The Sloan Digital Sky Survey and Beyond

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ABSTRACT
Our collaboration with Jim Gray has created some of the world's largest astronomy databases, and has enabled us to test many avant-garde ideas in practice. The astronomers have been very receptive to these and embraced Jim as a 'card carrying member' of their community. Jim's contributions have made a permanent mark on astronomy, and eScience in general.

Categories and Subject Descriptors
H.3.[Information Storage and Retrieval], J.2. [Physical Sciences and Engineering] Astronomy, H2.8. [Database Applications]

1. INTRODUCTION
Astronomy data has been doubling every year for the last 20 years. Most of this trend is due to the emergence of electronic sensors. The largest sky survey of the last decade, the Sloan Digital Sky Survey, the SDSS, has often been called the 'Cosmic Genome Project'. As the SDSS started, the size of the data set to be used for scientific analyses was in the Terabytes, frighteningly large for the early 90's. Our group at Johns Hopkins has been selected to build the science archive for the SDSS. In a few years we have realized that the task required a powerful search engine, with spatial search capabilities. Our experimental system, based on object oriented technologies, was good enough to develop an understanding what the eventual system should look like. However, it was also becoming increasingly clear that we will need to do something different.

2. MEETING JIM
One of the SDSS collaboration meetings in the mid 90-s took me to Seattle, where I had dinner with Charles Simonyi, then still at Microsoft, who saw the similarities between our problem and the TerraServer. He immediately called up Jim and arranged us to meet. A few weeks later I flew to San Francisco and visited Jim at BARC. We started a lively discussion about the TerraServer, how it could be turned inside out, and how spatial searches over the globe were similar and yet different from spatial searches over the sky. We spent a day on dissecting our problem.

Jim was immediately asking about our '20 queries'. The '20 queries' were a deceptively simple way to jump-start a dialog between a database expert and an astronomer (or as it turns out any scientist…). Jim said: "*give me your twenty most important questions you would like to ask from your data system, and I will design the system for you*". It was amazing to watch how well this worked.

Soon Jim came to Baltimore, looked into our computer room, and looked at the machines. After 30 seconds he noted, with a grin on his face, that we had the wrong database layout. We were stunned. He explained later that he also listened to the noise, and the disks were rattling too much, telling him that there was too much random disk access. We started mapping out what the hardware requirements are, projecting that in order to get an acceptable performance with a 1 terabyte data set we will need a GB/s sequential read speed from the disks, translating about 20 servers at the time. Jim was a firm believer in using 'bricks', the cheapest, simplest building blocks that money could buy. With the help of Jan Vandenberg, our system guru at Johns Hopkins we started to do many experiments with low-level disk IO on our inexpensive servers, and soon our disks became much quieter.

3. ASTRONOMY AND THE SKYSERVER
Towards the end of 2000 data started arriving from the SDSS telescope. Jim rolled up his sleeves, and said: "*let's get to work*". During Christmas and New Year's we have converted the whole object oriented database schema to SQL Server. We modified many of our loading scripts, by looking at Tom Barclay's TerraServer code, and soon we had a simple SQL Server version of the SDSS database [1].

The SDSS project was first very reluctant to even consider that we switch technologies, so for about a year the SQL Server database was a 'cowboy' implementation, not part of the official data release. Coincidentally, Intel has given us a pool of servers to experiment with the database, and they had a 'show and tell' meeting in San Francisco, a few months after the first bits of data started to come off the telescope. We decided to create a simple graphical interface on top of the database that would enable people to visually browse the sky. My son, Tamas, 13 at the time, came along for the Intel meeting, and he helped to man the booth, and told us that "*no self-respecting school kid would use such an interface*", it had to be visually much more stimulating…

Jim had one of his big laughs – then we looked at one another, and decided that we had our target audience! If astronomers were not ready, we would design a database and an integrated website for school kids. This was the moment when we set out to build the SkyServer, a connection of the database to the pixels on the sky. Obviously, the name was a play on TerraServer… We pitched it to the SDSS project as a tool for education and outreach. When the first batch of SDSS data became officially public, the SkyServer appeared side by side to the 'serious' database for astronomers. We wrote simple scripts to create the false color images from the raw astronomy data, and adopted the TerraServer scheme to build an image pyramid of tiles.

