Metagenomic analysis at the Edge with Jetson Xavier NX

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Abstract. Nanopore sequencing technologies and devices such as Min-ION Nanopore enable cost-effective and portable metagenomic analysis. However, performing mobile metagenomics analysis in secluded areas requires computationally and energetically efficient Edge devices capable of running the whole analysis workflow without access to extensive computing infrastructure. This paper presents a study on using Edge devices such as Jetson Xavier NX as a platform for running real-time analysis. In the experiments, we evaluate it both from a performance and energy efficiency standpoint. For the purposes of this article, we developed a sample workflow, where raw nanopore reads are basecalled and later classified with Guppy and Kraken2 software. To provide an overview of the capabilities of Jetson Xavier NX, we conducted experiments in various scenarios and for all available power modes. The results of the study confirm that Jetson Xavier NX can serve as an energy-efficient, performant, and portable device for running real-time metagenomic experiments, especially in places with limited network connectivity, as it supports fully offline workflows. We also noticed that a lot of tools are not optimized to run on such Edge devices, and we see a great opportunity for future development in that area.

Keywords: nanopore sequencing, edge computing, edge analytics, bioinformatics, Jetson Xavier NX, cloud computing, metagenomics

1 Introduction

In recent years, we've observed the rapid development of third-generation sequencing technologies that allow for cost-effective and portable metagenomic analysis with devices such as MinION. It is a miniaturized sequencing device developed by Oxford Nanopore Technologies (ONT). Its small dimensions, weight of 90 grams, cost of 1000\$, and ability to carry out sequencing experiments in less than an hour make it a perfect choice for use in mobile laboratories for various in-field applications such as real-time monitoring. So far, it has been successfully used for monitoring Zika outbreak in Brazil [15], Ebola virus in Kenya [14], Lassa virus outbreak in Nigeria [16], in freshwater [24] or sewage monitoring systems [6], for early detection of plant viruses in Africa [7] and African swine

2 P. Grzesik et al.

fever characterization [19]. It also has been tested in extreme conditions such as on International Space Station [9], and for studying microbial communities during an ice cap traverse expedition [13].

The portable metagenomics analysis, however, has to overcome a few challenges. The major one is having access to limited computational power at edge devices, where most of the bioinformatic tools require significant computing capabilities and are usually designed to run in cloud environments on multi-node clusters. Another challenge is the amount of data that has to be processed. According to official documentation [4], MinION can produce up to 15 GB of data per day, making it impossible to upload it to the cloud for further processing in scenarios where network connectivity is either not available or network throughput is very slow. The next important thing is energy consumption. For in-field applications in secluded areas, it might be challenging to have access to a reliable power supply, so such devices should operate on battery power or alternative energy sources such as solar panels. For that reason, it's important to use devices that offer a good ratio of computational power to energy consumption.

This paper aims to evaluate the feasibility, performance, and energy consumption of metagenomics analysis in the context of carrying it out on a low-cost constrained edge device in the form of Jetson Xavier NX. The paper is organized as follows. In section 2, we review the related works in the area. In section 3, we describe the considered analysis workflow along with bioinformatics tools used. Section 4 describes the testing environment with a focus on selected hardware. Section 5 contains a description of the testing methodology along with performance experiments that we carried out for selected scenarios. Finally, section 6 concludes the results of the paper.

2 Related Works

In the literature, there is little research concerning portable metagenomics analysis. In [17], Ko et al. describe the applications and challenges related to real-time mobile DNA analysis. The authors highlight time-sensitive and location-sensitive sequencing as two important areas for portable sequencing applications. They also cite energy management, data management, network management, and consumables management as the biggest challenges for portable DNA analysis. The authors also suggest potential ideas for addressing the aforementioned challenges.

