

Calculation of oscillation probabilities of atmospheric neutrinos using nuCraft

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Abstract

NuCraft (`nucraft.hepforge.org`) is an open-source Python project that calculates neutrino oscillation probabilities for neutrinos from cosmic-ray interactions in the atmosphere for their propagation through Earth. The solution is obtained by numerically solving the Schrödinger equation. The code supports arbitrary numbers of neutrino flavors including additional sterile neutrinos, CP violation, arbitrary mass hierarchies, matter effects with a configurable continuous Earth model, and takes into account the production height distribution of neutrinos in the Earth's atmosphere.

Keywords: neutrino oscillation; atmospheric neutrinos; sterile neutrinos; nuCraft

PROGRAM SUMMARY

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Authors: Marius Wallraff, Christopher Wiebusch

Program Title: nuCraft

Journal Reference:

Catalogue identifier:

Licensing provisions: Revised BSD License

Programming language: Python

Computer: IA32/x86-64 compatible

Operating system: all that are supported by SciPy, e.g., Linux, Windows, OS X

RAM: 134217728 bytes

Keywords: neutrino oscillation, sterile neutrino, atmospheric neutrino

Classification: 1.1 Cosmic Rays, 11.1 General, High-Energy Physics and Computing, 11.6 Phenomenological and Empirical Models and Theories

External routines/libraries: NumPy (1.5.1 or newer), SciPy (0.8.0 or newer)

Nature of problem: Calculation of oscillation probabilities of neutrinos that originate in cosmic-ray interactions in the Earth's atmosphere and propagate through the Earth, for realistic Earth and atmospheric models and multiple flavors (optionally including sterile neutrinos and CP violation).

Solution method: Direct solution of the Schrödinger equation for n flavors including matter effects, with sampling of the atmosphere.

Restrictions: Energy loss and absorption of neutrinos inside the Earth is not modeled; they have to be handled

independently.

Unusual features: Completely configurable oscillation parameters (including optional sterile flavors), configurable and realistic Earth model including atmosphere.

Running time: Roughly 100 neutrinos per second and CPU core (depends on energy and oscillation parameters).

1. Introduction

Neutrino oscillations have been a major research topic for many particle and astroparticle physicists over the last decades [1]. While neutrinos do not possess a mass in the minimum Standard Model of Particle Physics, many oscillation experiments have demonstrated that there are non-zero neutrino masses, and that their mass eigenstates differ from their flavor eigenstates. Despite the large progress that has been made in this field, there are still many open questions regarding neutrinos, including their absolute mass scale, their mass hierarchy, CP-violation, whether there are more than the three known flavors, and whether neutrinos are Majorana particles. Additionally, some neutrino properties are not yet very well measured, and neutrino oscillations are a good phenomenon to improve our knowledge of those.

NuCraft is a Python project designed to compute oscillation probabilities of atmospheric neutrinos that originate from cosmic-ray interactions in the Earth's atmosphere. Many experiments are able to detect and

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measure atmospheric neutrinos. While several tools to calculate oscillation probabilities exist, e.g., Prob3++ [2, 3] or GLOBES [4], nuCraft offers the advantage of a lightweight portable Python implementation and also improves the accuracy of calculations in some aspects. Beyond standard three-flavor oscillations, the code can handle an arbitrary number of additional flavors, e.g., sterile neutrinos [5]. A particular feature is the direct numerical solution of the Schrödinger equation with dynamically determined step sizes for the propagation through Earth. Included is also the smearing of the propagation length caused by different production heights of neutrinos in the atmosphere. This improves the description of down-going and horizontally arriving neutrinos. Furthermore, the density profile of the Earth is not modeled by shells of constant matter density but is instead varied continuously.

