

# Geometries for CAPTAIN

Daniel Palken, UC Davis physics REU student  
Christopher Grant, Ph.D., Professor Svoboda, advisors

## Abstract

Neutrinos interact as flavor eigenstates but propagate as mass eigenstates, meaning that a given neutrino essentially oscillates between the three flavors as it propagates through spacetime [1]. It is not necessarily the case that anti-neutrinos, despite being the anti-particles of neutrinos, must oscillate in the exact same manner [1]. Were anti-neutrinos not to oscillate as neutrinos, charge parity symmetry would be violated in a phenomenon known as CP violation [1]. A major experiment set up in part to test for CP violation in neutrinos and their anti-particles is the Long Baseline Neutrino Experiment (LBNE), scheduled to be operational at Fermilab in 2022 [2]. In the meantime, smaller experiments are being conducted in order to perform critical cross-section measurements. Among these is the Cryogenic Apparatus for Precision Tests of Argon Interactions with Neutrinos (CAPTAIN), being set up at Los Alamos National Lab (LANL) in New Mexico [3]. CAPTAIN consists of a hexagonal-cylindrical liquid argon Time Projection Chamber (TPC) housed in a cylindrical cryostat [3]. Before experiments are run with CAPTAIN, however, it is important to simulate detector performance in order to estimate the detector sensitivity. The TPC design and photomultiplier tubes (PMT's) placed around it must be optimized and evaluated. Developing these simulations requires having geometries as true as possible to the real-world, and the work this paper concerns itself with is the creation of those geometries in Geant4 to the best precision possible in the timeframe of UC Davis' 2013 physics REU program. The geometries ultimately setup included the TPC, the cryostat, the world housing them, a wire mesh covering the TPC on both ends used to detect charge, all constructed and/or filled with the proper materials. Particular attention has been paid to making the code not only readable but also easy to modify, so that any dimension can be altered intuitively at need.

## Background

Neutrinos are traditionally discussed in the context of their flavor eigenstates,  $\nu_e$ ,  $\nu_\mu$ , and  $\nu_\tau$ , in which they are observed interacting [1]. However, neutrinos propagate as the three mass eigenstates  $\nu_1$ ,  $\nu_2$ , and  $\nu_3$ , which contain the three flavor eigenstates in differing proportions [1]. It is possible to express the flavor eigenstates in terms of the mass eigenstates (or *vice versa*) through the Maki–Nakagawa–Sakata (MNS) matrix, analogous to the CKM matrix for quarks\* [1]:

---

\* In fact, neutrinos in this respect act exactly analogous to quarks with respect to their flavor and mass eigenstates. The only difference is that the flavor eigenstates of quarks,  $d'$ ,  $s'$ , and  $b'$  (for the negatively charged

$$\begin{pmatrix} \nu_e \\ \nu_\mu \\ \nu_\tau \end{pmatrix} = \begin{pmatrix} U_{e1} & U_{e2} & U_{e3} \\ U_{\mu1} & U_{\mu2} & U_{\mu3} \\ U_{\tau1} & U_{\tau2} & U_{\tau3} \end{pmatrix} \begin{pmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \end{pmatrix}$$

Equation 1

The MNS matrix is responsible for the phenomenon of neutrino oscillations, in which neutrinos shift back and forth in their likelihood to interact as each of the flavors, as they propagate through spacetime [1]. The algebra is a bit simpler with two neutrinos rather than three, and it is not difficult to derive the characteristics of the oscillation between two neutrinos using simple quantum mechanics [1]:

$$P_{\nu_e \rightarrow \nu_\mu} = \left( \sin^2(2\theta) \sin \left[ \frac{m_2^2 - m_1^2}{4E} t \right] \right)^2$$

Equation 2

Note the sinusoidal behavior that allows the muon neutrino to oscillate back into the electron neutrino after sufficient time. Also note that the degree to which a neutrino is likely to change flavor in the first place depends heavily on the  $\theta$  term, which, if zero, would forbid oscillations. Since neutrino oscillations have been observed in the past, it is clear that  $\theta$  is non-zero [4]. Lastly, note the dependence on the difference of squared masses between the heavier and lighter neutrino of the time, or effectively distance\*, over which the neutrino oscillates. It is this squared mass difference that makes the two-neutrino model a good approximation for the three-neutrino reality, as a result of the fact that two of the neutrinos (it is not clear which two, actually) are close in mass relative to the third [1].

