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# BigSeqKit: a parallel Big Data toolkit to process FASTA and FASTQ files at scale

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| **Abstract:** | Background. High-throughput sequencing technologies have led to an unprecedented explosion in the amounts of sequencing data available, which are typically stored using FASTA and FASTQ files. We can find in the literature several tools to process and manipulate those type of files with the aim of transforming sequence data into biological knowledge. However, none of them are well fitted for processing efficiently large files, likely in the order of terabytes in the following years, since they are based on sequential processing. Only some routines of the well-known seqkit tool are partly parallelized. In any case, its scalability is limited to use few threads on a single computing node.<br>Results. Our approach, BigSeqKit, takes advantage of an HPC-Big Data framework to parallelize and optimize the commands included in \emph{seqkit} with the aim of speeding up the manipulation of FASTA/FASTQ files. In this way, in most cases it is from tens to hundreds of times faster than several state-of-the-art tools. At the same time, our toolkit is easy to use and install on any kind of hardware platform (local server or cluster), and its routines can be used as a bioinformatics library or from the command line.<br>Conclusions. BigSeqKit is a very complete and ultra-fast toolkit to process and manipulate large FASTA and FASTQ files. It is publicly available at: https://github.com/citiususc/BigSeqKit |
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PAPER

# BigSeqKit: a parallel Big Data toolkit to process FASTA and FASTQ files at scale

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## Abstract

**Background**. High-throughput sequencing technologies have led to an unprecedented explosion in the amounts of sequencing data available, which are typically stored using FASTA and FASTQ files. We can find in the literature several tools to process and manipulate those type of files with the aim of transforming sequence data into biological knowledge. However, none of them are well fitted for processing efficiently large files, likely in the order of terabytes in the following years, since they are based on sequential processing. Only some routines of the well-known *seqkit* tool are partly parallelized. In any case, its scalability is limited to use few threads on a single computing node. **Results**. Our approach, *BigSeqKit*, takes advantage of an HPC-Big Data framework to parallelize and optimize the commands included in *seqkit* with the aim of speeding up the manipulation of FASTA/FASTQ files. In this way, in most cases it is from tens to hundreds of times faster than several state-of-the-art tools. At the same time, our toolkit is easy to use and install on any kind of hardware platform (local server or cluster), and its routines can be used as a bioinformatics library or from the command line. **Conclusions**. *BigSeqKit* is a very complete and ultra-fast toolkit to process and manipulate large FASTA and FASTQ files. It is publicly available at: https://github.com/citiususc/BigSeqKit.

**Key words**: FASTA/FASTQ files; Performance; Parallelism; Big Data

## Introduction

The history of modern DNA sequencing started several decades ago, and since then, has seen astounding growth in sequencing capacity and speed. From the first genomes with a few thousand bases, DNA sequencing has advanced to sequence the human genome of 3 billion bases. In recent years, next-generation sequencing (NGS) technology, also known as massive parallel sequencing (MPS), has made it possible to expand the amount of sequencing data available. For example, the Illumina NovaSeq 6000[1] platform can generate a maximum output of 6 Tb of data and read about 20 billion sequences per run. Note that sequences, commonly named *reads*, are composed of ASCII characters representing a nucleotide (base) from the sequence. In the DNA case, we can only find four possible bases (A - adenine, C - cytosine, G - guanine and T - thymine).

The NGS raw data are mainly stored in FASTA [1] and FASTQ [2] text-based file formats. In particular, nucleotide and protein sequences are typically stored in the FASTA file format, whereas FASTQ is the most widely used format for sequencing read data. An example of FASTA file is shown in Figure 1. A sequence in FASTA format begins with a single-line description about the sequence in the subsequent lines. The description line is distinguished from the sequence data by a greater-than (>) symbol at the beginning. On the other hand, the FASTQ format was designed to handle the quality metrics of the sequences obtained from the sequencers. In FASTQ every four lines describe a sequence or read. An example is displayed in Figure 2. The information provided per read is: identifier and an optional description (first line), sequence (second line), and the quality score of the read (fourth line). An extra field, represented by symbol '+', is used as separator between the data and the quality information (third line).

Manipulating these files efficiently is essential to analyze and interpret data in any genomics pipeline. Common operations on FASTA and FASTQ files include searching, filtering, sampling, dedu-

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[1] https://www.illumina.com/systems/sequencing-platforms/novaseq.html [accessed 28 feb 2023]

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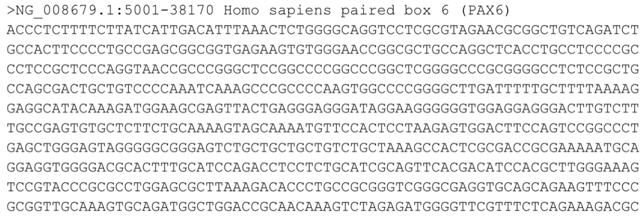
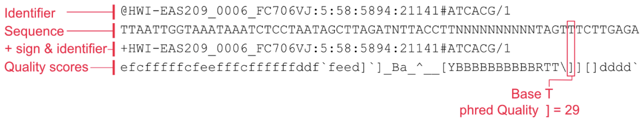


```
>NG_008679.1:5001-38170 Homo sapiens paired box 6 (PAX6)
ACCCTCTTTTCTTATCATTGACATTTAAACTCTGGGGCAGGTCCTCGCGTAGAACGCGGCTGTCAGATCT
GCCACTTCCCCTGCCGAGCGGCGGTGAGAAGTGTGGGAACCGGCGCTGCCAGGCTCACCTGCCTCCCCGC
CCTCCGCTCCCAGGTAACCGCCCGGGCTCCGGCCCCGGCCCGGCTCGGGGCCCGCGGGGCCTCTCCGCTG
CCAGCGACTGCTGTCCCCAAATCAAAGCCCGCCCCAAGTGGCCCCGGGGCTTGATTTTTGCTTTTAAAAG
GAGGCATACAAAGATGGAAGCGAGTTACTGAGGGAGGGATAGGAAGGGGGGTGGAGGAGGGACTTGTCTT
TGCCGAGTGTGCTCTTCTGCAAAAGTAGCAAAATGTTCCACTCCTAAGAGTGGACTTCCAGTCCGGCCCT
GAGCTGGGAGTAGGGGGCGGGAGTCTGCTGCTGCTGTCTGCTAAAGCCACTCGCGACCGCGAAAAATGCA
GGAGGTGGGGACGCACTTTGCATCCAGACCTCCTCTGCATCGCAGTTCACGACATCCACGCTTGGGAAAG
TCCGTACCCGCGCCTGGAGCGCTTAAAGACACCCTGCCGCGGGTCGGGCGAGGTGCAGCAGAAGTTTCCC
GCGGTTGCAAAGTGCAGATGGCTGGACCGCAACAAAGTCTAGAGATGGGGTTCGTTTCTCAGAAAGACGC
```

