar{\nu}_\tau$) with 50% of the events. The generators are provided with the custom double-differential/total cross section splines described in Section 1.2.1 and the parameters defining the sampling distributions. For each frame *OneWeight* and a reference weight are also calculated and stored using the weighting functions and a baseline atmospheric ν_τ flux + oscillation spline. The weight will later be calculated inside of the analysis framework

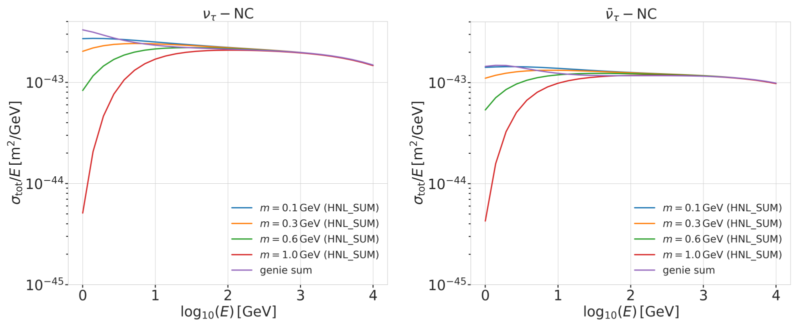

Figure 1.1: Custom HNL total cross sections for the four target masses compared to the total ($\nu_\tau/\bar{\nu}_\tau$ neutral current) cross section used for SM neutrino simulation production with GENIE.

PISA, based on the input OneWeight. In addition to the i3 file itself, a LeptonInjector configuration file is written which stores the needed information to produce event weights using LeptonWeighter. Optionally the script can also produce an hdf5 file with the same name in the same location. This will store a fixed set of keys, extracted from the i3 file.

We are using *volume mode*, for the injection of the primary particle on a cylindrical volume. The main generation/sampling happens in `VolumeLeptonInjector::DAQ` inside `LeptonInjector.cxx`. After writing the config (s) frame (currently not kept), the energy is sampled from a power law distribution, then the cosine(zenith) and azimuth angles are sampled from uniform distributions. The (x,y) position is sampled uniform in r, ϕ (for position on disk) and the z position is sampled from a uniform distribution. After the primary properties have been sampled the *EventProperties* is created and handed over to the `FillTree` functions which is where the custom HNL simulation happens:

add varied total cross-section for a few background HNL events

Cross Sections

The cross sections are calculated using a modified version of Carlos Argüelles' NuXSSplMkr, which is a tool to calculate neutrino cross sections from parton distribution functions (PDFs) and then produce splines that can be read and used with IceCube software. The main modification to calculate the cross sections for the ν_τ neutral current interaction into the new heavy mass state is the addition of a kinematic condition to ensure that there is sufficent energy to produce the heavy mass state. It is the same confition that needs to be fulfilled for the charged current case, where the outgoing lepton mass is non-zero. Following [2] (equation 7), the condition

[2]: Levy (2009), "Cross-section and polarization of neutrino-produced tau's made simple"

$$(1 + x\delta_N)h^2 - (x + \delta_4)h + x\delta_4 \leq 0, \tag{1.1}$$

is implemented for the neutral current case. Here $\delta_4 = \frac{m_4^2}{s-M^2}$, $\delta_N = \frac{M^2}{s-M^2}$, and $h \overset{def}{=} xy + \delta_4$, with x, y being the Bjorken variables, m_4 and M the mass of the heavy state and the target nucleon, respectively, and s the center of mass energy squared. Since the (SM) neutrino background simulation used for this analysis was created using GENIE (version 2.12.8), interfaced through the IceCube software package *genie-icetray*, with the GRV98LO PDFs, those were added as *GRV98lo_patched* to the