It being known something of the manner in which neutrinos oscillate, the question of whether anti-neutrinos operate in the same way remains unanswered [1]. While it would seem intuitive to claim that they must have the same mixing matrix, there is no particular reason why this must be so [1]. The mechanism by which anti-neutrinos could oscillate differently than neutrinos is subtle, and involves one of the four independent parameters which is required to express all nine entries in the MNS matrix,  $\delta$ . The MNS matrix of equation 1 can be expressed as:

$$U = \begin{pmatrix} \cos\theta_{12}\cos\theta_{13} & \sin\theta_{12}\cos\theta_{13} & \sin\theta_{13}e^{-i\delta} \\ -\sin\theta_{12}\cos\theta_{23} - \cos\theta_{12}\sin\theta_{23}\sin\theta_{13}e^{i\delta} & \cos\theta_{12}\cos\theta_{23} - \sin\theta_{12}\sin\theta_{23}\sin\theta_{13}e^{i\delta} & \sin\theta_{23}\cos\theta_{13} \\ \sin\theta_{12}\sin\theta_{23} - \cos\theta_{12}\cos\theta_{23}\sin\theta_{13}e^{i\delta} & -\cos\theta_{12}\sin\theta_{23} - \sin\theta_{12}\cos\theta_{23}\sin\theta_{13}e^{i\delta} & \cos\theta_{23}\cos\theta_{13} \end{pmatrix}$$

Equation 3

where the four independent parameters  $\theta_{12}$ ,  $\theta_{23}$ ,  $\theta_{13}$ , and  $\delta$  fully determine all of the mixing angles [1]. For a process that can occur in more than one different way, the rates for the process and the CP-reversed process (i.e. the process involving the

---

quarks) are the less commonly discussed ones, but are useful to bring up when discussing quarks in the context of flavor changing currents [1].

\* The neutrinos are so close to massless that they are almost always travelling at very nearly the speed of light.

corresponding anti-particles of opposite handedness) are not necessarily equal, meaning that CP violation is possible [1]. The reason the rates ultimately come out unequal, it is important to note, originates with the phase factor,  $\delta$ , which brings about a conjugating term in the amplitude so long as it is not 0 or 180 degrees. [1].

Despite the theoretical backing for CP violation in neutrinos, CP violation has yet to be observed experimentally for neutrinos. It is LBNE that the experimental community will turn to as an option among next generation experiments to make a measurement of CP-violation, if it exists to be observed [2]. For a “normal hierarchy” of neutrino masses (one in which the two flavor eigenstates with similar masses are below the third, called “normal” due to its analogousness with the quarks and charged leptons), the measured neutrino energy spectrum from a beam emitting neutrinos of energies described by the black histogram in figure 1 can be predicted according to its deviations from  $\delta = 0$  (the red curve) [1, 5]. Two such predictions for CP-violating  $\delta$  values,  $\delta = -\pi/2$  and  $\delta = \pi/2$  are shown in figure 1 [5].