**Figure 1.** Example of FASTA file showing the first part of the PAX6 gene (obtained from [3]).



```
@HWI-EAS209_0006_FC706VJ:5:58:5894:21141#ATCACG/1
TTAATTGGTAAATAAATCTCCTAATAGCTTAGATNTTACCTTNNNNNNNNNNTAGTTTCTTGAGA
+HWI-EAS209_0006_FC706VJ:5:58:5894:21141#ATCACG/1
efcfffffcfeefffcffffffddf`feed]`]_Ba_^__[YBBBBBBBBBBRTT\]][]dddd`
```

**Figure 2.** Example of FASTQ file format (obtained from [3]).

plication and sorting, among others. We can find several tools in the literature for FASTA/Q file manipulation such as *HTSeq* [4], *FASTX* [5], *fqtools* [6], *seqtk* [7], Biopython [8], samtools [9], *pyfadix* [10], *pyfastx* [11] and *seqkit* [12]. These tools can be classified according to how the sequences are parsed [11]. In the first category sequences are processed in order, which causes important overheads when extracting and randomly sampling sequences. That is the case of *HTSeq*, *FASTX*, *fqtools* and *seqtk*. In the second category we find tools that support random access to sequences by establishing an index file. Tools belonging to this category are more efficient in terms of performance and memory consumption. However, none of them are well fitted for processing large files of tens of GB (likely TBs in the near future) since they are based on sequential processing. The exception is *seqkit* that allows some routines to use a few threads but, in any case, its scalability is very limited.

To deal with this issue, in this paper we introduce *BigSeqKit*[2], a parallel toolkit to manipulate FASTA and FASTQ files at scale with speed and scalability at its core. *BigSeqKit* takes advantage of IgnisHPC [13, 14], a computing engine that unifies the development, combination and execution of HPC and Big Data parallel tasks using different languages and programming models. As it was demonstrated, IgnisHPC outperforms the state-of-the-art framework Spark [15] in terms of performance and scalability running applications that represent the most typical algorithmic patterns in Big Data and scientific computing.

*BigSeqKit* uses the *seqkit* routines as basis since that toolkit covers a wide range of utilities and is one of the most used by the bioinformatics research community. As a consequence, *BigSeqKit* will offer the same functionalities and command interface[3] than *seqkit*. *BigSeqKit* can be used from the command line, but it is at the same time a library, so its routines can also be called from a C/C++, Python, Go or Java application.

Another important characteristic of *BigSeqKit* is that it is fully containerized, which isolates the execution environment from the physical system and avoids dependency problems. As a consequence, *BigSeqKit* is very easy to install and can run on a local server or on any type of cluster since it supports some of the most important resource and scheduler managers (e.g., Mesos [16], Nomad [17] and Slurm [18]).

**Table 1.** Some of the most important IgnisHPC API functions.

| Type | Functions |
|---|---|
| Map | `map, flatmap, mapWithIndex, filter, keyBy, keys, values, mapPartitions, mapValues,` etc. |
| Reduce | `reduce, treeReduce, aggregate, treeAggregate, reduceByKey, aggregateByKey,` etc. |
| Group | `groupBy, groupByKey` |
| Sort | `sort, sortBy, sortByKey` |
| I/O | `parallelize,collect, top, take, saveAsObjectFile, saveAsTextFile, saveAsJsonFile,` etc |
| SQL | `union, join, distinct` |
| Math | `sample, sampleByKey, take, takeSample, count, countByKey, countByValue, max, min,` etc. |
| Balancing | `repartition, partitionByHash, partitionByRandom, partitionBy` |
| Persistence | `persist, cache, unpersist, uncache` |

## Background

IgnisHPC [13, 14] unifies the execution of Big Data and HPC workloads in the same computing engine. Unlike other frameworks such as Hadoop [19] and Spark [15], IgnisHPC has native support for multi-language applications using both JVM (Java Virtual Machine) and non-JVM-based languages. In this way, applications can be implemented using one or several programming languages following an API inspired by Spark's one.

The previous version of IgnisHPC supported natively C, C++, Java and Python. However, *seqkit* was implemented using the Go programming language. Since *BigSeqKit* parallelizes and optimizes the *seqkit* routines using IgnisHPC, it was necessary to add support for this language in the framework. Other solution would require to port the complete toolkit to a different language, which is a difficult and prone to errors task. It is worth noting that, to the best of our knowledge, nowadays IgnisHPC is the first parallel computing framework to include native support for this language. Considering Spark instead of IgnisHPC is not an option because, as it was demonstrated in [13], when using a non-native language code, data transfers between the JVM and external processes degrade noticeably the Spark's overall performance.

Go is a programming language with a simple syntax that was designed to be easy to learn and use. With the release of Go v1.18, the language included support for Generics, which allows the creation of functions, types, and methods that can work with any data type. This makes Go an effective and user-friendly way to implement Big Data interfaces. The implementation of Go in IgnisHPC is similar to that of C++, as both are compiled and statically typed languages. However, Go replaces the concept of inheritance with composition, which does not change the philosophy of use in IgnisHPC. Big Data functions are still accessible through the IgnisHPC API, and users can create their own code by implementing the same interfaces.

One of the key features of IgnisHPC is its use of containers to isolate and execute code. Containers are lightweight and portable, making it easy to run IgnisHPC on a variety of different clusters including both HPC (High-Performance Computing) and Big Data. IgnisHPC is also tolerant to failures, as the containers or processes can be easily restarted if there are issues. In particular, if some data is lost, IgnisHPC has enough information about how it was derived. In this way, only those operations needed to recompute the corresponding portion of data are performed.

We must highlight that although the IgnisHPC API[4] uses a se-

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[2] https://github.com/citiususc/BigSeqKit [accessed 28 feb 2023]

[3] https://bioinf.shenwei.me/seqkit/usage [accessed 28 feb 2023]

[4] https://ignishpc.readthedocs.io/en/latest/api.html [accessed 28 feb 2023]

quential notation, operations on data are performed in parallel. As we pointed out, the IgnisHPC API was inspired by the Spark API in such a way that IgnisHPC codes are easily understandable by users who are familiar with Spark. Table 1 shows a list of some of the most important functions supported by IgnisHPC. In particular:

- *Map functions:* The common characteristic to routines belonging to this type is that they apply the same function to each element in the data. As a result of the transformation, the output could be of different size with respect to the input.
- *Reduce functions:* `reduce` and `treeReduce` methods aggregate all the elements in the input data using a function. `aggregate` and `treeAggregate` are a sort of reduction where the type of the input and output data is different. In this case two functions are necessary, the first one is applied to each element in a data partition, and the second one combines the partial results obtained for each partition. `reduceByKey` and `aggregateByKey` are variations where the operation is performed only among elements with the same key in such a way that the final result is a set of unique pairs with values calculated using `reduce` or `aggregate` operations, respectively.
- *Group functions:* These methods group elements in a data frame according to their key value (`groupByKey`) or a user-defined function (`groupBy`).
- *Sort functions:* In order to sort elements, IgnisHPC provides three functions: `sort`, `sortByKey` and `sortBy`. The first method uses the natural order and does not need any additional function. `sortByKey` sorts the keys using their natural order. `sortBy` allows to use a user-defined function to specify the order of the elements. If the result of applying that function to two elements is *true*, then the first element should precede the second one. All methods support ascending and descending order.
- *SQL functions:* These functions operate on data frames. `union` concatenates two data frames, `join` merges elements of two data frames whose keys match, and `distinct` returns a new data frame after removing the duplicate records. These methods are necessary, for example, in many graph processing problems.
- *Other functions:* IgnisHPC implements several operations that return a value to the driver code, but they do not modify or generate new stored data. Spark refers to this type of operations as *actions*. For instance, IgnisHPC supports methods such as `count`, `take`, `takeSample` and `collect`. The most basic operation is `count` that returns the number of elements of a stored data collection. `collect` returns a collection with all the elements stored in the executors of a task. `take` applies a `collect` operation but obtains only the first *n* elements, where *n* is chosen by the user. `takeSample` returns a random sample of *n* elements from the distributed data, with or without replacement. Finally, another interesting routine is `parallelize`, which distributes the elements of a collection among the executors to form a distributed dataset. In this case new stored data is created.

It is worth noting that the IgnisHPC API functions allow users to parallelize a code with a high level of abstraction. In this way, it is only necessary to focus on data dependencies.

## Methods

As we commented previously, *BigSeqKit* speeds up the *seqkit* routines through parallelization and optimization techniques. Table 2 shows the routines supported by the current version of *BigSeqKit*. Despite most of the commands in *seqkit* are sequential, we can classify each command implementation into three categories according to its inherent parallelism:

- Independent: it is a embarrassingly parallel workload. As a consequence, the computation could be applied to all sequences in parallel. An example is `seq`, a function that transforms sequences. In this case, the transformation only affects each sequence individually.
- Partially dependent: computations could be done in parallel, but the method requires some type of consensus to obtain the result. For instance, `stats` should merge the partial results computed for each sequence to calculate some statistics of the considered FASTA/Q file.
- Dependent: dependencies between sequences prevent the method from being executed in parallel. As a consequence, *BigSeqKit* requires a complete new algorithm to perform the same command in parallel. `rmdup` is a good example because with the aim of removing duplicated sequences it is necessary to read all of them before generating a result.

The integration, parallelization and optimization of each *seqkit* command in IgnisHPC will be different depending on its category. More details are provided below.

### Independent routines

For these commands the computation can be applied to all sequences in parallel because there are no dependencies (communication) among them. In other words, routines belonging to this category can be processed using an embarrassingly parallel approach. Considering the IgnisHPC (and Spark) API, it is only necessary to use `map` functions to parallelize the computations. As we pointed out, the common characteristic to these API functions is that they apply the same operation to each element in the data.

The following *BigSeqKit* commands belong to this category: `seq`, `subseq`, `stats`, `fq2fa`, `fa2fq`, `translate`, `grep`, `locate`, `duplicate` and `replace` (see Table 2 for details).

### Partially dependent routines

As we mentioned, this category includes commands in which computations can be done in parallel using `map` functions, but the methods require some type of consensus to get the desired outcome. This consensus can be easily implemented using the IgnisHPC API. The following *BigSeqKit* commands belong to this category:

- `stats`: statistics can be generated in parallel but the final result must be unique, so all partial results must be merged using a reduction (`reduce` operation in the IgnisHPC API).
- `head`: sequences should know their position inside the file to check if they are inside the head window. To do that, it is necessary to use `mapWithIndex`, a special `map` operation included in the IgnisHPC API that allows each element to know its global index within a data structure.
- `head-genome`: similar to `head`, but not all sequences are valid. In order to determine the window, invalid sequences must be removed first.
- `range`: also similar to `head`. Sequences should know their position inside the file to check if they are within the range window.
- `grep`: although this command was included in the previous category, a command option (`-delete-matched`) limits the number of results to just one per search pattern. In such cases, it is necessary to remove the extra results.
- `faidx`: also similar to `head`, sequences compute their offsets inside the input file using `mapPartitionWithIndex` and exchange the information between executors to perform a parallel indexing operation with a simple `map`.

**Table 2.** List of commands included in both *BigSeqKit* and *seqkit*. Those commands with an asterisk support new functionalities not included in *seqkit*.

| | |
|---|---|
| **Basic commands** | |
| `seq` | Transform sequences (extract ID, filter by length, remove gaps, reverse complement, etc.) |
| `subseq` | Get subsequences by region/gtf/bed, including flanking sequences |
| `stats` | Simple statistics of FASTA/Q files: #seqs, min/max length, N50, Q20%, Q30%, etc. |
| `faidx`* | Create FASTA or FASTQ index file and extract subsequences |
| **Format conversion** | |
| `fa2fq` | Retrieve corresponding FASTQ records by a FASTA file |
| `fq2fa` | Convert FASTQ file to FASTA format |
| `translate` | Translate DNA/RNA to protein sequence |
| **Searching** | |
| `grep` | Search sequences by ID/name/sequence/sequence motifs |
| `locate` | Locate subsequences/motifs |
| **Set operations** | |
| `sample` | Sample sequences by number or proportion |
| `rmdup` | Remove duplicated sequences by ID/name/sequence |
| `common` | Find common sequences of multiple files by ID/name/sequence |
| `duplicate` | Duplicate sequences *N* times |
| `head` | Print first *N* FASTA/Q records |
| `head-genome` | Print sequences of the first genome with common prefixes in name |
| `pair` | Match up paired-end reads from two FASTQ files |
| `range` | Print FASTA/Q records in a range (start:end) |
| **Edit** | |
| `concat` | Concatenate sequences with the same ID from multiple files |
| `replace` | Replace name/sequence using a regular expression |
| `rename` | Rename duplicated IDs |
| **Ordering** | |
| `sort` | Sort sequences by ID/name/sequence/length |
| `shuffle` | Shuffle sequences |

## Dependent routines

Commands belonging to this category have an implementation in *seqkit* that by its nature cannot be parallelized. However, IgnisHPC allows us to define the implementation at a high level, which increases noticeably the productivity. Behaviors and functionalities will be preserved in *BigSeqKit* but through a complete new parallel implementation. In particular:

- `sample`: a sequential sampling can be performed in parallel if we split the sequences and run a sample for each partition. It was mathematically proven that sampling without replacement follows a hypergeometric function [20]. In this way, we can calculate the proportion of the sample that corresponds to each partition.
- `rmdup`: sequences are grouped (`groupBy` API function) using a hash with the ID, name or sequence. In those groups containing more than one element, a search for duplicates is carried out to remove them.
- `pair` and `concat`: sequences of the input files generate key-value pairs where the key is the ID and the value is the sequence with its index file (`map`). Pairs are unified by means of `union` and grouped using `groupByKey`. Afterwards, sequences in the same group are paired or concatenated if they belong to different files.
- `common`: the first stage of the command is the same one explained above for `pair` and `concat`. Then if a sequence can be found in all files, we check its index file, to avoid its deletion.
- `rename`: sequences are grouped (`groupBy`) using their ID, then IDs in the same group are renamed.
- `sort`: the sequential sort algorithm implemented in *seqkit* is replaced by a sample MergeSort [21] algorithm that can be efficiently executed in parallel in a distributed environment.
- `shuffle`: sequences shuffling can be implemented using the IgnisHPC API function `partitionByRandom`.