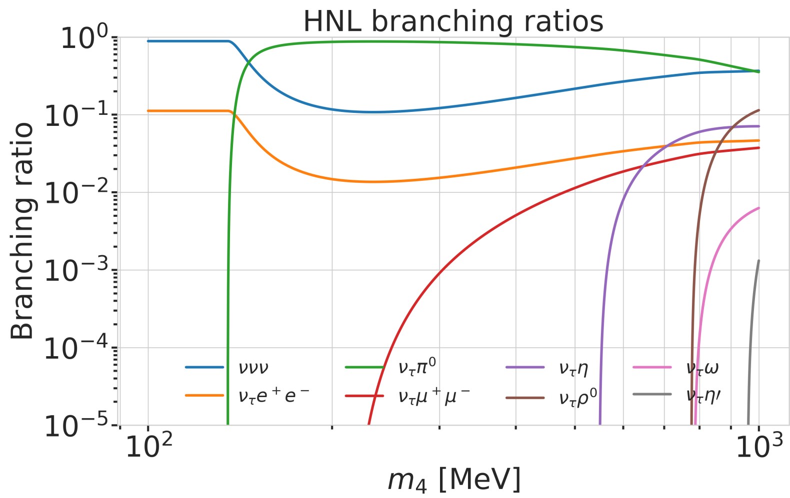

Figure 1.2: Branching ratios of the HNL within the mass range considered, calculated based on the results from [3]. Given the existing constraints on $|U_{e4}|^2$ and $|U_{\mu4}|^2$, we consider that the corresponding decay modes are negligible.

Channel	Opens [MeV]	Max BR [%]
$\nu_4 \longrightarrow \nu_\tau\nu_\alpha\bar{\nu_\alpha}$	0	100.0
$\nu_4 \longrightarrow \nu_\tau e^+e^-$	1	?
$\nu_4 \longrightarrow \nu_\tau\pi^0$	135	?
$\nu_4 \longrightarrow \nu_\tau\mu^+\mu^-$	211	?
$\nu_4 \longrightarrow \nu_\tau\eta$	548	?
$\nu_4 \longrightarrow \nu_\tau\rho^0$	770	?
$\nu_4 \longrightarrow \nu_\tau\omega$	783	?
$\nu_4 \longrightarrow \nu_\tau\eta'$	958	?

Table 1.1: xx

cross section spline maker, to ensure the best possibe agreement. Double-differential ($dsdxdy$) and total (σ) cross sections were produced for the four target HNL masses and then splined. The produced cross section splines are stored in the resources of the custom LeptonInjector module. Figure 1.1 shows the total cross sections that were produced compared to the cross section used for the production of the SM $\nu_\tau/\bar{\nu}_\tau$ neutral current background simulation .

Add comparions of SM cross sections between NuXSSplMkr and genie

Decay Channels

The accessible decay channels are dependent on the mass of the HNL and the allowed mixing. For this analysis, where only $|U_{\tau4}|^2 \neq 0$, the considered decay channels are listed in Table 1.1 and the corresponding branching ratios are shown in Figure 1.2. The indiviudal branching ratio for a specific mass is calculated as $\mathrm{BR}_i(m_4) = \Gamma_i(m_4)/\Gamma_{\mathrm{total}}(m_4)$, where $\Gamma_{\mathrm{total}}(m_4) = \sum \Gamma_i(m_4)$. The formulas to calculate the decay width show up in multiple references, but we chose to match them to [3], which also discusses the discrepencies in previous literature.

[3]: Coloma et al. (2021), "GeV-scale neutrinos: interactions with mesons and DUNE sensitivity"

2-Body Decay Widths The decay to a neutral pseudoscalar mesons is

$$\Gamma_{\nu_4 \to \nu_\tau P} = |U_{\tau4}|^2 \frac{G_F^2 m_4^3}{32\pi} f_P^2 (1 - x_p^2)^2, \tag{1.2}$$

with $x_P = m_P/m_4$ and

$$f_{\pi^0} = 0.130\,\text{GeV}, \qquad f_\eta = 0.0816\,\text{GeV}, \qquad C_2 = f_{\eta'} = -0.0946\,\text{GeV}, \tag{1.3}$$

while the decay to a neutral vector meson is given by

$$\Gamma_{\nu_4\to\nu_\tau V} = |U_{\tau 4}|^2 \frac{G_F^2 m_4^3}{32\pi}\left(\frac{f_V}{m_V}\right)^2 g_V^2 (1+2x_V^2)(1-x_V^2)^2, \tag{1.4}$$

with $x_V = m_V/m_4$,

$$f_{\rho^0} = 0.171\,\text{GeV}^2, \qquad f_\omega = 0.155\,\text{GeV}^2, \tag{1.5}$$

and

$$g_{\rho^0} = 1 - 2\sin^2\theta_w, \qquad g_\omega = \frac{-2\sin^2\theta_w}{3}, \qquad \sin^2\theta_w = 0.2229 \tag{1.6}$$

[4].