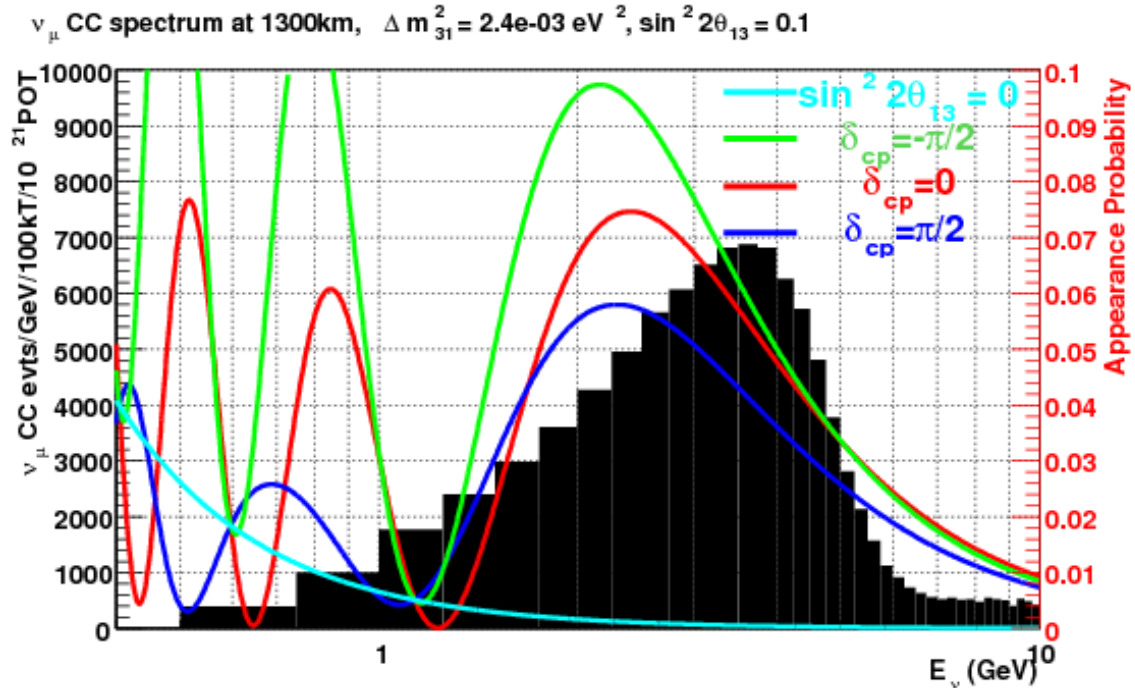


Figure 1 shows the means by which experimental physicists could hope to detect a non-zero value for  $\delta$ , which would be evidence for CP violation [5].

## CAPTAIN

While detecting CP-violations is a long term goal for future experiments such as LBNE, there is a lot of work to be done in the intervening time that will help researchers pursue a better understanding of the experiments to be performed at LBNE. CAPTAIN is being set up at LANL as an experiment with goals of doing

\* The opposing hierarchy in which the neutrino whose mass is significantly different from the other two is known as “inverted” [1].

comparatively basic tests in a liquid argon TPC involving first neutrons and ultimately neutrinos [3]. It is in these experiments that our understanding of particle physics can be both used and augmented, but all experiments taking place in CAPTAIN, while motivated by the larger picture partially detailed above, rely heavily on the specifics of the experimental setup itself.

## Technical Information

CAPTAIN's geometry in particular will have a great deal of bearing on the experimental results to emerge from the project. When neutrinos or neutrons interact with the liquid argon inside the TPC, they will ionize the argon, creating free electrons and argon ions. The ionized particles will then be guided upwards or downwards according to their charge by a properly aligned electric field. This is the mechanism by which a TPC works. When the ionized particles reach the top or bottom of the TPC chamber, they encounter a wire mesh, which can be used to pinpoint where the particles arrive. Since they are made to travel nearly straight lines up or down from where they became ionized, this charge detection gives  $\rho$ - and  $\phi$ -coordinates for the path in question. How long a given ionized particle will take to drift through liquid Argon to an end of the detector can then be calculated to determine a z-coordinate, and thus a three-dimensional picture of a charged particle's path is determined, as well as the particle's charge.

Charged particles, however, are not the only ones that will be crucial in determining the nature of whatever interactions might happen inside CAPTAIN's TPC. Scintillation photons, which carry no charge, and thus will go undetected by the TPC's wire mesh, will be emitted isotropically and scatter many times in the argon before making it to PMT's placed outside the TPC. Since some of the photons will not even make it to the outside before being absorbed back into the argon, the precise placement of the PMT's may have some influence on how many of those that do emerge are detected. Simulations can serve as a means of predicting how many photons, and of what energies, will make it to what points on the outside of the TPC for given events, provided the physics of the interactions as we understand it. If the real world results agree with the simulated ones, it is a good indication that the physics is correct, and the relevant aspects of the experimental setup have been adequately described to the simulation environment. Otherwise, it is an indication that either the experiment, the simulation, or the physics inside the simulation, has some inherent flaw. Either way, the first step to a successful interpretation of an experimental signal of any sort is to have simulated results to compare to. Since computational simulations are comparatively easier and substantially less expensive to run than the experiment itself, it is natural to run these prior to the experiment.