## Another implementation details

In order to parallelize and integrate the *seqkit* routines into IgnisHPC it was necessary to start considering the sequence parser. It takes a stream of characters in FASTA and FASTQ format and generates a data structure with the sequence representation. In *seqkit*, this stream can be represented by a file or the standard input. In *BigSeqKit*, this stream is implemented using the IgnisHPC iterators, which grant the users access to the data partitions. In this way, *BigSeqKit* will read the data from a file and split it in multiple partitions, which facilitates their parallel processing. As a result, the *seqkit* command arguments that affect file processing will have no effect in *BigSeqKit*. For example, the `-two-pass` option, which reads a file multiple times instead of storing all the sequences in memory, does not make sense in *BigSeqKit*. We must highlight that the fact of splitting the input files between several computing nodes in *BigSeqKit* means that the memory consumed by node is also split, which allows our tool to work with larger datasets. In addition, *BigSeqKit* also reduces the memory footprint by only storing the IDs and indices of each sequence.

Another important advantage of using IgnisHPC is how memory is handled. Users can choose a type of storage according to their particular case. For instance, if an input file is too large to be kept completely in the server memory, it could be stored compressed in memory or in disk. Performance would be lower, but it could be successfully processed. That scenario is not considered by *seqkit* that simply would raise an "out of memory" error. In particular, *BigSeqKit* supports the following storage options:

- *In-Memory:* it is the best performer since all data is stored in memory. It is the default option.
- *Raw memory:* data is stored in a memory buffer using a serialized binary format. Extra memory consumption is minimal and the buffer is compressed by Zlib.
- *Disk:* similar to raw memory but the buffer is stored as a POSIX file. Although the performance is significantly worse, it enables

working with vast amounts of data that cannot be entirely kept in memory.

On the other hand, `rmdup`, `common` and `pair` commands in *seqkit* use hash functions to check duplicates. It is well-known that hash functions can produce the same result for different values. This event is commonly known as a hash collision. However, *seqkit* does not check for collisions, so it is possible to generate incorrect results. *BigSeqKit* uses hashes to group sequences but then checks for collisions by comparing the real values.

Finally, *seqkit* and other state-of-the-art tools build index files (`faidx` routine) to speed up some other tasks (e.g., searches). Although *BigSeqKit* is also capable of creating those index files, it does not require them to improve its performance since data within IgnisHPC is already indexed. In other words, the index is created while reading the input file.

### New functionalities

*BigSeqKit* not only enables the parallelization of *seqkit* functions, but also improves its algorithms to provide benefits even for sequential executions and includes additional functionalities. In particular, the `faidx` command in *seqkit* implements indexing of FASTA files using the *samtools* format, but FASTQ files are not supported. *BigSeqKit* adds support for this type of files and generates an index file using the *samtools* format as well. Note that this is the most widespread format and is also supported by other state-of-the-art tools. Therefore, *BigSeqKit* allows indexing of both FASTA and FASTQ files using the same syntax than *seqkit*.

## How to use *BigSeqKit*

*BigSeqKit* can be used in two different ways. The first one is by means of a command-line interface (CLI). This approach is similar to the "command subcommand" structure adopted by *seqkit* [12]. In this way, it is only necessary to select a subcommand or routine (see a complete list in Table 2) and pass its arguments through command line. As we mentioned previously, to improve the usability and facilitate the adoption of *BigSeqKit*, it implements the same command interface than *seqkit*.

Since *BigSeqKit* runs within the IgnisHPC framework, it is necessary to send the *BigSeqKit* routine through the IgnisHPC submitter. For instance, if we are running *BigSeqKit* on a local server, the following expression uses the routine *seq* to print the name of the sequences included in a FASTA file to an output file:

```
ignis-submit ignishpc/full bigseqkit seq -n -o names.txt
     input-file.fa
```

Therefore, the syntax should be: `ignis-submit ignishpc/full bigseqkit <cmd> <arguments>`.

In addition, users can also specify through arguments the number of instances, cores and memory (in GB) to be used in the execution. By default, those values are set to 1. For example, we can execute the previous command using 2 cores:

```
ignis-submit ignishpc/full -p ignis.executor.cores=2
     bigseqkit seq -n -o names.txt input-file.fa
```

Unlike the other state-of-the-art tools, *BigSeqKit* can also be executed on a parallel cluster. Typical HPC clusters has Slurm [18] as the preferred resource manager, and Singularity [22] as container-based technology. In this case, users will send the job using the `ignis-slurm` submitter instead of `ignis-submit`.

On the other hand, *BigSeqKit* can also be used as a bioinformatics library. It is worth noting that *BigSeqKit* was implemented in Go language. However, thanks to the multi-language support provided by IgnisHPC, it is possible to call *BigSeqKit* routines from C/C++, Python, Java and Go applications without additional overhead. An example of Python code is shown in Figure 3. This example is equivalent to the previous one used in the explanation of the CLI. Since *BigSeqKit* has been created as a library, it only needs to be imported to be used. Functions in *BigSeqKit* do not use files as input, they use DataFrames instead, an abstract representation of parallel data used by IgnisHPC (similar to RDDs in Spark). Parameters are grouped in a data structure where each field represents the long names of a parameter. We must highlight that *BigSeqKit* functions can be linked (like system pipes using "|"), so the DataFrame generated by one can be used as input to another. In this way, integrate *BigSeqKit* routines in a more complex code is really easy.

```
1  import ignis
2  import bigseqkit
3
4  # Initialization of the framework
5  ignis.Ignis.start()
6  # Resources/Configuration of the cluster
7  prop = ignis.IProperties()
8  prop["ignis.executor.image"] = "ignishpc/go"
9  prop["ignis.executor.instances"] = "1"
10 prop["ignis.executor.cores"] = "2"
11 prop["ignis.executor.memory"] = "1GB"
12 # Construction of the cluster
13 cluster = ignis.ICluster(prop)
14 # Initialization of a Go Worker
15 worker = ignis.IWorker(cluster, "go")
16 # Sequence reading
17 seqs = bigseqkit.readFASTA("file.fa")
18 # Obtain Sequence names
19 names = bigseqkit.seq(seqs, name=True)
20 # Save the result
21 names.saveAsTextFile("names.txt")
22 # Stop the framework
23 ignis.Ignis.stop()
```

