Cloud Technologies for Microsoft Computational Biology Tools

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ABSTRACT

Executing large number of self-regulating tasks or tasks that execute minimal inter-task communication in analogous is a common requirement in many domains. In this paper, we present our knowledge in applying two new Microsoft technologies Dryad and Azure to three bioinformatics applications. We also contrast with traditional MPI and Apache Hadoop MapReduce completion in one example. The applications are an EST (Expressed Sequence Tag) series assembly program, PhyloD statistical package to recognize HLA-associated viral evolution, and a pairwise Alu gene alignment application. We give detailed presentation discussion on a 768 core Windows HPC Server cluster and an Azure cloud. All the applications start with a "doubly data parallel step" connecting independent data chosen from two parallel (EST, Alu) or two different databases (PhyloD). There are different structures for final stages in each application.

Categories and Subject Descriptors

C.4 PERFORMANCE OF SYSTEMS; D.1.3 Concurrent Programming; E.5 FILES; J.3 LIFE AND MEDICAL SCIENCES

General Terms
Algorithms, Performance.

Keywords

Cloud, bioinformatics, Multicore, Dryad, Hadoop, MPI

1. INTRODUCTION

There is increasing interest in approaches to data analysis in scientific computing as essentially every field is considering an exponential increase in the size of the data overflow.

The data sizes involve that parallelism is important to process the information in a well-timed fashion. This is generating acceptable interest in new runtimes and programming models that unlike conventional parallel models such as MPI, directly address the data-specific issues. Experience has shown that at least the initial (and often most time consuming) parts of data analysis are naturally data parallel and the processing can be made independent with possibly some collective (reduction) operation. This structure has forced the important MapReduce paradigm and many follow-on extensions. Here we observe four technologies (Dryad [1], Azure [2] Hadoop [8] and MPI) on three different bioinformatics application (PhyloD [3], EST [4, 5] and Alu clustering [6, 7]). Dryad is an implementation of extended MapReduce from Microsoft and Azure is Microsoft's cloud technology. All our computations were performed on Windows Servers with the Dryad and MPI work using a 768 core cluster Tempest consisting of 32 nodes each of 24-cores. Each node has 48GB of memory and four Intel six core Xenon E7450 2.4 Ghz chips. All the applications are (as is often so in Biology) "doubly data parallel" (or "all pairs" [24]) as the basic computational unit is replicated over all pairs of data items from the same (EST, Alu) or different sources (PhyloD). In the EST example, each parallel task executes the CAP3 program on an input data file separately of others and there is no "reduction" or "aggregation" necessary at the end of the computation, where as in the Alu case, a global aggregation is essential at the end of the independent computations to create the resulting distinction matrix that is fed into conventional high performance MPI. PhyloD has a alike initial stage which is followed by an aggregation step. In this paper we estimate the different technologies presentation they provide similar performance in spite of the dissimilar programming models. In section 2, we explain the three applications EST, PhyloD and Alu sequencing while the technologies are discussed in section 3 (without details of the well known Hadoop system). Section 4 presents some performance results. Conclusions are given in section 6 after a discussion of associated work in section 5.

2. APPLICATIONS

2.1 EST and its software CAP3

An EST (Expressed Sequence Tag) corresponds to envoy RNAs (mRNAs) transcribed from the genes residing on chromosomes. Each individual EST sequence represents a portion of mRNA, and the EST assembly aims to renovate full-length mRNA sequences for every expressed gene. Because ESTs match to the gene regions of a genome, EST sequencing has grow to be a standard practice for gene detection, particularly for the genomes of many organisms that may be too complex for whole-genome sequencing. EST is addressed by the software CAP3 which is a DNA sequence assembly program developed by Huang and Madan [4]. that performs a number of major assembly steps: these steps take in computation of overlaps, building of contigs, creation of multiple sequence alignments, and making of consensus sequences to a given set of gene sequences. The program reads a group of gene sequences from an input file (FASTA file format) and writes its output to several output files, as well as the standard output.

We have implemented a similar version of CAP3 using Hadoop , CGL-MapReduce, and Dryad but we merely report on a new Dryad study here.

2.2 PhyloD

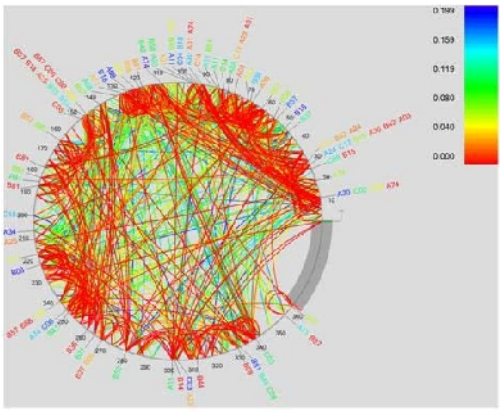

Figure 1. Pictorial representation of PhyloD output.

PhyloD is a statistical package to recognize HLA-associated viral development from the specified sample data. It is obtainable today as a web application and as downloadable source code . consecutively PhyloD jobs is a compute intensive process. PhyloD- Cloud is an attempt to influence Windows Azure as a computing platform and make a scalable web-based application to development PhyloD jobs. Users should be intelligent to submit sensibly large jobs with this web application with least manual association.

The package is used to get associations between HLA alleles and HIV codons and between codons themselves. The distinctiveness of PhyloD comes from the detail that it takes into reflection the phylogenic development of the codons for producing its results. The package takes as input the phylogenic tree in sequence of the codons, the information about being there or absence of HLA alleles and the information about presence or absence of HIV codons. It fits its inputs to a generative model and computes a 'p-value', a measure of the association between HLA alleles and the HIV codons. For a set of such computed p-values, the package may also compute a 'q-value' per p-value which is an indicative measure of the significance of the result. Figure 1 presents the output of one such run. Arcs indicate association between codons, colors indicate q-values of the most significant association between the two attributes.

At a high level, a run of PhyloD does the following: (i) calculate a cross product of input files to make all allele-codon pairs, (ii) For each allele-codon pair, calculate p value, and (iii) with the p values from the previous step, compute the q value for each allele- codon pair. The calculation of p value for an allele-codon pair can be completed separately of other p value computations and each such calculation can use the same input files. This gives PhyloD its "data-parallel" characteristics namely, (i) ability to separation input data into smaller logical parts and (ii) workers performing similar calculation on data partitions without to a large extent inter-process communication.

3. TECHNOLOGIES EXPLORED

3.1 Dryad

Dryad is a distributed execution engine for coarse grain data parallel applications. It combines the MapReduce programming style with dataflow graphs to resolve the computation tasks. Dryad considers computation tasks as directed acyclic graph (DAG) where the vertices symbolize computation tasks and with the edges performing as communication channels in excess of which the data flow from one vertex to another. The data is stored in (or partitioned to) local disks via the Windows common directories and meta-data files and Dryad schedules the carrying out of vertices depending on the data locality. Dryad also supplies the yield of vertices in local disks, and the other vertices which depend on these results, access them via the common directories. This enables Dryad to re-execute unsuccessful vertices, a step which improves the fault tolerance in the programming model.