Oliva et al. [20] focused on porting and benchmarking bioinformatics tools on an Android smartphone to evaluate the possibility of performing portable analytics on regular smartphones. In their evaluation, they managed to port and run 11 out of 23 considered tools successfully. In most cases, failures were caused by implementations relying on instruction sets unsupported on ARM architectures. They also conducted performance experiments. However, the paper does not include benchmark details for basecalling with Nanocall [10], which was the only basecaller that was successfully ported. They conclude the paper with the suggestion that in order to support real-time portable analytics on commodity smartphones, the development of optimized and dedicated tools will be needed.

In his research [22], Parker benchmarked a cluster of Raspberry Pi singleboard computers for the purposes of portable, scalable real-time analysis in comparison to a consumer laptop and a high-performance server. Evaluated analysis pipeline included tools such as Guppy, BLASTN, and Kraken. The author identified Raspberry Pi as a good candidate to run tasks such as BLASTN, where Guppy offered significantly lower performance and Kraken could only support tiny databases due to memory constraints of Raspberry Pi. The author concludes the paper with the observation that such computing clusters can be the right, inexpensive choice for carrying out several bioinformatics tasks.

D'Agostino et al., in their article [11], propose an architecture that combines edge and cloud computing for low-power and cost-effective metagenomics analysis. They evaluate the metagenomics workflow of basecalling and classification with Deepnano basecaller and Kraken software running on Intel System-on-Chip boards. They also consider various compression algorithms to reduce the amount of data that needs to be transferred to the cloud environment for further processing. The authors conclude the paper with the suggestion that while it is possible to run metagenomics sequencing on such devices directly at the edge, none of the tested SoCs could process data in real-time. For such applications, they suggest using fog-based architecture, with more computing nodes closer to the edge device.

Verderame et al. [25] proposed an edge-cloud architecture for metagenomics analysis. Authors in the paper focus on security aspects, providing an overview of security mechanisms handling authentication of devices and ensuring the confidentiality of processed and transmitted data. They evaluated the SSL overhead for MQTT protocol, which turned out to be around 8% of transmission time over using plain MQTT protocol.

Merelli et al. presented research [18] concerning the evaluation of the lowpower portable devices for metagenomics analysis in fog computing architecture, based on Intel System-on-Chip boards. They evaluated the performance of various boards during basecalling operations, both from a throughput and energy consumption perspective. In the tested scenario, they concluded that the system that would support real-time workflows could not be battery-powered and would require multiple SoCs to be able to process estimated output from a single Min-ION device.

In [12], Gamaarachchi provided an overview of a real-time, portable DNA sequence analysis using a System-on-Chip computer. The author highlights the challenges related to portable metagenomic analysis and presents optimizations to tools like minimap2, and introduces a replacement for Nanopolish in the form of f5c. The paper also includes a successful evaluation of the workflow on devices such as Jetson TX2 or Jetson Nano. However, the whole workflow does not include the basecalling step.

Palatnick et al., in [21], introduce a comprehensive metagenomic analysis tool dedicated to mobile devices running the iOS operating system. It offers the ability to align reads, perform variant calling and visualize results directly on an iPhone or an iPad. However, currently, it's impossible to perform basecalling

4 P. Grzesik et al.

directly on an iOS device, which makes it impossible to run the whole metagenomics workflow without having access to a separate device for sequencing with MinION. The author suggests that as soon as it's possible to connect MinION directly to these devices, iGenomics will be adjusted to execute the whole endto-end analysis pipeline.

In [23], Samarakoon et al. presents a corresponding metagenomic analysis tool but dedicated to Android devices. It has integrated multiple known tools (such as minimap2, Samtools, f5c, and Bedtools, to mention just a few) and allows building customizable analytical workflows. Currently, similarly to the iGenomics, it does not support basecalling directly on an Android smartphone and requires a separate device for basecalling and sequencing with MinION.

Based on the above, it can be concluded that there is a lot of interest in being able to perform metagenomic analysis workflow in a portable manner. However, based on research from D'Agostino [11] and Merelli [18], evaluated approaches and tools were not sufficient to run such workflows in a real-time manner. This paper aims to expand knowledge in that area and evaluate the capabilities of low-powered boards such as Jetson Xavier NX in the context of running such workflows on a constrained edge device in a real-time scenario.

