

# An efficient and robust parallel scheduler for bioinformatics applications in a public cloud: A bigdata approach

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## ABSTRACT

In bioinformatics, genomic sequence alignment is a simple method for handling and analysing data, and it is one of the most important applications in determining the structure and function of protein sequences and nucleic acids. The basic local alignment search tool (BLAST) algorithm, which is one of the most frequently used local sequence alignment algorithms, is covered in detail here. Currently, the NCBI's BLAST algorithm (stand-alone) is unable to handle biological data in the terabytes. To address this problem, a variety of schedulers have been proposed. Existing sequencing approaches are based on the Hadoop MapReduce (MR) framework, which enables a diverse set of applications and employs a serial execution strategy that takes a long time and consumes a lot of computing resources. The author, improves the BLAST algorithm based on the BLAST-BSPMR algorithm to achieve the BLAST algorithm. To address the issue with Hadoop's MapReduce framework, a customised MapReduce framework is developed on the Azure cloud platform. The experiment findings indicate that the suggested bulk synchronous parallel MapReduce-basic local alignment search tool (BSPMR-BLAST) algorithm matches bioinformatics genomic sequences more quickly than the existing Hadoop-BLAST method, and that the proposed customised scheduler is extremely stable and scalable.

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## 1. INTRODUCTION

According to research [1], [2], cloud computing has established itself as the future norm for data-intensive computing. According to [3], [4] cloud computing platforms allow on-demand access to shared, scalable, fault-tolerant, and reconfigurable computing resources with little administrative work and a low cost. In comparison to freestanding private computer clusters [5], [6] demonstrate how cloud computing platforms are a commonly desired and recognised method for running large data applications or high-performance computations (HPC). The cloud's resource management, virtual computing platforms, and elasticity all contribute to the ease with which data-intensive applications can be migrated to the cloud paradigm. Cai *et al.* [7], Okur and Büyükkeçeci [8] note that the frameworks required to enable the most efficient use of cloud resources at the lowest possible cost for data-intensive applications remain unresolved. Google's MapReduce framework discussed in [9] is a commonly used approach for performing distributed computations on the cloud. White [10] and Hadoop [11] present that implementations of Hadoop are based on the MapReduce architecture and are capable of supporting large-scale data applications. The MapReduce model employs a two-stage execution mechanism. The initial stage entails splitting or dividing the data to be

processed into little pieces. Each small bit of data is associated with a mapper. The mapper outputs  $\langle Key|Value \rangle$  pairs that are arranged according to the  $Key$  values. The Reduce workers are provided with the sorted values using the  $\langle Key|SortedList(Value) \rangle$  method. The Hadoop distributed file system is used to store the results of the reduce workers hadoop distributed file system (HDFS). In most public cloud setups, the Map and Reduce workers are virtual machines (VMs).

The researchers recognised the disadvantages of Hadoop MapReduce and examined several improvement strategies. Zhu *et al.* [12] discusses the use of Hadoop with CUDA to increase processing capacity and execution speed. Zhu *et al.* [12] proposes a research paradigm that facilitates appropriate use of graphics processing units (GPU). Dhiphale *et al.* [13] presents a cloud-based MapReduce model. Pipelining is used to improve execution performance and to enable elastic pricing. For scientific applications [14] proposed a framework based on parallel tempering called replica exchange statistical temperature molecular dynamics. Tang *et al.* [15] describe a unique dynamic Hadoop slot allocation technique for resolving the Hadoop resource provisioning problem that is not optimal. The result reported in Tang *et al.* [15] demonstrates that their technique significantly improves Hadoop's performance when handling many MapReduce jobs. The most often utilised technique is to increase execution effectiveness through scheduling practises, as described in [16]-[19].

