Real-time Position Reconstruction for the KamLAND-Zen Experiment using Hardware-AI Co-design

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Abstract

Monolithic liquid scintillator detector technology is the workhorse for detecting neutrinos and exploring new physics. The KamLAND-Zen experiment exemplifies this detector technology and has yielded top results in the quest for neutrinoless double-beta $(0\nu\beta\beta)$ decay. To understand the physical events that occur in the detector, experimenters must reconstruct each event's position and energy from the raw data produced. Traditionally, this information has been obtained through a time-consuming offline process, meaning that event position and energy would only be available days after data collection. This work introduces a new pipeline to acquire this information quickly by implementing a machine learning model, PointNet, onto a Field Programmable Gate Array (FPGA). This work outlines a successful demonstration of the entire pipeline, showing that event position and energy information can be reliably and quickly obtained as physics events occur in the detector. This marks one of the first instances of applying hardware-AI co-design in the context of $0\nu\beta\beta$ decay experiments.

1 Introduction

Liquid scintillator technology [6] [7] [3] [4] [13] [5] has been at the heart of recent searches for neutrino physics including solar neutrinos and neutrinoless double beta decay, a rare decay phenomenon. This technology probes for physics by emitting photons through energy excitations of the scintillator. The KamLAND-Zen (KLZ) experiment has used this technology to produce the world-leading results in the search for $0\nu\beta\beta$ decay [3]. KLZ features a spherical tank of liquid xenon scintillator, which is surrounded by a spherical array of 1,879 inner detector photomultiplier tubes (PMTs) and 247 outer detector PMTs (used for background rejection), as shown in Figure 1 LEFT. When a physics event occurs in the detector, it emits isotropic scintillation light. Each PMT capturing the scintillation light will provide two key readouts: the arrival time of the light and the integrated charge. Consequently, a single data point in KamLAND-Zen is represented as a point cloud with 2,126 points, where each point consists of five dimensions: the two PMT readout values plus the x, y, and z coordinates of the PMT's location. To search for neutrinoless double-beta decay, researchers must extract essential

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Figure 1: LEFT: A visual illustration of KamLAND-Zen's inner PMT Point Cloud Data. Image is originally from Reference [8]. RIGHT: Flow chart of FastPointNet. The top box shows the design and model testing flow. The middle box shows the flow from porting the PointNet model to the hardware. The bottom box shows the flow for executing and testing the hardware deployment of PointNet.

physical information, such as the event position within the detector and the event energy. This process is known as event reconstruction.

Traditionally, event reconstruction is performed offline. This means that data is first collected without any reconstruction over a period of time (usually $\mathcal{O}(1 \, day)$) and stored in an offline storage facility. A fitting algorithm is then applied to the stored data to generate the event's position and energy. Due to the episodic nature of offline reconstruction, neither event position nor energy information is available until $\mathcal{O}(1 \, day)$ later. In this paper, a pipeline for deploying a machine learning algorithm (PointNet) onto a Field Programmable Gate Array (FPGA)-a specialized type of computer used for reducing processing overhead-for online fast reconstruction of KLZ detector events is proposed. Since KLZ will be equipped with 120 data acquisition boards with RFSoC 4×2 FPGA chips, deploying algorithms onto FPGAs could enable real-time retrieval of event position and energy information. This pipeline relies on a key software package, cgra4ml [2], which allows the conversion from a machine learning design into its hardware representation. This work demonstrates the capabilities of this pipeline by deploying PointNet onto a single RFSoC 4×2 FPGA. Section 2 will discuss the proposed pipeline for deploying the algorithm to hardware and the decisions made regarding the application of machine learning. Section 3 will demonstrate the reconstruction results from the PointNet model and the latency of the deployed model. Lastly, Section 4 will summarize this toolchain and the applications of such a system.