2. Theory

2.1. Neutrino oscillation in vacuum

Neutrinos change their flavor during propagation in spacetime as a consequence of their weak-interaction flavor eigenstates ν_α not being identical to their mass eigenstates ν_j [6]; instead, they are a linear combination of each other, described by the unitary Pontecorvo-Maki-Nakagawa-Sakata (PMNS) matrix U :

$$\nu_\alpha = \sum_j U_{\alpha j} \nu_j$$

The PMNS matrix for $n \in \mathbb{N}$ neutrino flavors can be parameterized as a product of rotation matrices $R_{jk} \equiv R_{jk}(\theta_{jk}, \delta_{jk}) \in \mathbb{C}^{n \times n}$,

$$U = \prod_{j=1}^{n-1} \prod_{k=j+1}^n R_{jk},$$

$$(R_{jk})_{mn} = \hat{\delta}_{mn} \left((\hat{\delta}_{jm} + \hat{\delta}_{kn}) \cos(\theta_{jk}) + 1 - (\hat{\delta}_{jm} + \hat{\delta}_{kn}) \right) + (\hat{\delta}_{mj} \hat{\delta}_{nk} - \hat{\delta}_{mk} \hat{\delta}_{nj}) \sin(\theta_{jk}) \exp((-1)^{\hat{\delta}_{nk}} i \delta_{jk}),$$

with mixing angles $\theta_{jk} \in \mathbb{R}$, CP-violating Dirac phases $\delta_{jk} \in \{z \in \mathbb{C} \mid |z| = 1\}$, and Kronecker's delta $\hat{\delta}_{mn}$. This parametrization has to be given explicitly, because there is no clear canonical version for cases with $n > 3$, and rotation matrices do not commute in general. If neutrinos are Majorana particles, one also has to add CP-violating Majorana phases to the diagonal of the PMNS matrix, but those do not influence oscillation phenomena and are therefore omitted for this work. For antineutrinos, U has to be replaced by its complex conjugate.

Neutrinos originate from weak interactions, so they are generated in definite flavor eigenstates. Their propagation through vacuum is described by the time-dependent n -dimensional Schrödinger equation ($c = \hbar = 1$)¹:

$$i \frac{d}{dx} |v_j\rangle = \tilde{H}_0 |v_j\rangle$$

$$\tilde{H}_0 = \text{diag}(E_1, \dots, E_n)$$

In the ultra-relativistic limit, this is simplified using $E_j = \sqrt{p_j^2 + m_j^2} \approx E_\nu + \frac{m_j^2}{2E_\nu}$, which implies $v = c$ and $p_j = p_1$ for all j . Both approximations are fulfilled well for atmospheric neutrinos, but they do not necessarily hold for neutrinos of cosmological origin, which are not the scope of this work.

Terms proportional to the identity matrix do not cause migration from one eigenstate into another and can be omitted; using the PMNS matrix to translate the Schrödinger equation into the flavor bases yields

$$\frac{d}{dx} |v_\alpha\rangle = \frac{-i}{2E_\nu} H_0 |v_\alpha\rangle$$

$$H_0 = U \text{diag}(0, \Delta m_{21}^2, \dots, \Delta m_{n1}^2) U^\dagger.$$

Transition probabilities can then be obtained by

$$P_{\alpha \rightarrow \beta}(x) = |\langle v_\beta(0) | v_\alpha(x) \rangle|^2. \quad (1)$$

2.2. Matter effects

When propagating through matter, neutrinos are subject to coherent forward scattering, which can strongly influence the oscillation behavior [6]. The three known flavors of neutrinos can scatter on all particles via Neutral Current (NC) interactions, and ν_e and $\bar{\nu}_e$ can additionally scatter via Charged Current (CC) interactions on electrons without being absorbed. In contrast, sterile neutrinos do not interact via weak interactions per definition.