Wang *et al.* [20] presented a method for computing "Imprecise Applications" using MR frameworks. Reduce is run after the Map step in predictable MapReduce applications. In the case of inaccurate applications, the Reduce stage might be initiated using the Map stage's partial findings. Applications such as word frequency statistics and hot-word identification are considered imprecise. Executing inaccurate apps on well-known machine learning frameworks like Hadoop introduces latency. Running erroneous apps might result in additional expenditures on public cloud systems, where users are charged for all computations and storage services consumed. To address this shortcoming incorporated the check phase into the MapReduce framework in order to reduce costs and execution latencies [20].

In MR frameworks, iterative applications and certain graph-based applications performed poorly. Google introduced the Pregel framework for cloud computations in [21] for similar applications. Pregel is built on valiant's bulk synchronous parallel (BSP) computation model [22]. Kajdanowicz *et al.* [23] demonstrate that the Pregel framework outperforms MapReduce when calculating graph-based applications. Apart from the serial execution mechanism utilised in MR, several concerns remain unresolved, including node failure management capabilities, scheduling strategies, and multiway join processes.

The authors provide a framework for parallel computation MapReduce (PMR) in public cloud environments in this article. The MapReduce architecture of the BLAST-BSPMR enables parallel computation to accelerate the execution of the BSP model. The BLAST-BSPMR implements Map and Reduce workers by utilising Microsoft Azure VM computing environments. Multicore processors enable parallel computation in these virtualized computing environments. The BLAST-BSPMR proposal leverages this parallel execution feature to drastically lower the Map and Reduce worker nodes' computation times. In comparison to other MapReduce frameworks like Hadoop, the BLAST-Reduce BSPMR's phase is initiated when two or more worker nodes have completed their jobs. The BLAST-BSPMR function shown here is used to calculate the results of bioinformatics BLASTx applications.

Several strategies and scheduler are proposed by researchers to improve the performance of the MapReduce cloud computing framework proposed by Google in Dean *et al.* [9]. The work presented in Zhu, *et al.* [12] endures the closest similarity to our work presented here. Using CUDA codes the Map and Reduce worker tasks execute parallelly on the GPU's is achieved. The integration of Hadoop and GPU is achieved using the Hadoop Streaming, Pipes, JCUda and JNI approaches. The experimental investigation given in Jie Zhu *et al.* [12] demonstrates the effectiveness of the suggested approach on a private heterogeneous cloud environment using the word count application. The execution efficiency of the JCUda approach over Hadoop Streaming, Pipes and JNI is also proved. The major drawback of this approach is that such computational models are not suited for public cloud environments as GPU based VM environments are generally not offered. Public cloud environments like Amazon EC2 that offer such GPU based virtualized computing environments provide it at very high costs.

Dhiphale *et al.* [13] described the drawbacks of the conventional MapReduce frameworks as follows: the MapReduce framework adopts a sequential processing of the Map and Reduce stages. The scalability of the MapReduce is limited. The MapReduce framework provides no support for flexible pricing options. The MapReduce model provides no support for computing streaming data. To overcome these drawbacks a pipelined model is presented to parallelize the execution of the Map and Reduce phase. The MapReduce model proposed in [13] is realized on the Amazon public cloud. The spot instance offering of the Amazon cloud allows flexible pricing. The experimental study given here demonstrates the efficiency of the pipelining-based MapReduce model when compared to the conventional MapReduce model using the word count application. The major drawback of the model proposed in [13] is that the locality optimization is not

considered and hosting of additional data dependent applications like Smith Waterman and other bioinformatics application cannot be executed in a pipelined fashion.

The computation of certain data intensive applications like graph applications and iterative applications on MapReduce frameworks exhibit high computation time and cost. To support such applications, Google presented a proprietary cloud computing framework named Pregel that embraces the *BSP* computing model [21]. In Pregel, the graph computations are achieved using a set of super-steps. A super step is used to execute the user defined application or function in a parallel fashion using the data item from the database. Each data item from the database behaves as an agent. The Pregel system adopts vertex-centric execution strategy. The computation of each data item has a graph like representation in *BSP*. The vertexes in the Pregel deactivate post the computation operation and are reactivated only if additional data items are presented to them. Once all the vertexes are deactivated the computation is said to be complete. The local storage of the data items in the nodes executing the computation poses a problem. In the case the data item is large then a spilling-to-disk technique needs to be in [23].

