Challenges in AI/ML at the Intensity Frontier

SLAC SSI 2023 Taritree Wongjirad (Tufts University)

- What is the Intensity Frontier (IF)?
- A subset: Neutrino Experiments
- What are some of the physics questions we are after?
- What are the challenges to answering those questions?
 - w/ a bias on one question: measuring neutrino oscillations



The Intensity Frontier

From Snowmass 2013

"The Intensity Frontier explores fundamental physics with <u>intense sources</u> and <u>ultra-sensitive detectors</u>. It encompasses searches for <u>extremely rare processes</u> and for <u>tiny deviations from Standard Model expectations</u>. Intensity Frontier experiments use precision measurements to probe quantum effects. They typically investigate new laws of physics that manifest themselves at higher energies or weaker interactions than those directly accessible at high-energy particle accelerators."



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NEUTRINO FRONTIER

NF01: Neutrino Oscillations NF02: Understanding Experimental Neutrino Anomalies NF03: Beyond Standard Model (BSM) NF04: Neutrinos from natural sources NF05: Neutrino properties NF06: Neutrino Interaction Cross Sections NF07: Applications NF07: Applications NF08/TF11: Theory of Neutrino Physics NF09: Artificial Neutrino Sources NF10: Neutrino Detectors

RARE PROCESSES AND PRECISION MEASUREMENTS FRONTIER

RF1: Weak decays of b and c quarks RF2: Weak decays of strange and light quarks RF3: Fundamental Physics in Small Experiments RF4: Baryon and Lepton Number Violating Processes RF5: Charged Lepton Flavor Violation RF6: Dark Sector Studies at High Intensities RF7: Hadron Spectroscopy

Intensity Frontier 2.0 = Neutrino + Rare Process/Precision

Snowmass 21 Frontiers

NEUTRINO FRONTIER

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RARE PROCESSES AND PRECISION MEASUREMENTS FRONTIER

RF1: Weak decays of b and c quarks RF2: Weak decays of strange and light quarks RF3: Fundamental Physics in Small Experiments RF4: Baryon and Lepton Number Violating Processes RF5: Charged Lepton Flavor Violation RF6: Dark Sector Studies at High Intensities RF7: Hadron Spectroscopy

A very vast field to survey – I will stick closely to areas I am most familiar, i.e a subset of Neutrino Frontier

Neutrinos

Key properties

- No electric charge
- Interacts only via weak force (and gravity)
- Very, very small mass: <eV
- Come in three "flavors" -- named from what lepton made during certain interactions (Charged-Current)

Elementary Particles



Why Neutrinos

- The hope is that precision measurement of neutrino properties and behavior will show cracks in the SM which point the way to new physics
- These efforts center around the neutrino mass ...

Elementary Particles



Neutrino Oscillations: a brief History

- A long saga
- Starting with the Homestake Experiment (1970 until 1994) and culminating with measurements in Super-Kamiokande (1999) and the Sudbury Neutrino Observatory (2001)
- Showed that neutrinos can change flavor as they propagate



Homestake

Super-Kamiokande

SNO

Neutrino created in certain flavor ...



Mass induced Flavor Oscillations

- Several ways to explain neutrino flavor changing, but accepted model that has explained nearly all of the data* is that if <u>neutrinos have a non-zero mass</u>, <u>then the flavors of neutrinos can mix</u>
- Furthermore, constraints tell us that this mass is very small
- Is the neutrino mass mechanism different?







Ways to explaining very small Neutrino masses:

- Neutrinos are similar to the other leptons and quarks, i.e. are Dirac Fermions, and have a **very small coupling to the Higgs**
- Neutrinos are different Majorana Fermions and couple with a different Higgs Boson
- Neutrinos are Majorana and small mass due to effective couplings to new physics at a very different energy scale (See Saw Mechanisms)

* Quick def: A Majorana Neutrino would mean a neutrino and antineutrino are the same (Majorana condition: $\Psi_M^C = C\gamma_0\Psi_M^* = \Psi_M$)

From de Gouvea, PITP 2017

Other Questions

- Can we determine if the neutrino is **Dirac or Majorana**? (Yes! By seeing neutrino-less double beta decay)
- Neutrino flavors mix: will quantifying their **mixture give us hints for new symmetries**?