3.2 Azure

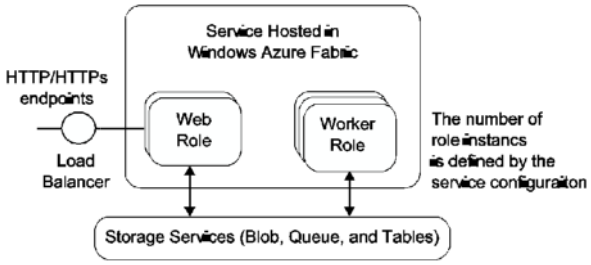

Figure 2. Architecture of a typical Azure application

Windows Azure platform is an internet-scale cloud computing and services platform hosted in Microsoft data centers. Dissimilar the distinctive cloud environments where the users are accessible with virtualized hardware mechanism such as load balancers, virtual servers (E.g. Amazon EC2) and cloud storage services such as Amazon S3 etc., Azure offers a set of discrete scalable components known as "roles" next to with a set of storage and communication components. The architecture of a distinctive Azure application is shown in figure 2. The web role and the worker role correspond to the giving out components of an Azure application. The web role is a web application easy to get to via HTTP or HTTPs endpoints and is hosted in an environment that supports subset of ASP.NET and Windows Communication Foundation (WCF) technologies. Worker position is the main dealing out individual in the Azure platform which can be used to execute functions written in managed code, scripts, or individual executables on data products. Both web position instances and worker role instances can right of entry the storage services.

Azure Queues are earliest in, First Out (not guaranteed) determined communication channels which can be used to build up composite communication patterns between a set of corporation worker roles and web roles. A set of tasks/jobs can be controlled as a set of messages in an Azure queue and a set of workers can be deployed to eliminate a message (a task/job) from the queue

and perform it. Azure provides three types of storage services Blob, Queue, and Table. The blob represents a perseverance storage services comprising of set of blocks. The user can store data (or partitioned data) in blobs and contact them from web and worker role instances. Azure Tables provides planned storage for maintaining service state. The Azure blobs and Queues have secure similarities to the Amazon Elastic Block storage and Simple Queue Service.

3.3 Old Fashioned Parallel Computing

One can execute many of the functionalities of Dryad or Hadoop using classic parallel computing together with threading and MPI. MPI in particular supports "Reduce" in MapReduce parlance through its collective operations. The "Map" operation in MPI, is immediately the simultaneous execution of MPI processes in between communication and synchronization operations. There are several significant differences such as MPI individual oriented towards memory to memory operations whereas Hadoop and Dryad are file oriented. This difference makes these new technologies far more robust and flexible. On the other the file orientation implies that there is much greater overhead in the new technologies. This is a not a problem for initial stages of data analysis where file I/O is separated by a long processing phase. However as discussed in [6], this feature means that one cannot execute efficiently on MapReduce, traditional MPI programs that iteratively switch between "map" and "communication" activities. We have shown that an extension CGL-MapReduce can support both classic MPI and MapReduce operations and we will comment further in section 4.3 on this. CGL-MapReduce has a larger overhead than good MPI implementations but this overhead does decrease to zero as one runs larger and larger problems.

Simple thread-based parallelism can also support "almost pleasingly parallel" applications but we showed that under Windows, threading was significantly slower than MPI for Alu sequencing. This we traced down to excessive context switching in the threaded case. Thus in this paper we only look at MPI running 24 processes per node on the Tempest cluster. Note that when we look at more traditional MPI applications with substantial communication between processes, one will reach different conclusions as use of hybrid threaded on node-MPI between node strategies, does reduce overhead [6].

4. PERFORMANCE ANALYSIS

4.1 EST and CAP3

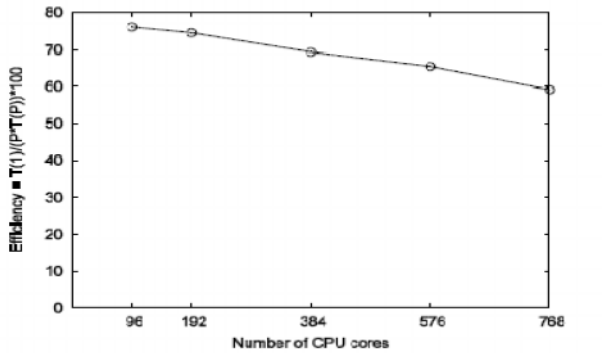

Figure 3. Efficiency vs. number of CPU cores of DryadLINQ implementation of the CAP3 application

We implemented a DryadLINQ application that performs CAP3 sequence assembly program in parallel. As discussed in section 2.1 CAP3 is a standalone executable that processes a single file containing DNA sequences. To execute a parallel application for CAP3 using DryadLINQ we accept the subsequent approach: (i) the input files are partitioned in the middle of the nodes of the cluster so that each node of the cluster stores approximately the identical number of input files; (ii) a "data-partition" (A text file for this application) is formed in each node containing the names of the input files accessible in that node; (iii) a DryadLINQ "partitioned-file" (a meta-data file implicit by DryadLINQ) is fashioned to point to the individual data-partitions to be originate in the nodes of the cluster.

Then we used the "Select" operation available in DryadLINQ to apply a function (developed by us) on each of these input sequence files. The function calls the CAP3 executable passing the input file name and other necessary program parameters as command line arguments. The function also captures the standard output of the CAP3 program and saves it to a file. Then it moves all the output files generated by CAP3 to a predefined location.

This application resembles a common parallelization obligation, where an executable, a script, or a function in a unique framework such as Matlab or R, needs to be useful on a group of data items. We can develop DryadLINQ applications similar to the above for all these use cases.
We measured the efficiency of the DryadLINQ implementation of the CAP3 application using a data set of 2304 input files by varying the number of nodes used for processing. The effect of this benchmark is exposed in figure 3. The set of input files we used for the over benchmark restricted different number of gene sequences in each, and hence it did not represent a consistent workload across the simultaneous vertices of the DryadLINQ application, because the time the CAP3 takes to development an input file varies depending on the number of sequences obtainable in the input file. The above individuality of the data produces lower efficiencies at advanced number of CPU cores as more CPU cores become idle towards the end of the calculation waiting for vertices that takes longer time to absolute. An architecture that supports scheduling of independent tasks/jobs among set of workers/processes depending on the priorities

of the tasks/jobs would perform an optimal scheduling of such a workload by scheduling tasks/jobs that takes longest to complete first. However, DryadLINQ and other MapReduce architectures do not hold up this performance, and in these architectures the scheduling of maps/reducers (in MapReduce) or vertices (in Dryad) is handled based on the ease of use of data and the calculation power and not by the priorities.