The MapReduce framework is been adopted by the Hadoop framework in Nguyen *et al.* [24] for computing on the cloud platform. The MapReduce paradigm employs a two-phase technique. The first phase divides the input data into little bits of data to be processed. Each small bit of data is associated with a mapper. The mapper outputs a <Key, Value> pair that is sorted according to the Key values. The reducer takes these sorted values as the <Key | SortedList (Value)>. These sorted values are stored in the Hadoop Distributed File System. Schatz [25] and CloudBurst make use of the Hadoop MapReduce framework as the computing platform. These alignment tools perform effectively for small base pair alignments requiring single-gap or un-gapped alignment. However, when huge base pairs are considered, these aligners perform poorly. Because all present cloud framework sequence aligners take the Hadoop framework into account, Hadoop suffers when iterative applications are hosted on the cloud framework. When considering multiway joins, Hadoop performs poorly. Since Hadoop framework executes sequentially, again there is degradation in the performance. The *BSP* based Pregel framework exhibits lower computation time for selective applications. In this paper the *BLAST – BSPMR* framework incorporates the MapReduce architecture and an execution strategy is conducted in parallel fashion as observed in the *BSP*.

## 2. METHOD

A cloud platform, *BLAST-BSPMR* is proposed that allows to apply bioinformatics application like gene sequencing. The *BLAST-BSPMR* uses MapReduce framework which works on a cloud computing environment. Azure VM is the Azure infrastructure as service (IaaS) which is used to deploy persistent VMs. Thus, the Map and Reduce worker nodes in *BLAST-BSPMR* are deployed on Azure VMs. Alignment of genomic sequences is performed using the *BLASTx* method. Here in *BLASTx*, a DNA query is compared to a protein database. The *BLAST-BSPMR* algorithm performs sequence alignment in two stages, namely the Map and Reduce phases. Since Hadoop framework is sequential, only when the Map phase is completed the Reduce phase gets executed. To prevent sequential execution, *BLAST-BSPMR* considers parallelizing the Map and Reduce phases. The Map and Reduce functions are meant to be executed in parallel and to make optimal use of the cores available in the worker VMs.

### 2.1. Basic local alignment search tool (BLAST) algorithm

Basic local alignment search tool (BLAST) is used to compare a query sequence with the database sequence to find similar sequences in the database. The BLAST consists of various sequence searching programmes (including *BLASTn*, *tBLASTn*, *BLASTx*, *BLASTp*, *tBLASTp*, and *tBLASTx*). Each application varies in its functionalities, but the core of the algorithm for all of them is basically the same. The BLAST algorithm consists of three steps. In the initial step, called as building the word list, the query sequence is split into small words of fixed size (*w*-mers), often *w* being 11. Therefore, if the length of the query sequence is *n*, then list of *n-w+1* words are being constructed. This step is illustrated in Figure 1. The second stage, referred to as the scan for hits, is where the BLAST algorithm looks for matches to the words (referred to as hits) in the database sequence. The BLAST algorithm employs the 'two-hit' strategy. If two non-overlapping word pairs are found to be within a distance *D* of one another, an extension is initiated. The next stage, dubbed extend the hits, involves the BLAST algorithm expanding the results in order to find longer related segment pairs. When the "two-hit" requirement is met, a gap-free extension in two directions is performed to locate an alignment known as a high-scoring segment pair (HSP). Figure 2 gives an example of gap-free extension. This is the seed-and-extend heuristic strategy for identifying high-scoring gene sequence alignments between the genomic query sequence and the database's genomic sequences.

