

When Database Systems Meet the Grid

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Abstract

We illustrate the benefits of combining database systems and Grid technologies for data-intensive applications. Using a cluster of SQL servers, we reimplemented an existing Grid application that finds galaxy clusters in a large astronomical database. The SQL implementation runs an order of magnitude faster than the earlier Tcl-C-file-based implementation. We discuss why and how Grid applications can take advantage of database systems.

Keywords: Very Large Databases, Grid Applications, Data Grids, e-Science, Virtual Observatory.

1. Introduction

Science faces a data avalanche. Breakthroughs in instruments, detector and computer technologies are creating multi-Terabyte data archives in many disciplines. Analysis of all this information requires resources that no single institution can afford to provide. In response to this demand, Grid computing has emerged as an important research area, differentiated from clusters and distributed computing. Many definitions of the Grid and Grid systems have been given [17]. In the context of this paper, we think of *the Grid as the infrastructure and set of protocols that enable the integrated, collaborative use of high-end computer, networks, databases, and scientific instruments owned and managed by multiple organizations, referred to virtual organizations* [18][27].

The need to integrate databases and database technology into the Grid was already recognized, in order

to support science and business database applications as well as to manage metadata, provenance data, resource inventories, etc. [16]. Significant effort has gone into defining requirements, protocols and implementing middleware to access databases in Grid environments [19][20][21][22][23]. Although database management systems (DBMS) have been introduced as useful tools to manage metadata, data, resources, workflows, etc [24][25][26], the presence of databases is minimal in *science* applications running on the Grid. Today the typical data-intensive science Grid application still uses flat files to process and store the data and cannot benefit from the power that database systems offer.

To evaluate the benefit of combining database and Grid technologies, this paper compares an existing file-based Grid application, MaxBCG [6], with an equivalent SQL implementation. This paper describes the MaxBCG algorithm and its relationship to the Sloan Digital Sky Survey (SDSS) and the Virtual Observatory (VO) project. Next, we describe in detail the file-based and database implementations, and compare their performance on various computer systems. Finally, we discuss how the SQL implementation could be run efficiently on a Grid system. We conclude by speculating why database systems are not being used on the Grid to facilitate data analysis.

2. Finding Galaxy Clusters for SDSS

Some Astronomy knowledge is needed to understand the algorithm's computational requirements [28]. Galaxies may be categorized by brightness, color, and redshift. Brightness is measured in specific wavelength intervals of light using standard filters. Color is the difference in brightness through two different filters. Due to the Hubble expansion of the Universe, the Doppler redshift of light from a galaxy is a surrogate for its distance from Earth.

Galaxy clusters are collections of galaxies confined by gravity to a compact region of the universe. Galaxy clusters are useful laboratories for studying the physics of the Universe. Astronomers are developing interesting new

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ways to find them systematically. The brightest galaxy in a cluster (BCG) is typically the most massive and so tends to be near the cluster center.

The Maximum-likelihood Brightest Cluster Galaxy algorithm [1], MaxBCG, finds galaxy clusters. It has been used to search the Sloan Digital Sky Survey (SDSS) catalog for Cluster candidates [2]. MaxBCG was originally implemented as Tcl scripts orchestrating the SDSS Astrottools package [3] and ran on the Terabyte Analysis Machine (TAM), a 5-node Condor cluster specifically tuned to solve this type of problem [4][5]. The same application code was integrated with the Chimera Virtual Data System created by the Grid Physics Network (GriPhyN) project to test Grid technologies [6]. As is common in astronomical file-based Grid applications, the TAM and Chimera implementations use hundreds of thousands of files fetched from the SDSS Data Archive Server (DAS) to the computing nodes.

SkyServer is the Web portal to the SDSS Catalog Archive Server (CAS) – the relational database system hosting the SDSS catalog data. All the data required to run MaxBCG is available in the SkyServer database. SDSS is part of the Virtual Observatory also known as the World Wide Telescope. The Virtual Observatory is being implemented in many countries [7]. It is developing portals, protocols, and standards that federate and unify many of the world’s astronomy archives into a giant database containing all astronomy literature, images, raw data, derived datasets, and simulation data integrated as a single intelligent facility [8].