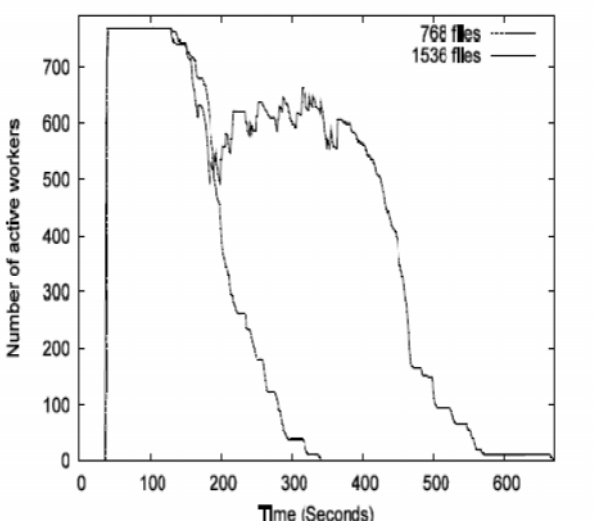

Figure 4. Number of dynamic tasks/CPU cores beside the running times of two runs of CAP3.

The primary graph in figure 4 equivalent to 768 files indicates that even though DryadLINQ starts all the 768 vertices at the same time they terminate at dissimilar times with long running tasks attractive approximately 40% of the overall time. The second graph (1536 files) shows that the higher than result has caused lower consumption of vertices when Dryad schedules 1536 vertices to 768 CPU cores. This is due to the way Dryad schedule tasks to compute nodes and we have discussed this behavior extensively in [10]. We would not expect the same behavior (for graph 2) in other MapReduce implementations such as Hadoop, however, still the non- uniformity of the processing time of parallel tasks and the simple scheduling adopted by the MapReduce runtimes may not produce optimal scheduling of tasks.

4.2 PhyloD

The parallel solution of PhyloD can be visualized as consisting of the following three different phases as shown in Figure 2 (left).

Initial – During this phase, the input files are collected from the user and copied to a shared storage available to all workers. Then a sufficient number of workers are instantiated, each with the information of the data partition it has to work on. To reduce the parallel overhead, a worker can process multiple allele-codon pairs. *ComputePartial* – Each worker processes its allotted partition and produces intermediate results. These results are again copied to a shared storage.

Summarize – During this phase, each of the intermediate results produced during the *ComputePartial* phase are aggregated and the final output is produced.

We developed an Azure application for the PhyloD application by utilizing Azure Web Role, Worker Role, Blob Container, Work Item Queue and Tracking tables described in sec. 3.2 generally and their use in PhyloD is shown in Figure 2 (Right). The web role is a simple ASP.NET application that allows clients to upload input files and provide other job parameters. A blob container is created per job which hosts the shared data between web and worker roles. The uploaded input files are copied to this container and an *Initial* work item is enqueued in the shared queue by the web role. Worker roles continuously poll the work item queue for new messages. A message encapsulates one of {*Initial*, *ComputePartial*, *Summarize*} work items. The evaluation of these work items is delegated to their respective processors. The processors return a Boolean result for the evaluation. The calling worker then removes the message from the queue or leaves it there based on the results of the evaluation.

While processing an *Initial* work item, a worker role first tries to locate the entry for this task in the JobSteps table. If the job step is not found then it means that the web role enqueued the work item and then encountered some error before creating the job step entry in the table storage. No further action is taken in this case and the job is marked 'Aborted'. If the job step entry is found and its status is 'Completed' we just remove this message from the queue. A 'Completed' status indicates that a worker has already processed this work item successfully but could not *delete* the message from the queue due to, for example, network errors or message timeout. After these checks are satisfied, the worker updates the status of parent job to 'In Progress'. It then enqueues multiple *ComputePartial* work items in the queue and also creates corresponding job. Each *ComputePartial* work item has the partition information. The worker then enqueues a *Summarize* work item and creates its corresponding job step. Finally, it updates the status of *Initial* job step to 'Completed' and removes the *Initial* work item from the queue. *ComputePartial* work items are processed by multiple worker roles simultaneously. Each worker processes its allotted partition of the input data and copies the intermediate results to the blob container. PhyloD engine works exclusively on files. So, a pre-processing task of copying the original input files to worker role's local storage is required for each *ComputePartial* work item. The worker follows similar checks for the status as in the *Initial* processing. Finally, the *Summarize* work item is processed. Intermediate results are aggregated to produce the final output which is again copied back to the blob container. The results can be downloaded via the web role. During the complete process, status information is updated in azure tables for tracking purposes.

We measured the running time of the PhyloD prototype by varying the number of worker roles used on Azure cloud, and calculated the efficiency in each worker assignment. As in CAP3 application describe in section 2.1, we also noticed in PhyloD lower efficiencies with higher number of workers, as shown in figure 6. In PhyloD the efficiency reduces to around 40% when we use 100 workers implying that more workers are idling waiting for few long running workers to finish. To verify the above observation we also measured the number of active worker role instances during the execution of the PhyloD application. Figure 7 shows that the less than 20 workers spend 30% of the time in processing long running PhyloD tasks which results lower efficiencies. Fixing this inefficiency in Azure is fairly straight forward as the tasks/jobs are dispatched via a queue which is accessed by the worker role instances to obtain a

task/job for processing. Unlike in Dryad and other MapReduce runtimes which require runtime level support to handle priorities in maps/reduces/ and vertices, in Azure the user can enqueue tasks based on their expected running times, so that tasks that takes longest will be processed at the beginning. We are currently developing a DryadLINQ application for the PhyloD data analysis where the set of tasks are directly assigned to a collection of vertices where each of them process some number of tasks and give intermediate results. Unlike in Azure

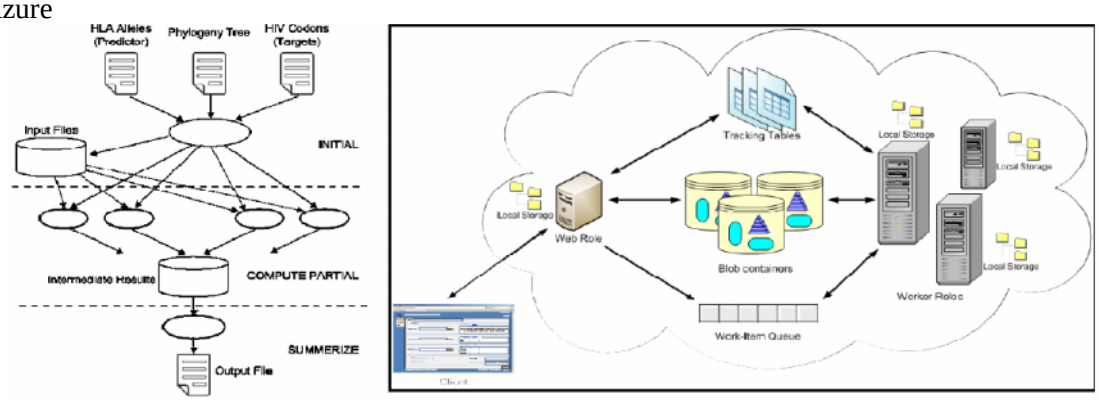

Figure 5. (Left) Three phases of the parallel solution (Right) The mapping of the parallel solution to a Azure application.