•	Do neutrinos exhibit	OD	ring the
	matter/anti-matter asy	physics - we need more information.	
	(but so far, SM neutrino CF		
•	How many neutrinos	ML/AI Techniques have already improved our ability to answer such questions with the experiments we have	
•	Do neutrinos have sho	 and we really on just begun 	
•	Neutrino experiments	require intense sources and large detectors – c	an searcl

for evidence of new particles (e.g. dark matter/dark sector)

Neutrino properties dictate how we search for them. Two key ones:

No electric charge => **observe** indirectly





Only Weak Force => *rare process*

Try to **observe and identity as many of the particles as possible** coming from neutrino interactions.

(Avoid background particles if possible: underground facilities, capabilities for rejection)

Need intense source of neutrinos and/or large detector

Neutrino Sources

Neutrinos are produced in several different sources – natural and artificial – and over a vast energy range



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Detector Types

A wide-variety. Here are four broad classes though experiments often mix elements.





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Accelerator Neutrino Experiments

Many of the research challenges that ML has highly impacted have to do with experiments accelerator neutrino experiments – and many in other experiments as well

Of their many physics goals, a primary objective is to make *precision measurements of neutrino oscillations*.

Example DUNE

one part of the program: $\nu_{\mu} \rightarrow \nu_{e}$ and $\bar{\nu}_{\mu} \rightarrow \bar{\nu}_{e}$ in order to look for **CP-violation**



Strongest oscillation effect expected after 1300 km: need really intense beam + large detector (40kt LArTPC)

Preferably large monolithic detector (scalable) with good particle discriminating power.



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Accelerator Neutrino Experiments



Both are Liquid Argon Time Projection Chambers - are class of tracking detectors



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Trackers

Promising applications of ML/AI in Neutrino physics applied to tracking detectors

Record 3D energy depositions as 2D projections which are very image-like: sensor measurements naturally arranges into regular 2D array.

Pattern of energy deposits can help us infer a lot: particle type, momentum





Segmented Scintillators: e.g. Nova/Minerva

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Challenges

ML/AI impacting research challenges common to many experiments

Reconstruction: are we getting all the information that we can from our data, precisely and accurately?

Simulation/Modeling: can we translate physics to observables faster? Can we better use data-driven methods?

Inference: are we testing our models against data as best as we can while accounting properly for and mitigating our model uncertainties?

Operations: are we saving the right events? Is the experiment running optimally? Can we detect and make decisions faster?



Reconstruction: are we getting all the information that we can from our data, precisely and accurately?

The bulk of the development in ML has been here





Reconstruction

Broadly, reconstruction involves a sequence of algorithms to take raw detector data to relevant observables.

Reduction of data into increasingly higher-level/summary representations.

Example: Reconstruction stages for parsing LArTPC data to find neutrinos





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ML Reconstruction

ML Approaches have been applied to several of these stages, effectively proposing higher-level outputs directly from low-level inputs.

Taking advantage of "data" as algorithm, i.e. intermediate representations (features) are learned through training a model to best output a given objective





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Neutrino Flavor/Interaction Classification



Two projections of neutrino interaction passed into Convolutional Neural Network to determine interaction type.

Used in analysis measuring

 $u_{\mu}
ightarrow
u_{e}$

oscillations, so signal are $\nu_e CC$ events

<u>35% increase</u> in signal efficiency over previous methods.

physics concept

JINST 11 P09001(2016)



Neutrino Flavor/Interaction Classification

Classification CNN also applied to **DUNE**: Upcoming oscillation experiment aiming to measure CP-violation

|CC ν_ρ |CC ν_e |CC ν_e

INC

CC DIS

1 nrotons

|2 protons N protons

0 charged pions

1 charged pions

2 charged pions

1 neutral pions

2 neutral pions

O neutral pions

N neutral pions

2 neutrons

O N neutrons

heutrino/
antineutrino

◯ |CC other

CC QE

oftmax

softmay

oftmay

output





(b) 2.2 GeV NC $1\pi^+$.





