Chapter 1

MASSIVE DATASETS IN ASTRONOMY

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Abstract

Astronomy has a long history of acquiring, systematizing, and interpreting large quantities of data. Starting from the earliest sky atlases through the first major photographic sky surveys of the 20th century, this tradition is continuing today, and at an ever increasing rate.

Like many other fields, astronomy has become a very data-rich science, driven by the advances in telescope, detector, and computer technology. Numerous large digital sky surveys and archives already exist, with information content measured in multiple Terabytes, and even larger, multi-Petabyte data sets are on the horizon. Systematic observations of the sky, over a range of wavelengths, are becoming the primary source of astronomical data. Numerical simulations are also producing comparable volumes of information. Data mining promises to both make the scientific utilization of these data sets more effective and more complete, and to open completely new avenues of astronomical research.

Technological problems range from the issues of database design and federation, to data mining and advanced visualization, leading to a new toolkit for astronomical research. This is similar to challenges encountered in other data-intensive fields today. These advances are now being organized through a concept of the Virtual Observatories, federations of data archives and services representing a new information infrastructure for astronomy of the 21^{st} century. In this article, we provide an overview of some of the major datasets in astronomy, discuss different techniques used for archiving data, and conclude with a discussion of the future of massive datasets in astronomy.

Keywords: Astronomy, Digital Sky Survey, Space Telescope, Data-Mining, Knowledge Discovery in Databases, Clustering Analysis, Virtual Observatory

1. INTRODUCTION: THE NEW DATA-RICH ASTRONOMY

A major paradigm shift is now taking place in astronomy and space science. Astronomy has suddenly become an immensely data-rich field, with numerous digital sky surveys across a range of wavelengths, with many Terabytes of pixels and with billions of detected sources, often with tens of measured parameters for each object. This is a great change from the past, when often a single object or a small sample of objects were used in individual studies. Instead, we can now map the universe systematically, and in a panchromatic manner. This will enable *quantitatively and qualitatively new science*, from statistical studies of our Galaxy and the large-scale structure in the universe, to the discoveries of rare, unusual, or even completely new types of astronomical objects and phenomena. This new digital sky, data-mining astronomy will also enable and empower scientists and students anywhere, without an access to large telescopes, to do first-rate science. This can only invigorate the field, as it opens the access to unprecedented amounts of data to a fresh pool of talent.

Handling and exploring these vast new data volumes, and actually making real scientific discoveries poses a considerable technical challenge. The traditional astronomical data analysis methods are inadequate to cope with this sudden increase in the data volume (by several orders of magnitude). These problems are common to all data-intensive fields today, and indeed we expect that some of the products and experiences from this work would find uses in other areas of science and technology. As a testbed for these software technologies, astronomy provides a number of benefits: the size and complexity of the data sets are nontrivial but manageable, the data generally are in the publicdomain, and the knowledge gained by understanding this data is of broad public appeal.

In this chapter, we provide an overview of the state of massive datasets in astronomy as of mid-2001. In Section 2., we briefly discuss the nature of astronomical data, with an emphasis on understanding the inherent complexity of data in the field. In Section 3., we present overviews of many of the largest

datasets, including a discussion of how the data are utilized and archived. Section 4. provides a thorough discussion of the virtual observatory initiative, which aims to federate all of the distributed datasets described in Section 3. into a coherent archival framework. We conclude this chapter with a summary of the current state of massive datasets in astronomy.

2. THE NATURE OF ASTRONOMICAL DATA

By its inherent nature, astronomical data are extremely heterogeneous, in both format and content. Astronomers are now exploring all regions of the electromagnetic spectrum, from gamma-rays through radio wavelengths. With the advent of new facilities, previously unexplored domains in the gravitational spectrum will soon be available, and exciting work in the astro-particle domain is beginning to shed light on our Universe. Computational advances have enabled detailed physical simulations which rival the largest observational datasets in terms of complexity. In order to truly understand our cosmos, we need to assimilate all of this data, each presenting its own physical view of the Universe, and requiring its own technology.

Despite all of this heterogeneity, however, astronomical data and its subsequent analysis can be broadly classified into five domains. In order to clarify later discussions, we briefly discuss these domains and define some key astrophysical concepts which will be utilized frequently throughout this chapter.

