CUDA Support in GNA Data Analysis Framework

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Abstract. Usage of GPUs as co-processors is a well-established approach to accelerate costly algorithms operating on matrices and vectors. We aim to further improve the performance of the Global Neutrino Analysis framework (GNA) by adding GPU support in a way that is transparent to the end user. To achieve our goal we use CUDA, a state of the art technology providing GPGPU programming methods.

In this paper we describe new features of GNA related to CUDA support. Some specific framework features that influence GPGPU integration are also explained. The paper investigates the feasibility of GPU technology application and shows an example of the achieved acceleration of an algorithm implemented within framework. Benchmarks show a significant performance increase when using GPU transformations.

The project is currently in the developmental phase. Our plans include implementation of the set of transformations necessary for the data analysis in the GNA framework and tests of the GPU expediency in the complete analysis chain.

Keywords: CUDA, GPGPU, parallel computing, data analysis, neutrino

1 Introduction

The neutrino is weakly interacting neutral fermion. There are three types of these particles ν_1 , ν_2 and ν_3 with masses m_1 , m_2 and m_3 , respectively. These particles interact with charged leptons (electron, muon and tau) with interaction strengths determined by elements $V_{\alpha i}$ of the lepton mixing matrix V, named after Pontecorvo-Maki-Nakagawa-Sakata.

Two facts, that neutrino masses are all different and that V is not a diagonal matrix, lead to a spectacular quantum mechanical phenomenon known as neutrino oscillations. Its firm experimental confirmation was celebrated by the 2015 Nobel Prize in physics and the 2016 Breakthrough Prize in Fundamental Physics [1,2,3].

Neutrino physics entered the stage of precision measurements and addressing remained open questions: neutrino mass hierarchy, if neutrino is Majorana particle, and others. Both require an accurate, fast and flexible tool for a combined analysis of neutrino world data. Our team began a development of the corresponding software GNA based on our experience in Daya Bay [4] ('Analysis D'), JUNO [5] and NOvA [6] experiments.

GNA is an universal tool for building comprehensive physical models and statistical data analysis, designed with neutrino experiments in mind. It was initially created as software for the JUNO and Daya Bay experiments in a flexible and efficient way. The name GNA stands for Global Neutrino Analysis, as the package introduces tools for the combined analysis of the physical data. The framework is described in more detail in the following section.

GPUs (Graphics Processing Units) are used today for a much wider range of problems than simply processing graphics, including data analysis in science [7,8]. Video cards can be used as co-processors on both personal computers and high-performance servers. There exist free tools that provide an interface for GPU programming such as CUDA [9], OpenACC [10] or OpenCL [11].

We have added CUDA support to the GNA framework in order to achieve better performance during the processing of vector data. With this architecture the input data is mapped on multiple threads that are executed in parallel. Because a GPU platform has hundreds of times more threads compared to modern CPUs it is especially suitable for running data-parallel algorithms.

The CUDA Toolkit is developed by NVIDIA and supports only NVIDIA graphics accelerators. This narrows the range of compatible acceleration devices compared to other tools. Nevertheless, the CUDA Toolkit provides a number optimized numerical routines. Also, NVIDIA GPUs are quite popular and are widely used in common desktop computers and laptops.

It this paper we describe the way in which CUDA is integrated in GNA, and its implications from both the end-user and developer points of view. Major implementation details are discussed. A review of our future plans for GPU-based development is also presented.

2 GNA Architecture

The computation process in GNA is represented by a directed graph in which nodes represent functions and edges present the data flow. Nodes are called transformations, which is an abstraction layer for C++ functions. They may have inputs (arguments) and have at least one output (return values). Transformations typically operate on data arrays. A computational graph describes how transformations interact with each other. Because transformations are encapsulated and have universal interfaces a high flexibility is achieved.

Data analysis in GNA consists of two stages:

- 1. Configuration stage on which the computational graph is created.
- 2. Computational stage on which graph is evaluated.

In the first stage the transformation instances are created, and outputs and inputs are bound together. This step is done only once within Python and is flexible, but may be inefficient. The actual calculation happens on the second

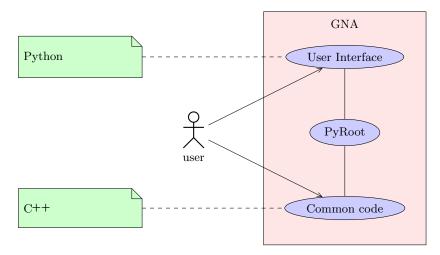


Fig. 1: GNA architecture schematic diagram.

step. Calculations are done within compiled C++ code and are usually executed repeatedly.