Updated architecture, multi-task output

SE-ResNet-34

Blocks 3-N

Improvement to previous selection. Used in sensitivity estimates for DUNE Technical Design Report



See talks by <u>S. Monsalve</u> on Computer vision techniques and <u>L. Whitehead</u> on Intensity Frontier Computer Vision Applications for more details

PhysRevD.102.092003



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SE-ResNet-34

Blocks 1-2

SE-ResNet-34

Blocks 1-2

SE-ResNet-34

Blocks 1-2

Q

View

View 1

View 2

input

1.1

SE-ResNet | SE-ResNet block 1 block 2

Low/Intermediate-level Representations

CNNs have also found use producing lower-level outputs for downstream algorithms.

Why? Didn't you show me how to get the answer already?

Reasons to produce low/intermediate-level representations

- Feed high-quality outputs more easily incorporated into downstream algorithms ("traditional" or ML-based)
- "Getting the right answer" uses physics which we have more confidence modeling: e.g. particle propagation in matter vs. to neutrino-nucleus interactions
- Can find side-bands in data to check for effects from <u>domain shift</u>, i.e training on sim, applying on data NB: Nova had a means for checking network using a control sample provided by another "near" detector

Examples:

- Producing 3D energy deposits from 2D projections
- Keypoints useful for seeding particle reconstruction
- Labeling hits by particle type
- Individual particle clusters

PhysRevD.102.092003



Signal Processing/ROI Finding



CNNs are helping to refine pre-preprocessing of waveforms

Mitigates detector effects that can remove signals

CNNs helping to also find lower energy signals: potentially addresses challenge of measuring low energy deposits associated to neutrons or providing charge calibration in DUNE





Low-Level "Hit" Finding

Options: 2D vs. 3D

2D Hit finding: Fit Gaussians to Waveforms in MicroBooNE LArTPC, <u>reduction of event data size</u> from 20 Megapixel image to ~15k hits

From 2D to 3D: producing 3D hits, or spacepoints, as first-level representation has advantages

- Primarily, clustering particles is easier as due to <u>less</u> overlap/close clusters in 3D
- Can use additional modality optical information
 - to reject backgrounds at earlier stage [JINST 16 P06043 (2021)]





PhysRevD.102.092003



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Low-Level "Hit" Finding

For inferring 3D spacepoints: requires solving an underspecified inverse problem – a prior is needed to make progress. E.g. sparsity [JINST 16 P06043 (2021)]



Example: track parallel to the wire plane \rightarrow Pixels for track all show up in same row



Highly degenerate combinations for matching pixels across wires to infer Y,Z position: leads to large number of ghost points





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Low-Level "Hit" Finding

Here DL is a good fit: learn patterns from data to form "prior" to better resolve degeneracies

LArMatch Net CNN represents content around given pixel and uses it to determine ghost/true









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Good triplet e 60

0.7

0.6

0.5

04

0

Keypoints

Certain 2D or 3D locations are useful to seed reconstruction

- Track starts and End
- Shower starts
- Location of Michel/Delta rays
- Neutrino Interaction vertex

Point Proposal Network (on 3D voxels): subpixel resolution and high classification accuracy





Different IF effort, *Minerva*, focused on understanding neutrino-nucleus interactions: mproved vertex finding using DNN + adversarial network to reduce bias from out-of-domain events <u>JINST 13 P11020 (2018)</u>

Automated architecture optimization

JINST 17 T08013 (2022)



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Intermediate Targets: Shower/Track labeling

Goal: separate pixels into track-like (proton, muon, pion) and shower-like (electron, photon)





Used architecture that can produce per-pixel labels.