3 Analysis workflow and software used

For the evaluation, we selected a workflow where after nanopore sequencing, reads in the form of FAST5 files are immediately basecalled to FASTQ format in real-time, which are further processed by classification software to identify microorganisms present in the tested sample. Fig. 1 presents the analyzed workflow.



Fig. 1: Metagenomic analysis workflow

For the basecalling step, several tools were considered. The first one was Deepnano-blitz [8], an open-source basecaller developed by Boža, V, based on bidirectional recurrent neural networks. Unfortunately, after preliminary testing on Jetson Xavier NX and Jetson Nano, we couldn't evaluate it since the implementation heavily relies on an instruction set not supported by processors powering testing boards. Next considered basecaller was Causalcall [28], another open-source basecaller, based on temporal convolutional network and CTC decoder. Unfortunately, similarly to Deepnano-blitz, we weren't successful in running it on Jetson Xavier NX. Next considered basecaller was Guppy [26], which is a closed-source, state-of-the-art basecaller developed by Oxford Nanopore Technologies. It offers support for GPU acceleration, including GPU on Jetson Xavier NX, and supports multiple basecalling models (fast and high accuracy). The last considered basecaller is Bonito [1], an open-source basecaller developed by Oxford Nanopore Technologies. Likewise the Deeepnano-blitz, it also uses a recurrent neural network. Even though the basecaller is open-sourced, some of its dependencies are not, and they were not available for the ARM architecture, which made running and evaluating Bonito impossible on Jetson Xavier NX.

For classification, we selected Kraken2 [27], which is a taxonomic classification tool that relies on a pre-built database of k-mers associated with the lowest common ancestor of all genomes that contain that k-mer. Based on that association, the classification algorithm then classifies each read by querying the database with each k-mer from a sequence. Then, based on the results, it constructs the classification for the given input. Kraken2 is an improved version of Kraken, offering smaller database sizes, faster classification speed, and faster database build times. It is important to note that the default Kraken2 database requires more than 30GB of memory, while the minified version of the default database requires 8 GB.

4 Testing Environment

The testing environment was based on a group of edge devices, where one of them served as a source of previously prepared MinION Nanopore reads in the form of FAST5 files. The other one served as a main analytical device that was responsible for carrying out the analysis workflow. It was also connected to an external SSD drive that served as storage for raw and basecalled reads. The main device was also powered through a power supply with an integrated current measurement circuit based on INA219 [2] current sensor connected to Raspberry Pi 4. Fig. 2 presents the diagram of the described system.

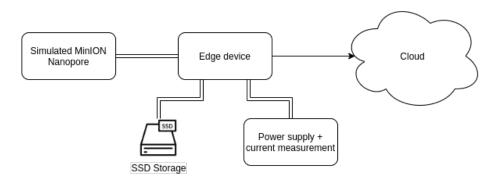


Fig. 2: Diagram of the testing environment.

6 P. Grzesik et al.

In this research, we focused on the performance evaluation of the analysis workflow of the presented system. Its central piece is the edge computing device, which was selected to be Jetson Xavier NX, due to offering enough RAM for classification with Kraken 2 and having access to integrated GPU that supports Guppy basecaller acceleration. One of the most important features of Jetson Xavier NX from the perspective of using it in the field is its energy efficiency. It offers five power consumption modes, 10W with either 2 or 4 CPU cores enabled and 15W with 2, 4 or 6 CPU cores enabled, which makes it possible to power it with a portable powerbank or by using solar panels. The full technical specification of Jetson Xavier NX is presented below [3]:

- CPU 6-core NVIDIA Carmel ARM®v8.2 64-bit CPU 6 MB L2 + 4 MB L3
- GPU NVIDIA VoltaTM architecture with 384 NVIDIA CUDA cores and 48 Tensor cores
- Memory 8 GB 128-bit LPDDR4x 51.2GB/s
- Storage SDHC card (32 GB, class 10)
- OS Ubuntu 18.04.5 LTS with kernel version 4.19.140-tegra

We also considered other low-powered single board computers. However, they were excluded after preliminary testing due to their limitations. While having access to GPU, Jetson Nano was not compatible with the GPU version of Guppy basecaller due to its lower compute capability. Its limited amount of RAM additionally makes running classification with Kraken2 more challenging. Raspberry Pi 4 was also considered, but its lack of GPU acceleration turned out to be a limiting factor for basecalling purposes.