The World-Wide Telescope is a prototypical data Grid application supporting a community of scholars cooperating to build and analyze a data Grid that integrates all astronomy data and literature. The MaxBCG search for clusters of galaxies is typical of the tasks astronomers will want to perform on this data Grid.

2.1 The Algorithm

The MaxBCG algorithm solves the specific astronomical problem of locating clusters of galaxies in a catalog of astronomical objects. It searches for galaxy clusters over a wide range of redshifts and masses. The search relies on the fact that the brightest cluster galaxies (BCG) in most clusters have remarkably similar luminosities and colors [9]. The MaxBCG algorithm works on a 5-dimensional space and calculates the cluster likelihood of each galaxy. The 5-space is defined by two **spatial** dimensions, Right Ascension, *ra*, and Declination, *dec*; two **color** dimensions, *g-r* and *r-i*; and one **brightness** dimension, *i*. The algorithm includes six steps:

Get galaxy list extracts the five-dimensions of interest from the catalog.

Filter calculates the unweighted BCG likelihood for each galaxy (unweighted by galaxy count) and discards unlikely galaxies.

Check neighbors weights the BCG likelihood with the number of neighbors.

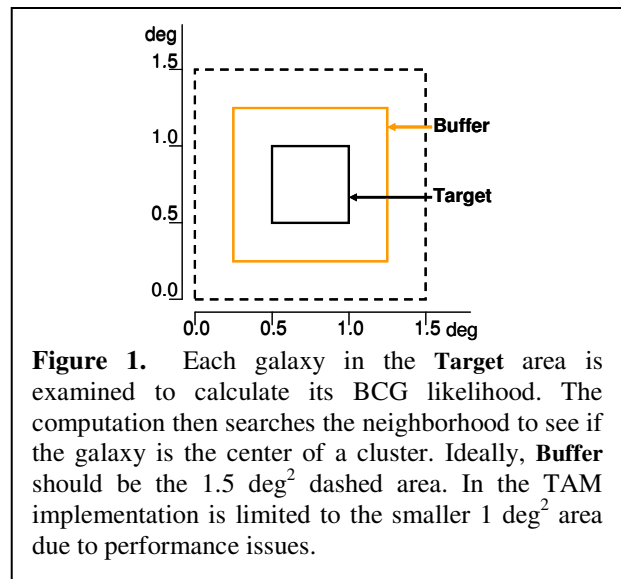
Pick most likely for each galaxy, determines whether it is the most likely galaxy in the neighborhood to be the center of the cluster.

Discard compromised results removes suspicious results and stores the final cluster catalog.

Retrieve the members of the clusters retrieves the galaxies that the MaxBCG algorithm determined are part of the cluster.

2.2 The TAM Implementation

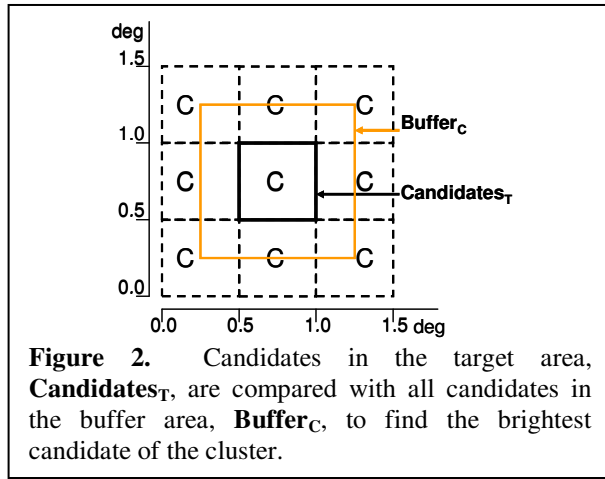
The MaxBCG algorithm was implemented as Tcl scripts driving Astrottools, which is an SDSS software package comprised of Tcl and C routines layered over a set of public domain software packages [3]. The CPU intensive computations are done by Astrottools using external calls to C routines to handle vector math operations. The algorithm ran on the TAM Beowulf cluster [4].