- Imaging data is the fundamental constituent of astronomical observations, capturing a two-dimensional spatial picture of the Universe within a narrow wavelength region at a particular epoch or instant of time. While this may seem obvious to most people—after all, who hasn't seen a photograph—astrophysical pictures (see, *e.g.*, Figures 1.1 and 1.2) are generally taken through a specific filter, or with an instrument covering a limited range of the electromagnetic spectrum, which defines the wavelength region of the observation. Astronomical images can be acquired directly, *e.g.*, with imaging arrays such as CCDs¹, or synthesized from interferometric observations as is customarily done in radio astronomy.
- Catalogs are generated by processing the imaging data. Each detected source can have a large number of measured parameters, including coordinates, various flux quantities, morphological information, and areal extant. In order to be detected, a source must stand out from the background noise (which can be either cosmic or instrumental in origin). The significance of a detection is generally quoted in terms of *σ*, which is

¹Charge Coupled Device—a digital photon counting device that is superior to photographic images in both the linearity of their response and quantum efficiency



Figure 1.1 A multiwavelength view of the Crab nebula, a supernova remnant that was first sighted by Chinese astronomers in 1054 AD. Clearly demonstrated in this montage of images are the different physical processes that are manifested in the different spectral regions. Image Credit: NASA/CXC/SAO.

a relative measure of the strength of the source signal relative to the dispersion in the background noise. We note that the source detection process is generally limited both in terms of the flux (total signal over the background) and surface brightness (intensity contrast relative to the background).

Coordinates are used to specify the location of astronomical sources in the sky. While this might seem obvious, the fact that we are sited in a non-stationary reference frame (*e.g.*, the earth rotates, revolves around the sun, and the sun revolves around the center of our Galaxy) complicates the quantification of a coordinate location. In addition, the Earth's polar axis precesses, introducing a further complication. As a result, coordinate systems, like Equatorial coordinates, must be fixed at a particular instant of time (or epoch), to which the actual observations, which are made at



Figure 1.2 Making the tradeoff between area and resolution. The image on the left is from the ground-based DPOSS survey (see below) of the field of M100, a nearby spiral galaxy. While the entire survey covers on-half of the entire sky, this single image is only one-millionth of the size of the entire sky (*i.e.* one microsky). The image on the right is a subset from the deepest optical image ever taken, the STIS clear image of the Hubble Deep Field South, image credit: R. Williams (STScI), the HDF-S Team, and NASA. This image is 10,000 times smaller than the DPOSS image, thus representing 100 picosky.

different times, can be transformed. One of the most popular coordinate systems is J2000 Equatorial, which is fixed to the initial instant (zero hours universal time) of January 1, 2000. One final caveat is that nearby objects (*e.g.*, solar system bodies or nearby stars) move on measurable timescales. Thus the date or precise time of a given observations must also be recorded.

Flux quantities determine the amount of energy that is being received from a particular source. Since different physical processes emit radiation at different wavelengths, most astronomical images are obtained through specific filters. The specific filter(s) used varies, depending on the primary purpose of the observations and the type of recording device. Historically, photographic surveys used filters which were well matched to the photographic material, and have names like O, E, J, F, and N. More modern digital detectors have different characteristics (including much higher sensitivity), and work primarily with different filter systems, which have names like U, B, V, R, and I, or g, r, i in the optical, and J, H, K, L, M, and N in the near-infrared.

In the optical and infrared regimes, the flux is measured in units of magnitudes (which is essentially a logarithmic rescaling of the measured flux) with one magnitude equivalent to -4 decibels. This is the result of the historical fact that the human eye is essentially a logarithmic detector, and astronomical observations have been made and recorded for many centuries by our ancestors. The zeropoint of the magnitude scale is determined by the star Vega, and thus all flux measurements are relative to the absolute flux measurements of this star. Measured flux values in a particular filter are indicated as B = 23 magnitudes, which means the measured B band flux is $10^{0.4 \times 23}$ times fainter than the star Vega in this band. At other wavelengths, like x-ray and radio, the flux is generally quantified in standard physical units such as ergs cm⁻² s⁻¹ Hz⁻¹. In the radio, observations often include not only the total intensity (indicated by the Stokes I parameter), but also the linear polarization parameters (indicated by the Stokes Q, and U parameters).