The generalized scheme of the framework is shown on Figure 1. GNA has a Python user interface (UI) that is used for building computation chains. The implementation of all transformations and the way they interact are described in C++. These two parts are linked via PyRoot.

The user may manage the computational process by using transformations already implemented in GNA. Transformations may also be written by users themselves and added into the framework environment.

2.1 Transformation

A transformation is an encapsulated wrapper for a function that converts input data into output.

Figure 2 schematically displays several kinds of transformations. Transformations may or may not have inputs (marked by arrows on the left side) and must have at least one output (marked by arrows on the right side). Inputs and outputs generally refer to data arrays. In addition to inputs transformation may also depend on variables. A variable is a small input data type which usually refers to a single number.

Actual data is allocated on the transformation outputs. Input data cannot be changed inside the transformation, it is a read-only state for the output it is connected to. It enables us to ensure that data will not be modified by following transformations after it is computed. A transformation is computed only once and the result may be used multiple times afterwards. It will be re-computed only if any of the variables or inputs it depends on were modified.

There is a set of predefined transformations implemented in the GNA framework. Because transformations are independent from each other the set may be

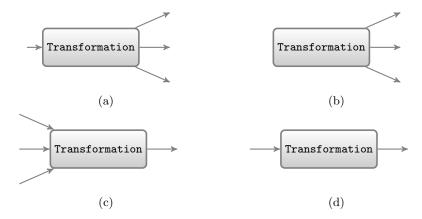


Fig. 2: Example of transformation kinds. Intermediate transformation (a) with a single input and multiple outputs. Initial transformation (b) with multiple outputs. Intermediate transformation (c) with multiple inputs and single output. Intermediate transformation (d) with single input and single output.

straightforwardly extended by the users. The guidelines on how to do this are provided in the framework documentation [12].

The typical computational chain that produces prediction for the reactor antineutrino experiments contains hundreds of nodes and is evaluated within a time frame on the order of 0.1 seconds to seconds. The prediction is a histogram with 300 bins and depends overall on 250 independent parameters. The prediction is then used in the process of multidimensional minimization, which takes around 30 minutes for 15 free parameters or around 6 hours for all the model parameters, most of which are constrained. Statistical analysis requires repeated minimization and may take several days to evaluate confidence intervals. MC based methods, such as Feldman-Cousins, require millions of minimization procedures and may take months when executed on a cluster. The framework is also suitable for building more complex graphs with evaluation times on the order of seconds to hours.

2.2 Computational graph

A computational graph is formed by a chain of transformations with inputs connected to outputs. Figure 3 displays a simple example of such a graph. This scheme shows that the same output may refer to and be referred by any number of inputs. The graph may be configured in an arbitrary way, as long as data types of the outputs are compatible with the requirements of the transformation they are connected to.

The graph is constructed using Python. Users describe the way transformations are chained via Python script or from the command line interface. The result of any transformation may be read at any moment through the Python interface.

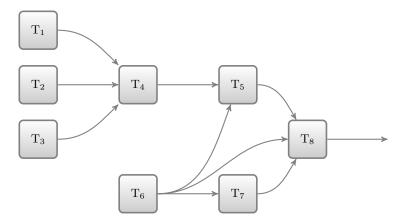


Fig. 3: Schematic example of the GNA computational graph.

Lazy evaluation means that the output of a transformation is computed on demand if the output is read by a caller. In the case when the output of an intermediate transformation is accessed only preceding transformations are evaluated, not the entire graph.

2.3 Parallelism opportunities

Parallel computing is a well-known method to speed up the computational process. There are methods to achieve performance increases on different levels. The most efficient and safe method is to divide input data into smaller independent datasets and execute the analysis on a distributed system [13,14]. However, in real-world cases analysis of those datasets often takes a long time. Due to this fact acceleration at an individual dataset level is also needed, and may be implemented for multi-core CPUs or GPUs [15]. In this paper we consider the prospects for acceleration of computations in GNA on a framework level using GPGPU.