Over the next year everyone realized that the SkyServer engine was much more robust and scalable. Ani Thakar at JHU did a superhuman effort to convert the whole existing framework over to SQL Server[2]. Jim insisted on two-phase loading, i.e. we load each new batch of data into its own separate little database, then run a lot of data cleaning code, and only accept the data if it passed all the tests. This foresight turned out to be enormously useful: once the data started coming 'through the hose', we could recover from errors (and there were lots of those...) much more easily. Soon we had the framework and the ability of loading hundreds of GB of data in a reasonable amount of time. This marks the transition of the SkyServer team from 'cowboys' to 'ranchers'.

Curtis Wong of Microsoft came along and redesigned the SkyServer's interface. His seemingly minor modifications of our style sheets had a huge impact on the whole look-and-feel of the site. Suddenly the site 'came alive'. Many volunteers (former students like Steve Landy, physics teachers like Rob Sparks, and many others) helped adding contents. Jordan Raddick, a science writer, joined our team and created a whole new branch of the website with educational exercises and formal class materials for K-12. Astronomers also realized the power of the visual tools and the site started to become popular even in astronomy circles.

The next major evolutionary step came with the emergence of .NET web services. Jim invited our whole team to San Francisco, to the VSLive, where .NET was introduced. Our students (Tanu Malik and friends) entered a world-wide programming contest and their entry won the second prize. The JHU team created a set of services, called SkyQuery[3], that can perform queries across geographically separated databases. Jim built a prototype for the ImageCutout, which became the core of the next generation user interfaces for the SkyServer, on how images and database content can be integrated[4].

3.1 Going Native

During his sabbatical in the early 2000s Jim has picked up a few astronomy textbooks, took them along on his sailboat and in a remarkably short time he turned 'native', he very quickly understood the important concepts of astronomy and was able to participate in reformulating research ideas to elegant SQL and work with us side-by-side in not only database related problems but in astronomy research. We have written many papers together where his ideas were also very relevant for the astronomy part[5]. At the same time he was teaching us databases and computer science, and had several of our students as interns at BARC.

As Jim started spending a large fraction of his time working on astronomy, on one of his famous slides he noted: "*I love working with astronomers, since their data is worthless*!" Of course, he meant it in the most complimentary sense – the data could be freely distributed and shared, since there were no financial implications and legal constraints.

Jim participated in many of the SDSS meetings, and he became a much beloved member of our community. His contributions were very much appreciated, and in recognition of his work an asteroid is about to be named after him.

3.2 Spatial Searches

Soon after the SkyServer was launched, it was obvious that astronomers wanted to perform various spatial searches for objects on the sky. Also, the whole survey had a rather complex geometry. In order to describe this we needed an extensive framework for spatial operations. Over the years with several of my students and postdocs (in particular Peter Kunszt) we have written a fast package for spatial searches, called Hierarchical Triangular Mesh (HTM)[6]. With Jim's help we built an interface to SQL Server, and soon we were performing blazingly fast searches over the sky. This became one of the most characteristic features of the SkyServer. These tools made it into the 'shrink-wrap' package of SQL Server 2005 as a demo on how to interface SQL to external software[7,8].

Jim was very excited about these spatial computations, since these demonstrated extremely well one of his main convictions: "*when you have lots of data, you have to take the computations to the data rather than data to the computations*!" Being Jim, there is nothing closer to the data than the database, thus this meant that the computations had to be done inside the database[9].

As the spatial searches grow in complexity, it became apparent that we needed even more extensive capabilities. Jim and I ended up writing a complex computational geometry library, all in SQL!!! Needless to say, I cannot think of another person who would even have thought of such an idea, not to mention implementing it. Today this library has been finally converted to C# by Tamas Budavari and George Fekete, but still much of the code in SkyServer is Jim's original.

Jim realized that there are two different types of spatial problems: one relates to searches over a localized, relatively small region, the other involves a fuzzy (probabilistic) spatial join over much of the celestial sphere. He came up with the idea of organizing the data along latitude zones, and was able to write the whole query joining two tables with hundreds of millions of rows as a single SQL statement, letting the optimizer doing its magic[10]. This was one of the finest example of SQL wizardry I have ever seen! He worked with Maria Nieto-Santisteban to create parallel implementations of this across many servers, and the performance is nothing short of stunning[11,12]. These ideas are forming the basis of our next generation SkyQuery engine that were are building now.

