GrayWulf: Scalable Clustered Architecture for Data Intensive Computing

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Abstract

Data intensive computing presents novel challenges for traditional computing architectures that have focused on FLOPS. CPU speeds have surpassed IO capabilities of both commodity clusters and traditional supercomputers. We present the architecture of a database cluster targeted at data-intensive computations with petascale data sets. The goal of our design is to build a balanced system in terms of IO capability, following Amdahl's Laws. The system is built from commodity servers, similar to the well-known BeoWulf architecture. The GrayWulf name pays tribute to Jim Gray who was actively involved in its early design. The hardware at JHU exceeds one petabyte of disk space, and has 70GB/sec aggregate IO bandwidth. Our benchmarks are based on data from the petascale Pan-STARRS project, building the largest sky survey to date. The benchmarks involve sequential searches over hundreds of terabytes.

1. Problem Statement

The nature of high performance computing is changing. While a few years ago much of high-end computing involved maximizing CPU cycles per second allocated for a given problem; today it revolves around performing computations over large data sets. This means that efficient data access from disks and data movement across servers is an essential part of the computation. Data sets are doubling every year, growing slightly faster than Moore's Law[1]. As a result, a new challenge is emerging, as many groups in science (but also beyond) are facing analyses of data sets in tens of terabytes, eventually extending to a petabyte since disk access and data-rates have not grown with their size. There is no magic way to manage and analyze such data sets today. The problem exists both on the hardware and the software levels.

The requirements for the data analysis environment are (i) scalability, including the ability to evolve over a long period, (ii) performance, (iii) ease of use, (iv) some fault tolerance and (v) most important—*low entry cost*.

Database-Centric Computing

Many of the typical data access patterns in science require a first, rapid pass through the data, with relatively few CPU cycles carried out on each byte. These involve filtering by a simple search pattern, or computing a statistical aggregate. Such operations are quite naturally performed within a relational database, and expressed in SQL. So a traditional relational database fits these patterns extremely well.

The picture gets more complicated when one needs to run more complex algorithms on the data, not necessarily easily expressed in a declarative language. Examples of such applications can include complex geospatial queries, processing time series data, or running the BLAST algorithm for gene sequence matching.

The traditional approach of bringing the data to where there is an analysis facility is inherently not scalable, once the data sizes exceed a terabyte, due to network bandwidth, latency, and cost. It has been suggested [2] that the best approach is to bring the analysis to the data. If the data are stored in a relational database, nothing is closer to the data than the CPU of the database server. It is quite easy today with most relational database systems to import procedural (or object oriented) code and expose their methods as user defined functions within the query.

This approach has proved to be very successful in many of our reference applications, and while writing class libraries linked against SQL was not always the easiest coding paradigm, its excellent performance made the coding effort worthwhile.

Typical data-intensive scientific workloads

Over the last few years we have implemented several eScience applications, in experimental data-intesive physical sciences applications such as astronomy, oceanography and water resources. We have been monitoring the usage and the typical workloads corresponding to different types of users. When analyzing the workload on the publicly available multi-terabyte Sloan Digital Survey SkyServer database[6], it was found that most user metrics have a *1/f* power law distribution[7].

Of the several hundred million data accesses most queries were very simple, single row lookups in the data set, which heavily used indices such as on position over the celestial sphere (nearest object queries). These made up the high frequency, low volume part of the power law distribution. On the other end there were analyses which did not map very well on any of the precomputed indices, thus the system had to perform a sequential scan, often combined with a merge join. These often took over an hour to scan through the multi-terabyte database. In order to submit a long query, users had to register with an email address, while the short accesses were anonymous.

We have noticed a pattern in-between these two types of accesses. Long, sequential accesses to the data were broken up into small, templated queries, typically implemented by a simple client-side Python script, submitted once in every 10 seconds. These "*crawlers*" had the advantage of returning data quickly, and in small buckets. If the inspection of the first few buckets hinted at an incorrect request (in the science sense), the users could terminate the queries without having to wait too long.

The "power users" have adopted a different pattern. Their analyses involved complex, multi-step workflows, where the end result was approached in a multi-step, hit-and-miss fashion. Once the workflow was finalized, they executed it over the whole data set, by submitting a large job into a batch queue.

In summary, most scientific analyses are done in a exploratory fashion, where "everything goes", and few predefined patterns apply. Users typically want to experiment, try innovative things that often do not fit preconceived notions, and would like to get rapid feedback on the momentary approach.