2 Methods

An overview of the entire pipeline may be found in Figure 1 RIGHT. The flow chart has three phases: 1) design phase, 2) software-to-hardware port phase, and 3) FPGA execution phase. Each phase includes various subprocedures as outlined in the flow chart. The first step was to design and train PointNet over a dataset of 100,000 KLZ simulated events [3]. The shape of each point in the dataset is described in Section 1. In addition to the five dimensions, an additional binary trigger dimension is added based on whether or not the PMT received a light signal: when event energy is low, it is possible that some PMTs will not receive any light signal. To reconstruct the physics inside the detector, a mapping of these six features to four outputs is desired: the three spatial coordinates of the vertex of the physics event and the energy of the event. More rigorously, this model takes the form:

$$f(\mathbf{x}): \mathbb{R}^{6 \times 2126} \to \mathbb{R}^4 \tag{1}$$

The network architecture selected for this purpose was based on PointNet, an architecture particularly suited for data involving point clouds—data structures that preserve spatial semantics while remaining invariant to permutation [15]. Because the events in the dataset are point clouds, PointNet is a sound architecture for fitting Equation 1. The PointNet model was built using Tensorflow-Keras [1], and the training parameters are listed in Table 5. The training/validation split for the data was 0.7/0.3, respectively. The implementation the PointNet model may be found in Appendix A.2.

The next step involved quantizing the PointNet model, which required defining the bit precision for the input, output, and layer parameters of the PointNet architecture. This step was critical due to the strict resource constraints of the FPGA, necessitating the compression of the model to minimize its physical utilization. Moreover, transitioning the machine learning model from software to hardware requires specifying the bit allocation for each layer of the FPGA. High-level quantization provides these parameters, enabling the fine-tuning of resource allocation for optimal performance without directly interfacing with the FPGA. A description of the implemented layers in the compressed model may be found in Appendix A.3. After training and quantizing the model using QKeras [9], a hyperparameter search was conducted to obtain layer-level bit parameters. The hyperparameter search was executed to minimize the mean squared error (MSE) between the predicted and true event position and energy of each event in the validation split. The loss function used was an MSE function:

$$\mathcal{L} = \text{MSE}(x) + \text{MSE}(y) + \text{MSE}(z) + \text{MSE}(\text{energy})$$
(2)

The script for the hyperparameter search may be found in Appendix A.1.

Having established the quantized model and its optimal parameters, the next step was to port the model to a format that was compatible with the cgra4ml library, a software framework that facilitates the export of a complicated machine learning model to the AMD Vivado platform. Vivado then synthesized the model into an FPGA representation compatible with the RFSoC 4×2 FPGA development board. A similar RFSoC 4×2 chip will be adopted by the KamLAND-Zen experiment for their future upgrades. After synthesizing the model using the resources found in Table 4, AMD Vitis deployed the model onto the RFSoC 4×2 board. The model's performance and reconstruction speed were estimated after the deployment step, and these results are described in Section 3. In summary, the pipeline involves three phases: the design and quantization phase, software to hardware port using cgra4ml and Vivado, and the execution and evaluation phase using Vitis.

3 Results

This section describes the three key results of deploying the PointNet model onto an FPGA. As discussed in Section 2, quantizing the PointNet model yielded the number of bits required for each layer when deploying the model to the FPGA. The results from the hyperparameter search are shown in Table 8. Using the results of this hyperparameter search, the optimal parameters for compression were selected: eight bits of integer precision and twelve bits of mantissa precision. The specific information regarding each layer may be found in Appendix A.4.

Having established the best kernel and bias quantization parameters, the next step was to port the PointNet model from Tensorflow-Keras to cgr4ml. Using cgra4ml and Vivado, the model was exported and synthesized for use in the RFSoC 4×2 board. The synthesized model is shown in Figure 2 RIGHT. Training the ported model yielded the accuracy shown in Figure 2 LEFT. Unfortunately, the optimal parameters found in the hyperparameter search were not used to train the ported model since they were incompatible with cgra4ml. The authors are working directly with the cgra4ml developers to deploy the most optimal model onto the FPGA as part of their future work. Instead, eight bits of mantissa precision were used with zero bits of integer precision.