Figure 4 shows a part of a computational graph for the JUNO experiment implementing the neutrino oscillation probability calculation (see section 4.1). There are multiple OscProb transformation instances in the graph computing the neutrino oscillation probability for various distances L, each of them depending on a vector neutrino energy E_{ν} . For the most practical cases E_{ν} may be computed only once. OscProb transformation instances are independent from each other and bound to different parameters (variables) that may change their output. Parallel technologies are applicable for graphs with such a structure, since no data writing collision is possible.

The OscProb transformation, as well as most of the framework modules, provide multi-dimensional array operations which are particularly suitable for multi-threaded systems such as GPUs or multi-core CPUs if their elements are computed independently.

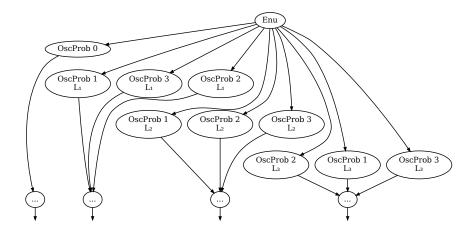


Fig. 4: Neutrino oscillation probability calculation scheme. A part of JUNO computational graph.

3 CUDA overview

CUDA (Compute Unified Device Architecture) is an architecture for parallel data processing for NVIDIA GPUs. The average GPU has hundreds of times more threads compared to modern CPUs. Threads run in parallel in SIMT (Single Instruction, Multiple Threads) [16] manner as GPUs were originally created for image processing — a vivid example of SIMT algorithms.

The CUDA Toolkit [17] has a set of specialized libraries optimized for their purposes, such as cuBLAS (linear algebra), cuRAND (random number generators), cuDNN (deep neural networks), etc. It also provides high-level abstractions to manage computational processes on GPUs, and low-level methods to tune it.

GPGPU's main performance limitations are memory allocation and data transfers, as the co-processor is an independent physical device. The copying of data from Host (CPU and RAM) to Device (GPU) or vice versa is slow. Nevertheless, it is a powerful tool for accelerating algorithms that contain operations with the same instruction applied to each element of an array, and producing independent output.

4 GPU acceleration

4.1 Neutrino oscillation probability

In this section we consider an opportunity of achieving better performance for a distinct transformation that calculates the neutrino oscillation probability [18].

The general formula for oscillation probability in vacuum, the probability that neutrino flavor changes from ν_{α} to ν_{β} after travelling distance L, reads as follows:

$$P(\nu_{\alpha} \to \nu_{\beta}) = \delta_{\alpha\beta} - 4 \sum_{i>j} \operatorname{Re}(V_{\alpha i}^* V_{\beta i} V_{\alpha j} V_{\beta j}^*) \sin^2 \frac{\Delta m_{ij}^2 L}{4E_{\nu}} + 2 \sum_{i>j} \operatorname{Im}(V_{\alpha i}^* V_{\beta i} V_{\alpha j} V_{\beta j}^*) \sin \frac{\Delta m_{ij}^2 L}{2E_{\nu}},$$

where E denotes neutrino energy, L is a distance between neutrino source and detector, $V_{\alpha i}$ is a complex unitary matrix called a Pontecorvo-Maki-Nakagawa-Sakata (PMNS) matrix, and $\Delta m_{ij}^2 = m_i^2 - m_j^2$ is a neutrino mass splitting.

Within GNA the oscillation probability is implemented as a set of transformations for each formula item respectively. Each transformation input is a vector of neutrino energy values E_{ν} .

The computations for different energy values are identical and independent from each other, therefore they can run in parallel on a GPU. It should be noted that the input array (neutrino energy), in most realistic cases, is known beforehand and will be copied to the GPU only once while the computation is performed for different oscillation parameter values.

The following features were used to port the oscillation probability code to GPU:

- CUDA Streams [19],
- datasets are divided into smaller sizes to organize overlapped execution,
- asynchronous memory copying.

After porting the oscillation probability the result was verified: a difference between GPU and CPU output results is within the roundoff accuracy of the double precision floating point numbers.

Results of the test with input energy vectors of sizes 10^4 and 10^6 elements are presented in table 1. The calculation is performed with double precision on Intel Core i7-6700HQ CPU and NVIDIA GeForce GTX 970M GPU. It should be noted that a size of 10^4 elements corresponds to the JUNO experiment's case. First row contains the ratio of the full computation times for CPU-only

Input data size, elements	10^{4}	10^{6}
CPU time / (GPU computing + transfer time)	0.017	1.39
\ensuremath{CPU} time / \ensuremath{GPU} computing-only time	20.90	26.46

Table 1: Benchmarks for oscillation probability calculation on CPU and GPU with input vectors sizes of 10^4 and 10^6 elements.

and GPU-oriented (including data transfer costs) versions of the algorithm. The second row contains the ratio of the computation times (without data transfer costs in GPU-based case).