Genomic Query Sequence: TCGACAGACGAGTT

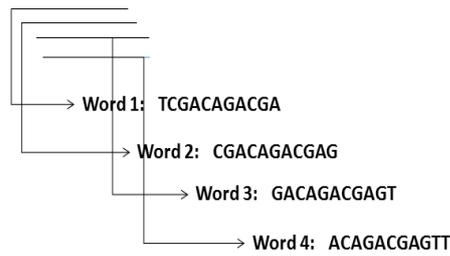


Figure 1. Build word list

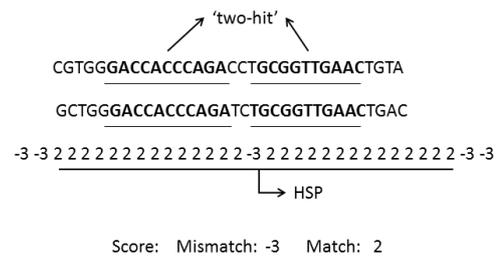


Figure 2. Build word list

## 2.2. BLASTon the proposed parallelized MapReduce framework

The genomic sequence database was initially split into trivial chunks of static size and scheduled over the virtual Azure computing nodes in the current work. Numerous computing nodes can process the chunks in parallel. The three core BLAST processes (building word lists, scanning, and extension) were then reorganised and run concurrently. It takes longer in two stages, according to the BLAST algorithm: searching for matching terms in the genome database and extending the seeds. Thus, the proposed BLAST-BSPMR framework is employed to parallelize the BLAST algorithm, thereby increasing the calculation's overall efficiency. The BLAST-BSPMR technique is implemented in three stages: data storage in Azure blob storage, genomic sequence preparation, and genomic sequence parallelization. The first stage involves transferring the genomic database and query sequence to Azure blob storage. The second level preprocesses each computational worker node's genetic data. The third stage performs further accurate matches, extension, and statistics on the preprocessed sequence seeds prior to giving them as input to the BLAST-BSPMR algorithm. The sections that follow describe the suggested method's several stages.

### 2.2.1. Pre-processing of gene sequence data

As stated in the basic procedure of the NCBI BLAST algorithm, the first criterion the BLAST algorithm is to generate a word list for the BLAST-BSPMR method. The purpose of identifying words with a high correlation coefficient during the pre-processing of genomic sequence data is to simplify calculations or computations concerning accurate/correct matches and seed expansion. This technique accelerates the third phase of sequence alignment. Due to the fact that the research query data consists of nucleic acid sequences, the lengths of the genomic query and database sequences are  $x$  and  $y$ , respectively, and the number of words is  $x-10$  and  $y-10$ . The following stages must be followed in the pre-processing of genomic sequence data: Stages of mapping, sorting, shuffle, and reduction. The author generates a statistic of nucleobases (ATGC) with the highest occurrence number using a Map scheme on each word in the Map stage, such as  $\langle T, 4 \rangle$ , where  $T$  indicates the most often occurring nucleobase and  $4$  denotes the number. The output of Map is sorted by the frequency of each nucleobase during the sort stage. In the shuffle phase, the sort stage's results are jumbled and merged. If the frequency of nucleobase  $T$  in the word  $qs_i (i = 0, 11, \dots, 10y + 1, \dots)$  in the genomic query sequence is  $num1$  and the count of nucleobase  $T$  in the word  $db_i (i = 0, 11, \dots, 10y + 1, \dots)$  in the genomic database sequence is  $num2$ ,  $qs_i$  will combine with all  $db_i$ , and rank them according to the size of  $num1 + num2$ . List of all  $db_i$  combined with  $qs_i$  as items in the BLAST-BSPMR algorithm's word list in the final stage of Reduce, based on the output of the shuffle stage. The following step is to save the results to Azure Blob Storage for later analysis.

### 2.2.2. Alignment of gene sequences in parallel

The word list for the scanner is produced from preprocessed genomic sequencing data. The three basic steps in the parallel alignment of genomic sequences using a word list and a scanner are exact word matches, seed expansion, and statistical significance during seed expansion. To facilitate parallelization of genomic sequence alignment, the generated word list and scanner should be distributed among a large number of virtual processing nodes. The flow chart in Figure 3 depicts the parallelization of the BLAST-BSPMR method with MapReduce.