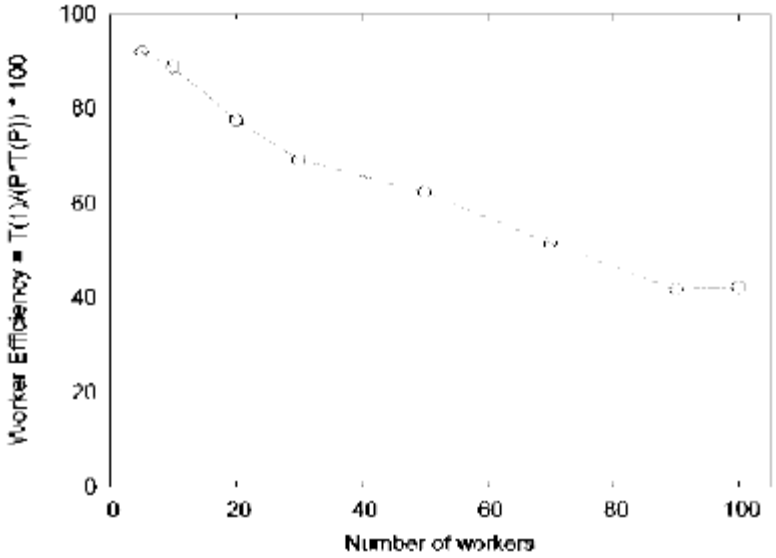

Figure 7. Number of dynamic Azure workers for the period of a run of PhyloD application.

implementation, in Dryad case, the intermediate results can directly be transferred to a vertex for aggregation to produce the final output.

4.3 Alu Sequence Classifications

4.3.1 Complete Problem with MPI and MapReduce

This application uses two highly parallel traditional MPI applications MDS (Multi-Dimensional Scaling) and Pairwise (PW) Clustering algorithms described in Fox, Bae et al. [6]. The latter identifies sequence families as relatively isolated as seen for example in figure8. MDS allows visualization by mapping the high dimension sequence data to three dimensions for visualization.

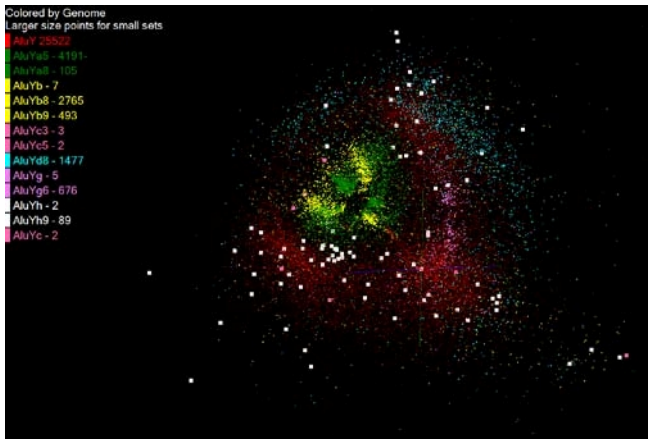

Figure 8. Alu: Display of Alu families from MDS calculation from 35339 sequences using SW-G distances. The younger families AluYa, AluYb show tight clusters

MDS has a very formulation as it finds the best set of 3D vectors $\underline{x}(i)$ such that a weighted least squares sum of the difference between the sequence dissimilarity D(i,j) and the Euclidean distance $|\underline{x}(i) - \underline{x}(j)|$ is minimized. This has a computational complexity of $O(N^2)$ to find 3N unknowns for N sequences. It can be heuristically solved in severa ways including Expectation Maximization and use of traditional excellent χ^2 minimization methods. The latter are used here.

The PWClustering algorithm is an well-organized MPI parallelization of a robust EM (Expectation Maximization) method by means of annealing (deterministic not Monte Carlo) initially developed by Ken Rose, Fox [14, 15] and others [16]. This improves in excess of clustering methods like Kmeans which are responsive to false minima. The original clustering work was based in a vector space (like Kmeans) where a cluster is distinct by a vector as its middle. However in a main advance 10 years ago [16], it was exposed how one could use a vector free approach and function with just the distances D(i,j). This method is obviously most normal for problems like Alu sequences where at this time global sequence position (over all N sequences) is difficult but D(i,j) can be specifically calculated. PWClustering also has a time complexity of O(N2) and in perform we discover all three steps (Calculate D(i,j), MDS and PWClustering) take similar times (a few hours for 50,000 sequences) even though searching for a lot of clusters and refinement the MDS can increase their execution time extensively. We have presented performance results for MDS and PWClustering elsewhere [6, 17] and for large datasets the efficiencies are high (showing sometimes super linear speed up). For a node design reason, the

early distance calculation phase reported under has efficiencies of approximately 40-50% as the Smith Waterman computations are memory bandwidth inadequate. The more complex MDS and PWClustering algorithms show more computation per data access and high efficiency.

4.3.2 Structure of all pair distance processing

The Alu sequencing problem shows a fine known factor of 2 matter present in many $O(N^2)$ parallel algorithms such as those in straight simulations of astrophysical stems. We originally calculate in parallel the Distance D(i,j) connecting points (sequences) i and j. This is complete in parallel over all processor nodes selecting criteria I < j (or j > i for higher triangular case) to evade calculating both D(i,j) and the equal D(j,i). This can need considerable file relocate as it is not likely that nodes requiring D(i,j) in a presently step will discover that it was intended on nodes where it is desirable.

The MDS and PWClustering algorithms described in section 4.3.1, need a meticulous parallel disintegration where each of N processes (MPI processes, threads) has 1/N of sequences and for this subset {i} of sequences stores in memory D({i},j) for all sequences j and the subset {i} of sequences for which this node is accountable. This implies that we require D(i,j) and D(j,i) (which are equal) stored in dissimilar processors/disks. This is a fine known group operation in MPI called also gather or scatter but we did not utilize this in current work. Some what we intended our first calculation of D(i,j) so that professionally we only calculated the autonomous set but the data was stored so that the presently MPI jobs could proficiently right of entry the data needed. We chose the simplest approach where the initial phase formed a single file investment the full set of D(i,j) stored by rows – all j for each consecutive value of i. We commented in preface that the initial phase is “doubly data parallel” over i and j whereas the MPI algorithms have the simple data parallelism over just a single sequence index i; there is further the typical iterative communication-compute phases in both MDS and PWClustering that implies one needs extensions of MapReduce (such as CGL-MapReduce) if you wish to execute the whole problem in a single programming paradigm. In both MDS and PWClustering, the only MPI primitives needed are MPI Broadcast, AllReduce, and Barrier so it will be quite elegantly implemented in CGL-MapReduce.