**Figure 3.** Example of Python code using the *BigSeqKit* routines.

The code starts initializing the IgnisHPC framework (line 5 in the figure). Next, a cluster of containers is configured and built (lines from 7 to 15). Multiple parameters can be used to configure the environment such as image, number of containers, number of cores and memory per container. In this example, we will use 1 node (instances) and 2 cores by node. After configuring the IgnisHPC execution environment, the *BigSeqKit* code actually starts. First, we read the input file (line 17). There is a different function for reading FASTA and FASTQ files. All the input sequences are stored as a single data structure. The next stage consists of printing the name of the sequences included in the FASTA file (line 19). The function takes as parameters the sequences and the options that specify its behavior. Finally, the names of the sequences are written to disk. It is important to highlight that lazy evaluation is performed, so functions are only executed when the result is required to be saved on disk.

## Experimental Results

In this section we analyze the performance results obtained by *BigSeqKit* with respect to other state-of-the-art tools. In particular, we have considered *samtools*, *pyfastx* and *seqkit* for their performance and number of commands supported. Experiments were

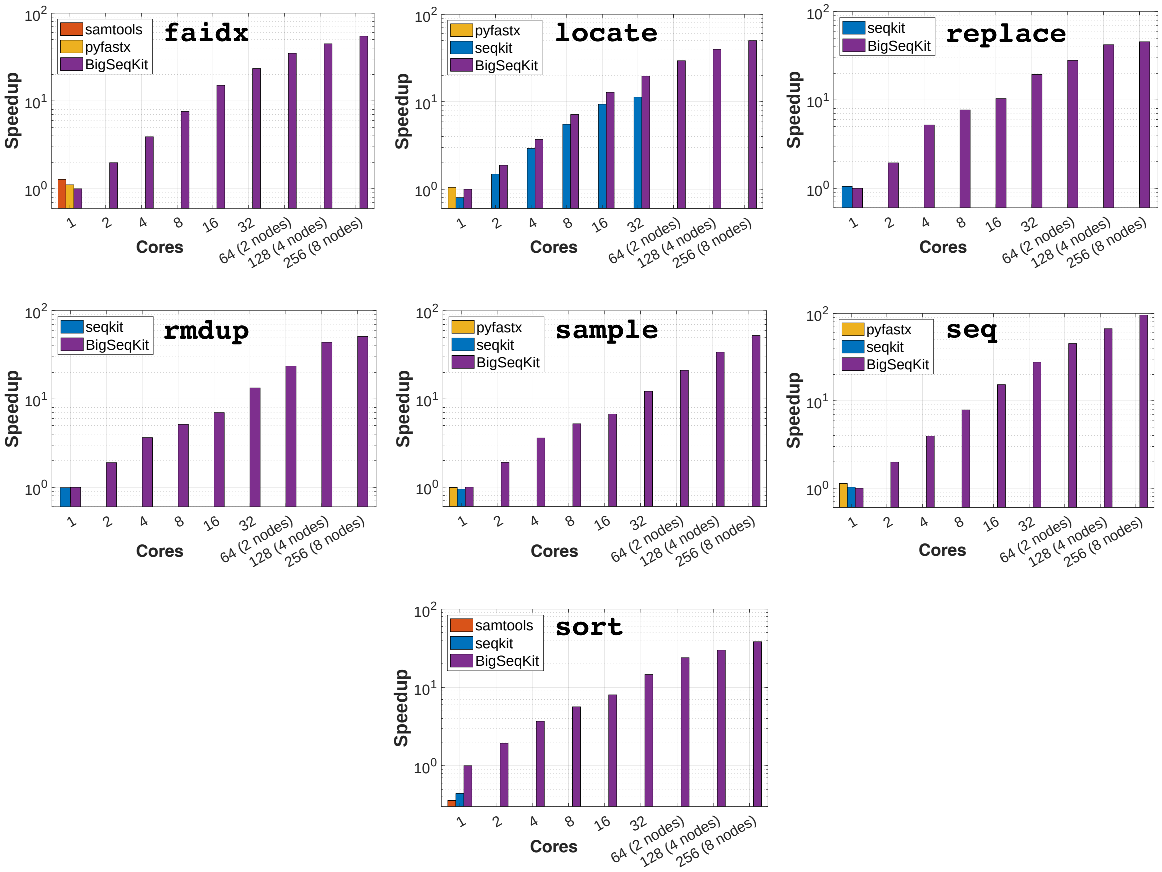

**Figure 4.** Speedups (in log scale) obtained by *BigSeqKit* and other state-of-the-art tools with respect to the *BigSeqKit* sequential time when executing different commands using $D_4$ as input. Note that `locate` was parallelized in *seqkit*.

conducted using up to 8 computing nodes of the FinisTerrae III [5] supercomputer installed at CESGA (Spain). Each node contains a 32-core Intel Xeon Ice Lake 8352Y @2.2GHz processor and 256 GB of memory interconnected with Infiniband HDR 100. It is a Linux cluster running Rocky Linux v8.4 (kernel v4.18.0). We have used SingularityCE v3.9.7 (containers), IgnisHPC v2.2, *pyfastx* v0.8.4, *samtools* v1.16.1 and *seqkit* v2.3.1 (with Slurm as cluster manager).

The performance evaluation was carried out using as input five different FASTA/FASTQ files that cover a wide variety of characteristics. The main features of these files are the following:

- $D_1$ (`m64013e_210227_222017.hifi_reads` - FASTA - 24 GB): Number of sequences: 1.2M, Minimum length: 85, Average length: 19.7K, Maximum length: 48.5K.
- $D_2$ (`SRR642648_1.filt` - FASTQ - 24.1 GB): Number of sequences: 98.7M, Minimum length: 100, Average length: 100, Maximum length: 100.
- $D_3$ (`Homo_sapiens.GRCh38.dna_sm.toplevel` - FASTA - 59.7 GB): Number of sequences: 639, Minimum length: 970, Average length: 98.8M, Maximum length: 248.9M.
- $D_4$ (`ERR4667750` - FASTQ - 79.1 GB): Number of sequences: 318.1M, Minimum length: 101, Average length: 101, Maximum length: 101.
- $D_5$ (`uniprot_trembl` - FASTA - 104 GB): Number of sequences: 229.9M, Minimum length: 7, Average length: 351.6, Maximum length: 45.3K.