U-(*Res*)*Net builds in paths for features at multiple resolution to flow*

PhysRevD.99.092001

Clustering/reco algorithms for tracks and showers are different due to much different topologies

NB: Improvements from per-image class-balancing and importance weighting for pixels with neighbors of a different class

For an approach using Graph Neural Networks see:

EPJ Web of Conferences (CHEP 2021) 251, 03054 (2021)



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Checking Output on Data



- Sample: stopping muons
- Score distributions similar
- Robust to moderate difference in images as shown by peak pixel distributions



Acquired sample of cosmic particles that come to rest in the detector – both in data and simulation

Mostly muons, many of which decay into electrons

Use to check track and shower labeling



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Sparse Submanifold Convolutions

LArTPC (and many other experiments) have sparse data, i.e. a vast majority (90%+) of sensor output is zero or below threshold.

For CNNs - a lot of wasted computation where operations performed on input with all zeros.

Can perform efficient convolutions on sparse representation of images, i.e. a list of above threshold pixels, but this efficiency is lost due to information "bleeding" across image

Sparse *submanifold* convolutions (SSC) preserve sparsity – and thus efficiency – by requiring that new information produced only at locations of original input.



Sparsity reduced with regular convolutions



Sparsity conserved with submanifold convolutions

arxiv:1711.10275



Sparse Submanifold Convolution Application

A SSC Network trained as an upgrade for MicroBooNE

- Performance improvement: Showers acc. $95.9\% \rightarrow 99.6\%$ and track $97.4\% \rightarrow 99.2\%$
- Why? Hypotheses: no need to determine dominating background class, information maintains locality, larger input so less information loss due to being on the boundary
- Much more efficient: 10x lower in CPU time ($\sim 5 \rightarrow \sim 0.5$ s), 6x less RAM ($\sim 6 \rightarrow \sim 1$ GB)
- **Deployable**: Fit onto more FermiGrid nodes, can run on entire event image





Output of network on entire wireplane image

PhysRevD.103.052012

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Sparse SSNet for LArTPC analysis

Sparse SSNet key in search for $\nu_e CC$ 1 electron + 1 proton exclusive channel

Aim was to search for signs of a low-energy electron neutrino excess – another experiment (MiniBooNE) had seen such an anomaly in the same neutrino beam line [PhysRevD.103.052002]

Shower+track pixels fed into a mixture of DL and traditional algorithms

Algorithms relatively simple: using neighboring shower and track pixel clusters [JINST 16. P02017 (2021)]

Analysis competitive with other reco. algorithms for given LEE signal model





Clustering+Classification: Sparse Mask-RCNN

A key task is clustering hits (2D or 3D) into individual particles or into meaningful groups of particles

For detectors near the surface, neutrino interactions are a very small fraction of the cosmic background that passes through the detector



A modified version of the *Detectron* network trained to locate cosmic clusters and neutrino interactions.



Changed several components of this network to use *sparse submanifold convolutions*



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Sparse Mask-RCNN for addressing backgrounds

Output from network can be used in minimal selection scheme to augment baseline cosmic taggers

Note that baseline tagger already good, but incorporates timing information from optical sensors to use (non-)coincidence between clusters and the beam



Reasons to believe Mask-RCNN and similar object detection methods will have trouble with particles within interactions

2022 JINST 17 P09015



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Object Detection Methods for Individual Particles

Issues derive from mismatch between bounding box and trajectories

- Two distinct objects can have essentially the same bounding box
- Objects often overlap
- These type of top-down detection methods often have trouble with small objects
- Potentially solvable with rotatable boxes ...





SPICE

Instance+Semantic Segmentation

• Three component loss: pull together points that belong to the same cluster, keep distance between clusters, and regularization



Equation credit: Dae Hyun K. @ Stanford

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SPICE Output

Network learns to push spacepoints from same particle into ball and provides a centroid and radius to cluster the ball





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Shower Clustering

One challenge to shower clustering is that at the lower (<~1 GeV neutrino energies) of DUNE or for experiments like MicroBooNE showers are actually disconnected



One strategy is to use SPICE to find contiguous shower sub-clusters and then piece together entire shower



- Interpret each fragment as a graph node + edges connect nodes in the same cluster
- Cast the problem to a classification of node (e.g. particle type) and edge (clustering)





Interaction Clustering





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Interaction Clustering

Can extend this to clustering interactions



Performance remains high, even with higher multiplicities of interactions



Addresses a big challenge in DUNE: high multiplicity of neutrino interactions in the near detector!