4.3.3 Smith Waterman Dissimilarities

We recognized samples of the human and Chimpanzee Alu gene sequences using Repeatmasker [18] with Repbase Update [19]. We have been slowly growing the size of our projects with the existing major samples having 35339 and 50000 sequences and these need a humble cluster such as Tempest (768 cores) for dispensation in a sensible time (a few hours as shown in section 4.3.6). Note from the conversation in section 4.3.2, we are aiming at underneath problems with a million sequences -- fairly sensible today on TeraGrid and alike facilities known basic study steps scale like O(N2). We used open source version NAligner [20] of the Smith Waterman – Gotoh algorithm SW-G [21, 22] modified to ensure low start up effects by each thread/processing large numbers (above a few hundred) at a time. Memory bandwidth required was condensed by storing data items in as few bytes as probable. In the following two sections, we just discuss the initial phase of calculating distances D(i,j) for each pair of sequences so we can efficiently use either MapReduce and MPI.

4.3.4 Dryad Implementation

We developed a DryadLINQ application to execute the calculation of pair wise SW-G distances for a known set of genes by adopting a common grain task disintegration approach which requires least amount inter-process communicational necessities to improve the higher communication and synchronization costs of the parallel runtime. To make clear our algorithm, let's think an example where N gene sequences produces a pair wise distance matrix of size NxN. We decay the calculation task b allowing for the resultant matrix and groups the overall calculation into a block matrix of size DxD where D is a multiple (>2) of the available computation nodes. Due to the regularity of the distances D(i,j) and D(j,i) we merely calculate the distances in the blocks of the higher triangle of the block matrix as shown in figure 9 (left). Diagonal blocks are specially handled and calculated as full sub blocks. As number of diagonal blocks D and total number D(D+1)/2, there is no significant compute overhead added. The blocks in the higher triangle are partitioned (assigned) to the accessible compute nodes and an "Apply" operation is used to perform a function to compute (N/D)x(N/D) distances in every block, where d is defined as N/D. After computing the distances in every block, the function calculates the transpose matrix of the outcome matrix which corresponds to a block in the lower triangle, and writes together these matrices into two output files in the local file system. The names of these files and their block numbers are communicated back to the main program. The main program sort the files based on their block number s and perform another "Apply" operation to join the files equivalent to a row of blocks in a single big row block as shown in the figure 9 (right).

4.3.5 MPI Implementation of Distance Calculation

The MPI edition of SW-G calculates pair wise distances using a set of each single or multi-threaded processes. For N gene sequences, we require to calculate half of the values (in the lower triangular matrix), which is a total of M = N x (N-1) /2 distances. At a elevated level, calculation tasks are consistently divided amongst P processes and perform in parallel. Explicitly, calculation workload per process is M/P. At a low level, each calculation task can be additional divided into subgroups and sprint in T simultaneous threads. Our implementation is considered for flexible utilize of shared memory multicore system and distributed memory clusters (tight to medium tight coupled communication technologies such threadingand MPI). We offer options for any combinations of thread vs. process vs. node but in earlier papers [6, 17], we have shown as discussed in section 3.3 that threading is much slower than MPI for this class of problem. We explored two different algorithms

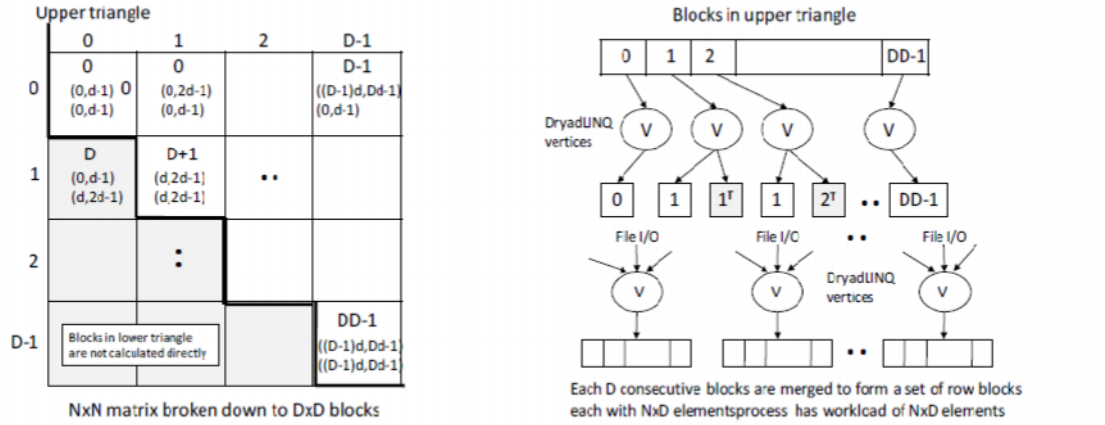

Figure 9. Task disintegration (left) and the DryadLINQ vertex hierarchy (right) of the DryadLINQ implementation of SW-G pair wise distance computation application.

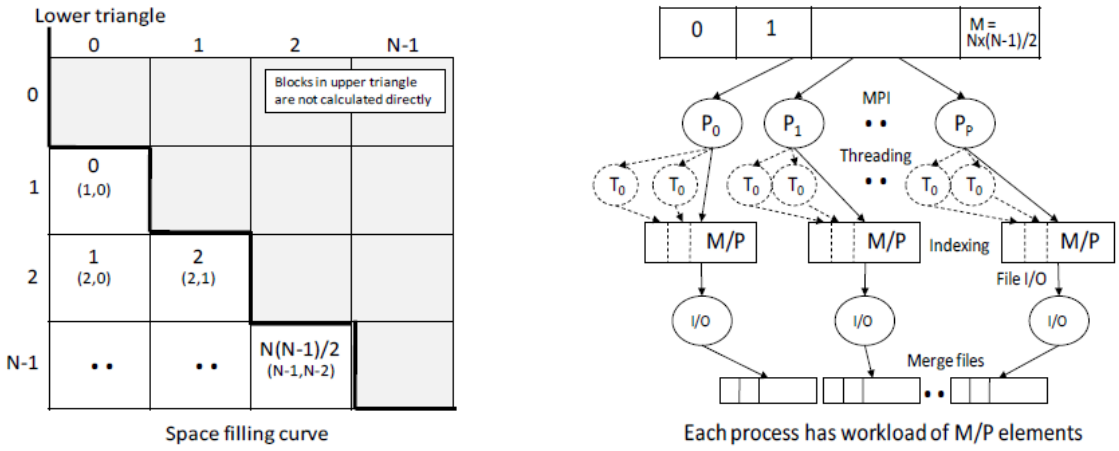

Figure 10. Space Filling MPI Algorithm: Task decomposition (left) and SW-G implementation calculation (right).