When data transfer is taken into account the acceleration for the 10^6 sample size is not significant. For the smaller sample the acceleration is not enough to cover the overhead due to data transfer.

When data transfer is not taken into account the achieved acceleration is at least $\times 20$ compared to CPU case. Since the neutrino energy is computed only once and then stored the latter is the more realistic case for this task.

The speed-up is expected to be more significant for larger datasets. At the same time the data transfer overhead should be considered and handled appropriately in any case.

It should also be noted that single precision floating point operations are typically much faster (dozens of times) on most GPUs when compared to double precision. For CPUs the single precision is only twice as faster. Therefore a significant speed-up is expected for cases when single precision is sufficient.

4.2 Computational chains with GPU-oriented transformations

The original CPU computational scheme was modified in such a way that switching between CPU- and GPU-oriented transformation modes is transparent for the end user. The transformation is still a single object with two function definitions: one for the CPU and another for the GPU. On the UI side the GPU computation is enabled by setting a single flag that changes the target device of the transformation and switches the active function. Thus, users are enabled to work with the GPU mode of GNA without any special knowledge about GPGPU.

In order to handle data transfer we implemented a C++ wrapper for the GPU array and defined several frequently used mathematical operations. The portion of the framework that contains CUDA is built as a separate shared library. Then the main code is built with this library as a dependency. This way GPU functions may be called from the common C++ code. GPU related code may be switched off completely by a special flag during the compilation of the framework.

Since memory allocation is one of GPGPU's limitations within GNA, all required memory for both the GPU and CPU is allocated during the configuration stage to avoid extra time costs in the runtime.

As described earlier, inputs are simply the views on the data of the corresponding outputs of preceding transformations. The same feature is implemented for the GPU arrays. There is no additional allocation on the GPU for the inputs as it refers to the output it is bound to. The only exception to this rule is the first GPU-oriented transformation in the computational subchain: an extra GPU memory allocation for its inputs occurs because we need to transfer data from Host memory to the Device.

We have extended the GNA internal data storage objects in order to maintain a synchronized copy of Host data on the Device. The synchronization is done in

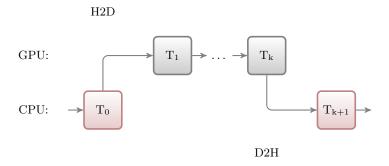


Fig. 5: Schema of mixed (CPU and GPU) computational chain.

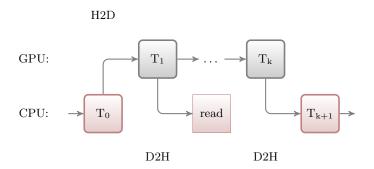


Fig. 6: Reading an intermediate result from the GPU chain.

a lazy manner, i.e. it happens only when the unsynchronized Host data is read from Device and vice versa.

Figure 5 shows the computation scheme in which the chain contains a subset of GPU-based transformations. Only two data transfers between the Host and the Device take place in this case: at the beginning of GPU subchain and at the end of it. We minimize communication between Host and Device to cut the time costs due to data copying since it is an expensive operation. The status of GPU function, which indicates whether or not it was executed successfully, is available on the Host side after the transformation computation is finished. Device-To-Device data transfers may occur inside the transformations implementation, but they are not considered to be costly.

Extra data transfers from Device to Host may be triggered by the user, reading the data at any point of the computational chain as is shown in Figure 6. In this case an extra data transfer occurs. The backward transfer is not needed. Because user-triggered reading may occur during a debugging procedure or for the plotting of data, the data transfer overhead in not significant in this case when compared to the actual data analysis.

5 Future work

The major shortcoming of the current GPU support implementation is the lack of fault tolerance. In the case of GPU failure the computation will be aborted.

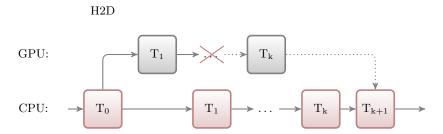


Fig. 7: Computational process recovery on CPU after GPU fault.