As example to illustrate the benefits of our tool, we will evaluate the following utilities (see Table 2 for a complete list of commands): `faidx` builds an index for FASTA/FASTQ files, `locate` locates sequences following some search pattern, `replace` replaces a name/sequence using a regular expression, `rmdup` removes duplicated sequences, `sample` selects sequences by number or proportion, `seq` transforms sequences (extract ID, filter by length, etc.) and removes gaps, and `sort` sorts sequences by ID/name/sequence/length. We will also include the performance results of the corresponding utilities, if exist, for *samtools*, *pyfastx* and *seqkit*. Each result was computed as the median of five experiments. For the sake of reproducibility, all the codes and scripts used for performing the benchmarks are freely available at the *BigSeqKit* repository.

First, in order to provide an overall idea about the scalability and performance of *BigSeqKit* with respect to the other state-of-the art tools, we will show the speedups obtained for the $D_4$ dataset using different number of cores. The behavior is very similar when considering the other datasets. Results in log scale are displayed in Figure 4. Speedups were calculated using as reference the sequential execution (1 core) of the corresponding *BigSeqKit* command. According to the results, several conclusions can be made. It can be observed that the scalability of *BigSeqKit* is quite good, reaching speedups up to 27.7× and 95.7× (`seq` command) using one server (32 cores) and eight computing nodes (256 cores), respectively.

While *samtools* and *pyfastx* routines are always processed sequentially, *seqkit* uses a multi-threaded approach to (partly) parallelize some commands. However, its scalability is limited to use a few threads on a single server (computing node). This is the case of `locate`. Its best speedup only reaches 11.3× (32 cores) while this value increases until 19.6× with *BigSeqKit*. If eight nodes are used, *BigSeqKit* is 49.9× faster than the sequential execution.

For all the commands studied, *BigSeqKit* clearly outperforms *samtools*, *pyfastx* and *seqkit*. There are only a few cases using one

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[5] https://www.cesga.es/en/infrastructures/computing/ [accessed 28 feb 2023]

**Table 3.** Execution times (seconds) using different number of cores: `faidx` command. Highlighted in blue, fastest time and number of times faster than sequential *BigSeqKit*.

| | **1** | **2** | **4** | **8** | **16** | **32** | **64 (2 nodes)** | **128 (4 nodes)** | **256 (8 nodes)** |
|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | | | | | | | | | |
| *samtools* | 86.2 [1.03×] | – | – | – | – | – | – | – | – |
| *pyfastx* | 109.2 [0.81×] | – | – | – | – | – | – | – | – |
| *seqkit* | 75.4 [1.17×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 88.4 | 46.0 | 35.3 | 26.3 | 19.4 | 16.3 [5.4×] | 13.6 | **12.3 [7.2×]** | 12.5 |
| $D_2$ | | | | | | | | | |
| *samtools* | 165.6 [1.06×] | – | – | – | – | – | – | – | – |
| *pyfastx* | 177.9 [0.99×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 175.9 | 90.8 | 67.4 | 50.3 | 39.1 | 31.4 [5.6×] | 23.4 | 19.1 | **15.5 [11.3×]** |
| $D_3$ | | | | | | | | | |
| *samtools* | 210.0 [0.77×] | – | – | – | – | – | – | – | – |
| *pyfastx* | 131.2 [1.23×] | – | – | – | – | – | – | – | – |
| *seqkit* | 131.8 [1.23×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 161.9 | 83.9 | 61.7 | 24.5 | 17.5 | 15.7 [10.3×] | 13.6 | **13.4 [12.1×]** | 14.7 |
| $D_4$ | | | | | | | | | |
| *samtools* | 538.4 [1.27×] | – | – | – | – | – | – | – | – |
| *pyfastx* | 615.5 [1.11×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 684.2 | 346.6 | 175.2 | 90.3 | 45.4 | 29.3 [23.3×] | 19.6 | 15.3 | **12.5 [54.7×]** |
| $D_5$ | | | | | | | | | |
| *samtools* | 771.0 [1.08×] | – | – | – | – | – | – | – | – |
| *pyfastx* | 634.3 [1.31×] | – | – | – | – | – | – | – | – |
| *seqkit* | 1,096.2 [0.76×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 829.8 | 361.3 | 179.4 | 89.3 | 49.4 | 30.3 [27.4×] | 23.6 | 19.3 | **16.5 [50.3×]** |

**Table 4.** Execution times (seconds) using different number of cores: `locate` command. Highlighted in blue, fastest time and number of times faster than sequential *BigSeqKit*.

| | **1** | **2** | **4** | **8** | **16** | **32** | **64 (2 nodes)** | **128 (4 nodes)** | **256 (8 nodes)** |
|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | | | | | | | | | |
| *pyfastx* | 11,523.5 [1.0×] | – | – | – | – | – | – | – | – |
| *seqkit* | 12,822.9 | 6,385.0 | 3,210.9 | 1,731.4 | 940.5 | 612.4 [18.8×] | – | – | – |
| *BigSeqKit* | 11,486.2 | 6,286.1 | 3,180.0 | 1,637.3 | 850.9 | 470.6 [24.4×] | 264.6 | 156.9 | **110.3 [104.1×]** |
| $D_2$ | | | | | | | | | |
| *pyfastx* | 8,841.2 [1.2×] | – | – | – | – | – | – | – | – |
| *seqkit* | 12,319.8 | 6,909.4 | 3,335.9 | 1,746.2 | 997.3 | 971.2 [10.5×] | – | – | – |
| *BigSeqKit* | 10,168.6 | 5264.5 | 2711.5 | 1412.2 | 814.6 | 545.4 [18.6×] | 384.7 | 293.5 | **234.9 [43.3×]** |
| $D_3$ | | | | | | | | | |
| *pyfastx* | 13,075.3 [1.1×] | – | – | – | – | – | – | – | – |
| *seqkit* | 14,281.6 | 8,161.7 | 5,009.6 | 3,184.1 | 1,832.4 | 1,054.9 [14.1×] | – | – | – |
| *BigSeqKit* | 14,834.2 | 8,223.3 | 4,572.8 | 2,585.6 | 1,494.6 | 872.1 [17.0×] | 532.8 | 365.9 | **262.5 [56.5×]** |
| $D_4$ | | | | | | | | | |
| *pyfastx* | 30,028.3 [1.05×] | – | – | – | – | – | – | – | – |
| *seqkit* | 39,640.5 | 21,257.6 | 10,803.1 | 5,715.1 | 3,369.7 | 2,795.2 [11.3×] | – | – | – |
| *BigSeqKit* | 31,615.2 | 16,832.1 | 8,531.9 | 4,433.3 | 2,466.8 | 1,609.9 [19.6×] | 1,074.7 | 794.6 | **633.5 [49.9×]** |

core where the speedups of these tools are slightly greater than 1. For instance, executing the `faidx` routine with *samtools* and *pyfastx*. However, other commands such as `sort` and `sample` are processed faster with *BigSeqKit* even using one core.