The TAM MaxBCG implementation takes advantage of the parallel nature of the problem by using a divide-and-conquer strategy which breaks the sky in 0.25 deg² fields. Each field is processed as an independent task. Each of these tasks require two files: a 0.5 x 0.5 deg² **Target** file that contains galaxies that will be evaluated and a 1 x 1 deg² **Buffer** file with the neighboring galaxies needed to test for the presence of a galaxy cluster. Ideally the **Buffer** file would cover 1.5 x 1.5 deg² = 2.25 deg² to find all neighbors within 0.5 deg of any galaxy in the **Target** area and estimate the likelihood that a galaxy is the brightest one in a cluster. But the time to search the larger **Buffer** file would have been unacceptable because the TAM nodes did not have enough RAM storage to hold the larger files: the compromise was to limit the buffer to cover only to 1 x 1 deg² areas [Figure1].

A **Target** field of 0.25 deg^2 contains approximately 3.5×10^3 galaxies. Initially, every galaxy in the catalog is a possible BCG. The observed brightness and color of each candidate is compared with entries in a **k-correction** table, which contains the expected brightness and color of a BCG at 100 possible redshifts. This comparison yields a (perhaps null) set of plausible redshifts for each candidate BCG. If, at any redshift, a galaxy has even a remote chance of being the right color and brightness to be a BCG, it is passed to the next stage.

Given a candidate galaxy, the next stage uses the **Buffer** file to compute the number of neighbor galaxies at every redshift. This *every redshift* search is required because the color window, the magnitude window, and the search radius all change with redshift. The BCG likelihood is computed at each redshift. The maximum likelihood, over the entire range of redshifts for the object with at least one neighbor, is recorded in the BCG **Candidates** file, **C**. About 3% of the galaxies are candidates to be a BCG.



In order to determine whether a candidate galaxy is a BCG, rather than just a member of the cluster, the algorithm compares it with the neighboring **candidates** which are compiled into the **Buffer_C** file [Figure 2]. Ideally, each candidate should be compared with all candidates within 0.5 deg as this corresponds to a reasonable low redshift cutoff. However, as explained earlier [Figure 1], TAM is restricted to $1 \times 1 \text{ deg}^2$ area to meet its computation time and storage budget, leaving only a 0.25 deg buffer surrounding the $0.5 \times 0.5 \text{ deg}^2$. The algorithm finds approximately 4.5 clusters per target area (0.13% of the galaxies are BCGs).

The last step is to retrieve the galaxies in the cluster. A galaxy is considered to be part of the cluster if it is inside a radius of 1 Mpc (3.26 million light years, converted into degrees using the redshift) of the BCG and inside the R_{200} radius containing 200 times the background mass density. The R_{200} radius is derived from the cluster mass (number of galaxies) using a lookup table. In the TAM

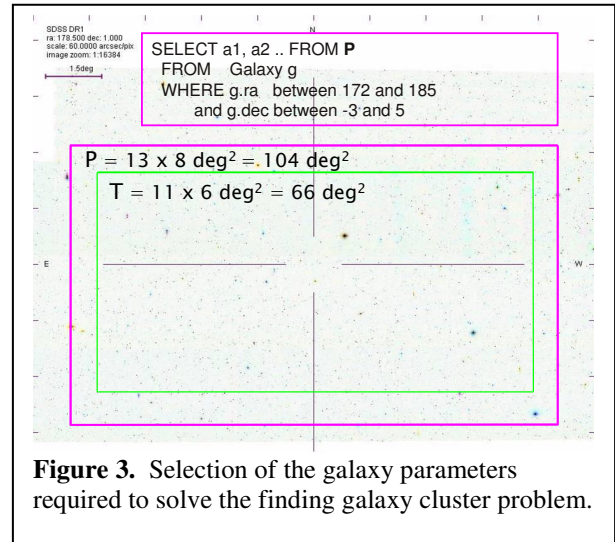
implementation these spherical neighborhood searches are reasonably expensive as each one searches the **Buffer** file.