We are planning to add a feature of switching the computation between CPU and GPU modes automatically during runtime as is shown in Figure 7. It is assumed that the deceleration of the algorithm execution is more preferred than aborting it.

Another planned feature is adding checkpoints for the GPU side of the framework. It will decrease latency time for recovering the computation crashed on GPU side. This implies that data will regularly be synchronized between Host and Device. Since this may lead to an additional overhead the existence and frequency of the checkpoints will be configurable.

In order to use a GPU for the computational chain in a real analysis a subset of existing transformations should be ported to the GPU. Not every algorithm will be ported, however. The choice will be made based on analysis of the computational chains of the Daya Bay and JUNO experiments. As a sufficient set of transformations is ported we will benchmark the GPU-enabled version of GNA on several realistic computational schemes with various configurations and floating point precision settings.

Since the data transfer costs may negate performance improvement of GPU-enabled computational chain the actual choice of the configuration should be made and tested by the end-user, based on a particular computational chain. Specialized benchmarking tools will be implemented in GNA to simplify this task.

6 Conclusion

In this paper we describe the GPU support within the GNA framework implemented via the CUDA architecture with transparency for the end-user. For the particular case of neutrino oscillation probability it has been demonstrated that

the achieved acceleration may be of order of $\times 20$ for double precision floating point numbers.

While the realistic acceleration for the large computational chains may be lower and may depend on a particular chain, the prospects look very promising. Significant improvement is expected when single precision is sufficient for the task. An acceleration obtained in case of single precision is usually much higher for GPUs compared to CPUs. The corresponding studies and benchmarks will be performed in further work.

The solutions to the major problems and limitations, such as memory allocation and data transfer are discussed.

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References

- 1. T. Ohlsson, Nuclear Physics B 908, 1 (2016).
- 2. T. Kajita, Reviews of Modern Physics 88, 030501 (2016).
- 3. A. B. McDonald, Reviews of Modern Physics 88, 030502 (2016).
- 4. Daya Bay, F. P. An et al., Phys. Rev. **D95**, 072006 (2017), 1610.04802.
- 5. JUNO, F. An et al., J. Phys. G43, 030401 (2016), 1507.05613.
- 6. NOvA, P. Adamson et al., Phys. Rev. Lett. 118, 231801 (2017), 1703.03328.
- M. Al-Turany, F. Uhlig, and R. Karabowicz, Journal of Physics: Conference Series 219, 042001 (2010).
- 8. A. Fatkina, O. Iakushkin, and N. Tikhonov, Application of GPGPUs and multicore CPUs in optimization of some of the MpdRoot codes, in <u>25th Russian Particle Accelerator Conf.</u>(RuPAC'16), St. Petersburg, Russia, November <u>21-25</u>, <u>2016</u>, pp. <u>416-418</u>, JACOW, Geneva, Switzerland, <u>2017</u>.
- 9. J. Nickolls, I. Buck, M. Garland, and K. Skadron, Queue 6, 40 (2008).
- 10. R. Farber, Parallel programming with OpenACC (Newnes, 2016).
- 11. L. Howes and A. Munshi, Khronos Group (2015).
- 12. GNA group, GNA documentation, http://gna.pages.jinr.ru/gna/.
- 13. M. Ballintijn, R. Brun, F. Rademakers, and G. Roland, arXiv preprint physics/0306110 (2003).
- 14. I. Gankevich, Y. Tipikin, and V. Korkhov, Subordination: Providing resilience to simultaneous failure of multiple cluster nodes, in <u>Proceedings of International Conference on High Performance Computing Simulation (HPCS'17)</u>, pp. 832–838, NJ, USA, 2017, Institute of Electrical and Electronics Engineers (IEEE).

- 15. O. Iakushkin, A. Fatkina, A. Degtyarev, and V. Grishkin, Application of multicore architecture to the MPDRoot package for the task tof events reconstruction, in <u>International Conference on Computational Science and Its Applications</u>, pp. 428–437, Springer, 2017.
- 16. E. Lindholm, J. Nickolls, S. Oberman, and J. Montrym, IEEE micro 28 (2008).
- 17. Nvidia, CUDA, (2007).
- 18. C. Giunti and C. W. Kim, <u>Fundamentals of neutrino physics and astrophysics</u> (Oxford university press, 2007).
- 19. J. Gómez-Luna, J. M. González-Linares, J. I. Benavides, and N. Guil, J. Parallel Distrib. Comput **72**, 1117 (2012).