These processes induce an effective squared mass:

$$\frac{d}{dx} |v_\alpha\rangle = \frac{-i}{2E_\nu} (H_0 + A) |v_\alpha\rangle \quad (2)$$

$$A = \text{diag}(A_{\text{CC}} + A_{\text{NC}}, A_{\text{NC}}, A_{\text{NC}}, 0, \dots)$$

$$A_{\text{CC}} = \pm 2 \sqrt{2} G_{\text{F}} E_\nu Y_e \rho / m_{\text{N}}$$

$$A_{\text{NC}} = \mp \sqrt{2} G_{\text{F}} E_\nu Y_{\text{N}} \rho / m_{\text{N}},$$

¹Technically, as neutrinos are spin 1/2-particles, one has to use a more general relativistic wave equation, but it can be shown that they all converge on what looks like a Schrödinger equation [6].

where G_F is Fermi's constant, Y_e is the electron fraction ($Y_e = Y_p = 1 - Y_n$), ρ is the mass density, and m_N is the mean of the proton mass and the neutron mass [6]. The upper signs hold for particles, the lower for antiparticles. The reason for A_{NC} only to depend on the neutron density is that in electrically neutral and unpolarized matter, proton and electron potentials cancel out.

In some publications, matter effects are classified as either caused by the Mikheyev-Smirnov-Wolfenstein (MSW) effect or by parametric enhancement to gain phenomenological insights [7]. The work presented here correctly handles both, but the effects cannot be separated because they both originate from A when numerically solving the Schrödinger equation.

2.3. The interaction picture

Numerical algorithms for solving ordinary differential equations generally work better the smoother the solutions are, such that the internal time steps can be chosen large without losing precision. The solution for the Schrödinger equation (2) however is in most cases similar to the plane-wave solution for vacuum oscillations. To significantly reduce the number of time steps that the solvers need in these cases, the Schrödinger equation can be transformed into the interaction basis, in which the vacuum solution is a constant function [8]:

$$\begin{aligned} \frac{d}{dx} |v_{\text{inter}}\rangle &= \frac{-i}{2E_\nu} \tilde{A} |v_{\text{inter}}\rangle \\ |v_{\text{inter}}\rangle &= \exp(-iH_0 x) |v_\alpha\rangle \\ \tilde{A} &= \exp(-iH_0 x) A \exp(iH_0 x) \end{aligned} \quad (3)$$

The additional computations that are needed per time step are relatively expensive, but in most cases they are more than compensated for by the reduced number of steps required.

3. Program

NuCraft is fully written in Python and is compatible with both Python 2 (tested with 2.6 and above) and Python 3 (tested with 3.3). It relies on the libraries NumPy [9] and SciPy [10] and especially uses a SciPy wrapper around the ODE solver ZVODE [11]. Using ZVODE, it directly solves the Schrödinger equation (3) in the interaction picture. The nuCraft source code is available at [12] under the revised BSD license (3-clause version).

The project nuCraft consists of two classes, NuCraft and EarthModel. NuCraft is a class with three helper methods ConstructMassMatrix,

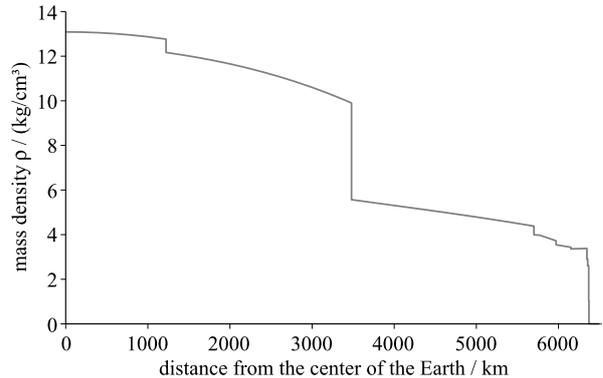


Figure 1: Mass density of the Earth as a function of the distance to Earth's center according to the Preliminary Reference Earth Model. The plot shows the values that are used in the code by default and without further simplifications.

ConstructMixingMatrix and InteractionAlt as well as the main methods CalcWeights and CalcWeightsLegacy, with the latter solving the Schrödinger equation in the original basis of equation (2). The legacy method does not perform the transformations described in subsection 2.3 and is therefore easier to read and faster in cases where vacuum oscillations are weak in comparison to matter effects (e.g., for sterile neutrinos at very high neutrino energies), but generally, it is substantially slower and does not offer all features, so its use is discouraged. EarthModel is an auxiliary class that allows for convenient and flexible specification of the parameters of the Earth that are relevant for oscillation effects of atmospheric neutrinos; see section 4.