5 Performance Experiments

During experiments, we decided to measure the basecalling and classification capabilities of the Jetson Xavier NX board with different power modes set. For each experiment scenario, we recorded the number of bases or signals processed per second, as well as average power consumption, to assess if these processes could be carried out in real-time while offering energy-efficiency that allows the system to be battery-powered and usable in a portable manner. For evaluating power consumption, we used a dedicated INA219 sensor with Raspberry Pi to collect data, but after evaluating its results against outputs from tegrastats [5] module available on Jetson Xavier NX, we decided to use data from tegrastats to simplify the testing environment, as the values reported were very similar. We measured power every second during the experiment and computed the average to obtain the final value. To carry out experiments, we used a subset of the Klebsiella pneumoniae reads dataset that was used for benchmarking in [26]. During the experiments, we used Guppy in the 4.0.14 version and Kraken2 in the 2.1.1 version.

7

5.1 Basecalling

During the basecalling evaluation step, we considered two separate Guppy models, fast and high accuracy. Both of them were dedicated to basecalling reads obtained with flow cell using chemistry R9.4.1. We observed that the fast model offers up to 10 times higher throughput, which can be seen on Fig 3 and Fig 4, while also recording lower average power consumption, presented on Fig 5 and Fig 6. We did not observe significant differences between all three 15W power modes when using GPU acceleration. However, we observed that from an energyefficiency standpoint, it might be better to use a 10W power mode, as the ratio of samples per second to average power is higher in that scenario. We also observed that basecalling without GPU acceleration is not feasible on Jetson Xavier NX, with throughput being lower in that scenario more than 50 times.

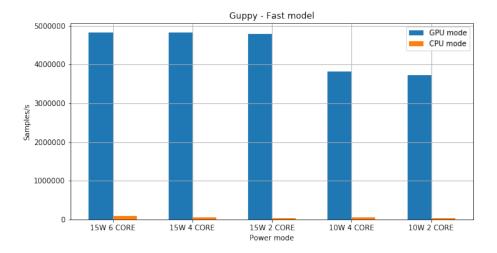


Fig. 3: Samples per second basecalled with Guppy fast model.

5.2 Classification

During classification experiments, in order to accommodate for the fact that Jetson Xavier NX offers only 8 GB of memory, we built a custom Kraken2 database that takes only up to 6 GB of RAM, which made running the experiments on Jetson Xavier NX feasible. As input data, we used the results obtained during the basecalling step in the form of FASTQ files. We observed an almost linear change in basepairs processed per second with changing the number of available cores in different power modes, which can be seen in Fig. 7, with 42,4 Mbp processed per second with 15W 6 CORE mode. However, as can be seen in Fig. 8, average power does not follow similar linear change, and the most efficient from

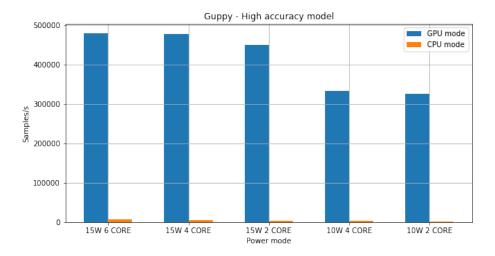


Fig. 4: Samples per second basecalled with Guppy high accuracy model.