The “Space Filling” MPI algorithm is shown in figure 10, where the data decomposition strategy runs a "space filling curve through lower triangular matrix" to produce equal numbers of pairs for each parallel unit such as process or thread. It is essential to chart indexes in every pairs group back to equivalent matrix coordinates (i, j) for constructing full matrix presently on. We implemented a extraordinary function "PairEnumertator" as the convertor. We tried to bound runtime memory convention for presentation optimization. This is completed by writing a triple of i, j, and distance value of pair wise arrangement to a stream writer and the system flashes accumulated consequences to a local file occasionally. As the final stage, individual files are merged to form a full distance matrix. Next we describe the “Block Scattered” MPI algorithm shown in figure 11. Points are divided into blocks such that each processor is responsible for all blocks in a simple decomposition illustrated in the figure 11 (Left). This also illustrates the initial computation, where to respect symmetry, we calculate half the D (α, β) using the following criterion:

If β >= α, *we only calculate D(*α,β*) if* α+β *is even while in the lower triangle,* β < α, *we only calculate D(*α,β*) if* α+β *is odd* termed "Space Filling" and "Block Scattered" below. In each case, we must calculate the independent distances and then build the full matrix exploiting symmetry of D(i,j).

This approach can be applied to points or blocks. In our implementation, we applied to blocks of points -- of size (N/P)x(N/P) where we use P MPI processes. Note we get better load balancing than the "Space Filling" algorithm as each processor samples all values of β. This computation step must be followed by a communication step illustrated in Figure 11 (Right) which gives full strips in each process. The latter can be straightforwardly written out as properly ordered file(s).

	Alu data # sequences			Cap3 data	
	Original		Replicated (subset of original 50k)	Medium size Files kb	
	50k	35k	10k, 20k,30k,40k,50k	Set A	Set B
Standard Deviation	26.91	30.99	26.49	129.06	189.29
Min	150	150	151	213	213
Max	479	462	467	869	869
Average	296.09	294.89	296.31	438.59	455.59
Data points	50000	35399	10000	2304	1152

Table 1: Mean and Standard Deviation of Alu & CAP3 data

4.3.6 Alu SW-G Distance Calculation Performance

We present a summary of results for both Dryad and MPI computations of the Alu distance matrix in figures 12 and 13. We used several data sets and there is inhomogeneity in sequence size throughout these sets quantified in table 1. Two of 35,339 and

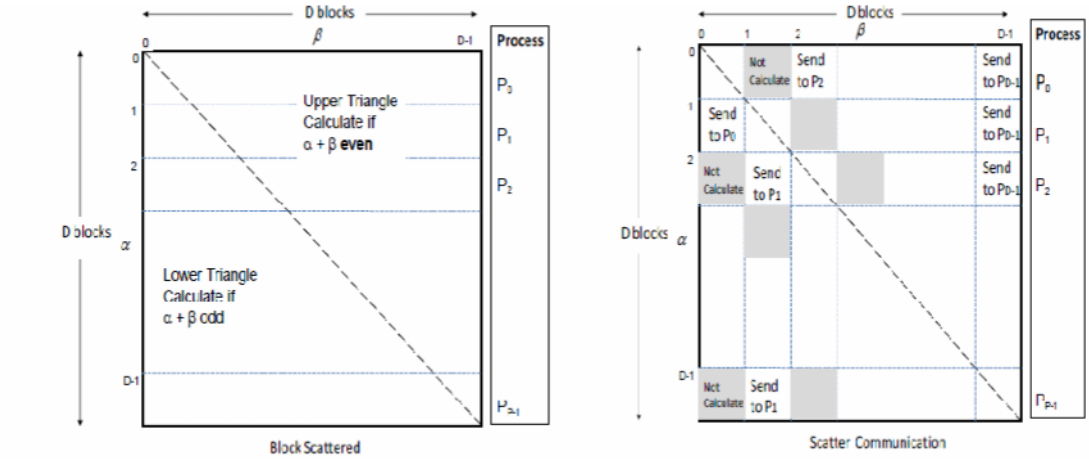

Figure 11. Block Scattered MPI Algorithm: Decomposition (Left) and Scattered Communication (Right) to construct full matrix.

Figure 12. Performance of Dryad implementation of SW-G (note that the Y-axis has a logarithmic scale)

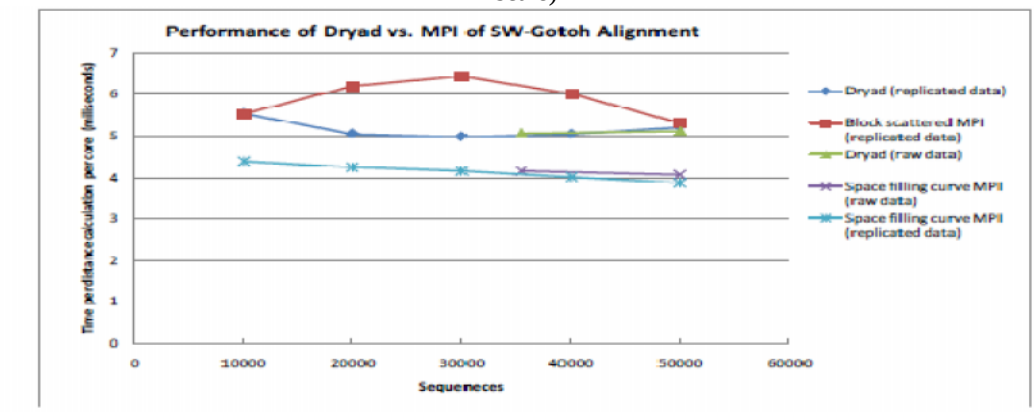

Figure 13. Comparison of Dryad and MPI on SW-G alignment on replicated and original raw data samples

50,000 sequences were comprised of distinct sequences while we also prepared datasets allowing us to test scaling as a function of dataset size by taking 10,000 sequences and replicating them 2-5 times to produce 10K, 20K, 30K, 40K, 50K "homogeneous" or replicated datasets.