[4]: Tiesinga et al. (2021), "CODATA recommended values of the fundamental physical constants: 2018"

3-Body Decay Widths The (invisible) decay to three neutrinos is

$$\Gamma_{\nu_4\to\nu_\tau\nu_\alpha\bar{\nu_\alpha}} = |U_{\tau 4}|^2 \frac{G_F^2 m_4^5}{192\pi^3}, \tag{1.7}$$

while the decay to two charged leptons (using $x_\alpha = (m_\alpha/m_4)^2$) of the same flavor reads

$$\Gamma_{\nu_4\to\nu_\tau l_\alpha^+ l_\alpha^-} = |U_{\tau 4}|^2 \frac{G_F^2 m_4^5}{192\pi^3}\left[C_1 f_1(x_\alpha) + C_2 f_2(x_\alpha)\right], \tag{1.8}$$

with the constants defined as

$$C_1 = \frac{1}{4}(1 - 4s_w^2 + 8s_w^4), \qquad C_2 = \frac{1}{2}(-s_w^2 + 2s_w^4), \tag{1.9}$$

the functions as

$$f_1(x_\alpha) = (1 - 14x_\alpha - 2x_\alpha^2 - 12x_\alpha^3)\sqrt{1-4x_\alpha} + 12x_\alpha^2(x_\alpha^2 - 1)L(x_\alpha), \tag{1.10}$$

$$f_2(x_\alpha) = 4[x_\alpha(2+10x_\alpha - 12x_\alpha^2)\sqrt{1-4x_\alpha} + 6x_\alpha^2(1-2x_\alpha+2x_\alpha^2)L(x_\alpha)], \tag{1.11}$$

and

$$L(x) = \ln\left(\frac{1 - 3x_\alpha - (1-x_\alpha)\sqrt{1-4x_\alpha}}{x_\alpha(1+\sqrt{1-4x_\alpha})}\right). \tag{1.12}$$

1.2.2 MadGraph5 3-Body Decays

The code to produce the 3-body decay kinematics is MadGraph4 v3.4.0 based on the decay diagrams calculated with FeynRules 2.0 using the Lagrangians derived in [3]. The Universal FeynRules Outpur (UFO) from `effective_HeavyN_Majorana_v103` were used for our calculation. For each meass and corresponding decay channel, we produce $1e06$ decay kinematic variations (rest frame) and store those in a text file.

[3]: Coloma et al. (2021), "GeV-scale neutrinos: interactions with mesons and DUNE sensitivity"

variable	distribution	range
energy	E^{-2}	$[2, 10^4]$ GeV
zenith	uniform (in $\cos(\theta)$)	[180 °, 80 °]
azimuth	uniform	[0 °, 360 °]
vertex (x, y)	uniform	$r = 600$ m
vertex z	uniform	[-600, 0] m
m_{HNL}	fixed	[0.3, 0.6, 1.0] GeV
L_{decay}	L^{-1}	[0.0004, 1000.0] m / [1.0, 1000.0] m

Table 1.2: Sampling distributions of HNL simulation generation.

1.2.3 Sampling Distributions

This is the description of the signal simulation generator used to (re-)start simulation production in December 2023. The underlying sampling distributions are listed in Table 1.2. Judging from how the generation/processing efficiency was for the 190607 set, we target $1e04$ files per set with $5e05$ events per file at generation, resulting in a maximum of $5e09$ events per set at generation level. Note here that the actual number of events per set at generation might be a little lower since some events won't be allowed if they don't have enough energy to produce the HNL.