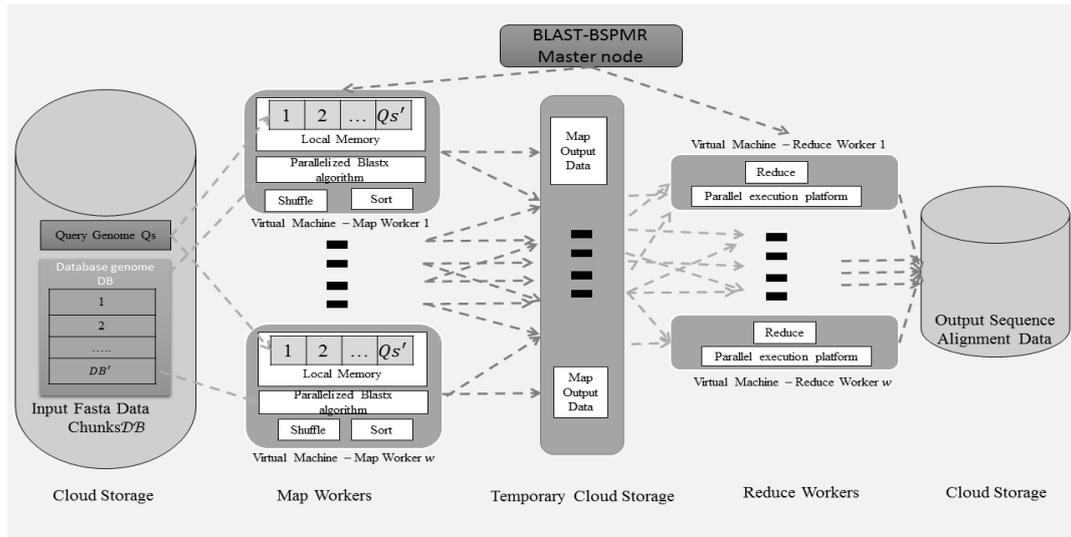


Figure 3. The Parallelized BLAST-BSPMR model

### 2.2.3. The steps required in aligning the BLAST-BSPMR method in parallel

- Each Azure virtual computer node will receive the list of words and scanner, and the gene sequence will be aligned using a BLAST-BSPMR MapReduce Job.
- During the Map phase, each Map task reads the scanner and a list of words from local memory to build accurate matches for items with a high correlation; items that satisfy the matching conditions are saved as words in the following extension.
- Following scanning, the restored bits from second step 2) will go through three processes in each computing node: they will initiate a simple match extension without space, they will use DP to find a match extension with vacancies, and they will finally obtain alignment results that satisfy the given conditions.
- The results of the comparison will be arranged according to the score acquired during the shuffle phase.
- The Reduce phase transfers the genomic sequence alignment findings to Azure Blob Storage in their original format.