3.3 The Virtual Observatory

It was around 2001 that people started to explore the idea of a Virtual Observatory[13,14]. Given the fact that most of the world's astronomy data is public ('worthless'), and is on-line, the time seemed to be right to develop a framework where all this data appeared as part of a single system. Jim was an enthusiastic supporter of this idea and from the very first moment he has been an active participant in all the discussions about the design of the VO. His ideas are right at the heart of the current service-based architecture of the VO. He has been instrumental in starting the National Virtual Observatory, NVO. His advice helped us to avoid many pitfalls that we would have undoubtedly fallen into otherwise. He has helped many different groups all over the world to get started in bringing their data into databases. One finds his astronomy collaborators from Edinburgh to Beijing, Pasadena, Munich and Budapest. He bought several '*sneakernet*' boxes, inexpensive servers that were traveling around to world to transport data. He was highly amused by the fact that in spite of the delays due to postal services and customs the bandwidth still exceeded those of the networks[15].

3.4 A Model for Digital Publishing

The SkyServer turned out to be a ground-breaking exercise in publishing and curating digital scientific data. We learned that if once a dataset is released, it cannot be changed, it must be treated like an edition of a printed book, as one should not destroy the old copies when a new one appears on the shelves. To this date, we carry forward all the old releases of the SDSS data.

We also made a huge effort to capture all the relevant information in the database. We built tools for supporting physical units and descriptions automatically by the database, using markup tags in the comments of our SQL scripts. Recently we have just archived all the emails sent during the project in a free-text searchable database, the only record of the technical decisions made during the project.

We were anxious to see how scientists interacted with the database. It was clear, that analyses must be done as close to the data as possible, but it is also dangerous to allow general users to create and run their own functions inside a shared, public database. Nolan Li, one of our graduate students and Wil O'Mullane, a senior programmer in our group came up with a clever idea of giving users their own server-side databases, where they are free to do anything, and yet they can link to the main database as well. Jim immediately embraced the idea and has been instrumental in turning it into the generic data-space that it is today[16].

We were logging the traffic from day one, and we were amazed to watch how traffic was growing, and how a New York Times article resulted in a huge spike. It was gratifying to see that after these spikes traffic leveled off at a higher level than before – many people liked what they saw. The analysis of the SkyServer traffic demonstrated that most of the 1 million users of the system are non-astronomers, and that there is a power law with no obvious breaks in any of the usage statistics[17]. Jim liked to quote: "*you have nothing to fear but success or failure*". Of course, he never intended to fail….

4. BEYOND ASTRONOMY

It became clear that Virtual Observatories will emerge on every scale of the physical world, from high energy physics to nanotech, molecular biology, environmental observatories, our planet Earth, all the way to the Universe. Many of the unknown issues are quite similar and they revolve around our inability to deal with the increasing amounts of data[18].

As a result we started to consider the broader implications of the SkyServer work. The SDSS is one of the projects that mark a transition to a new kind of science. Science itself has evolved over the centuries, from empirical to analytic, then computational-X, where X marks many of the scientific disciplines. With the emergence of these large experiments, like SDSS where even the data collection is done via computers, a paradigm shift is happening. We are entering the era when there is so much data that brute force is not enough. We need to approach even the design of the experiments differently, with an algorithmic perspective. Data management and databases are inevitable in this new world, where business becomes eBusiness and science turns into eScience[19].

The SDSS data provided an amazing opportunity to explore and experiment with how scientists will adopt to new tools and new technologies. In the same spirit, Jim experimented with how these tools and technologies can carry over to other disciplines. He consciously started to develop connections in the molecular biology and genomics community. I came along for some of his trips when he visited the Whitehead Institute or NCBI, and it was amazing how similar many of the problems were to those we had to deal with in astronomy. It was great to see how Jim was able to go 'native' in biology with the same ease as he did in astronomy, and how his '20 queries' immediately cut through the communication gap between different communities. The same thing happened when he started to work with oceanographers from MBARI and NEPTUNE.