- Spectroscopy, Polarization, and other follow-up measurements provide detailed physical quantification of the target systems, including distance information (*e.g.*, redshift, denoted by *z* for extragalactic objects), chemical composition (quantified in terms of abundances of heavier elements relative to hydrogen), and measurements of the physical (*e.g.*, electromagnetic, or gravitational) fields present at the source. An example spectrum is presented in Figure 1.3, which also shows the three optical filters used in the DPOSS survey (see below) superimposed.
- Studying the time domain (see, *e.g.*, Figure 1.4) provides important insights into the nature of the Universe, by identifying moving objects (*e.g.*, near-Earth objects, and comets), variable sources (*e.g.*, pulsating stars), or transient objects (*e.g.*, supernovae, and gamma-ray bursts). Studies in the time domain either require multiple epoch observations of fields (which is possible in the overlap regions of surveys), or a dedicated synoptic survey. In either case, the data volume, and thus the difficulty in handling and analyzing the resulting data, increases significantly.
- Numerical Simulations are theoretical tools which can be compared with observational data. Examples include simulations of the formation and evolution of large-scale structure in the Universe, star formation in our Galaxy, supernova explosions, *etc.* Since we only have one Universe and cannot modify the initial conditions, simulations provide a valuable tool in understanding how the Universe and its constituents formed and have evolved. In addition, many of the physical processes that are involved in



Figure 1.3 A spectrum of a typical z > 4 quasar PSS 1646+5524, with the DPOSS photographic filter transmission curves (J, F, and N) overplotted as dotted lines. The prominent break in the spectrum around an observed wavelength of 6000 Angstroms is caused by absorption by intergalactic material (that is material between us and the quasar) that is referred to as the Ly α forest. The redshift of this source can be calculated by knowing that this absorption occurs for photons more energetic than the Ly α line which is emitted at 1216 Angstroms.

these studies are inherently complex. Thus direct analytic solutions are often not feasible, and numerical analysis is required.

3. LARGE ASTRONOMICAL DATASETS

As demonstrated below, there is currently a great deal of archived data in Astronomy at a variety of locations in a variety of different database systems systems. In this section we focus on ground-based surveys, ground-based observatories, and space-based observatories. We do not include any discussion of information repositories such as the Astrophysics Data System² (ADS), the Set of Identifications, Measurements, and Bibliography for Astronomical Data³ (SIMBAD), or the NASA Extragalactic Database⁴ (NED), extremely valuable as they are. This review focuses on more homogeneous collections of data from digital sky surveys and specific missions rather than archives which are more appropriately described as digital libraries for astronomy.

Furthermore, we do not discuss the large number of new initiatives, including the Large-Aperture Synoptic Survey Telescope (LSST), the California

²http://adswww.harvard.edu/

³http://cdsweb.u-strasbg.fr/Simbad.html

⁴http://ned.ipac.caltech.edu



Figure 1.4 Example of a discovery in the time domain. Images of a star, PVO 1558+3725, seen in the DPOSS plate overlaps in J (= green, top) F (= red, middle) and N (\approx near-infrared, bottom). Since the plates for the POSS-II survey were taken at different epochs (*i.e.* they were taken on different days), that can be separated by several years (the actual observational epoch is indicated below each panel), we have a temporal recording of the intensity of the star. Notice how the central star is significantly brighter in the lower right panel. Subsequent analysis has not indicated any unusual features, and, as a result, the cause, amplitude, and duration of the outburst are unknown.

Extremely Large Telescope (CELT), the Visible and Infrared Survey Telescope⁵ (VISTA), or the Next Generation Space Telescope⁶ (NGST), which will provide vast increases in the quality and quantity of astronomical data.

3.1 GROUND-BASED SKY SURVEYS

Of all of the different astronomical sources of data, digital sky surveys are the major drivers behind the fundamental changes underway in the field. Primarily

⁵http://www.vista.ac.uk

⁶http://www.ngst.stsci.edu/

this is the result of two factors: first, the sheer quantity of data being generated over multiple wavelengths, and second, as a result of the homogeneity of the data within each survey. The federation of different surveys would further improve the efficacy of future ground- and space-based targeted observations, and also open up entirely new avenues for research.

In this chapter, we describe only some of the currently existing astronomical archives as examples of the types, richness, and quantity of astronomical data which is already available. Due to the space limitations, we cannot cover many other, valuable and useful surveys, experiments and archives, and we apologize for any omissions. This summary is not meant to be complete, but merely illusory.