The goal of the research described in this paper has been to set up as accurate a geometry as possible using the C++-based Geant4 coding toolkit, which can in turn be used in simulations carried out by future collaborators on the CAPTAIN project.

## Design of Geometries

Geant4's creators provide with the software several examples for both novice and experienced users of what can be done with it. There are seven novice examples, and the geometry files that I created for CAPTAIN started with the second of these as a template, though by the end of the process, nearly everything pertaining to the geometry was changed or added on in its specifics. The benefit of starting with this template, however, was that nearly everything else (i.e. those aspects not pertaining to the geometry) about the simulation, including the code for visualizing it, remains the same, and thus, while the geometry files (now named ExN02DetectorConstruction and ExN02WireParameterization) can be easily transplanted, they also come with a bunch of code capable of visualizing them and having particles interact with them.

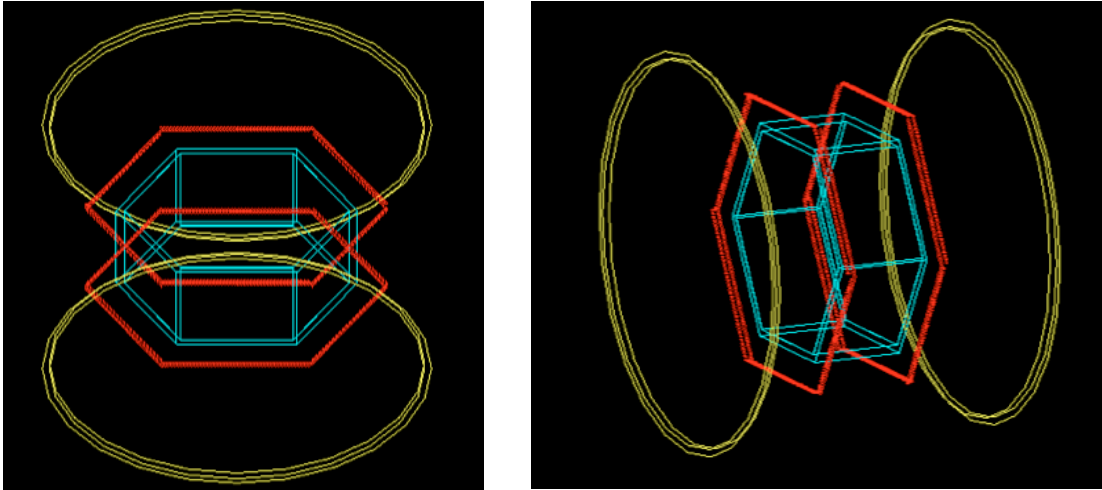
The elements of which all the materials relevant to the geometries are made are established in the ExN02DetectorConstruction File. Nitrogen (N), oxygen (O), carbon (C), manganese (Mn), phosphorous (P), sulfur (S), silicon (Si), chromium (Cr), nickel (Ni), and iron (Fe) are all defined, and then used to make air (N, O) and stainless steel SS304 (N, C, Mn, P, S, Si, Cr, Ni, Fe). Copper (Cu) and liquid argon (Ar) at 79 K are defined as their own materials.