For information regarding the usage of the classes and methods, such as input parameters and output formats, please see docstrings and inline documentation.

4. Earth Model

As detailed in subsection 2.2, the oscillation probabilities in matter depend on the parameters mass density ρ and electron fraction Y_e . By default, nuCraft assumes the Earth to be spherical and uses the mass density values given by the Preliminary Reference Earth Model (PREM) [13]. The default electron fraction is 0.4957 in the mantle (including the crust) and 0.4656 in the inner and outer core. The density profile is shown in figure 1. It has been parameterized using 50 grid points that are interpolated by a linear spline. During the solution of the Schrödinger equation, the minimizer step size is determined dynamically. Therefore, the density change between two steps is calculated quasi continuously.

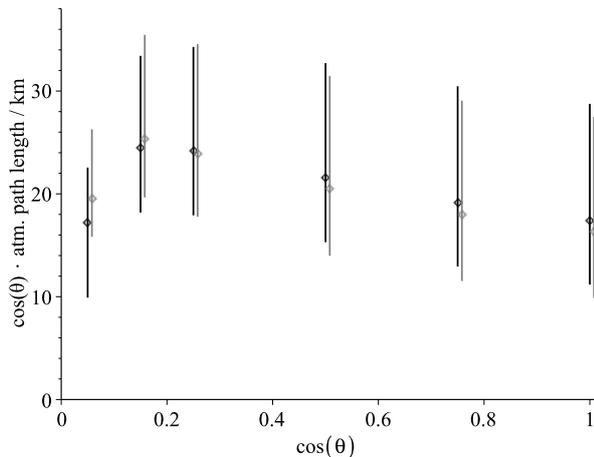


Figure 2: Expectation values and widths (defined as the 68% probability range around the expectation value) of the neutrino path length in the atmosphere as function of the cosine of the zenith angle at two energies. Black corresponds to 200 GeV, gray to 2 GeV; gray has been shifted to the right by 0.008.

The customization of the Earth model can be done by the aforementioned class `EarthModel`. Electron fractions in the three regions can be adjusted independently with a keyword argument, new density profiles can either be added to the dictionary `models` inside `EarthModel`, or can be loaded from a text file; an example file is provided with the code. Together with a trivial change in `nuCraft`'s main class, this class can also be used to employ non-symmetrical Earth models, e.g., for use with reactor neutrino experiments; an explanation of the required changes can be found in the `README` file.

5. Atmosphere

Neutrinos are produced in the Earth's atmosphere at different heights. For short neutrino path lengths and correspondingly shallow zenith angles, the variation of the production height becomes significant. For atmospheric neutrinos in an experiment, the original production height is not known, so the oscillation path length will be smeared out by the distribution of production heights. As a result, the oscillation pattern becomes less pronounced.

`NuCraft` uses the atmospheric model described in [14]. This model gives neutrino rates from meson and muon decays as functions of energy at six discrete zenith angle values, with no closed-form solution. The difference of the production heights between 2 GeV and 200 GeV is small compared to the width of their distributions (see figure 2). For the goal to model the dom-

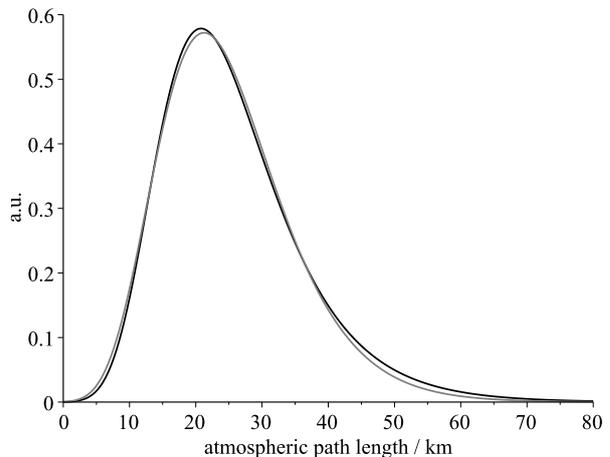


Figure 3: Exemplary unnormalized probability density function for the neutrino path length in the atmosphere at 2 GeV and $\cos(\theta) = 0.75$ (black; corresponding to a path length of 9556 km without atmosphere), and log-normal distribution fitted to it (gray).

inant smearing effect, it was decided to fix the energy at 2 GeV for the calculation. The modified oscillation probability is not expected to depend strongly on the the specific shape of the distribution of production heights because the variance of heights over which the oscillation is averaged is large.