### 2.3. Proposed BLAST alignment on the parallelized MapReduce model BLAST-BSPMR

Let  $DB$  denote a bioinformatics sequence of the genome database and  $Qs$  the genomic query sequence. The *BLAST – BSPMR* is positioned on a public cloud platform namely azure consist of a master node, Map and Reduce worker computing nodes. The master computing node of *BLAST – BSPMR* initializes  $cw$  Map and Reduce worker computing nodes using the virtual computing nodes. Every virtual computing node is presumed to  $C$  CPU cores available for task/job computation. Let  $TIE_{VM\_inz}$  represent the time spent initialising the virtual platform. The sequence  $DB$  is a bioinformatics database that is divided into  $DB'$  tiny chunks of sequence data with overlapping portions. A database's short bit of data sequence and the  $Qs$  are then transmitted as input key, value pairs to the Map computing nodes. The key value pairings that take into account the reference small bit of data  $DB'$  are denoted as  $(kd, vd)$ , where  $kd$  is the key and  $vd$  which contains the genomic data with overlapping offsets. The key-value pair corresponding to the genome query sequence  $Qs$  is indicated by  $(kqs, vqs)$ , where  $kqs$  is the key and  $vqs$  is the genome query sequence. Each of the  $cw$  computing Map workers divides the query sequence  $Qs$  into  $Qs'$  little bits of data and stores them in the available local memory storage. The sequence alignment is performed using the BLASTx algorithm in parallel using the  $C$  cores taking into account  $DB'$  and each and every  $Qs'$ . The BLASTx algorithm is parallelized to reduce the time required to complete genomic sequence alignments. Let  $TIE_{MS}$  denote the average time taken by the  $cw$  Map compute nodes to complete a task. The mappers give alignment positions between  $Qs$  and database small bit of data of  $DB'$  along with the computed score as a result of their post computations. Multiple alignment places and computed score, i.e.,  $vms$  combined with the small bit of data id of  $DB'$  i.e.,  $kms$  are saved in the memory in the following manner:  $list(kms, vms)$ . The BLAST-BSPMR Mapfunction is represented as  $map((kd, vd), (kqs, vqs)) \rightarrow list(kmp, vmp)$ . The  $cw$  Map computing worker nodes obtain intermediate genomic data i.e.,  $list(kmp, vmp)$  and perform shuffle and sort operations. The reduce step considers the collection of all non-overlapping and non-redundant

alignment results, i.e.,  $list(vgd)$ . Allow  $TE_{RS}$  is the average time spent by the  $cr$  Reduce computing worker nodes to complete the storage procedure (gather the results). The total time required for the BLAST-BSPMR to align the genomic sequence using a cloud-based platform  $Qs$  against the database,  $DB$  is calculated as,

$$E = TE_{VM_{inz}} + TE_{MS} + TE_{RS} \tag{1}$$

the BLAST-BSPMR cloud platform is depicted in Figure 3.

### 3. RESULTS AND DISCUSSION

The machine was configured with a 64-bit version of Windows 10 Enterprise, 16 GB of RAM, and an i-5 quad core processor. We conducted an experimental investigation comparing the proposed BLAST-BSPMR gene sequencing model to the existing Hadoop-BLAST sequencing model on the following parameters: speedups, throughput, and sequence alignment completion time using the dot net framework 4.0 and C# 6.0 programming language for the proposed work and java programming language for the existing Hadoop.

It is considered to compare the performance of BLAST-BSPMR with Hadoop-BLAST. With a single VM computing node, Hadoop-BLAST and BLAST-BSPMR can be deployed. The Microsoft Azure cloud platform hosts the BLAST-BSPMR. The Hadoop-BLAST application is built on top of the Hadoop MapReduce framework. The Hadoop-BLAST is deployed using Apache Hadoop & YARN 2.6.0. In the deployments, identical configurations of VM computing nodes are taken into account. The *BLAST – BSPMR* model is hosted on Microsoft’s Azure cloud considering A3 VM instances. Each A3 VM instance consists of 4 virtual computing cores, 7 GB of RAM and 120 GB of local hard drive space. The *BLAST – BSPMR* model deployed on the Azure cloud platforms are comprised of a master node and a worker node for the purpose of performing Map and Reduce operations/tasks. Using Azure HDInsight. It enables deployment and provisioning of Apache Hadoop clusters on the Azure cloud platform. The Apache Hadoop & YARN version 2.6.0 is considered for performance evaluation. The master node of the azure cluster runs on the Windows Server 2012 R2 operating system. One worker node of A3 VM instances is considered for the Hadoop deployment. For evaluation, the non-redundant protein genomic database is used. The initial investigations employ a continuous non-redundant protein genomic sequence and four nucleotide query sequences of varying sizes. The first experiment conducted with the reference and varied query genomic sequences are summarized in Table 1. Figure 4 shows the execution time and Figure 5 shows the speedup and throughput and Figure 6 shows the average speedup and throughput. The results show that the proposed BLAST-BSPMR aligner, which is running on Azure, outperforms Hadoop-BLAST. For both BLAST-BSPMR and Hadoop-BLAST, the execution time increases as the query file length grows. The second experiment is conducted using varied non-redundant protein genomic sequence and constant query sequences of nucleotide. The total time (including the Map and Reduce stages) taken to execute the alignment is monitored using Table 2 for the BLASTx sequence alignment computation on the BLAST-BSPMR and Hadoop-BLAST. The results obtained are summarized in Table 3. The total time required to complete sequence alignment (as depicted in Figure 7) is recorded. The results show that the proposed BLAST-BSPMR aligner, which is running on Azure, outperforms Hadoop-BLAST. Figure 8 shows the speedup and throughput for the experiment 1 and Figure 9 depicts the average speedup and throughput obtained for the experiment 2. As the database file size increases, the execution time also increases for both BLAST-BSPMR and Hadoop-BLAST.