1.2.4 Weighting Scheme

The weighting for the HNL signal simulation happens in a custom stage of PISA. The only input is the stored OneWeight and the variable physics parameter $|U_{\tau 4}|^2$, which is the mixing strength of the new heavy mass state and the tau sector. The custom re-weighting is needed to go from the used sampling PDF (1/L with fixed range in lab frame decay length) to the target PDF (exponential defined by proper lifetime of the HNL). For each event the re-weighting factor is calculated using the gamma factor

$$\gamma = \frac{\sqrt{E_{\mathrm{kin}}^2 + m_{\mathrm{HNL}}^2}}{m_{\mathrm{HNL}}}, \tag{1.13}$$

with the HNL mass m_{HNL} and it's kinetic energy E_{kin}. The speed of the HNL is calculated as

$$v = c \cdot \sqrt{1 - \frac{1}{\gamma^2}}, \tag{1.14}$$

where c is the speed of light. With these the lab frame decay length range can be converted into the rest frame lifetime range for each event

$$\tau_{\mathrm{min/max}} = \frac{s_{\mathrm{min/max}}}{v \cdot \gamma}. \tag{1.15}$$

The proper lifetime of each HNL event can be calculated using the total decay width Γ_{total} shown in Figure **??** and the chosen mixing strength $|U_{\tau 4}|^2$ as

$$\tau_{\mathrm{proper}} = \frac{\hbar}{\Gamma_{\mathrm{total}}(m_{\mathrm{HNL}}) \cdot |U_{\tau 4}|^2}, \tag{1.16}$$

where $\hbar$ is the reduced Planck constant. Since the decay length/lifetime of the events is sampled from an inverse distribution instead of an exponential as it would be expected from a particle decay we have to re-weight accordingly to achieve the correct decay length/lifetime distribution. This is done by using the wanted exponential distribution

$$\mathrm{PDF}_{\mathrm{exp}} = \frac{1}{\tau_{\mathrm{proper}}} \cdot e^{\frac{-\tau}{\tau_{\mathrm{proper}}}}, \tag{1.17}$$

and the inverse distribution that was sampled from

$$\mathrm{PDF}_{\mathrm{inv}} = \frac{1}{\tau \cdot (\ln(\tau_{\mathrm{max}}) - \ln(\tau_{\mathrm{min}}))}. \tag{1.18}$$

The lifetime re-weighting factor is calculated as

$$w_{\mathrm{lifetime}} = \frac{\mathrm{PDF}_{\mathrm{exp}}}{\mathrm{PDF}_{\mathrm{inv}}} = \frac{\Gamma_{\mathrm{total}}(m_{\mathrm{HNL}}) \cdot |U_{\tau 4}|^2}{\hbar} \cdot \tau \cdot (\ln(\tau_{\mathrm{max}}) - \ln(\tau_{\mathrm{min}})) \cdot e^{\frac{-\tau}{\tau_{\mathrm{proper}}}}. \tag{1.19}$$

Adding another factor of $|U_{\tau 4}|^2$ to account for the mixing at the interaction vertex the total re-weighting factor becomes

$$w_{\mathrm{total}} = |U_{\tau 4}|^2 \cdot w_{\mathrm{lifetime}}, \tag{1.20}$$

which can be applied on top of flux and oscillation weight to get the final HNL weight for a given mixing (and mass).

1.3 Model Dependent Simulation Distributions

1.3.1 Generation Level

1.3.2 Final Level

Detecting Low Energetic Double Cascades

2

2.1 Reconstruction

2.1.1 Table-Based Minimum Likelihood Algorithms

2.1.2 Double Cascade Hypothesis

2.1.3 Modification to Low Energy Events

2.2 Performance

2.2.1 Energy/Decay Length Resolution

2.2.2 Double Cascade Classification

Search for an Excess of Heavy Neutral Lepton Events

3

The measurement performed in this thesis is the search for an excess of HNL events in the 10 years of IceCube DeepCore data. In principle the two physics parameters to be probed are the mass of the HNL, m_4, and the mixing between the fourth heavy mass state and the SM τ sector, $|U_{\tau 4}|^2$. Since the mass itself influences the production and decay kinematics of the event and the accessible decay modes, individual mass sets were produced as described in Section 1.2. The mass slightly influences the energy distribution, while the mixing both changes the overall scale of the HNL events and the shape in energy and PID. IceCube DeepCore is suited to measure the excess which appears around and below 20 GeV, due to its production from the atmospheric tau neutrinos. The measurement will be performed for the three mass sets individually, while the mixing is the parameter that can be varied continuously and will be measured in the fit.