Based on the fit values in [14] the height distributions have been reproduced at each given zenith angle θ . They are described reasonably well by log-normal distributions (figure 3) with two fitted parameters μ and σ . To be able to interpolate to other zenith angle values, the fit results of these parameters were then parameterized as functions of the zenith angle, using a polynomial for μ and a power function plus a linear polynomial for σ . Close to the horizon ($|\cos(\theta)| \lesssim 0.05$), [14] gives no reliable prediction. As the height distribution is up-down symmetric, the parameterization is smoothly interpolated between up-going and down-going particles, using the value of $|\cos(\theta)| = 0.05$ at the horizon.

By default, `nuCraft` computes eight equally likely production heights based on the quantile function of the log-normal parametrization. Specifically, it uses the central values of the eight equally-sized subintervals of $[0, 1]$. The average oscillation probability for the eight heights is obtained efficiently: The oscillation probability is computed for the lowest height and then modified using analytically computed vacuum oscillation probabilities from the seven higher heights for the path length differences to the lowest height. The chosen value of eight has been found as a good compromise between precision and speed and is sufficient for a rea-

sonable smearing. Alternative options are (1) production at a configurable fixed height, (2) a random height sampled from the continuous production height distribution, or (3) to fully propagate eight neutrinos at eight equally likely production heights (see above) through Earth. The last option is slow and meant for debugging purposes only.

6. Performance

NuCraft prioritizes accuracy and flexibility over speed; moreover, Python is not the best choice for high-performance computing. Nonetheless, its speed can compete with similar tools written in C++ because of extensive use of highly optimized NumPy and SciPy functions. Figure 4 can be used to estimate the calculation speed. However, we note that the speed depends strongly on the neutrino energy, zenith angle, and the Earth model.

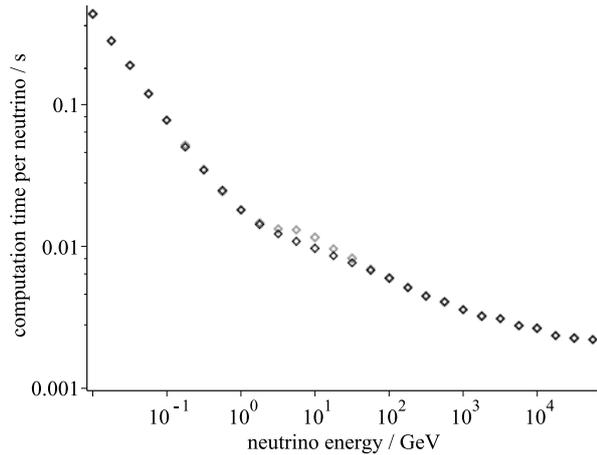


Figure 4: Time in seconds needed per oscillation probability computation in dependence of neutrino energy for the standard three-flavor model, for muon neutrinos (gray) and muon antineutrinos (black), distributed uniformly in $\cos(\theta)$. The feature at about 10 GeV is caused by matter effects. Times were measured using a single core of an AMD Phenom II X6 1055T CPU.

An initial comparison to Prob3++, written in C++, shows that nuCraft is about a factor 1000 slower. This large difference can be attributed to the Earth modeling because Prob3++ uses four layers of constant density, only. As the execution speed of Prob3++ scales linearly with the number of layers, an Earth modeling as accurate as nuCraft would lead to a substantially reduced computing speed comparable to nuCraft.