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End-to-End 3D Voxel-based DL Chain





Going back to raw 2D images – potentially still useful in conjunction with reconstruction in 3D

Here shower object missing trunk because of detector issues: In two planes beginning of shower obscured for different reasons





U-plane missing because of effect involving long ionization clouds moving past induction wire



V-plane obscured due to unresponsive wires



Y-plane clearly shows ionization between shower and vertex \rightarrow suggests shower is from electron





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Provide "Prong CNN" both a masked "prong image" containing only those pixels consistent with 3D cluster

AND

"Context" image with crop around interaction

(cosmic tagged clusters are masked in both)

Allow network to recognize and estimate upstream clustering errors

*Nova does something similar



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Performance Metrics

Validation Sample Accuracy Statistics



*Output of network used in next-generation MicroBooNE analysis - that combines larmatch outputs + 3D clustering: early results suggest its competitive with current state-of-art analysis for nue-inclusive selection



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Doing image manipulations to study use of context



Prong under consideration seems attached to vertex, but gap potentially obscured

However, there is a second shower in the context image



electron score = -3.63, photon score = -0.03

Remove second photon, prong photon score drops



plane 1 all

electron score = -1.53 photon score = -0.25

Using such physics is good - but must be careful with understanding biases coming from neutrino interaction generator

Currently exploring



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Lot's of progress over less than a decade or so

... still lot's of areas to tackle for which lot's of ongoing effort

Simulation/Modeling: can we translate physics to observables faster? Can we better use data-driven methods?

Inference: are we testing our models against data as best as we can while accounting properly for and mitigating our model uncertainties?

Operations: are we saving the right events? Is the experiment running optimally? Can we detect and make decisions faster?

Fast ML on FPGAs to implement special rare process triggers

frai.2022.855184



Simulation/Modeling: can we translate physics to observables faster? Can we better use data-driven methods?

Like in other frontiers, generating simulated data is a bottleneck of analyses

- Individual events can take upwards of ~5 mins/event+ for MicroBooNE TPC with simulated cosmics + neutrino interaction
- Data driven methods are used to get better estimate: in MicroBooNE and SBN experiments which are on surface, cosmic background data is collected and used in simulated data by adding neutrino interaction – but cannot save enough of these events due to processing and storage constraints



Simulations - Generative Models

Score-based Generative Modeling shows promise for generating LArTPC-like images



Model generation as the reverse of a diffusion process bringing data images to noise



Simulations - Generative Models

Which set, left or right, is training images – which are generated?



More details in next Wed. talk: "Generative Model Applications 3"



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Simulations - Data Driven/Differentiable

Differentiable (surrogate) simulations save time by allowing a way to possible reweight MC events rather than generating additional samples with variation in detector physics parameters

Also enables simulation-based inference for a number of exciting applictions



https://arxiv.org/abs/2211.01505



Accelerating Development: Are we providing enough tools to the community to enable new ideas and new contributors?



LArTPC Neutrino Interaction (Simulation) Dataset

MicroBooNE has released some LArTPC simulations: cosmic data overlaid with simulated neutrino interaction





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LArTPC Neutrino Interaction (Simulation) Dataset