Amdahl's laws

Amdahl has established several laws for building a balanced computer system [8]. These were reviewed recently[9] in the context of the explosion of data. The paper pointed out that contemporary computer systems IO subsystems are lagging CPU cycles. In the discussion below we will be concerned with two of Amdahl's Laws:

A balanced system

- *needs one bit of IO for each CPU cycle*
- *has 1 byte of memory for each CPU cycle*

These laws enumerate a rather obvious statement– in order to perform continued generic computations, we need to be able to deliver data to the CPU, through the memory. Amdahl observed that these ratios need to be close to unity and this need has stayed relatively constant.

For large data sets the only way we can even hope to accomplish the analysis if we follow a maximally sequential read pattern. The sequential IO rate has grown somewhat faster as the density of the disks has increased by the square root of disk capacity. For commodity SATA drives the sequential IO **is** typically 60MB/sec, compared with 20MB/sec 10 **y**ears ago. Nevertheless, compared to the increase of the data volumes and the CPU speedups, this increase is not fast enough to conduct business as usual. Just loading a terabyte at this rate takes 4.5 hours. Given this sequential bottleneck, the only way to increase the disk throughput of the system is to add more and more disk drives and to eliminate obvious bottlenecks in the rest of the system.

Scale-up or scale-out?

A 20-30TB data set is too large to fit on a single, inexpensive server. One can scale-up, buying an expensive multiprocessor box with many fiber channel (FC) Host Channel Adapters (HCA) and a FC disk array, easily exceeding the $1M price tag. The performance of such systems is still low, especially for sequential IO. To build a system with over one GB/sec sequential IO speed one needs at least 8 FC adapters. While this may be attractive for management, the entry cost is not low!

Scaling out using a cluster of disks attached to each computing node provides a much more cost effective and high throughput solution, very much along the lines of BeoWulf designs. The sequential read speed of a properly balanced mid-range server with many local disks can easily exceed a GB/sec before saturation[10]. The cost of such a server can

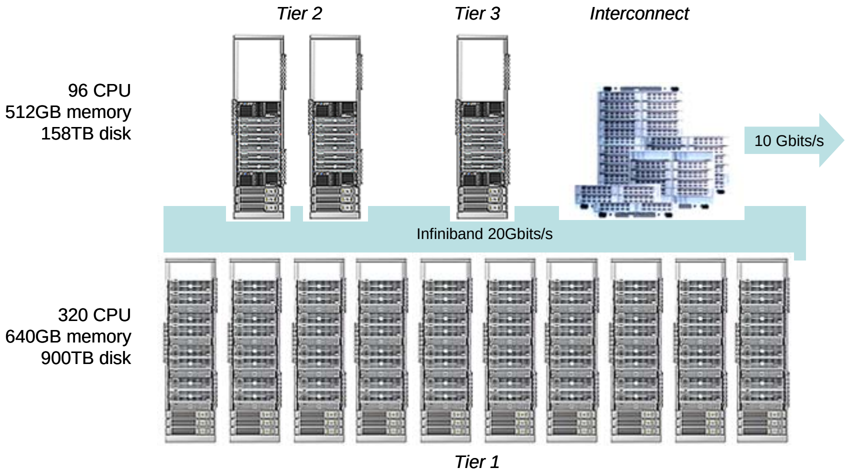


Figure 1. Schematic diagram of three tiers of the GrayWulf architecture. All servers are interconnected through a QLogic Infiniband switch. The aggregate resource numbers are provided for the bottom and the top two tiers, respectively.

be kept close to the $10,000 range. On the other hand managing an array of such systems, and manually partitioning the data can be quite a challenge. Given the success of the BeoWulf concept for academic research, we believe that the dominant solution in this environment will be deployed locally. Given the scarcity of space at universities it also needs to have a high packing density. In this challenge we would like to show that:

(i) *a scaled-out, database–centric system provides a good platform to perform typical data intensive computations*
(ii) *such a system can be built in from quite inexpensive components*
(iii) *the aggregate IO performance of such a system can be extremely competitive, reaching tens of GBytes/sec.*

2. The Hardware Configuration

We are building a combined hardware and software platform from commodity components to perform large-scale database-centric computations.
The system should

a) *scale to petabyte-size data sets*
b) *provide a very high sequential IO bandwidth*
c) *support most eScience access patterns*
d) *provide simple tools for database design*
e) *provide tools for fast data ingest*

Modular, layered architecture

Our cluster consists of modular building blocks, in three tiers. Having multiple tiers provides a system with a certain amount of hierarchical spread of memory and disk storage. The low level data can be spread evenly among server nodes on the lowest tier, all running in parallel, while query aggregations are done on more powerful servers in the higher tiers.