Once the **Buffer** and **Target** files are loaded into RAM the algorithm is CPU-bound. The 600 MHz CPUs of the TAM could process a **Target** field of 0.25 deg^2 in about a thousand seconds. Processing the many target fields is embarrassingly parallel, so the time scales linearly with the number of target areas being processed. TAM is composed of 5 nodes, each one a dual-600-MHz PIII processor nodes each with 1 GB of RAM. The TAM cluster could process ten target fields in parallel.

2.3 SQL Server DBMS Implementation

We implemented the same MaxBCG algorithm using the SDSS CAS database [10]. This new implementation includes two main improvements. First, it uses a finer k-correction table with redshift steps of 0.001, instead of 0.01. Second, it uses a 0.5 deg buffer on the target field. Although these two improvements give better scientific results, would have increased the TAM processing time by a factor of about 25. The implementation is available from [29].

As described in Section 2.2, the TAM approach builds two files, **Target** and **Buffer**, for each 0.25 deg^2 target field. The SQL application processes much larger pieces of the sky all at once. We have been using a target area of $11 \text{ deg} \times 6 \text{ deg} = 66 \text{ deg}^2$ inside a buffer area of $13 \text{ deg} \times 8 \text{ deg} = 104 \text{ deg}^2$; but, in principle the target area could be much larger. Larger target areas give better performance because the relative buffer area (overhead) decreases [Figure 3]. Using a database and database indices allows this much large area because the database scans the areas using high-speed sequential access and spatial indices rather than keeping all the data in the RAM.



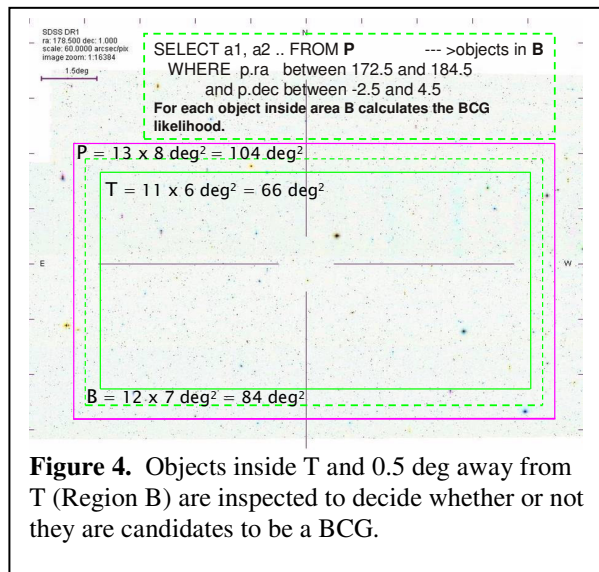
The SQL application does not extract the data to files prior to doing the processing. It uses the power of the

database system to SELECT the necessary data and to do some processing and filtering inside the database. The processing requires basically one SELECT statement to extract the 5 parameters of interest from the general Galaxy table. Each of these rows or galaxies is JOINED with the 1000-row redshift lookup k-correction table to compute the BCG likelihood. This process eliminates candidates below some threshold very early in the computation.

These two steps are fairly simple and fast. The next step, counting the number of neighbors to estimate the BCG likelihood, is a bit more complex.

Neighborhood searches are usually very expensive because they imply computing distances between all pairs of objects in order to select those within some radius. Relational databases are well suited to look for objects meeting some criteria. However, when the searches are spatial, they usually require a special indexing system. We used the techniques described in [11] to perform the neighborhood searches. We tried both the Hierarchical Triangular Mesh (HTM) [12] and the zone-based neighbor techniques. As explained below, the *Zone* index was chosen to perform the neighbor counts because it offered better performance.