Table 1. Experiment data used to compare BLAST-performance BSPMR's to that of BLAST-Hadoop with varied size of query genome

No	Database Genome	Size (GB)	Query Genome	Size (kb)
1	nr.01(non-redundant protein)	2.99	Nucleotide sequence	16
2	nr.01(non-redundant protein)	2.99	Nucleotide sequence	32
3	nr.01(non-redundant protein)	2.99	Nucleotide sequence	64
4	nr.01(non-redundant protein)	2.99	Nucleotide sequence	128

Table 2. Experiment data used to compare BLAST-performance BSPMR's to that of BLAST-Hadoop with varied size of database genom

No	Database genome	Size (GB)	Query genome	Size (kb)
1	nr.40 (non-redundant protein)	0.078	Nucleotide sequence	128
2	nr.04 (non-redundant protein)	0.299	Nucleotide sequence	128
3	nr.05 (non-redundant protein)	1.075	Nucleotide sequence	128
4	nr.01 (non-redundant protein)	2.99	Nucleotide sequence	128



Figure 4. Sequence alignment execution time

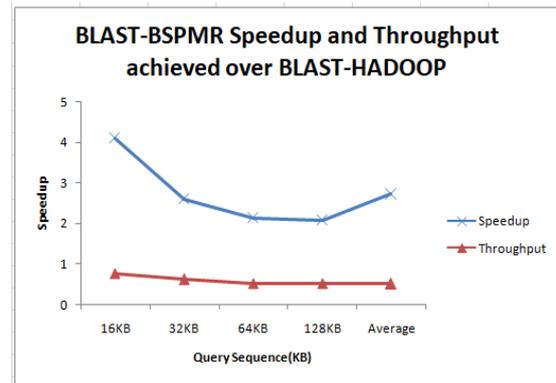


Figure 5. Speedup and throughput

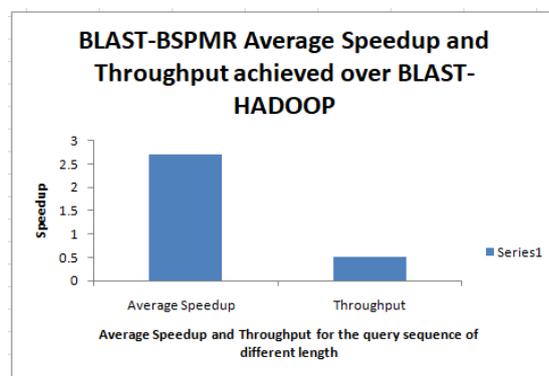


Figure 6. Average speedup and throughput

Table 3. Speedup and throughput for varied query genome

Seg. File Size	Speedup	Throughput
16 KB	4.1	76%
32 KB	2.6	62%
64 KB	2.14	53%
128 KB	2.07	53%
<b>Average</b>	<b>2.72</b>	<b>51%</b>
0.078 GB	7.067	85.0%
0.299 GB	3.35	70.0%
1.075 GB	2.16	53.8%
2.99 GB	2.07	51.8%
<b>Average</b>	<b>3.66</b>	<b>65.15%</b>