Tables from 3 to 9 display, for all the datasets, the execution times of *BigSeqKit* and the other state-of-the-art tools when running `faidx`, `locate`, `replace`, `rmdup`, `sample`, `seq` and `sort` utilities, respectively. Speedups with respect the sequential execution of the corresponding *BigSeqKit* command are shown between brackets. Highlighted in blue is shown the fastest time overall and the corresponding speedup.

For all the experiments conducted, *BigSeqKit* is always the fastest tool both considering a single server (one node) or several computing nodes. In any case, let's take a look in detail of the behavior for each command:

- `faidx` (Table 3): *BigSeqKit* speedups range from 5.4× to 27.4× considering a single server (32 cores), and from 7.2× to 54.7× with 8 nodes. It means, for example, building the index file for our largest dataset $D_5$ (104 GB) in just 30.3 seconds (single server), while *samtools*, *pyfastx* and *seqkit* require 12.8, 10.6 and 18.3 minutes, respectively. As mentioned previously, the `faidx` routine in *seqkit* does not support FASTQ files ($D_2$ and $D_4$).
- `locate` (Table 4): the searching routines, `grep` and `locate`, are very expensive in terms of computations. Note that considering sequential processing, `locate` takes more than 3 hours to process our smallest dataset $D_1$ independently of the tool considered. This time increases to more than 8 hours for $D_4$. *seqkit* has a multi-thread version of `locate`, which obtains speedups from 10.5× to 18.8×. These speedups are always lower to the ones obtained by *BigSeqKit* on a single server. When using 8 nodes, *BigSeqKit* achieves noticeable speedups up to 104.1×. In this way, *BigSeqKit* reduces to only about 10 minutes the time necessary to execute the `locate` command with $D_4$.
- `replace` (Table 5): this routine (or an equivalent) is not supported by *samtools* and *pyfastx*. In this case, *BigSeqKit* is tens of times faster than *seqkit*, reaching speedups up to 45.6×.
- `rmdup` (Table 6): this routine is also not supported by *samtools* and *pyfastx*. The performance results are similar to the ones obtained by `replace`. That is, *BigSeqKit* is tens of times faster than *seqkit*, achieving a maximum speedup of 51.1× when removing the duplicated sequences in $D_4$.
- `sample` (Table 7): operation not supported by *samtools*. *BigSeqKit* is again faster than the other tools, increasing the speedups as the input datasize grows. It can be observed that *BigSeqKit* is able to sample sequences in a few seconds.
- `seq` (Table 8): operation not supported by *samtools*. Performance results are similar to the `sample` ones in such a way that *BigSeqKit* filters sequences by ID in few seconds, achieving a maximum speedup of 95.7×.

**Table 5.** Execution times (seconds) using different number of cores: `replace` command. Highlighted in blue, fastest time and number of times faster than sequential *BigSeqKit*.

| | 1 | 2 | 4 | 8 | 16 | 32 | 64 (2 nodes) | 128 (4 nodes) | 256 (8 nodes) |
|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | | | | | | | | | |
| *seqkit* | 132.4 [1.02×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 134.5 | 69.5 | 36.1 | 25.0 | 18.7 | 12.7 [10.6×] | 13.1 | 13.6 | 12.5 [10.8×] |
| $D_2$ | | | | | | | | | |
| *seqkit* | 395.7 [1.04×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 410.6 | 213.5 | 110.1 | 74.5 | 56.9 | 29.7 [13.8×] | 16.8 | 13.9 | 13.5 [30.4×] |
| $D_3$ | | | | | | | | | |
| *seqkit* | 410.5 [0.99×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 406.7 | 209.5 | 109.4 | 74.0 | 56.1 | 29.5 [13.8×] | 15.3 | 13.6 | 12.9 [31.5×] |
| $D_4$ | | | | | | | | | |
| *seqkit* | 543.7 [1.05×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 570.3 | 293.5 | 109.4 | 74.0 | 55.1 | 29.4 [19.4×] | 20.3 | 13.5 | 12.5 [45.6×] |

**Table 6.** Execution times (seconds) using different number of cores: `rmdup` command. Highlighted in blue, fastest time and number of times faster than sequential *BigSeqKit*.

| | 1 | 2 | 4 | 8 | 16 | 32 | 64 (2 nodes) | 128 (4 nodes) | 256 (8 nodes) |
|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | | | | | | | | | |
| *seqkit* | 178.9 [1.01×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 180.5 | 94.3 | 50.2 | 35.1 | 27.1 | 15.8 [11.4×] | 14.8 | 14.4 | 13.8 [13.1×] |
| $D_2$ | | | | | | | | | |
| *seqkit* | 320.6 [1.04×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 333.3 | 174.7 | 93.5 | 65.9 | 49.9 | 26.5 [12.6×] | 15.9 | 14.1 [23.6×] | 15.0 |
| $D_3$ | | | | | | | | | |
| *seqkit* | 515.5 [0.91×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 469.5 | 246.7 | 182.7 | 127.5 | 96.1 | 51.4 [9.1×] | 27.4 | 20.9 | 20.6 [22.8×] |
| $D_4$ | | | | | | | | | |
| *seqkit* | 729.9 [0.99×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 720.5 | 378.5 | 197.5 | 139.7 | 102.9 | 54.0 [13.3×] | 30.5 | 16.4 | 14.1 [51.1×] |

**Table 7.** Execution times (seconds) using different number of cores: `sample` command. Highlighted in blue, fastest time and number of times faster than sequential *BigSeqKit*.

| | 1 | 2 | 4 | 8 | 16 | 32 | 64 (2 nodes) | 128 (4 nodes) | 256 (8 nodes) |
|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | | | | | | | | | |
| *pyfastx* | 308.2 [0.67×] | – | – | – | – | – | – | – | – |
| *seqkit* | 196.1 [1.05×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 205.7 | 108.2 | 57.8 | 36.4 | 27.1 | 17.3 [11.9×] | 15.1 | 15.4 | 14.1 [14.6×] |
| $D_2$ | | | | | | | | | |
| *pyfastx* | 458.7 [1.12×] | – | – | – | – | – | – | – | – |
| *seqkit* | 492.4 [1.04×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 514.5 | 271.7 | 143.8 | 98.1 | 76.1 | 42.2 [12.2×] | 36.1 | 30.1 | 26.4 [19.5×] |
| $D_3$ | | | | | | | | | |
| *pyfastx* | 450.2 [0.88×] | – | – | – | – | – | – | – | – |
| *seqkit* | 491.7 [0.80×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 394.3 | 207.8 | 105.2 | 70.5 | 52.7 | 26.1 [15.1×] | 22.1 | 19.2 | 14.3 [27.6×] |
| $D_4$ | | | | | | | | | |
| *pyfastx* | 1,929.1 [0.99×] | – | – | – | – | – | – | – | – |
| *seqkit* | 1,996.7 [0.96×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 1,912.8 | 1,000.5 | 529.3 | 365.8 | 283.4 | 156.3 [12.2×] | 90.4 | 56.2 | 36.5 [52.4×] |