The concept behind the zone-indexing schema is to map the celestial sphere into stripes of certain height called *Zones*. Each object at position (ra, dec) is assigned to a *Zone* by using the fairly simple formula $Zone = \text{floor}((dec + 90) / h)$, where h is the *Zone* height.

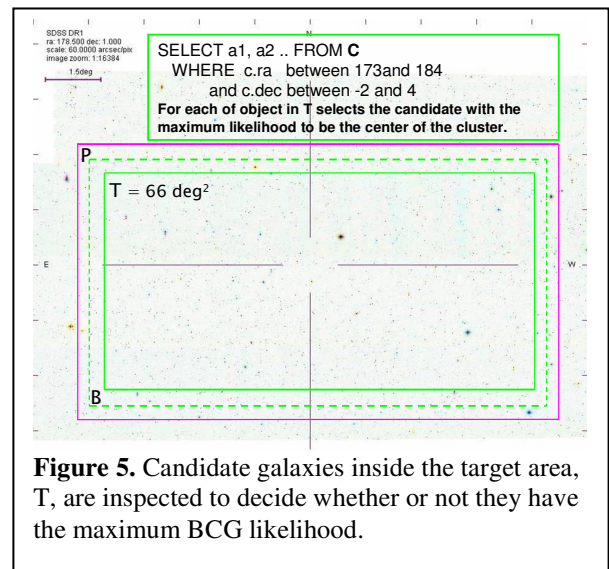


Zone-indexing has two benefits. First, using relational algebra the algorithm performs the neighborhood searches by joining a *Zone* with itself and discarding those objects beyond some radius. This pure SQL approach avoids the cost of using expensive calls to the external C-HTM

libraries to do the spatial searches. Second, the data and computation partition very easily by assigning different *Zones* to each SQL Server and running the MaxBCG code in parallel.

The SQL MaxBCG algorithm works as follows. Given a target area T, all objects inside T and up to 0.5 deg away from T (buffer area B) are inspected to decide whether they are candidates to be the brightest cluster galaxy [Figure 4]. Searches for neighbors include all objects inside P which guarantees 0.5 deg buffer for objects near the border. This computation is therefore more accurate than the TAM version which used only a 0.25 deg buffer only. Area T differs from area B because deciding whether a candidate is the brightest cluster galaxy requires knowledge about candidate neighbors within 0.5 deg. To avoid unnecessary dependencies, we do in advance what will be required later. This task generates a **Candidates** table C.

In the next stage, all **candidate** galaxies in target area T are inspected to decide whether or not they have the maximum likelihood to be the brightest galaxy of their cluster. This neighbor search is done only among objects in the **Candidate** table, C [Figure 5]. This step creates a **Cluster** catalog where the likelihood of all candidates has been properly computed using 0.5 deg buffer around each candidate.



Processing a target field of 66 deg² as described above, requires about 5 hours with a dual 2.6 GHz machine running Microsoft SQL Server 2000. However, SQL Server is usually I/O bound instead of CPU bound so algorithm performance will not scale exactly with CPU speed.

Table 1. SQL Server cluster performance, with no partitioning and with 3-way partitioning.					
	Task	elapse (s)	cpu (s)	I/O	Galaxies on each partition
No Partitioning	spZone	563.7	210.2	102,144	1,574,656
	fBCGCandidate	15,758.2	15,161.0	562	
	fIsCluster	2,312.7	6,58.5	16,043	
	total	18,635	16,030	118,749	
3-node Partitioning					
P1	spZone	285.5	65.5	46,758	729,234
	fBCGCandidate	6,099.1	5,850.7	209	
	fIsCluster	286.6	189.4	2,910	
	total	6,671.2	6,105.6	49,877	
P2	spZone	325.4	77.9	50,519	898,916
	fBCGCandidate	8,210.7	7,907.7	306	
	fIsCluster	451.8	306	476	
	total	8,987.9	8,291.6	51,301	
P3	spZone	326.3	65.6	46,275	719,900
	fBCGCandidate	6,121.5	5,783.5	283	
	fIsCluster	189.4	158.1	1,955	
	total	6,637.2	6,007.2	48,513	
Partitioning Total		8,988	20,404	149,691	2,348,050
Ratio 1node/3node		48 %	127 %	126 %	