3.1 Final Level Sample

3.1.1 Expected Rates/Events

Add final level composition for benchmark mixing/all masses?

3.1.2 Analysis Binning

describe binning and bin masking

add 3D expectation and/or S/sqrt(B) plots

3.2 Statistical Analysis

3.2.1 Test Statistic

The measurements are performed by comparing the weighted MC to the data. Through variation of the nuisance and physics parameters that govern the weights, the best matching set of parameters can be found. The comparison is done using a modified χ^2 defined as

$$\chi^2_{\mathrm{mod}} = \sum_{i \in \mathrm{bins}} \frac{(N_i^{\nu} + N_i^{\mu} + N_i^{\mathrm{HNL}} - N_i^{\mathrm{obs}})^2}{N_i^{\nu} + N_i^{\mu} + N_i^{\mathrm{HNL}} + (\sigma_i^{\nu})^2 + (\sigma_i^{\mu})^2 + (\sigma_i^{\mathrm{HNL}})^2} + \sum_{j \in \mathrm{syst}} \frac{(s_j - \hat{s}_j)^2}{\sigma^2_{s_j}}, \tag{3.1}$$

as the test statistic (TS), where N_i^{ν}, N_i^{μ}, and N_i^{HNL} are the expected number of events in bin i from neutrinos, atmospheric muons, and HNL, while N_i^{obs} is the observed number of events in bin i. The expected number of events from each particle type is calculated by summing the weights of all events in the bin $N_i^{\mathrm{type}} = \sum_i^{\mathrm{type}} \omega_i$, with the statistical uncertainty being $(\sigma_i^{\mathrm{type}})^2 = \sum_i^{\mathrm{type}} \omega_i^2$. The expected Poisson error is calculated using the combined expectation of neutrinos, atmospheric muons, and HNL events. The additional term in Equation 3.1 is included to apply a penalty term for prior knowledge of the systematic uncertainties of the parameters where they are known. s_j are the systematic parameters that are varied in the fit, while $\hat{s_j}$ are their nominal values and σ_{s_j} are the known uncertainties.

Do I want/need to include the description of the KDE muon estimation?

3.2.2 Systematic Uncertainties

Treatment of Detector Response Uncertainties via a Likelihood-Free Inference Method

[5]

[5]: Fischer et al. (2023), "Treating detector systematics via a likelihood free inference method"

Copy paste from OVS PRD about hypersurfaces (and interpolation of those):

To evaluate the expected impact of detection uncertainties, data sets are produced with different variations of detector response, processed to the final level of selection, and then they are parameterized following a model of the uncertainties to evaluate how the final sample would look like for any reasonable choice of parameters. The parametrizations are done at the analysis bin level, assuming that every effect considered is independent and that they can be approximated by a linear function. Under these assumptions we can compute a reweighting factor in every bin that depends on N parameters, which correspond to the number of systematic effects being considered, plus an offset c, as

$$f(p_1, ..., p_N) = c + \sum_{n=1}^{N} m_n \Delta p_n . \tag{3.2}$$

Here m_n are the reweighting factors obtained from simulation sets with a systematic variation and Δp_n is the test value of a specific systematic variation.

The fit of the parameters m_n is done over all systematic MC sets, reducing the uncertainty on the MC prediction in each bin as a side effect since the error on the fitted function is smaller than the statistical error from the nominal MC set. The set of all fitted functions in all histogram bins are called "hypersurfaces". An example of such a fit from a single bin, projected onto one dimension, is shown in Fig. **??**.