Photographic plates have long endured as efficient mechanisms for recording surveys (they have useful lifetimes in excess of one hundred years and offer superb information storage capacity, but unfortunately they are not directly computer-accessible and must be digitized before being put to a modern scientific use). Their preeminence in a digital world, however, is being challenged by new technologies. While many photographic surveys have been performed, *e.g.*, from the Palomar Schmidt telescope⁷ in California, and the UK Schmidt telescope in New South Wales, Australia, these data become most useful when the plates are digitized and cataloged.

While we describe two specific projects, as examples, several other groups have digitized photographic surveys and generated and archived the resulting catalogs, including the Minnesota Automated Plate Scanner⁸ (APS; Pennington et al., 1993), the Automated Plate Measuring Machine⁹ (APM; McMahon and Irwin, 1992) at the Institute of Astronomy, Cambridge, UK, the coordinates, sizes, magnitudes, orientations, and shapes (COSMOS; Yentis et al., 1992) and its successor, SuperCOSMOS¹⁰, plate scanning machines at the Royal Observatory Edinburgh. Probably the most popular of the digitized sky surveys (DSS) are those produced at the Space Telescope Science Institute¹¹ (STScI) and its mirror sites in Canada¹², Europe¹³, and Japan¹⁴.

DPOSS The Digitized Palomar Observatory Sky Survey¹⁵ (DPOSS) is a digital survey of the entire Northern Sky in three visible-light bands, formally

⁷A Schmidt telescope has an optical design which allows it to image a very wide field, typically several degrees on a side. This is in contrast to most large telescopes which have field of views that are measured in arcminutes.

⁸http://aps.umn.edu/

⁹http://www.ast.cam.ac.uk/~mike/casu/apm/apm.html

¹⁰http://www.roe.ac.uk/cosmos/scosmos.html

¹¹http://archive.stsci.edu/dss/

¹²http://cadcwww.dao.nrc.ca/dss/

¹³http://archive.eso.org/dss/dss/

¹⁴http://dss.nao.ac.jp

¹⁵http://dposs.caltech.edu/

indicated by g, r, and i (blue-green, red, and near-infrared, respectively). It is based on the photographic sky atlas, POSS-II, the second Palomar Observatory Sky Survey, which was completed at the Palomar 48-inch Oschin Schmidt Telescope (Reid et al., 1991). A set of three photographic plates, one in each filter, each covering 36 square degrees, were taken at each of 894 pointings spaced by 5 degrees, covering the Northern sky (many of these were repeated exposures, due to various artifacts such as the aircraft trails, plate defects, *etc.*). The plates were then digitized at the Space Telescope Science Institute (STScI), using a laser microdensitometer. The plates are scanned with 1.0"pixels, in rasters of 23,040 square, with 16 bits per pixel, producing about 1 Gigabyte per plate, or about 3 Terabytes of pixel data in total.

These scans were processed independently at STScI (for the purposes of constructing a new guide star catalog for the HST) and at Caltech (for the DPOSS project). Catalogs of all the detected objects on each plate were generated, down to the flux limit of the plates, which roughly corresponds to the equivalent blue limiting magnitude of approximately 22. A specially developed software package, called SKICAT (Sky Image Cataloging and Analysis Tool; Weir et al. 1995) was used to analyze the images. SKICAT incorporates some machine learning techniques for object classification and measures about 40 parameters for each object in each band. Star-galaxy classification was done using several methods, including decision trees and neural nets: for brighter galaxies, a more detailed morphological classification may be added in the near future. The DPOSS project also includes an extensive program of CCD calibrations done at the Palomar 60-inch telescope. These CCD data were used both for magnitude calibrations, and as training data sets for object classifiers in SKICAT. The resulting object catalogs were combined and stored in a Sybase relational DBMS system; however, a more powerful system is currently being implemented for more efficient scientific exploration. This new archive will also include the actual pixel data in the form of astrometrically and photometrically calibrated images.

The final result of DPOSS will be the Palomar Norris Sky Catalog (PNSC), which is estimated to contain about 50 to 100 million galaxies, and between 1 and 2 billion stars, with over 100 attributes measured for each object, down to the equivalent blue limiting magnitude of 22, and with star-galaxy classifications accurate to 90% or better down to the equivalent blue magnitude of approximately 21. This represents a considerable advance over other, currently existing optical sky surveys based on large-format photographic plates. Once the technical and sci-

entific verification of the final catalog is complete, the DPOSS data will be released to the astronomical community.

As an indication of the technological evolution in this field, the Palomar Oschin Schmidt telescope is now being retrofitted with a large CCD camera (QUEST2) as a collaborative project between Yale University, Indiana University, Caltech, and JPL. This will lead to pure digital sky surveys from Palomar Observatory in the future.