Figure 5 shows an example oscillogram computed with nuCraft by calculating probabilities for one neutrino per grid point. In this example, one additional

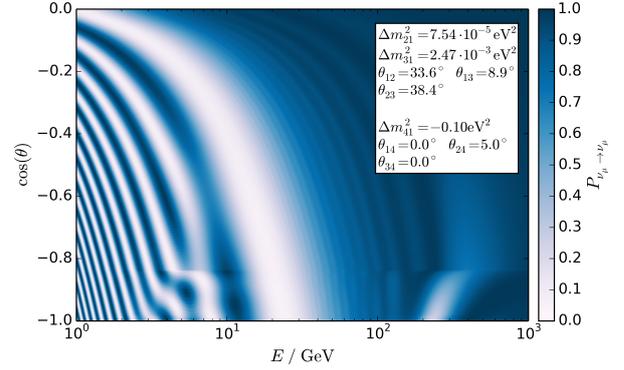


Figure 5: Example plot of muon neutrino disappearance probabilities computed with nuCraft in dependence of neutrino energy and zenith angle, including one sterile flavor. The hierarchy of the sterile neutrino was inverted ($\Delta m_{42}^2 < 0$) to not have the matter resonances in the antiparticle channel. All relevant parameters are given in the plot.

(sterile) neutrino flavor is added to the known three flavors.

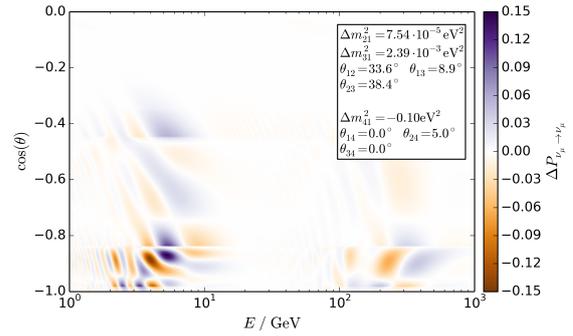


Figure 6: Difference of the oscillation probability for the default Earth model as implemented in nuCraft and an Earth model with 4 layers of constant density. All oscillation parameters are identical to fig. 5

The effect of the Earth modeling is demonstrated in figure 6. The more accurate description can lead to substantial differences up to 15% in oscillation probabilities.

Figure 7 shows the result of the smearing of the production height. Overall, the effect is small. However, close to the horizon, changes up to 10% are visible.

The accuracy of the calculation is limited by the numerical solution of the Schrödinger equation. The accuracy is automatically estimated for each neutrino, using the sum of the survival and all oscillation probabilities to other flavors. This corresponds to a test of unitarity. For the default configuration the accuracy is better than 0.05%, which can be changed using the numPrec keyword argument. Close to the horizon, further un-

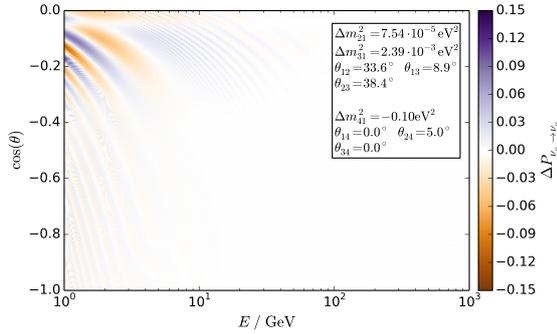


Figure 7: Difference of the oscillation probability for the modeling of the atmosphere as implemented in nuCraft to a fixed production height. All oscillation parameters are identical to fig. 5

certainties arise from the modeling of the atmospheric production heights.

The neglect of the oblateness of the Earth only has small effects. The absolute error in length has its maximum at about $\cos(\theta) = -0.55$, but the more relevant relative error in the length barely exceeds 0.5% at its peak at $\cos(\theta) = -0.1$ (using the WGS 84 model [15]). As oscillation probabilities scale with $\frac{1}{E}$, this error in length is substantially smaller than energy resolutions of typical experiments.

At very high energies, where neutrino interactions in the Earth become relevant for conventional neutrinos but not for sterile neutrinos, the propagation including sterile flavors can not be decoupled from oscillations.

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