The event counts coming from different flavors and interactions have a different response to varying the same detector parameter. Therefore, the hypersurfaces in each bin are fit separately for three groups of events:

- $(\nu_{\mathrm{all}} + \bar{\nu}_{\mathrm{all}})$ NC + $(\nu_e + \bar{\nu}_e)$ CC: These events all produce cascade signatures in the detector.
- $(\nu_\tau + \bar{\nu}_\tau)$ CC: These interactions may differ from the previous group because they have a production threshold of $E_\nu \gtrsim 3.5\,\mathrm{GeV}$ and also produce muons with a branching ratio of 17%.
- $(\nu_\mu + \bar{\nu}_\mu)$ CC: These interactions produce track-like signatures.

The distribution of χ^2/d.o.f. from the fits in all analysis bins is used as a diagnostic to ensure that the fitted, linear hypersurfaces provide a good estimate for the expected number of events for the full range of simulated detector configurations. We find that the means of these χ^2/d.o.f. distributions are all consistent with 1.0 as expected from good fits for each of the three categories described above (NC + ν_e CC, ν_τ CC and ν_μ CC). Attempts to use higher order polynomial fits did not yield a significantly improved χ^2/d.o.f., and in fact often rendered the fits less stable.

To produce the histograms for fitting the hypersurfaces, a choice must be made for the values of flux, cross section and oscillation parameters. We found that the hypersurface fits are sensitive to the choice of parameters that have correlations with the effect they encode. Most notably, this effect is observed between the mass splitting and DOM optical efficiency as demonstrated in Fig. **??**, which shows the difference between fitted hypersurface gradients for the DOM efficiency dimension for two values of Δm^2_{32}.

This problem arises because we are only fitting the hypersurfaces in reconstructed phase space, without accounting for the different true energy and zenith distributions of MC in each analysis bin, which change with each detector systematic variation. To mitigate this problem, we fit the hypersurfaces for 20 different values in mass splitting between $1.5 \times 10^{-3}\,\mathrm{eV}^2$ and $3.5 \times 10^{-3}\,\mathrm{eV}^2$, and then apply a piece-wise linear interpolation to all slopes, intercepts and covariance matrix elements. The oscillation parameter fit can then dynamically adapt the hypersurfaces for each value of Δm^2_{32} that is tested using these interpolated functions. The effects of other parameter choices were evaluated as well, but none were found to introduce a significant bias.

Free Parameter Selection

Copy paste from OVS PRD about systematic impact test:

We decide which systematic uncertainties must be included in the fit by studying the potential bias they would produce in the oscillation parameters and the change on the test statistic χ^2_{mod} if we neglected them. We create data sets with their observed quantities set equal to their expected values for a wide range of values for θ_{23} and Δm^2_{32} and perform two fits: one where the oscillation parameters are fixed to their true value and one where they are left free. In both fits, the systematic parameter being tested is fixed to a value off from its nominal expectation by either 1σ or by an educated guess, if the uncertainty is not well defined. Parameters are included in the analysis when this test creates a significant bias in the oscillation parameters, which is conservatively defined as a difference larger than 2×10^{-2} between the test statistics of the two fits.

Copy paste from OVS PRD about detector systematic nominal, prior, and ranges:

As motivated in Section **??**, the DOM efficiency is constrained by a Gaussian prior to the value of 1.0 ± 0.1. The ice model parameters are unconstrained in the fit, and allowed to vary within conservative ranges determined from calibration data. The hole ice model parameters are bounded within the ranges $-2.0 < p_0 < 1.0$ and $-0.2 < p_1 < 0.2$. The bulk ice model parameters are bounded within $-0.90 <$ Absorption < 1.10 and $-0.95 <$ Scattering < 1.15.

Add table with all systematic uncertainties used in this analysis (in the analysis chapter).

add final level effects of varying the axial mass parameters (or example of one)

add final level effects of varying the DIS parameter (or example of one)

3.3 Analysis Checks

3.3.1 Asimov Inject/Recover Tests

3.3.2 Sensitivity

3.3.3 Ensemble Tests

3.4 Results

3.4.1 Best Fit Parameters

3.4.2 Upper Limits

3.4.3 Post-Fit Data/MC Agreement

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