In the ExN02DetectorConstruction file, the bulk of the geometry is set up. For all of the geometrical elements, a number of constants are defined at the top of the header file. These specify a desired unit, and then the user can easily change the value associated with each constant to alter the dimensions or other features of the geometry as easily as possible. Lined up next to these constants are commented areas where the user can keep track of the source for each of the values used if he chooses. Currently, some are taken from the schematics drawn up for the design of CAPTAIN, and others are merely guesses. In Figure 2 below, for example, the height of the TPC should be specified in millimeters (the units can be changed through the .cc file if desired), and the value of 320.0 is taken from a set of schematics for the TPC.

```
// TIME PROJECTION CHAMBER (TPC):  
// TPC specs:  
#define TPC_HEIGHT_MM           320.0 // source: schematics  
#define TPC_EDGE_TO_EDGE_DIAMETER_MM 750.0 // guess  
#define TPC_THICKNESS_INCHES    1.0 // guess
```

Figure 2 shows a small sample of the code used to easily set adjustable parameters relevant to the geometries. Including those relevant to the materials, there are 74 such variables which can be easily altered from the ExN02DetectorConstruction.hh file.

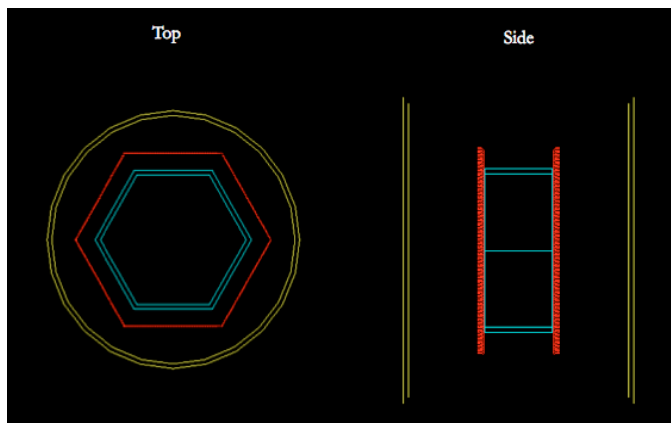
The outermost “mother volume” is simply the “World,” a box filled with air in which everything else exists. The side length is the box’s only adjustable parameter.



Figures 3a (left) and 3b (right) show different views of the set up. Only the edges of shapes are shown by the visualization program, so two circles opposing one another represent a cylinder. The red specs are too small to distinguish here, but they are also circles representing the cylindrical wires of the mesh.

The cryostat is presently the outermost piece of equipment geometry constructed. It is a circular cylinder with a small thickness but otherwise hollow on the inside. The radius parameter provided is for the outer radius of the cryostat, from which its thickness is subtracted off to get the inner radius. It is made of stainless steel, and another cylinder identical to it in shape and in size equal to its inner radius is positioned inside it and filled with liquid argon\*. Adjustable parameters include the radius, height, thickness, start and spanning angles (these should be set to 0 and 360 degrees, respectively), and X, Y, and Z offsets from the center of the world.

Inside the cryostat is the TPC, a regular hexagonal cylinder made of copper whose outer thickness, like that of the cryostat, is what is specified by the diameter parameter provided for it. The inner radius is obtained by subtracting the thickness



off. Positioned inside the TPC is an inner volume that is filled with liquid argon, just as the cryostat. Adjustable parameters include the height, diameter between any two opposing edges (which determines the side length), thickness, start and

every layer of wire mesh on each side of the  
 stating each layer of the wire mesh relative to  
 each layer is given its own parameterization and  
 es relative to the cryostat.

Figure 4a (left) gives a top view and 4b (right) a side view of the geometries constructed.

spanning angles (which should, again, be set to 0 and 360 degrees respectively), and X, Y, and Z offsets from the center of the cryostat.

The wire mesh is constructed as an array of parameterized volumes, which Geant4 has a framework built in for. This means that the wires are each copies of one another, but with altered features, in this case lengths and positions. It also means that each wire in a given parameterization is given a copy number, ranging from 0 to the number of wires that are in that parameterization minus one. This is important, as in a simulation, when a signal is seen from a wire of a given copy number and

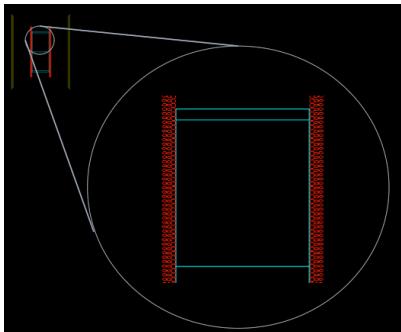


Figure 5, a close up on figure 4b showing the ends of the wires, oriented so that they are all visible end-on.