Another public dataset of 3D voxels along with simple 2D projections



https://arxiv.org/abs/2006.01993

● osf.io/vruzp/ 👬 OSF**HOME 🗸** LArTPC 2D/3D - Simulation - Particle Se.. t Metadata Analytics Files Wiki Registrations Particle Imaging in Liquid Argon (PILArNet) / I ArTPC 2D/3D - Simulation - Particle Segmentation & Clustering Contributors: DeepLearnPhysics Date created: 2018-12-04 06:43 PM | Last Updated: 2020-07-02 01:31 PM Identifier: DOI 10.17605/OSF.IO/VRUZP Category: 🛢 Data Description: This sub-project is organized by DeepLearnPhysics (www.deeplearnphysics.org), and is a part of a bigger project to share public imaging detector. It is particularly aimed for developing pixel-level particle classification technique for pixel-type (=3D readout) LArTPC. License: CC-By Attribution 4.0 International

https://osf.io/vruzp



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- ML techniques have already impacted the physics program of several neutrino experiments
- Many develops across experiments should provide further impact
- Developments have been somewhat focused on reconstruction
- But there are still other research challenges that ML might help to advance
- Cross pollination between experiments and frontiers will surely accelerate progress









LArTPC Primer



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Recording wire signals over time, detector produces image-like data



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Capture 3 projection images with wire planes

Can solver inverse problem to recover 3D energy deposits

lonization signals on wires coincident in time provide info for (Y,Z) position

X position given by time delay from light signal





wire number

Example of data event in MicroBooNE. View of same event for each projection.

Color scale indicates amount of ionization electrons seen on wire at given time



Flavor determined from finding partner lepton (muon,electron) produced in interaction Neutrino energy inferred from momenta of resulting particles





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Neutrino Oscillation Analysis



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Neutrino Oscillations

Neutrino oscillations occur because

- neutrinos have mass
- and flavor states are mixture of mass states

Neutrinos <u>created/interact</u> in flavor states They <u>propagate</u> in their mass states

Don't have to line up!



Neutrino Oscillation: 2-flavor example

Neutrino oscillations occur because

- neutrinos have mass
- and flavor states are mixture of mass states





Neutrino Oscillation: 2-flavor example

Let's start with a neutrino created in flavor state $| u_{\mu} angle$


Neutrino Oscillation: 2-flavor example

Probability of transition from flavor ν_{μ} to ν_{e} :

$$P(\nu_{\mu} \to \nu_{e}) = |\langle \nu_{e} | U_{PNMS} U(t) U_{PNMS}^{-1} | \nu_{\mu} \rangle|^{2}$$
$$= \sin^{2} 2\theta \sin^{2} \left(([1.27 \text{ GeV } \text{km}^{-1}] \Delta m^{2} \frac{L}{E}) \right) \text{ osc}_{of L}$$

Key signature is oscillatory prob function of L/E





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Neutrino Oscillation: 2-flavor example

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Key signature is oscillatory prob function of L/E





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Neutrino nucleon Interactions

Never scattering on a free quark.

Dominant interactions at u_{μ} at $E_{\nu} \sim 1 \text{ GeV}$ (typical flavor and energy for accelerator ν)







Want to know state at time, *t*, so we need to apply the propagator, U(t), on the $|\nu_{\mu}\rangle$ in the mass basis

$$U(t)U_{PMNS}^{-1}|\nu_{\mu}\rangle = -\sin\theta e^{-iE_{1}t}|\nu_{1}\rangle + \cos\theta e^{-iE_{2}t}|\nu_{2}\rangle$$
$$E = \sqrt{p^{2} + m^{2}}$$

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$$E = \sqrt{p^{2} + m^{2}}$$

what we have are two states oscillating at slightly two frequencies due to the slightly different masses



with a slight shift in frequency, you get periods where two waves in phase for some time, and out of phase for others

Want to know state at time, *t*, so we need to apply the propagator, U(t), on the $|\nu_{\mu}\rangle$ in the mass basis

$$U(t)U_{PMNS}^{-1}|\nu_{\mu}\rangle = -\sin\theta e^{-iE_{1}t}|\nu_{1}\rangle + \cos\theta e^{-iE_{2}t}|\nu_{2}\rangle$$
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what we have are two states oscillating at slightly two frequencies due to the different masses

Classical analogue is the beat-frequency phenomenon





Cherenkov

Other experiments analyze the pattern of Cherenkov Radiation to infer particle momenta and type.

Spatial arrange of optical sensors not grid-like





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