The lowest, tier 1 building block is a single 2U sized Dell 2950 server, with two quad core 2.66GHz CPUs. Each server has 16 GB of memory, two PCIe PERC6/E dual-channel RAID controllers and a 20 Gbit/sec QLogic SilverStorm Infiniband HCA, with a PCIe interface. Each server is connected to two MD1000 SAS disk boxes that contain a total of 30-750GB, 7,200rpm SATA disks. Each disk box is connected to its dedicated controller. There are two mirrored 73GB, 15,000rpm disks residing in internal bays, connected to a controller on the motherboard. These contain the operating system and the rest of the installed software. Thus, each of these modules contain a total of 22.5TB of data storage.

Four of these units with UPS power is put in a rack. The whole lower tier consists of 10 such racks, with a total of 900TB of data space, and 640 GB of memory. Tier 2 consists of four Dell R900 servers with 16 cores each and 64 GB of memory, connected to three of the MD1000 disk boxes, each populated as above. There is one dual channel PERC6/E controller for each disk box. The system disks are two mirrored 73GB SAS drives at 10,000 rpm and a 20Gbit/sec SilverStorm Infiniband HCA. This layer has a total of 135TB of data storage and 256GB of memory. We also expect that data sets that need to be sorted and/or rearranged will be moved to these servers, utilizing the larger memory.

Finally, tier 3 consists of two Dell R900 servers with 16 cores, 128GB of memory, each connected to a single MD1000 disk box with 15 disks, and a SilverStorm IB card. The total storage is 22.5TB and the memory is 256GB. These servers can also run some of the resource intensive applications, complex data intensive web services (still inside the SQL Server engine using CLR integration) requiring more physical memory than available on the lower tiers.

	server	*core*	*mem[GB]*	*disk[TB]*	*Count*
Tier 1	2950	8	16	22.50	40
Tier 2	R900	16	64	33.75	4
Tier 3	R900	16	128	11.25	2
total		**416**	**1152**	**1057.50**	**46**

Table 1. Tabular description of the three tiers of the cluster with aggregates for cores, memory and disk space within our GrayWulf system.

The Infiniband interconnect is through a Qlogic SilverStorm 9240 288 port switch, with across-sectional aggregate bandwidth of 11.52 Tbit/s. The switch also contains a 10 Gbit/sec Ethernet module that connects any server to our dedicated single lambda National Lambda Rail connection over the Infiniband fabric, without the need for dedicated 10 Gbit Ethernet adapters for the servers.

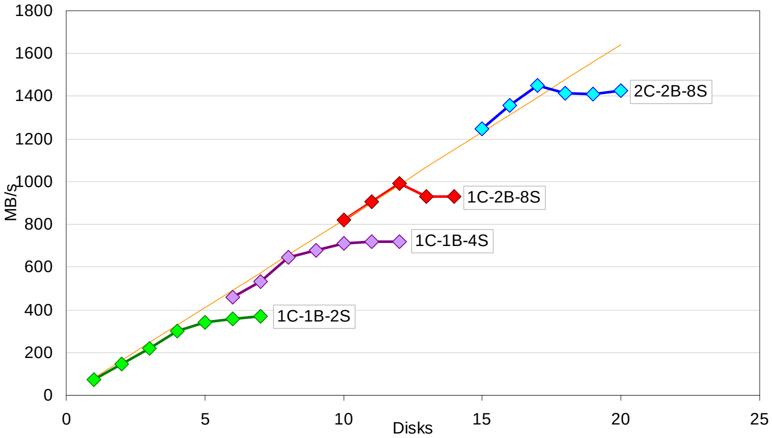


Figure 3. Throughput measurements corresponding to different controller, bus, and disk configurations.

Storage layout: Balanced IO bandwidth

The most important consideration when we designed the system (besides staying within our budget) was to avoid the obvious choke points in terms of streaming data from disk to CPU, then across the interconnect layer. These bottlenecks can exist all over the system: the storage bus (FC, SATA, SAS, SCSI), the storage controllers, the PCI buses, system memory itself, and in the way that software chooses to access the storage.

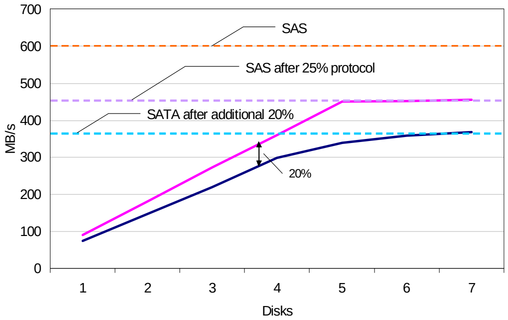


Figure 2. Behavior of SAS lanes showing the effects of the various protocol overheads relative to the idealized bandwidth.