USNO-A2 The United States Naval Observatory Astrometric (USNO-A2) catalog¹⁶ (Monet et al., 1996) is a full-sky survey containing over five hundred million unresolved sources down to a limiting magnitude of $B \sim 20$ whose positions can be used for astrometric references. These sources were detected by the Precision Measuring Machine (PMM) built and operated by the United States Naval Observatory Flagstaff Station during the scanning and processing of the first Palomar Observatory Sky Survey (POSS-I) O and E plates, the UK Science Research Council SRC-J survey plates, and the European Southern Observatory ESO-R survey plates. The total amount of data utilized by the survey exceeds 10 Terabytes.

The USNO-A2 catalog is provided as a series of binary files, organized according to the position on the sky. Since the density of sources on the sky varies (primarily due to the fact that our galaxy is a disk dominated system), the number of sources in each file varies tremendously. In order to actually extract source parameters, special software, which is provided along with the data is required. The catalog includes the source position, right ascension and declination (in the J2000 coordinate system, with the actual epoch derived as the mean of the blue and red plate) and the blue and red magnitude for each star. The astrometry is tied to the ACT catalog (Urban et al., 1997). Since the PMM detects and processes at and beyond the nominal limiting magnitude of these surveys, a large number of spurious detections are initially included in the operational catalog. In order to improve the efficacy of the catalog, sources were required to be spatially coincident, within a 2" radius aperture, on the blue and red survey plate.

SDSS The Sloan Digital Sky Survey¹⁷ (SDSS) is a large astronomical collaboration focused on constructing the first CCD photometric survey of the North Galactic hemisphere (10,000 square degrees—one-fourth of the entire sky). The estimated 100 million cataloged sources from this sur-

¹⁶http://ftp.nofs.navy.mil/projects/pmm/a2.html

¹⁷http://www.sdss.org/

vey will then be used as the foundation for the largest ever spectroscopic survey of galaxies, quasars and stars.

The full survey is expected to take five years, and has recently begun full operations. A dedicated 2.5m telescope is specially designed to take wide field (3 degree x 3 degree) images using a 5 by 6 mosaic of 2048x2048 CCD's, in five wavelength bands, operating in scanning mode. The total raw data will exceed 40 TB. A processed subset, of about 1 TB in size, will consist of 1 million spectra, positions and image parameters for over 100 million objects, plus a mini-image centered on each object in every color. The data will be made available to the public (see, *e.g.*, Figure 1.5 for a public SDSS portal) at specific release milestones, and upon completion of the survey.

During the commissioning phase of the survey data was obtained, in part to test out the hardware and software components. Already, a wealth of new science has emerged from this data.

The Sloan Digital Sky Survey (SDSS) is a joint project of The University of Chicago, Fermilab, the Institute for Advanced Study, the Japan Participation Group, The Johns Hopkins University, the Max-Planck-Institute for Astronomy (MPIA), the Max-Planck-Institute for Astrophysics (MPA), New Mexico State University, Princeton University, the United States Naval Observatory, and the University of Washington.

There is a large number of experiments and surveys at aimed at detecting time-variable sources or phenomena, such as gravitational microlensing, optical flashes from cosmic gamma-ray bursts, near-Earth asteroids and other solar system objects, *etc.* A good list of project web-sites is maintained by Professor Bohdan Paczynski at Princeton¹⁸. Here we describe several interesting examples of such projects.

MACHO The MACHO project¹⁹ was one of the pioneering astronomical projects in generating large datasets. This project was designed to look for a particular type of dark matter collectively classified as Massive Compact Halo Objects (*e.g.*, brown dwarfs or planets) from whence the project's name was derived. The signature for sources of this type is the amplification of the light from extragalactic stars by the gravitational lens effect of the intervening MACHO. While the amplitude of the amplification can be large, the frequency of such events is extremely rare. Therefore, in order to obtain a statistically useful sample, it is necessary to photometrically monitor several million stars over a period of several

¹⁸http://astro.princeton.edu/faculty/bp.html

¹⁹http://wwwmacho.anu.edu.au/



Figure 1.5 A public portal into the Sloan Digital Sky Survey, which is the cosmic equivalent to the Human Genome project.

years. The MACHO Project is a collaboration between scientists at the Mt. Stromlo and Siding Spring Observatories, the Center for Particle Astrophysics at the Santa Barbara, San Diego, and Berkeley campuses of the University of California, and the Lawrence Livermore National Laboratory.