parameterization, it can easily be figured out at which position that wire is at, and a dimension of an event's location can be determined. The wires themselves are simply narrow cylinders. The parameter for the spacing between them refers to that between the closest points on adjacent wires' edges, so a value of 0 will have the wires just touching. The number of wires is not fixed, but rather self-adjusts according to the

hexagonal plane that the wires are desired to occupy, and

the length within that plane that a wire takes up, equal to its diameter plus the spacing between wires. Reasonably small values for the wires size and spacing will result in thousands of wires. The values for the sizes have been set larger for visual aid in the figures presented here. The wire mesh goes on both sides of the TPC, and is in an adjustable

number of layers, but the same number will appear on each side, so long as an even number is provided for the total. Adjustable parameters include the total number of layers (this should be an even number), the layers per parameterization (2 is the ideal value here, generally), the relative rotational orientations of adjacent parameterizations, the spacing between layers, the height of the "lowest" layer above the TPC, a length extension variable that makes all the wires uniformly longer if an irregular hexagon is desired, an inner radius (making this variable non-zero will result in hollow wires), outer radius, maximum wire length (the shortest wire in the regular hexagon will be half this length), spacing between adjacent wires in the same layer, and start and spanning angles (should be 0 and 360 degrees).

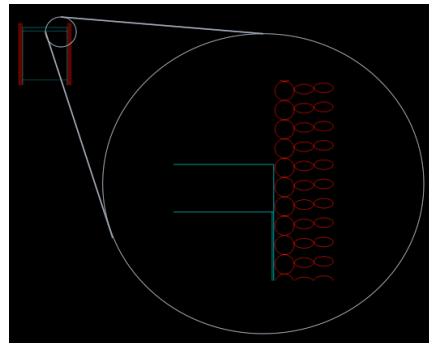


Figure 6, a further close up on figure 5 showing the cylindrical shape of the wires.

## Conclusions and Future Research

Having used the first few weeks for unrelated work and taken some time to acquaint myself with Geant4, I found myself short of time to actually run the simulations that comprise the next step now that the geometries are in place. However, the code should be easily adaptable to anyone who does wish to use it for CAPTAIN simulations, now that all of the primary pieces of equipment are set up in the virtual environment. While the geometries are not exactly as they will be (one end of the cryostat bows out, for example, and then there are countless other minute details which could theoretically impact simulated or experimental results. Hopefully, however, having taken care of the major parts of the experimental setup, any simulations will provide a good reflection of what will one day be made experimental reality.

Future simulations would likely entail adding a few photon detection boxes (essentially PMT's) to the outside of the TPC and then shooting neutrons or neutrinos of various energies and baseline distances (in the case of the neutrinos) at the TPC. The particles will interact according to the physics that the designers of Geant4 at CERN included, and should produce both charged particles and photons. These will produce signals on both the wire mesh and the PMT's, which can be looked at in order to gain an understanding of exactly what the output signals from a given beam intensity and location might be. In the future, these can ideally be further improved upon and ultimately held up to experimental results.



## References

1. D. Griffiths, Introduction to Elementary Particles, Second, Revised Edition ed. (WILEY-VCH, 2001).
2. M. Diwan, R. Svoboda and J. Strait, 2012.
3. C. Bromberg et. al. 2013.
4. A. Aguilar, L. B. Auerbach, R. L. Burman, D. O. Caldwell, E. D. Church, A. K. Cochran, J. B. Donahue, A. Fazely, G. T. Garvey, R. M. Gunasingha, R. Imlay, W. C. Louis, R. Majkic, A. Malik, W. Metcalf, G. B. Mills, V. Sandberg, D. Smith, I. Stancu, M. Sung, R. Tayloe, G. J. VanDalen, W. Vernon, N. Wadia, D. H. White and S. Yellin, Physical Review D 64 (11), 112007 (2001).
5. J. Hewett et. al. 2011.