Resolving the same target area of 66 deg^2 with only one of the TAM CPUs using the file-oriented approach required about 73 hours (1000 s per each 0.25 deg^2 field), but that computation had only a 0.25 deg surrounding buffer and only 100 redshift steps. TAM would require about 25 times longer to do the equivalent SQL-calculation with a 0.5 deg buffer and redshift steps of 0.001.

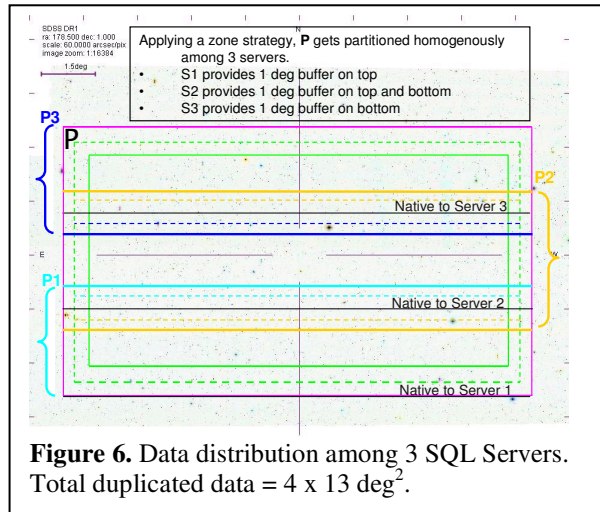
2.4 SQL Server Cluster

The SQL implementation can run either on a single SQL Server or on a cluster of SQL Servers. As mentioned

before, the problem is intrinsically parallel; each target area T can be processed in parallel. Using the *Zone* strategy described in section 2.3, a single target area may be processed in parallel by distributing the *Zones* among several servers allowing parallel execution of MaxBCG on different partitions of the target area [Figure 6].

When running in parallel, the data distribution is arranged so *each server is completely independent* from the others. We achieve this by duplicating some data and processing on different servers. The duplicated computations are insignificant compared to the total work involved when processing big volumes of data, or equivalently, big areas of the sky. We benchmarked this partitioning approach using a Microsoft SQL Server 2000 cluster composed of 3 nodes, each one a dual 2.6 GHz Xeon with 2 GB of RAM.

Table 1 shows the elapsed times, CPU times, and I/O operations used by SQL Server when solving MaxBCG with and without partitioning. **SpZone** is the task that arranges the data in *Zones* so the neighborhood searches are efficient. This task assigns a ZoneID and creates a clustered-index on the data. **fBCGCandidate** is the main task. It includes the BCG likelihood computations. Here is where the main neighborhood searches are performed to estimate properly the BCG likelihood. The fact that the I/O density is low during **fBCGCandidate** indicates the required data is usually in memory, which is always highly desired. Finally, **fIsCluster** screens the **Candidates** table and decides whether or not a candidate is a BCG. Although not included in Table 1, we also have the function that collects the galaxies that belong to a



cluster. This is a fairly simple and fast operation which searches for neighboring galaxies within some radius for each detected cluster.

The union of the answers from the three partitions is identical to the BCG candidates and clusters returned by the sequential (one node) implementation. Overall the parallel implementation gives a 2x speedup at the cost of 25% more CPU and I/O (including the cost of rezoning).

2.5 Time Performance

Tables 2 and 3 present a side-by-side comparison showing that the relational database solution is about 40 times faster per node than the file-based approach. For the specific cluster configurations considered here the 3-node SQL Server approach is about 20 times faster than the 5-node TAM.