The disks: A single 7,200 rpm 750 GB SATA drive can sustain about 75 MB/sec sequential reads at the outer cylinders, and slighly less on the inner parts.

The storage interconnect: We are using Serial Attached SCSI (SAS) to connect our SATA drives to our systems. SAS is built on full-duplex 3 Gbit/sec “lanes”, which can be either point-to-point (i.e. dedicated to a single drive), or can be shared by multiple drives via SAS “expanders”, which behave much like network switches. Prior parallel SCSI standards like Ultra320 accommodated only expensive native SCSI drives, which are great for IOPS-driven applications, but are not as compelling for petascale, sequentially-accessed data sets. In addition to supporting native SAS/SCSI devices, SAS also supports SATA drives, by adopting a physical layer compatible with SATA, and by including a Serial ATA Tunneling Protocol within the SAS protocol. For large, fast, potentially low-budget storage applications, SATA over SAS is a terrific compromise between enterprise-class FC and SCSI storage, and the inexpensive but fragile "SATA bricks" which are particularly ubiquitous in research.

The SCSI protocol itself operates with a 25% bus overhead. So for a 3 Gbit/sec SAS lane, the real-world sustainable throughput is about 225 MB/sec. The SATA Tunneling Protocol introduces an additional 20% overhead, so the real-world SAS-lane throughput is about 180 MB/s with SATA drives.

The disk enclosures: Each Dell MD1000 15-disk enclosure uses a single SAS "4x" connection. 4x is a bundle of four 3 Gbit/sec lanes, carried externally over a standard Infiniband-like cable with Infiniband-like connectors. This 12 Gbit/sec connection to the controller is very nice relative to common 4 Gbit/sec FC interconnects. But with SATA drives, the actual sustainable throughput over the 12 Gbit/sec is only 720 MB/sec. Thus we have already introduced a moderate bottleneck relative to the ideal ~1100 MB/sec throughput of our 15x750 MB/sec drives.

The disk controllers: The LSI Logic based Dell PERC6/E controller has dual 4x SAS channels, and has a feature set which is common among contemporary RAID controllers. Why do we go to the trouble and the expense of using one controller per disk enclosure when we could easily attach one dedicated 4x channel to each enclosure using a single controller? Our tests show that the PERC6 controllers themselves saturate at about 800 MB/sec, so to gain additional throughput as we add more drives, we need to add more controllers. It is convenient that a single controller is so closely matched to a SATA-populated enclosure.

The PCI and memory busses: The Dell 2950 servers have two "x8" PCI Express connections and one "x4" connection, rated at 2000 MB/sec and 1000 MB/s half-duplex speeds respectively. We can safely use the x4 connection for one of our PERC6 controllers since we expect no more than 720 MB/s from these. These 2000 MB/sec-each x8 connections are plenty for one of the PERC6 controllers, and just enough for our 20 Gbit/sec DDR Infiniband HCAs. Our basic tests suggest that the 2950 servers can read from memory at 5700 MB/sec, write at 4100 MB/sec, and copy at 2300 MB/sec. This is a pretty good match to our 1440 MB/sec of disk bandwidth and 2000 MB/sec Infiniband bandwidth.

In Figure 3, we present our measurements of the saturation points of various components of the GrayWulf's IO system. The labels on the plots designate the number of controllers, the number of disk boxes, and the number of SAS lanes for each experiment. The "1C-1B-2S" plot shows a pair of 3 Gbit/sec SAS lanes saturating near the expected 360 MB/sec mark. "1C-1B-4S" shows the full "4x" SAS connection of one of the MD1000 disk boxes saturating at the expected 720 MB/sec. "1C-2B-8S" demonstrates that the PERC6 controller saturates at just under 1 GB/sec. "2C-2B-8S" shows the performance of the actual Tier 1 GrayWulf nodes, right at twice the "1C-1B-4S" performance.

The full cluster contains 96 of the 720 MB/sec PERC6/MD1000 building blocks. This translates to an aggregate low-level throughput of about 70 GB/sec. Even though the bandwidth of the interconnect is slightly below that of the disk subsystem, we do not regard this as a major bottleneck, since in our typical applications the data is first filtered and/or aggregated, before it is sent across the network for further stream aggregation. This filtering operation will result in a reduction of the data volume to be sent across the network (for most scenarios) thus a factor of 2 lower network throughput compared to the disk IO is quite tolerable.