From Figure 2, it is clear that the neural network was able to recover the spatial coordinates and energy of the event in distribution. The average MSE error across all batches during validation was 978.40. This error was higher than the results from the quantization step (366.25) since the best-performing model from quantization was incompatible with cgra4ml. Table 1 summarizes the error for each label across different experiments, along with the nominal reconstruction error from the traditional method for comparison. A more detailed description of these errors may be found in Appendix A.5. The QKeras model produced a spatial resolution close to the nominal values while outperforming the nominal energy resolution. The cgra4ml-ported model performed worse on position reconstruction yet outperformed the traditional method on energy reconstruction.

3.1 FPGA Latency Results

The primary motivation for deploying PointNet onto an FPGA was to enable fast reconstruction; therefore, understanding the latency–defined as the time taken to obtain a result from the network after input—is crucial for evaluating the model's performance. The latency for the untrained model was 6,996.7 ms per batch and 6,980.9 ms per batch for the trained model. These values are averaged

Experiment	Avg. Validation MSE	x Error (cm)	y Error (cm)	z Error (cm)	E Error (MeV)
Traditional Method [11]	N/A	13.7	13.7	13.7	0.14
QKeras	366.25	20	21	21	0.06
cgra4ml	987.40	34	34	36	0.06

Table 1: Training Results



Figure 2: LEFT: Performance of cgra4ml-ported PointNet model. The bottom four panes show the reconstruction of the event's location and energy; the blue histogram shows the true position/energy from the simulated dataset while the yellow histogram shows the machine-learning-reconstructed positions and energy. The top four panes show the histograms of the difference in the prediction versus the true labels. The red lines show the Gaussian fit from the SciPy library [16]. RIGHT: The Vivado synthesis of PointNet on the RFSoC 4×2 FPGA. The cyan-colored region shows the utilized FPGA resources on the chip.

over 20 runs with a batch size of 16 events. This indicates a 436.3 ms inference speed per event. This represents a significant reduction in the time required to obtain key physics information, from approximately $\mathcal{O}(1 \ day)$ in offline reconstruction to $\mathcal{O}(1 \ s)$ in on-FPGA reconstruction. Future work will focus on optimizing the model to accelerate reconstruction speed to $\mathcal{O}(1 \ ms)$. Given that KamLAND-Zen collects roughly one data point per millisecond, achieving $\mathcal{O}(1 \ ms)$ reconstruction would allow for real-time event position and energy reconstruction as KLZ collects data. Considering this demonstration was performed on a single FPGA and that the next-generation KamLAND-Zen detector will consist of 120 FPGAs, achieving an inference time on the order of $\mathcal{O}(1 \ ms)$ is feasible with proper optimization.

4 Summary

This paper presents a pipeline for deploying a PointNet model onto an FPGA for real-time event reconstruction of position and energy in the KamLAND-Zen experiment. While position reconstruction accuracy was worse compared to the traditional method, the energy resolution was improved. A key advantage of this approach is the significant reduction in latency to obtain reconstruction results from several days to just a few seconds. Future work will involve collaborating with the cgra4ml developers to port the best-performing model and optimizing the model structure for faster inference speed. In the long term, this framework will be integral to the deployment of 120 data acquisition boards in the next generation of the KamLAND-Zen experiment.

5 Broader Impacts

In this section, the broader impacts of this work are discussed.