Even if one were willing to wait 20 times longer, TAM nodes do not have enough memory to handle z-steps of 0.001 and a buffer of 0.5 deg. As mentioned before, a single TAM CPU takes 1000 s to process a target field of 0.25 deg² with a buffer of 0.25 deg and z-steps of 0.01 TAM performance is expected to scale lineally with the number of fields.

Table 2. Time scale factors for converting the TAM test case to the SQL server test case.

	TAM	SQL Server	Scale Factor
CPUs used	1	2	0.5
CPU	600 MHz	2.6 GHz	~ 0.25
Target field	0.25 deg ²	66 deg ²	264
z- steps	0.01	0.001	25
Buffer	0.25 deg	0.5 deg	
Total Scale Factor			825

Table 2 compares both configurations and provides the scale factor to convert the TAM test case into the SQL test case. We normalize for the fact that the TAM CPU is about 4 times slower by dividing by 4 -- in fact much of the time is spent waiting for disk so this is being generous to the TAM system which had a comparable disk subsystem. Even with that the ratio is about 2 hours to about 2 days.

Table 3. Scaled TAM vs. Measured SQL Server performance for a target field of 66 deg².

Cluster	Nodes	Time(s)	Ratio
TAM	1	825,000	44
SQL Server	1	18,635	
TAM	5	165,000	18
SQL Server	3	8,988	

2.6 Performance Analysis

What makes things run faste in SQL than in the file-based application? We wish we knew but we can no longer run the original code so we can only make educated guesses (one of the authors wrote the original code).

First, the SQL implementation discards candidates early in the process by doing a natural JOIN with the k-correction table and filtering out those rows where the likelihood is below some threshold. This reduces the number of operations for subsequent INNER JOINs with the k-correction table and other tables. The SQL design uses the redshift index as the JOIN attribute which speeds the execution. So, early filtering and indexing are a big part of the answer. Second, the main advantage comes from using the *Zone* [11] strategy to index the data and speed up the neighborhood searches.

The SQL design could be further optimized. The iteration through the galaxy table uses SQL cursors which are very slow. But there was no easy way to avoid them. Our tests used a galaxy table of roughly 1.5 million rows (44 bytes each). About 1.2 million of those galaxies need to be joined with the k-correction table (1000 rows x 40 bytes). Joining this in memory would require at least 80 GB. A possible optimization is to define some sort of sky partitioning algorithm that breaks the sky in areas that can fit in memory, 2 GB in our case. Once an area has been defined, the MaxBCG task is scheduled for execution. This approach would be similar to the cluster implementation described in section 2.4 but at the level of cluster nodes since different computer may have different memory resources.

3. Discussion

This work demonstrates that using a relational database management system and SQL can improve computational performance on data-intensive applications. But performance is not the only advantage of using general database management systems rather than implementing custom applications. There is no magic in a relational DBMS; anything it does can also be done in a custom application (e.g. one implemented in TCL and C!). In fact, a quality custom solution should outperform a general-purpose DBMS.

The SQL implementation of MaxBCG was considerable simpler than the Tcl-Astrotools implementation primarily because it leveraged the features of the SQL system for data access, indexing, and parallelism.

The scientist, in our case an astronomer, should be free to focus on the science and minimize the effort required to optimize the application. Database management systems are designed to do fast searches, workload balancing and manage large data volumes and certainly will do a better job compared to what an average

scientist could code. Database management systems allow simultaneous data access from different applications providing a good sharing environment.

So, the first lesson to learn for scientists working in data-intensive disciplines like astronomy, biology, etc. is that database systems are powerful tools to analyze big volumes of data and share results with others. On the other hand, the community researching database systems should ask itself why scientists are so reluctant to use database technologies.

As stated in the introduction, although the potential benefits of using database systems on the Grid has been recognized [16], their actual use as analysis tools is minimal. To our knowledge, most of the data-intensive applications that run on the Grid today focus on moving hundreds of thousands of files from the storage archives to the thousands of computing nodes. Many of these applications, like the one described in this paper, could solve the same problem more efficiently using databases.