The other factor to note is that for our science application the relevant calculations take place at the backplanes of the individual servers, and the higher level aggregation requires a much lower bandwidth at the upper tiers.

3. The Software Used

The cluster is running Windows Enterprise Server 2008 and the database engine is SQL Server 2008 that is automatically deployed across the cluster. We built a middleware that is used for resource tracking, data partitioning and workflow execution.

Low level IO testing, monitoring tools

We use a combination of Jim Gray's *MemSpeed* tool, and *SQLIO* [11]. MemSpeed measures system memory performance itself, along with basic buffered and unbuffered sequential disk performance. SQLIO can perform various IO performance tests using IO operations that resemble what SQL Server's. Using SQLIO, we typically test sequential reads and writes, and random IOPS, but we're most concerned with sequential read performance.

Performance measurements presented here are typically based on SQLIO's sequential read test, using 128 KB requests, one thread per system processor, and 32-deep requests per thread. We believe that this resembles the typical table scan behavior of SQL Server's Enterprise Edition. We find that the IO speeds that we measure with SQLIO are very good predictors for SQL Server's real-world IO performance.

The full-scale GrayWulf system is rather complex, with many components performing tasks in parallel. We need a detailed performance monitoring subsystem that can track and quantitatively measure the behavior of the hardware. We need the performance data in several different contexts:

- track and monitor the status of computer and network hardware in the "traditional" sense
- as a tool to help design and tune individual SQL queries, monitor level of parallelism
- track the status of long-running queries, particularly those that are heavy consumers of CPU, disk, or network resources in one or more of the GrayWulf machines

The performance data are acquired both from the well-known "PerfMon" (Windows Performance Data Helper) counters and from selected SQL Server Dynamic Management Views (DMVs). To understand the resource utilization of different long-running queries, it is useful to be able to relate DMV performance observations of SQLServer objects such as filegroups with PerfMon observations of per-processor CPU utilization and logical disk IO.

Performance data for SQL queries are gathered by a C# program that monitors SQL Trace events and samples performance counters on one or more SQL Servers. The data is aggregated in a SQL database, where performance data is associated with individual SQL queries. This part of the monitoring represented a particular challenge in a parallel environment, since there is no easy mechanism to follow process identifiers for remote subqueries. Data gathering is limited to "interesting" SQL queries, which are annotated by specially-formatted SQL comments whose contents are also recorded in the database.

4. Description of Solution

In this proposal we would like to demonstrate how we can use simple building blocks, a commercial database software, combined with our own middle-ware, running in the Windows environment to solve real-world data-intensive problems at the scale of hundreds of Terabytes. The key to this performance (at the sub $700K cost) is the usage of locally attached disks, and a careful selection of the low level system components, combined with a good data layout strategy.

We have three reference applications, each corresponding to a different kind of data layout, and thus a different access pattern. These range from computational fluid dynamics to astronomy, each consisting of datasets close to or exceeding 100TB. Our proposed benchmarks will use these data sets in their proper scientific context, and demonstrate that the GrayWulf system is capable of delivering the necessary throughput to do the science.

5.1. Immersive Turbulence

The first application is in computational fluid dynamic, CFD, to analyze large hydrodynamic simulations of turbulent flow. The state-of-the-art simulations have spatial resolutions of 4096^3 and consist of hundreds if not thousands of timesteps. While current supercomputers can easily run these simulations it is becoming increasingly difficult to perform subsequent analyses of the results. Each timestep over such a spatial resolution can be close to a terabyte. Storing the data from all timesteps requires a storage facility reaching hundreds of terabytes. Any analysis of the data requires the users to analyze these data sets, which requires accessing the same compute/storage facility. As the cutting edge simulations become ever larger, fewer and fewer scientists can participate in the subsequent analysis. A new paradigm is needed, where a much broader class of users can perform analyses of such data sets.

A typical scenario is that scientists want to inject a number of particles (5,000-50,000) into the simulation and follow their trajectories. Since many of the CFD simulations are performed in Fourier space, over a regular grid, no labeled particles exist in the output data. At JHU we have developed a new paradigm to interact with such data sets using a web-services interface [12].

A large number of timesteps are stored in the database, organized along a convenient three-dimensional spatial index based on a space-filling curve (Peano-Hilbert, or z-transform). The disk layout closely preserves the spatial proximity of grid cells, making disk access of a coherent region more sequential. The data for each timestep is simply ***sliced*** across *N* servers, shown as scenario (a) on Figure 4. The slicing is done along a partitioning key derived from the space filling curve.