He was among the first to realize how the data explosion is changing not only sciences, but scientific computing as well. As the amount of data is growing faster than our ability to transfer, the only feasibly way to keep up is to take the computations to the data[20]. This goes against the trends seen in supercomputing today where the machines are becoming increasingly CPU intensive, while the ability to read and write data is lagging behind. Lots of lively discussions with Jim and Gordon (Bell) about this problem resulted in a short paper that outlines what is wrong with today's computing architectures[21]. I am immensely proud of having participated in the paper. Our group at JHU is now working very hard to implement the vision outlined there, in building a machine especially tailored for data-intensive computations that would make Jim very happy.

4.1 Sensor Networks

We realized that the data explosion in astronomy was due to the electronic CCD detectors that replaced photographic plates. As semiconductor manufacturing matured, every year brought a new generation of bigger and more sensitive detectors that could be replaced without affecting the telescopes themselves. Much the same way gene chips, and gene sequencers have industrialized molecular biology. The revolution in Earth Observing, satellite imagery has been due to the improved imaging devices as well. The commonality is that whenever an inexpensive sensing device appears that is on an exponential growth path, leapfrogging over previous generations, a scientific revolution is imminent.

Such a revolution is taking place now with inexpensive wireless sensor networks, also sometimes called '*smartdust*'. It is expected that in five years there will be more sensors on-line than computers. Intel's Berkeley Lab was among the first to develop such devices. My wife Kathy Szlávecz is a soil biologist, who is interested in the soil ecosystem as a whole. She has been painstakingly taking data of environmental parameters for many years. Jim connected her to the Berkeley people, and after Kathy's seminar at the Intel Lab we came away with a shoebox of 'Berkeley Motes'. At the same time Johns Hopkins hired Andreas Terzis, a computer scientist specializing in wireless sensors, and thus a new collaboration formed. On a shoestring budget, we were building a small sensor network to study soil moisture and temperature.

Jim realized that in this field almost everyone is entirely focused on the first phase of the problem: collecting the data. In astronomy we have learned the hard way that with exponential data growth one should worry about the data processing and analysis even at the beginning, otherwise it will be difficult to catch up once the big data stream opens up[22].

He was also very interested in how flexible the SkyServer framework was. Another aspect of environmental science is that scientists are very interested in long term trends and averages, while they still want to retain all the raw data to 'dive in' wherever something unusual is found. So once again, we 'rolled up our sleeves' and in a matter of weeks converted the SkyServer framework to an end-to-end system to handle data from environmental science[23]. We had to write code to deal with time series and in-database calibrations. Soon we had help from Stuart Ozer, who built an OLAP data cube for the sensor data, as far as we know the first ever in a scientific application[24].

5. A COLLABORATOR AND FRIEND

Over the years, as our collaboration has intensified, the days started with Jim's phone calls while walking from home to BARC, followed by several back and forth calls until the early morning hours on the East Coast. Very often we were still talking at 3am my time or 7am his time. We spent a lot of time together, chasing bugs and arguing about code.

Jim had an uncanny ability to 'go for the jugular', to see what is the single most important issue or bottleneck. I had the privilege to meet some of the top physicists of the 20th Century, including Richard Feynman and Yakov Zeldovich. Jim's mind worked the same way as theirs, he could solve a problem on the 'back of an envelope', as they say.

He was very good in getting results published. When the time came that he felt we should write a paper, he got the 'itch', and started with a quick draft, helping all his collaborators who (like me) have a writer's block, to get up to speed. He was very generous, he often did more work than his share, but he still insisted on others, in particular young people, to become lead authors. I have seen him mentoring many students. He was always very patient and encouraging, trying to get them excited and lead by example.

Jim would never give up hands-on work. If he did not have time to write code and 'tinker' with databases, it was not a good day for him. He had an inexhaustible source of energy. When everyone was falling over, he still kept going, drawing everybody with him. One day we kept going at a spurious SQL bug starting at 7am at BARC and not even standing up except for coffee, until it was 11pm (only when we found the bug, of course). By that time most restaurants were closed, but Jim kept going on North Beach at night until we found a nice Italian restaurant, and we had a proper dinner.

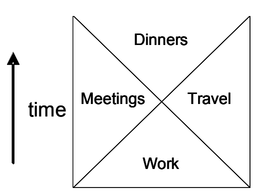

Figure 1. The world of science according to Jim.

He used to draw me a rectangle, with two diagonals splitting it into four pieces, and saying jokingly: "*this is our life*". The vertical axis shows the arrow of time. And he asked: "*Alex, where are we on this diagram?*" He did everything to keep the work part to occupy as big a piece as possible.