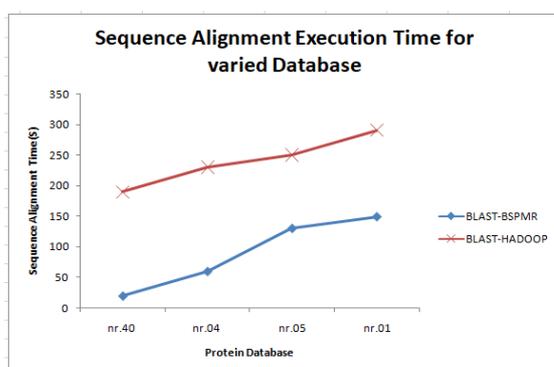


Figure 7. Sequence alignment execution time for varied non-redundant protein database

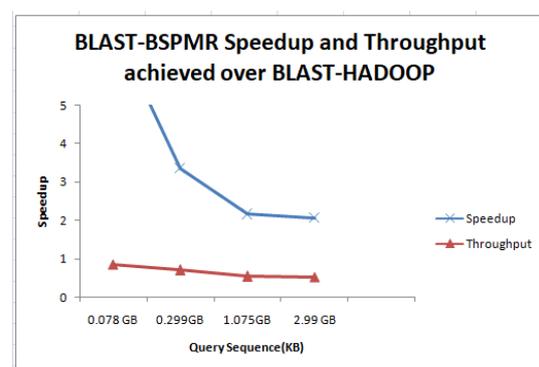


Figure 8. Speedup and throughput for varied non-redundant protein database

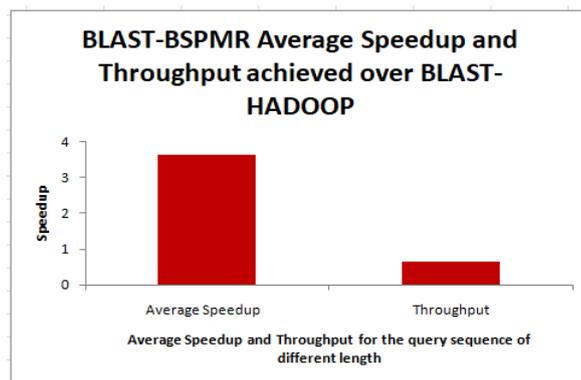


Figure 9. Average speedup and throughput non-redundant protein database

#### 4. CONCLUSION

Aligning genomic sequences is a straightforward technique for managing and analysing bioinformatics data. The author describes the proper methods for aligning sequences using the BLAST algorithm, which is the most widely used tool for aligning local sequences. Currently, the BLAST algorithm given by NCBI (stand-alone) is unable to handle dynamic biological data in the terabyte range. Cloud platforms are used to address issues such as data storage and data-intensive computation. Biosequencing analysis of genetic data is a critical application. In this study, the author evaluates many existing schedulers. The existing scheduler has issues which are expensive with aligning genomic data sequences. Existing bioinformatics sequence aligners that make use of or embrace Hadoop MapReduce suffer from the concerns discussed in this study. In this paper, the proposed BLAST-BSPMR algorithm is employed to align sequences. For biosequence alignment, the BLASTx algorithm is used, and a parallel MapReduce execution approach based on Azure cloud is used in the BLAST-BSPMR cloud platform. The Map and Reduce framework are executed in parallel to take use of the cloud computing platform's virtual machine-based design. Additionally, the research compares the proposed BLAST-BSPMR technique to previously published system sequence alignments. Experiments are carried out with a variety of non-redundant proteins and nucleotide query sequence files of various sizes. Experiments are presented to demonstrate the efficiency of the BLASTx algorithm. Through an experimental study, a comparison with Hadoop-BLAST for sequence alignment is presented. When comparing the BLAST-BSPMR results to the Hadoop-BLAST results, the BLAST-BSPMR results show a significant improvement. The authors plan to test their theory on a variety of redundant databases in the future such as SwissProt protein, and REFSEQ and also run varied application that are available in NCBI such as BLASTn, and BLASTp on our proposed BSPMR Scheduler to further analyse the robustness and efficacy of our scheduler.

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