We believe there is a basic reason for the absence of database technology in the Grid science community. While it is relatively easy to deploy and run applications coded in C, Fortran, Tcl, Python, Java, etc.; it is difficult to find resources to do the equivalent tasks using databases. Grid nodes hosting big databases and facilities where users can have their own database with full power to create tables, indexes, stored procedures, etc. are basically nonexistent. However, such facilities are needed to minimize the distance between the stored data and the analysis nodes, and in this way to guarantee that is the code that travels to the data and not the data to the code.

With the motivation of minimizing the distance between the SDSS CAS databases and analysis computing nodes, we implemented the SDSS Batch Query System, CasJobs [13][14]. The next section describes CasJobs and our work to develop an efficient Grid-enabled implementation of MaxBCG that instead of transferring hundreds of thousands of files over the network [6], leverages database technologies as parallel querying processing and indexing.

4. CasJobs, MaxBCG and Data Grids

CasJobs is an application available through the SkyServer site [15] that lets users submit long-running SQL queries on the CAS databases. The query output can be stored on the server-side in the user's personal relational database (MyDB). Users may upload and download data to and from their MyDB. They can correlate data inside MyDB or with the main database to do fast filtering and searches. CasJobs allows creating new tables, indexes, and stored procedures. CasJobs provides a collaborative environment where users can form groups and share data with others.

MaxBCG can be run using CasJobs, but that implementation is equivalent to the one described in section 2.3, which uses only one server. We want to take

it one step further. Inspired by our SQL Server cluster experience, we plan to implement an application able to run in parallel using several systems. So for example when the user submits the MaxBCG application, upon authentication and authorization, the SQL code (about 500 lines) is deployed on the available Data-Grid nodes hosting the CAS database system. Each node will analyze a piece of the sky in parallel and store the results locally or, depending on the policy, transfer the final results back to the origin. We aim for a general implementation that makes it easy to bring the code to the data, avoids big data transfers, and extrapolates easily to solve other problems.

At the moment, two different organizations host the CAS database and the CasJobs system; Fermilab (Batavia, IL, USA) and The Johns Hopkins University (Baltimore, MD, USA). In the near future, the Inter-University Centre for Astronomy and Astrophysics (IUCCA) in Pune, India, will also host the system. Other organizations have showed interest in DB2 implementations of the CAS database. These are institutions with different access policies, autonomous and geographically distributed. CasJobs is accessible not only through the Web interface but also through Web services. Once the GGF DAIS protocol [21] becomes a final recommendation, it should be fairly easy to expose CasJobs Web services wrapped into the official Grid specification. We are working on issues of security, workflow tracking, and workload coordination, which need to be resolved to guarantee quality of service. Autonomy, geographical distribution, use of standards and quality of service are the key characteristics that a system requires in order to be accepted as a Grid system [27].

5. Conclusion

This paper presents a typical astronomical data-intensive application which aims to find galaxy clusters in SDSS catalog data. It demonstrates that using a database cluster achieves better performance than a file-based Tcl-C implementation run on a traditional Grid system. It also describes future work to "gridify" the implementation.

It points out that even though database systems are great tools for data-intensive applications, and even though one of the main goals of the Grid is providing infrastructure and resources for such applications, there are virtually no database management systems on the Grid to do effective data analysis.

In current Grid projects, databases and database systems are typically used only to access and integrate data, but not to perform analytic or computational tasks. Limiting usage in this manner neglects a strength of database systems, which is their ability to efficiently index, search, and join large amounts of data – often in parallel. It is a mistake to move large amounts of data to the query, when you can move the query to the data and execute the query in parallel. For this reason, it would be

useful for nodes on the Grid to support different Database Management Systems so that SQL applications could be deployed as easily as traditional Grid applications coded in C, Fortran, etc.

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