In figure 12, we present Dryad results for the replicated dataset showing the dominant compute time compared to the small partition and merge phases. Further for the Block Scattered MPI approach, the final "scatter" communication takes a negligible time. Figure 13 compares the performance of Dryad and the two MPI approaches on the homogeneous (10K – 50K) and heterogeneous (35K, 50K) datasets. We present the results as the time in milliseconds per distance pair per core. This is measured total time of figure 12 multiplied by number of cores and divided by square of dataset size i.e. it is time a single core would take to calculate a single distance. Then "perfect scaling in dataset size or number of nodes" should imply a constant value for this quantity. We find that for Dryad and MPI, the replicated dataset time is roughly constant as a function of sequence number and the original 35339 and 50,000 sequence samples are just a little slower than the replicated case. Note from table 1, that there is little variation in measure of inhomogeneity between replicated and raw data. A surprising feature of our results is that the Space Filling MPI algorithm is faster than the Block Scattered approach. Dryad lies in between

the two MPI implementations and is about 20% slower on the replicated and heterogeneous dataset compared to Space-Filling MPI. We are currently investigating this but given the complex final data structure, we see that it is impressive that the still preliminary Dryad implementation does very well.

In figure 14, we show that Dryad scales well with number of nodes in that time per distance pair per core is roughly constant on the 10K replicated SW-G data and consistent with Dryad replicated data points in figure 13. In table 1, we showed that SW-G is more homogeneous than CAP3 in that standard deviation/mean is lower. However we also got reasonable scaling in figure 3 for CAP3 which corresponds to data set A of table 1 while preliminary results for the more heterogeneous "Set B", also shows good scaling from 192 to 576 cores. The dependence on data homogeneity is very important and needs better study and perhaps dynamic scheduling or more sophisticated scattering of data between processes to achieve statistical load balance. We study the effect of inhomogeneous gene sequence lengths for SW-G pairwise distance calculation applications. These results also present comparisons of Hadoop and Dryad on identical hardware rebooted with Linux and Windows respectively. The data sets used were arbitrarily generated with a known indicate sequence length (400) with changeable standard deviations subsequent a ordinary distribution of the sequence lengths.

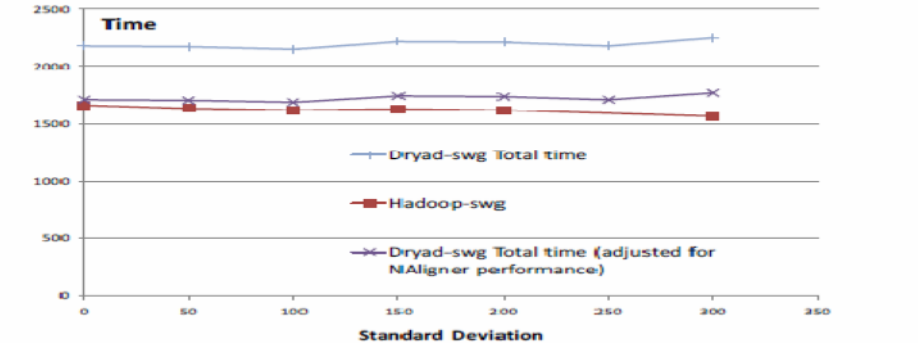

Figure 14. Performance of Dryad for SW-G Alignment on 10K data sample as a function of number of cores

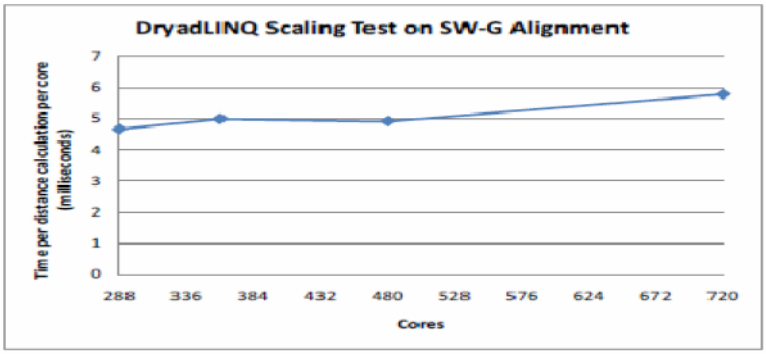

Figure 15. Performance of Dryad vs. Hadoop for SW-G for inhomogeneous data as a function of standard deviation with mean sequence length of 400

Each data set contained a set of 10000 sequences and a 100 million pairwise distance calculations

to perform. Sequences of changeable lengths are arbitrarily distributed across the data set. The Dryad-adjusted consequences represent the raw Dryad results familiar for the routine difference of the NAligner (C#) and JAligner (Java) base Smith-Waterman arrangement programs. As we observe from the figure 15, together the Dryad implementation as well as the Hadoop completion performed adequately, without presentation significant act degradations for high standard variation. In detail the Hadoop implementation showed small improvements in the execution times. The suitable performance can be credited to the fact that the sequences with changeable lengths are arbitrarily distributed across the data set, generous a normal load balancing to the succession blocks. The Hadoop implementations' trivial performance development can be recognized to the universal pipeline arrangement of map tasks that Hadoop performs. In Hadoop, the administrator can identify the map task capacity of a exacting worker node and then Hadoop global scheduler schedules the map tasks straight on to those placeholders when person tasks finish in a great deal better granularity than in Dryad. This allows the Hadoop implementation to carry out normal global level load balancing.

5. RELATED WORK

There have been several papers discussing data analysis using a variety of cloud and more traditional cluster/Grid technologies with the Chicago paper [23] influential in posing the broad importance of this type of problem. The Notre Dame all pairs system [24] clearly identified the "doubly data parallel" structure seen in all of our applications. We discuss in the Alu case the linking of an initial doubly data parallel to more traditional "singly data parallel" MPI applications. BLAST is a well known doubly data parallel problem and has been discussed in several papers [25, 26]. The Swarm project [5] successfully uses traditional distributed clustering scheduling to address the EST and CAP3 problem. Note approaches like Condor have significant startup time dominating performance. For basic operations [27], we find Hadoop and Dryad get similar performance on bioinformatics, particle physics and the well known kernels. Wilde [28] has emphasized the value of scripting to control these (task parallel) problems and here DryadLINQ offers some capabilities that we exploited. We note that most previous work has used Linux based systems and technologies. Our work shows that Windows HPC server based systems can also be very effective.

6. CONCLUSIONS

We have studied three data analysis problems with four different technologies. The applications each start with a "doubly data- parallel" (all pairs) phase that can be implemented in MapReduce, MPI or using cloud resources on demand. The flexibility of clouds and MapReduce suggest they will become the preferred approaches. We showed how one can support an application (Alu) requiring a detailed output structure to allow follow-on iterative MPI computations. The applications differed in the heterogeneity of the initial data sets but in each case good performance is observed with the new cloud technologies competitive with MPI performance. The easy structure of the data/compute flow and the smallest amount inter-task communicational necessities of these "pleasingly parallel" applications enabled them to be implemented by means of a extensive variety of technologies. The sustain for managing big data sets, the perception of affecting computation to data, and the improved quality of services provided by the cloud technologies, make simpler the implementation of several problems in excess of traditional

systems. We discover that dissimilar programming constructs accessible in cloud technologies such as autonomous “maps” in MapReduce, “homomorphic Apply” in Dryad, and the “worker roles” in Azure are all appropriate for implementing applications of the type we inspect. In the Alu case, we demonstrate that Dryad and Hadoop can be planned to arrange data for make use of in presently parallel MPI/threaded applications used for additional investigation. Our Dryad and Azure work was all performed on Windows machines and achieved very large speed ups (limited by memory bandwidth on 24 core nodes). Similar conclusions would be seen on Linux machines as long as they can support the DryadLINQ and Azure functionalities used. The current results suggest several follow up measurements including the overhead of clouds on our Hadoop and Dryad implementations as well as further comparisons of them.