Spatial and temporal interpolation functions are implemented inside the database that can compute the velocity field at an arbitrary spatial and temporal coordinate. A scientist with a laptop can insert thousands of particles into the simulation by requesting the velocity filed at those locations. Given the velocity values, the laptop can then integrate the particles forward, and again request the velocities at the updated location and so on. The resulting trajectories of the particles have been integrated on the laptop, but they correspond to the velocity field inside the simulation spanning hundreds of terabytes. This is digital equivalent of launching sensors into a vortex of a tornado, like the scientists in the movie “Twister”.

This computing model has been proven extremely successful; we have so far ingested a 1024^3 simulation into a prototype SQL Server cluster, and created the above mentioned interpolating functions configured as a TVF (table valued function) inside the database[13]. The data has been made publicly available. We also created a Fortran(!) harness to call the web service, since most of the CFD community is still using that language.

SkyQuery

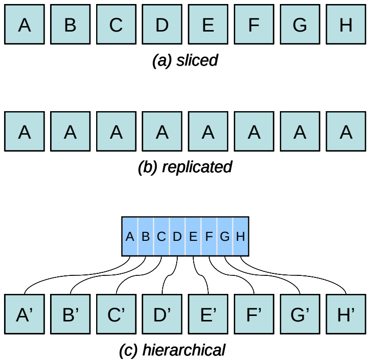
The *SkyQuery*[14] service has been originally created as part of the National Virtual Observatory. It is a universal web services based federation tool, performing cross-matches (fuzzy geospatial joins) over large astronomy data sets. It has been very successful, but has a major limitation. It is very good in handling small areas of the sky, or small user-defined data sets. But as soon as a user requests a cross-match over the whole sky, involving the largest data sets, generating hundreds of millions of rows, its efficiency rapidly deteriorates, due to the slow wide area connections.

Co-locating the data from the largest few sky surveys on the same server farm will give a dramatic performance improvement. In this case the cross-match queries are running on the backplane of the database. We have created a zone-based parallel algorithm that can perform such spatial cross-matches in the database[15] extremely fast. This algorithm has also been shown to run efficiently over a cluster of databases. We can perform a match between two datasets (2MASS, 400M objects and USNOB, 1B objects) in less than 2 hours on a single server. Our reference application for the GrayWulf is running *parallel queries*, and merging the result set, using a paradigm similar to the MapReduce algorithm[5].

Making use of threads and multiple servers we believe that on the JHU cluster can achieve a 20-fold speedup, yielding a result in a few minutes instead of a few hours. We use our spatial algorithms to compute the common sky area of the intersecting survey footprints then split this area equally among the participating servers, and include this additional spatial clause in each instance of the parallel queries for an optimal load balancing. The data layout in this case is a simple N-way ***replication*** of the data, as shown as part (b) on Figure 4. The relevant database that contains all the catalogs is about 5TB, thus a 20-way replication is still manageable. The different query streams will be aggregated on one of the Tier 3 nodes.

Pan-STARRS

The Pan-STARRS project[3] is a large astronomical survey, that will use a special telescope in Hawaii with a 1.4 gigapixel camera to sample the sky over a period of 4 years. The large field of view and the relatively short exposures will enable the telescope to cover three quarters of the sky 4 times per year, in 5 optical colors. This will result in more than a petabyte of images per year. The images will then be processed through an image segmentation pipeline that will identify individual detections, at the rate of 100 million detections per night. These detections will be associated with physical objects on the sky and loaded into the project’s database for further analysis and processing. The database will contain over 5 billion objects and well over 100 billion detections. The projected size of the database is 30 terabytes by the end of the first year, growing to 80 terabytes by the end of year 4.



(a) sliced

(b) replicated

(c) hierarchical

Figure 4. Data layouts over the GrayWulf cluster, corresponding to our reference applications. The three scenarios show (a) sliced, (b) replicated and (c) hierarchical data distributions.

Expecting that most of the user queries will be ran against the physical object, it is natural to consider a ***hierarchical*** data layout, shown of section (c) on Figure 4. The star schema of the database naturally provides a framework for such an organization. The top level of the hierarchy contains the objects, which are logically partitioned into *N* segments, but they physically stored on one of the Tier 2 servers. The corresponding detections (much larger in cardinality) are then sliced among the N servers in the lowest Tier (A’,B’, etc).