**Table 8.** Execution times (seconds) using different number of cores: `seq` command. Highlighted in blue, fastest time and number of times faster than sequential *BigSeqKit*.

| | 1 | 2 | 4 | 8 | 16 | 32 | 64 (2 nodes) | 128 (4 nodes) | 256 (8 nodes) |
|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | | | | | | | | | |
| *pyfastx* | 151.8 [0.56×] | – | – | – | – | – | – | – | – |
| *seqkit* | 234.4 [0.36×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 84.4 | 43.5 | 22.5 | 11.6 | 6.3 | 4.8 [17.6×] | 4.7 | 3.7 | 3.5 [24.1×] |
| $D_2$ | | | | | | | | | |
| *pyfastx* | 209.4 [1.15×] | – | – | – | – | – | – | – | – |
| *seqkit* | 234.0 [1.03×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 240.9 | 128.5 | 65.0 | 34.6 | 19.5 | 10.7 [22.5×] | 6.1 | 4.3 | 4.0 [60.2×] |
| $D_3$ | | | | | | | | | |
| *pyfastx* | 400.5 [0.90×] | – | – | – | – | – | – | – | – |
| *seqkit* | 541.2 [0.67×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 360.2 | 182.7 | 93.4 | 48.1 | 27.1 | 20.2 [17.8×] | 8.6 | 5.1 [65.5×] | 5.5 |
| $D_4$ | | | | | | | | | |
| *pyfastx* | 901.2 [1.13×] | – | – | – | – | – | – | – | – |
| *seqkit* | 981.7 [1.03×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 1,014.7 | 508.8 | 257.1 | 129.1 | 66.3 | 36.6 [27.7×] | 22.5 | 15.2 | 10.6 [95.7×] |

- `sort` (Table 9): this routine was not included in *pyfastx*. In general, the performance of *samtools* and *seqkit* is poor. As a result, for example, *BigSeqKit* sorts $D_4$ using a single server 39.8× and 33× faster than *samtools* and *seqkit*, respectively. These

**Table 9.** Execution times (seconds) using different number of cores: `sort` command. Highlighted in blue, fastest time and number of times faster than sequential *BigSeqKit*.

| | 1 | 2 | 4 | 8 | 16 | 32 | 64 (2 nodes) | 128 (4 nodes) | 256 (8 nodes) |
|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | | | | | | | | | |
| *samtools* | 1,590.3 [0.10×] | – | – | – | – | – | – | – | – |
| *seqkit* | 169.0 [0.97×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 164.4 | 86.2 | 46.2 | 33.5 | 24.2 | 14.5 [11.3×] | 13.8 | 13.5 | **12.9 [12.7×]** |
| $D_2$ | | | | | | | | | |
| *samtools* | 1,672.5 [0.25×] | – | – | – | – | – | – | – | – |
| *seqkit* | 1,050.5 [0.40×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 422.8 | 221.6 | 117.6 | 81.7 | 62.1 | 34.9 [12.1×] | 21.5 | 15.8 | **13.2 [32.0×]** |
| $D_3$ | | | | | | | | | |
| *samtools* | 1,203.5 [0.44×] | – | – | – | – | – | – | – | – |
| *seqkit* | 497.5 [1.05×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 523.8 | 272.5 | 144.2 | 100.7 | 77.6 | 43.2 [12.1×] | 26.5 | 18.6 | **15.8 [33.1×]** |
| $D_4$ | | | | | | | | | |
| *samtools* | 3,835.1 [0.36×] | – | – | – | – | – | – | – | – |
| *seqkit* | 3,122.2 [0.44×] | – | – | – | – | – | – | – | – |
| *BigSeqKit* | 1,377.3 | 708.5 | 372.5 | 243.7 | 171.5 | 94.6 [14.6×] | 57.6 | 46.0 | **36.0 [38.3×]** |

speedups increase to 106.5× and 86.7× when considering 8 computing nodes.

## Conclusions

Current state-of-the-art tools such as *seqkit*, *pyfastx* and *samtools* are not ready for processing and manipulating very large FASTA and FASTQ files because all of them are mainly based on sequential processing. To that end, we have presented *BigSeqKit*, which parallelizes and optimizes the *seqkit* routines using the IgnisHPC computing framework. Since *seqkit* was programmed in Go, IgnisHPC was extended to support that language. As a consequence, IgnisHPC is nowadays the first parallel computing framework that supports Go. *BigSeqKit* can be easily installed on a local server or on a cluster. In addition, it can be used from the command line or as a library. Thanks to the multi-language support of IgnisHPC, *BigSeqKit* routines can be called from C/C++, Python, Java and Go codes.

Regarding the experimental results, *BigSeqKit* clearly outperforms *seqkit*, *pyfastx* and *samtools* for all the tasks considered. On a single server, *BigSeqKit* is overall tens of times faster than those state-of-the-art tools, reaching speedups with respect to the *BigSeqKit* sequential time up to 27.7×. Considering an 8-nodes cluster, *BigSeqKit* is even faster, reaching speedups higher than 100×. It means that most of the tasks can be performed in just a few seconds.

As future work we plan to add also the remainder *seqkit* commands not included in the current version of *BigSeqKit*: `sliding`, `sana`, `fx2tab`, `tab2fx`, `convert`, `amplicon`, `fish`, `split`, `split2`, `restart` and `mutate`. Note that all of them are independent routines, so their implementation using IgnisHPC will be straightforward.

## Availability of source code and requirements

- Project name: BigSeqKit
- Project home page: `https://github.com/citiususc/BigSeqKit`
- Operating system(s): Linux
- Programming language: Go
- Other requirements: IgnisHPC 2.2
- License: GNU GPL-3.0

## Availability of supporting data and materials

The datasets supporting the results of this article are available in: $D_1$ was obtained from the PacBio repository, $D_2$ and $D_4$ from the International Genome Sample Resource (accession ids, SRR642648_1.filt and ERR4667750) [23], $D_3$ from Ensembl [24] (assembly accession id, GCA_000001405.20), and $D_5$ from UniProtKB - release 2022_03.

## Declarations

### List of abbreviations

(CLI) Command-Line Interface, (HPC) High-Performance Computing, (JVM) Java Virtual Machine, (NGS) Next-Generation Sequencing, (MPS) Massive Parallel Sequencing.

### Ethical Approval

Not applicable.

### Consent for publication

Not applicable.

### Competing Interests

The authors declare that they have no competing interests.

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### Author’s Contributions

**César Piñeiro**: Methodology, Software Development, Conducted Experiments, and Contributed to Writing.
**Juan C. Pichel**: Conceptualization, Methodology, Supervision, Writing and Revision.

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