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REFERENCES

[1] M. Isard, M. Budiu, Y. Yu, A. Birrell, D. Fetterly, “Dryad:Distributed data-parallel programs from sequential building blocks,” European Conference on Computer Systems, March 2007.
[2] Microsoft Windows Azure, http://www.microsoft.com/azure/windowsazure.mspx
[3] C. Kadie, PhyloD. Microsoft Computational Biology Tools x?title=Phy loD
[4] X. Huang, A. Madan, “CAP3: A DNA Sequence Assembly Program,” Genome Research, vol. 9, no. 9, pp. 868-877, 1999.
[5] S. L. Pallickara, M. Pierce, Q. Dong, and C. Kong, “Enabling Large Scale Scientific Computations for Expressed Sequence Tag Sequencing over Grid and Cloud Computing Clusters”, PPAM 2009 EIGHTH INTERNATIONAL ONFERENCE ON PARALLEL PROCESSING AND APPLIED MATHEMATICS Wroclaw, Poland, September 13-16, 2009
[6] G. Fox, S.H. Bae, J. Ekanayake, X. Qiu, H. Yuan Parallel Data Mining from Multicore to Cloudy Grids Proceedings of HPC 2008 High Performance Computing and Grids workshop Cetraro Italy July 3 2008 WriteupJan09_v12.pdf
[7] M.A. Batzer, P.L. Deininger, 2002. "Alu Repeats And Human Genomic Diversity." Nature Reviews Genetics 3, no. 5: 370-379. 2002
[8] Apache Hadoop, http://hadoop.apache.org/core/
[9] Y.Yu, M. Isard, D. Fetterly, M. Budiu, Ú. Erlingsson, P. Gunda, J. Currey, “DryadLINQ: A System for General Purpose Distributed Data-Parallel Computing Using a High-Level Language,” Symposium on Operating System Design and Implementation (OSDI), CA, December 8-10, 2008.
[10] J. Ekanayake, A. S. Balkir, T. Gunarathne, G. Fox, C. Poulain, N. Araujo, R. Barga. "DryadLINQ for Scientific Analyses", Technical report, Submitted to eScience 2009.
[11] Source Code. Microsoft Computational Biology Tools. http://mscompbio.codeplex.com/SourceControl/ListDownl oadableCommits.aspx
[12] J. Ekanayake, S. Pallickara, “MapReduce for Data Intensive Scientific Analysis,” Fourth IEEE International Conference on eScience, 2008, pp.277-284.
[13] T. Bhattacharya, M. Daniels, D. Heckerman, B. Foley, N. Frahm, C. Kadie, J. Carlson, K. Yusim, B. McMahon, B Gaschen, S. Mallal, J. I. Mullins, D. C. Nickle, J. Herbeck, C. Rousseau, G. H. Lear. PhyloD . Microsoft Computational Biology Web Tools.

[14] K. Rose, "Deterministic Annealing for Clustering, Compression, Classification, Regression, and RelatedOptimization Problems", Proceedings of the IEEE, vol. 80, pp. 2210-2239, November 1998.
[15] Kenneth Rose, Eitan Gurewitz, and Geoffrey C. Fox "Statistical mechanics and phase transitions in clustering" Phys. Rev. Lett. 65, 945 - 948 (1990)
[16] T Hofmann, JM Buhmann "Pairwise data clustering by deterministic annealing", IEEE Transactions on Pattern Analysis and Machine Intelligence 19, pp1-13 1997
[17] Geoffrey Fox, Xiaohong Qiu, Scott Beason, Jong Youl Choi, Mina Rho, Haixu Tang, Neil Devadasan, Gilbert Liu "Biomedical Case Studies in Data Intensive Computing" Keynote talk at The 1st International Conference on Cloud Computing (CloudCom 2009) at Beijing Jiaotong University, China December 1-4, 2009
[18] A. F. A. Smit, R. Hubley, P. Green, 2004. Repeatmasker. http://www.repeatmasker.org
[19] J. Jurka, 2000. Repbase Update: a database and an electronic journal of repetitive elements. Trends Genet. 9:418-420 (2000).
[20] Source Code. Smith Waterman Software. http://jaligner.sourceforge.net/naligner/.
[21] O. Gotoh, An improved algorithm for matching biological sequences. Journal of Molecular Biology 162:705-708 1982.
[22] T.F. Smith, M.S.Waterman,. Identification of common molecular subsequences. Journal of Molecular Biology 147:195-197, 1981
[23] I. Raicu, I.T. Foster, Y. Zhao, Many-Task Computing for Grids and Supercomputers,: Workshop on Many-Task Computing on Grids and Supercomputers MTAGS 2008 17 Nov. 2008 IEEE pages 1-11 Computing on Campus Grids," IEEE Transactions on Parallel and Distributed Systems, 13 Mar. 2009, DOI 10.1109/TPDS.2009.49.
[24] C. Moretti, H. Bui, K. Hollingsworth, B. Rich, P. Flynn, D.Thain, "All-Pairs: An Abstraction for Data Intensive Computing on Campus Grids," IEEE Transactions on Parallel and Distributed Systems, 13 Mar. 2009, DOI 10.1109/TPDS.2009.49
[25] M. C. Schatz "CloudBurst: highly sensitive read mapping with MapReduce", Bioinformatics 2009 25(11):1363-136 doi:10.1093/bioinformatics/btp236
[26] K. Keahey, R. Figueiredo, J. Fortes, T. Freeman, M.Tsugawa, "Science clouds: Early experiences in Cloud computing scientific applications". In Cloud Computing and Applications 2008 (CCA08), 2008.
[27] J. Ekanayake, X. Qiu, T. Gunarathne, S. Beason, G. Fox "High Performance Parallel Computing with Clouds and Cloud Technologies", Technical Report August 25 2009 http://grids.ucs.indiana.edu/ptliupages/publications/CGLCloudReview.pdf
[28] M. Wilde, I. Raicu, A. Espinosa, Z. Zhang1, B. Clifford, M. Hategan, S. Kenny, K. Iskra, P. Beckman, I. Foster, "Extreme-scale scripting: Opportunities for large task parallel applications on petascale computers", SCIDAC 2009, Journal of Physics: Conference Series 180 (2009). DOI: 10.1088/1742-6596/180/1/012046