5. Experiments and measurements

We propose to perform a series of tests to show the performance of our system:

1. **Establish the low level IO speeds**. We will run a sequence of tests using the Microsoft tool SQLIO under various parameters to measure the low level sequqntial IO using different disk and controller configurations (for a preview see Fig. 3.) In separate experiments, we establish the speed of the Infiniband interconnect, both at the operating syste level and at the application level (SQL to SQL streaming).
2. **Sequential scan of Pan-STARRS data**. We will use simulated data that we used for the system testing since the telescope will only become fully operational at the end of this calendar year. The data will involve the P2Detection table, which is partitioned across many servers. We will replicate data across 25 servers, in excess of 200TB. We will perform a set of range queries, both on indexed and unindexed quantitites, with a selectivity of approximately 2%. The output will be collected on a set of Windows application nodes connected through the Infiniband.
3. **Deliver the Pan-STARRS data to Chicago**. In collaboration with the UIC group we will use the Sector environment to transfer the resulting 4TB of data to an application server in Chicago. We will send the data both buffered at JHU, and as a direct data stream from SQL.
4. **Extract a subset of the turbulence data**. We will run a subset extraction query on the turbulence data, partitioned and replicated over 25 servers for an aggregate data volume of 120TB. We deliver the result to an HPC cluster residing at JHU. The benchmark will select a sub-cube of our 1024^3 simulation at a given timestep, and extract the pressure for a subset of the $64x256^3$ sub-regions for further computing and visualization.
5. **Distributed join across a geographic divide**. We will use the SkyQuery dataset, replicated across 20 servers at JHU to perform a streaming join with another large table residing at Chicago (UIC) and compare the performance to a local join. This represents one of the most frequent query patterns in the astronomy community's use of the National Virtual Observatory.

The quantitative measurements will be done though capturing various system counters (PerfMon) both at the operating system level and at the database server level, at the 10 sec granularity. The resulting data stream will be captured in a database and the various statistical analyses will be evaluated afterwards.

6. Claims

In this section we would like to consider several well-studied architectures for scientific High Performance Computing and calculate their Amdahl numbers for comparison. The ***Amdahl RAM number*** is calculated by dividing the total memory in Gbytes with the aggregate instruction cycles in units of GIPS (1000 MIPS). The Amdahl IO number is computed by dividing the aggregate sequential IO speed of the system in Gbits/sec by the GIPS value. A ratio close to 1 indicates a balanced system in the Amdahl sense.

We consider first a typical University BeoWulf cluster, consisting of 50 3GHz dual-core machines, each with 4GB of memory and one SATA disk drive with 60MB/sec. Next, we consider a typical desktop used by the average scientist, doing his/her own data analysis. Today such a machine has 2 3GHz CPUs, 4GB of memory and 3 SATA disk drives, which provide an aggregate sequential IO of about 150MB/sec, since they all run off the motherboard controller. A virtual machine in a commercial cloud would have a single CPU, say at 3GHz, 4GB RAM, but a lower IO speed of about 30MB/sec per VM instance[4].

Let us consider two hypothetical machines used in today's scientific supercomputing environments. An approximate configuration "SC1" for a typical BlueGene-like machine was obtained from the LLNL web pages[16]. The sequential IO performance of an IO-optimized BlueGene/L configuration with 256 IO nodes has been measured to reach 2.6 GB/sec peak[17]. A simple minded scaling this result to the 1664 IO nodes in the LLNL system gives us the hypothetical 16.9 GB/sec figure used in the table for "SC1". The other hypothetical supercomputer, "SC2," has been modeled on the Cray XT-3 at the Pittsburgh Supercomputer Center. The XT-3 IO bandwidth is currently limited by the PSC Infiniband fabric[18]. We have also attempted to get accurate numbers from several of the large cloud computing companies – our efforts have not been successful, unfortunately.

The Graywulf IO numbers have been estimated from our single-node measurements of sequential IO performance and our typical reference workloads. Table 2 shows that our GrayWulf architecture excels in aggregate IO performance as well as in the Amdahl IO metric, in some cases well over a factor of 50. It is interesting that the desktop of a data

System	CPU count	GIPS [GHz]	RAM [GB]	diskIO [MB/s]	Amdahl	
					RAM	IO
BeoWulf	100	300	200	3000	0.67	0.080
Desktop	2	6	4	150	0.67	0.200
Cloud VM	1	3	4	30	1.33	0.080
SC1	212992	150000	18600	16900	0.12	0.001
SC2	2090	5000	8260	4700	1.65	0.008
GrayWulf	416	1107	1152	70000	1.04	0.506

Table 2. The two Amdahl numbers characterizing a balanced system are shown for a variety of systems commonly used in scientific computing today. Amdahl numbers close to 1 indicate a balanced architecture.

intensive user comes closest to the GrayWulf IO number of 0.5.