Jim and I met rather late in our careers. At that point in life people usually establish good working relationships, but deep friendships form much earlier. But for whatever reason, we quickly connected, became very close friends, and we had these amazing, rare conversations where the bandwidth went way beyond the spoken word.

His love of life and his love of work irradiated all of us near him. My friendship and collaborations with Jim took my career in new, entirely different directions, away from astrophysics and into eScience. He impacted lives of many others around him in the same way. All of us who had the privilege to call Jim a friend are working very hard to turn at least some of the projects we dreamed about together into reality.

6. ACKNOWLEDGMENTS

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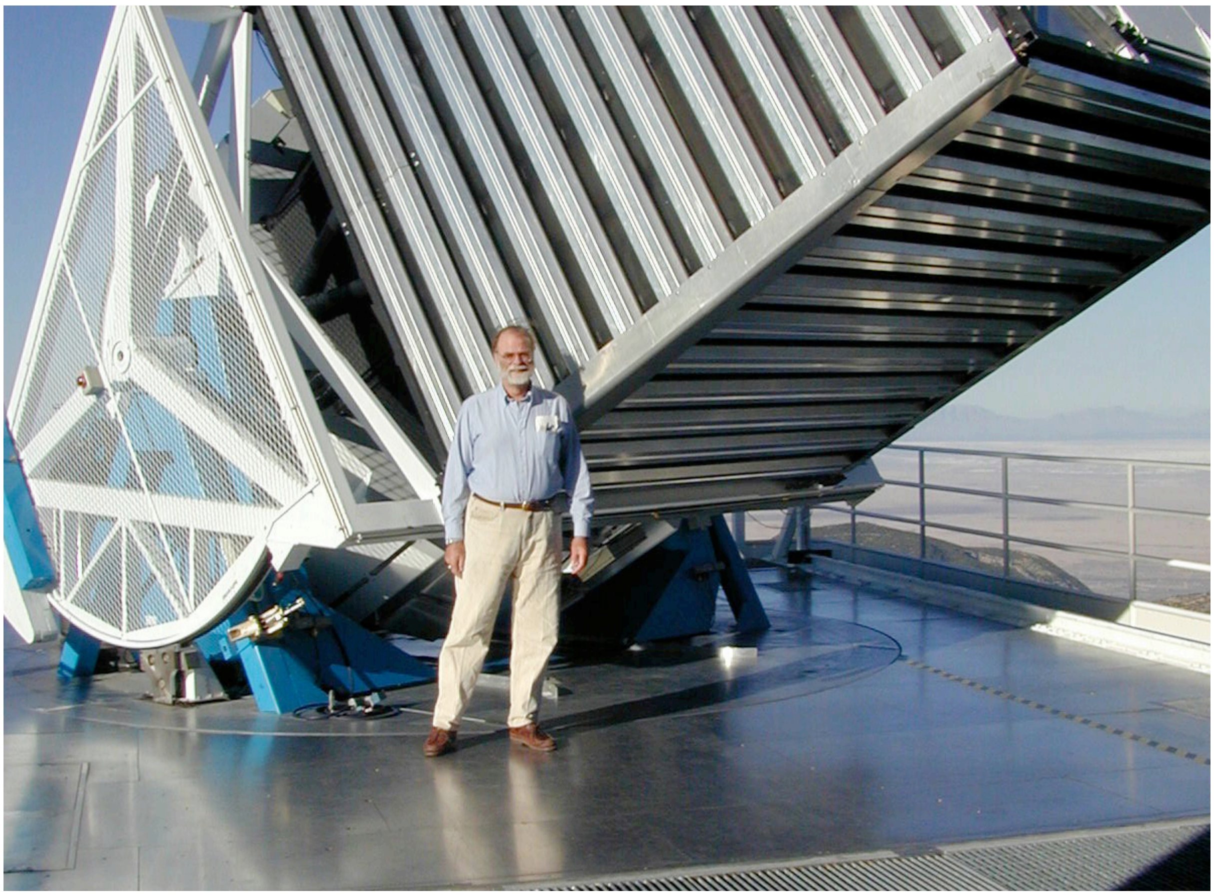

Figure 2. Jim Gray in front of the SDSS telescope