5.1 Limitations

This work has some limitations. One major limitation is that the model's accuracy was not tested against permutations of the dataset. Moreover, this model was only trained on one dataset. It is also possible that the model was overfit. Therefore, to make the model's results more robust, a k-fold analysis of the accuracy would need to be completed. Another major limitation is that the model was trained on simulated detector physics, which may not accurately reflect the true reconstruction physics in the detector. While the deployed model's computational efficiency is unaffected by dataset size, it is affected by the number of inputs; increasing the number of inputs (PMTs) increases the number of compute resources necessary during both the design and deployment phases. This work is limited in its application and thus cannot be used for harmful acts.

5.2 Societal Impacts

The application of this work is limited to the context of the KLZ experiment, thus it cannot pose any societal harm. However, the models that are developed throughout the work are computationally expensive to train. Using shared compute resources that are energy-efficient may help mitigate the energy used to train these models. See Table 3 for the compute resources used in this work.

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A Appendix / supplemental material

A.1 Optimization Hyperparameter Search Script

This is the script used to search for the optimal quantization parameters:

A.2 Tensorflow Model Implementation

Below is a layer-level description of the Sequential Tensorflow model implementation used to fit Equation 1:

- 1. 1D Convolutional Layer (64 filters, kernel size 1)
- 2. 10% dropout layer
- 3. ReLU layer
- 4. 1D Convolutional Layer (64 filters, kernel size 1)
- 5. 10% dropout layer
- 6. ReLU layer
- 7. 1D Convolutional Layer (512 filters, kernel size 1)
- 8. Global Average Pooling 1D
- 9. Dense Layer (256 points, leaky ReLU activation)
- 10. 0% or 10% Dropout Layer
- 11. Dense Layer (64 points, leaky ReLU activation)
- 12. Dense Layer (4 points)

A.3 QKeras Model Implementation

Below is a layer-level description of the Sequential Tensorflow QKeras model design:

- 1. 1D Convolutional Layer (64 filters, kernel size 1, kernel and bias quantizers use quantized_relu)
- 2. Quantized Activation Layer (8 bits mantissa precision)
- 3. 1D Convolutional Layer (64 filters, kernel size 1, kernel and bias quantizers use quantized_relu)
- 4. Quantized Activation Layer (8 bits mantissa precision)
- 5. 1D Convolutional Layer (512 filters, kernel size 1, kernel and bias quantizers use quantized_relu)
- 6. Global Average Pooling 1D

- 7. Dense Layer (256 points, leaky ReLU activation, kernel and bias quantizers use quantized_relu)
- 8. Quantized Activation Layer (8 bits mantissa precision)
- 9. Dense Layer (64 points, leaky ReLU activation, kernel and bias quantizers use quantized_relu)
- 10. Quantized Activation Layer (8 bits mantissa precision)
- 11. Dense Layer (4 points, kernel and bias quantizers use quantized_relu)

A.4 cgra4ml-Ported Model Implementation

Below is a description of the XModel implementation used in the cgra4ml-ported model. Note that the mantissa bit precision used across all layers is 8 for the input, 8 for the kernel, and 16 for the bias.

- 1. XBundle. Core is XConvBN (0 integer bit precision for kernel and bias, 64 filters, 1 kernel size, activation is ReLU XActivation)
- 2. XBundle. Core is XConvBN (0 integer bit precision for kernel and bias, 64 filters, 1 kernel size, activation is ReLU XActivation)
- 3. XBundle. Core is XConvBN (0 integer bit precision for kernel and bias, 512 filters, 1 kernel size, activation is ReLU XActivation). Pool is Global Averaging with no activation. Flatten is true
- 4. XBundle. Core is XDense (0 integer bit precision for kernel and bias, 256 points, activation is ReLU activation with negative slope of 0.125)
- 5. XBundle. Core is XDense (0 integer bit precision for kernel and bias, 64 points, activation is ReLU activation with negative slope of 0.125)
- 6. XBundle. Core is XDense (0 integer bit precision for kernel and bias, 6 points, no activation)