In this paper we wanted to make a few simple claims:

- *Data-intensive scientific computations today require a large sequential IO speed more than anything else.*
- *As we consider higher and higher end systems, their IO rate does not keep up with the CPUs.*
- *It is possible to build balanced IO intensive systems using commodity components*
- *These systems satisfy criteria in today's data-intensive environment similar to those that made the original BeoWulf idea so successful*
- *Database-centric computing can perform at high enough IO rates necessary to today's petascale scientific challenges*

Our specific claims include the following:

- *We will reach an aggregate sequential IO speeds in excess of 30GBytes/sec*
- *We will use several different applications, each with data sizes between 10TB to 200TB to demonstrate the generic nature and scalablility of our approach*
- *We will show that the IO rates are in excess of 70% of the maximum delivered by the hardware*
- *We will demonstrate how to build a scalable petabyte system with these metrics for well under the budget of $1M*

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8. References

[1] G. Moore, "Cramming more components onto integrated circuits", Electronics Magazine, 38, No 8, 1965.

[2] A.S. Szalay, J. Gray, "Science in an Exponential World", Nature, 440, pp 23-24, 2006.

[3] Pan-STARRS: Panoramic Survey Telescope and Rapid Response System, http://pan-starrs.ifa.hawaii.edu/

[4] M. Palankar, A. Iamnitchi, M. Ripeanu and S. Garfinkel,"Amazon S3 for Science Grids: a Viable Solution?" DADC'08 Conference, Boston, MA, June 24 2008.

[5] J. Dean and S. Ghemawat, "MapReduce: Simplified Data Processing on Large Clusters", 6th Symposium on Operating System Design and Implementation, San Francisco, 2004.

[6] A.R. Thakar, A.S. Szalay, P.Z. Kunszt, J. Gray, "The Sloan Digital Sky Survey Science Archive: Migrating a Multi-Terabyte Astronomical Archive from Object to Relational DBMS", *Computing in Science and Engineering*, V5.5,Sept 2003, IEEE Press. pp. 16-29, 2003.

[7] V. Singh, J. Gray, A.R. Thakar, A.S. Szalay, J. Raddick, W. Boroski, S. Lebedeva and B. Yanny, "SkyServer Traffic Report – The First Five Years", Microsoft Technical Report, MSR-TR-2006-190, 2006.

[8] http://en.wikipedia.org/wiki/Amdahl's_law

[9] G. Bell, J. Gray, and A.S. Szalay, "Petascale Computational Systems: Balanced Cyber-Infrastructure in a Data-Centric World", *IEEE Computer*, 39, pp 110-113, 2006.

[10] T. Barclay, W. Chong, J. Gray, "TerraServer Bricks – A High Availability Cluster Alternative," Microsoft Technical Report, MSR-TR-2004-107, 2004.

[11] J. Gray, B. Bouma, A. Wonders, “Performance of Sun X4500 under Windows, NTFS and SQLServer 2005”, http://research.microsoft.com/~gray/papers/JHU_thumper.doc

[12] Y. Li, E. Perlman, M. Wan, Y. Yang, C. Meneveau, R. Burns, S. Chen, G. Eyink and A. Szalay, “A public turbulence database and applications to study Lagrangian evolution of velocity increments in turbulence”, submitted to J. Comp. Phys, 2008.

[13] E. Perlman, R. Burns, Y. Li and C. Meneveau, “Data exploration of turbulence simulations using a database cluster”, In *Proceedings of the Supercomputing Conference* (SC’07), 2007.

[14] T. Budavari,T., T. Malik, A.S. Szalay, A. Thakar, J. Gray, “SkyQuery – a Prototype Distributed Query Web Service for the Virtual Observatory”, Proc. ADASS XII, ASP Conference Series, eds: H.Payne, R.I. Jedrzejewski and R.N.Hook, 295, 31, 2003.

[15] J. Gray, M.A. Nieto-Santisteban, A.S. Szalay, “The Zones Algorithm for Finding Points-Near-a-Point or Cross-Matching Spatial Datasets,” Microsoft Technical Report, MSR-TR-2006-52, 2006.

[16]https://computing.llnl.gov/?set=resources&page=SCF_resources#bluegenel

[17] H. Yu, R. K. Sahoo, C. Howson, G. Almasi, J. G. Castanos, M. Gupta J. E. Moreira, J. J. Parker, T. E. Engelsiepen, R. Ross, R. Thakur, R. Latham, and W. D. Gropp, "High Performance File I/O for the BlueGene/L Supercomputer," in Proc. of the 12th International Symposium on High-Performance Computer Architecture (HPCA-12), February 2006.

[18] Ralph Roskies, private communication