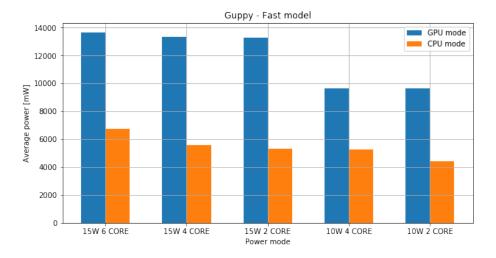


Fig. 5: Average power during basecalling with Guppy fast model.

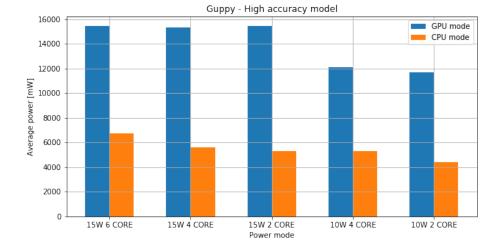


Fig. 6: Average power during basecalling with Guppy high accuracy model.

an energy standpoint is 15W 6 CORE mode. As Kraken2 does not support GPU acceleration, we could not evaluate the potential benefits of taking advantage of Jetson Xavier NX's GPU.

6 Results Summary and Concluding Remarks

Considering the results presented in the previous chapter, we observe that GPU acceleration provides improvements over the CPU only computations in the range of 45 to 70 times more samples processed per second while consuming only 2 to 3 times more energy. Given the fact that the theoretical maximum of MinION Nanopore is around 2,300,000 signals per second (512 pores with around 4,500 signals read per second per pore), with real-world scenarios resulting in less than 2,000,000 signals per second, we can conclude that Jetson Xavier NX, even with the lowest power configuration of 10W with 2 enabled cores, can perform basecalling in real-time. In fact, it might be able to support basecalling in real-time from two MinION sequencing runs as it can basecall up to 3,826,260 signals per second according to our experiments while requiring only as little as 10W power supply. However, when a high accuracy model of Guppy is required, then even on the highest power mode 15W 6 CORE, Jetson Xavier NX can only process up to 480,000 samples per second, which means that it cannot keep up with real-time sequencing, but can still be useful if only few sequencing experiments are performed during the day. We also observed that basecalling is a more computationally expensive process than classification. In our experiment, 1,000,000 of signals processed translated to roughly 89,525 bases, which means that the classification process is orders of magnitude faster than basecalling and is not a limiting factor for real-time metagenomic analysis at the edge. The clas-

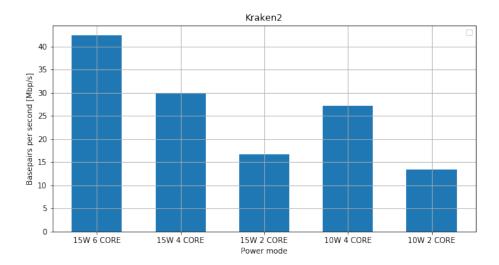


Fig. 7: Basepairs processed per second during classification with Kraken2.

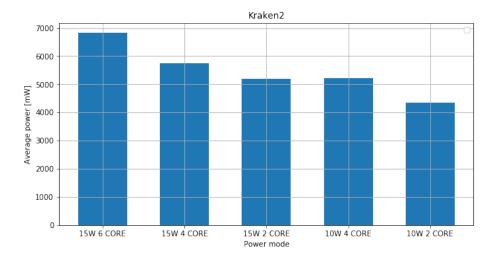


Fig. 8: Average power during classification with Kraken2.

sification process can be run successfully on such edge devices, as long as the database that we're using for classification can fit into just 8 GB of memory available on Jetson Xavier NX.

Given the above results, we conclude that computing capabilities, small size, and low energy consumption make Jetson Xavier NX a suitable edge device for portable metagenomics analysis, especially in places with limited network connectivity as whole analysis can be done fully offline. It is important to note that it is still challenging to run alternative open-source basecallers. Many bioinformatics tools are designed for high-performance clusters in cloud environments, which suggests that there is still a lot of room for improvement and development in that area.

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