A.5 Model Prediction Error

From the KLZ collaboration, the approximate nominal spatial resolution is reported to be approximately ± 13.7 cm in the z direction [11], and this work assumes that this error is the same for the x and y dimensions as well. When reporting a model's error, the histogram of differences between the model's predicted and true labels of the x, y, z, and energy is considered: an example of this may be found in Fig. 2 LEFT. Then, a Gaussian distribution is fitted onto this histogram using the SciPy Python package [16]. From this fit, the 1-sigma result is reported for each spatial coordinate as well as the energy. In addition, the nominal energy resolution of KLZ is 7.2%/MeV [11]. From Figure 2 LEFT, the mean energy of the events from the dataset is approximately 2 MeV; therefore, the KLZ 1-sigma energy resolution is approximated as 0.14 MeV.

A.6 Other Tables

Characteristic	Detail
Authors	Charles r. Qi, Hao Su, Kaichun Mo, Leonidas J. Guibas
Model Date	2017
Training Algorithms	See appendices 5 and 6
Paper and Citation	See reference [15]
Primary Intended Users	Fitting point cloud data
Primary intended users	Researchers
Evaluation factors	Total Mean-Squared-Error (MSE) between target and predicted
	x, y, z, and energy
Dataset	Simulated dataset from the KLZ collaboration
Data Motivation	Simulated data includes true labels of physics events, which is necessary for PointNet training
Data Preprocessing	Inject data label "PMT label," which describes whether the PMT
	was triggered. PMT has label 0 or 1. Label 0 is registered if both
	charge and time labels are identically 0. Reshape data into (x, y,
	z, label, time, charge) format.
Ethical Considerations	The way PointNet is applied is limited to the scope of the experi- ment and thus does not present ethical issues.

Table 2: PointNet Model Card Based on Reference [14]

Table 3: Compute Resources Used for Design and cgra Port Phases

Hardware	Hardware Used
Compute Name	UCSD Expanse Cluster
GPU (Graphics Processing Unit)	NVIDIA Tesla V100 32GB VRAM
CPU cores	4
RAM (Random Access Memory)	64GB

Table 4: FPGA Deployment Computer Resources

Hardware/Software	Hardware Used
GPU (Graphics Processing Unit) CPU RAM (Random Access Memory) Storage	Radeon Graphics AMD Ryzen 7 5700G with Radeon Graphics 12GB 500 GB
Swap Memory Vivado Version Vitis Version	2022.2 2022.2

Parameter	Value	Reasoning
Epochs	50	Loss curve suggested that at least 30 epochs was necessary to reach convergence
Batch Size	128	Larger batch size improved training results
Learning rate	1e-3	Stable learning rate
Training/Validation Split	0.7/0.3	N/A
Optimizer	AdamW [10] [12]	Commonly-used optimizer

Table 6 [.]	cgra4m]	Port Trainin	g Hyperparameters
rubie o.	ogra mir	1 ont manning	5 Hyperpurumeters

Parameter	Value	Reasoning
Epochs	50	Quantization phase also used 50 epochs
Batch Size	128	Larger batch sizes would not train due to insufficient amount of RAM
Learning rate Training/Validation Split	1e-3 0.7/0.3	Stable learning rate
Optimizer	AdamW [10] [12]	Commonly-used optimizer

Table 7: Implemented Assets and Licensing

Asset	License or Permission
AMD Vivado	University License
AMD Vitis	University License
cgra4ml	Apache-2.0 License
KLZ Dataset	KLZ Collaboration
RFSoC 4×2 Development Board	Board may be used for academic purposes only

Mantissa Precision	Integer Precision	Activation Integer Preci- sion	Loss (MSE(x) + MSE(y) + MSE(z) + MSE(energy)
8	0	0	404
8	0	8	9018
8	8	0	306
8	8	8	62099
8	12	0	368
8	12	8	18470
12	0	0	476
12	0	8	1670
12	8	0	362
12	8	8	19492
12	12	0	375
12	12	8	2265

Table 8: Quantization Hyperparameter Results