The MACHO project built a two channel system that employs eight 2048x2048 CCDs, which was mounted and operated on the 50-inch telescope at Mt. Stromlo. This large CCD instrument presented a high data rate (especially given that the survey commenced in 1992) of approximately several Gigabytes per night. Over the course of the survey, nearly 100,000 images were taken and processed, with a total data volume exceeding 7 Terabytes. While the original research goal of finding microlensing events was realized (essentially by a real-time data-analysis system), the MACHO data provides an enormously useful resource for studying a variety of variable sources. Unfortunately, funding was never secured to build a data archive, limiting the utility of the data primarily to only those members of the MACHO science team. Another similar project is the OGLE-II²⁰, or the second Optical Gravitational Lensing Experiment, which has a total data volume in excess of one Terabyte.

ROTSE The Robotic Optical Transient Search Experiment²¹ is an experimental program to search for astrophysical optical transients on time scales of a fraction of a second to a few hours. While the primary incentive of this experiment has been to find the optical counterparts of gamma-ray bursts (GRBs), additional variability studies have been enabled, including a search for orphan GRB afterglows, and an analysis of a particular type of variable star, known as an RR Lyrae, which provides information on the structure of our Galaxy.

The ROTSE project initially began operating in 1998, with a four-fold telephoto array, imaging the whole visible sky twice a night to limiting flux limit of approximately 15.5. The total data volume for the original project is approximately four Terabytes. Unlike other imaging programs, however, the large field of view of the telescope results in a large number of sources per field (approximately 40,000). Therefore, reduction of the imaging data to object lists does not compress the data as much as is usual in astronomical data. The data is persisted on a robotic tape library, but insufficient resources have prevented the creation of a public archive.

The next stage of the ROTSE project is a set of four (and eventually six) half meter telescopes to be sited globally. Each telescope has a 2 degree field of view and operations, including the data analysis, and it will be fully automated. The first data is expected to begin to flow during 2001 and the total data volume will be approximately four Terabytes. The limiting flux of the next stage of the ROTSE experiment will be approximately 18 – 19, or more than ten times deeper than the original experiment. The ROTSE (and other variability survey) data will provide important multi-epoch measurements as a complement to the single epoch surveys (*e.g.*, DPOSS, USNOA2, and the SDSS). Other examples of similar programs include the Livermore Optical Transient Imaging System (LOTIS) program²², which is nearly identical to the original ROTSE experiment, and its successor, Super-LOTIS.

NEAT Near Earth Asteroid Tracking (NEAT) $program^{23}$ is one of several programs that are designed to discover and characterize near earth objects (*e.g.*, Asteroids and comets). Fundamentally, these surveys cover thousands of square degrees of the sky every month to a limiting flux depth

²⁰http://astro.princeton.edu/~ogle

²¹http://www.umich.edu/~rotse

²²http://hubcap.clemson.edu/~ggwilli/LOTIS/

²³http://neat.jpl.nasa.gov/

of approximately 17 - 20, depending on the survey. All together, these programs (which also include Catalina²⁴, LINEAR²⁵, LONEOS²⁶, and Spacewatch²⁷) generate nearly 200 Gigabytes of data a night, yet due to funding restrictions, a large part of this data is not archived. NEAT is currently the only program which provides archival access to its data through the skymorph project²⁸ (see Figure 1.6 for the skymorph website). All told, these surveys have around 10 Terabytes of imaging data in hand, and continue to operate. The NEAT program has recently taken over the Palomar Oschin 48-inch telescope, which was used to generate the two POSS photographic surveys, in order to probe wider regions of the sky to an even deeper limiting flux value.

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Figure 1.6 The skymorph web-site, which provides access to the data from the NEAT program.

2MASS The Two Micron All-Sky Survey²⁹ (2MASS) is a near-infrared (J, H, and K_S) all sky survey. The 2MASS project is a collaboration between the The University of Massachusetts, which constructed the observatory

²⁴http://www.lpl.arizona.edu/css/

²⁵http://www.ll.mit.edu/LINEAR/

²⁶http://asteroid.lowell.edu/asteroid/loneos/loneos_disc.html

²⁷http://www.lpl.arizona.edu/spacewatch/

²⁸http://skys.gsfc.nasa.gov/skymorph/skymorph.html

²⁹http://www.ipac.caltech.edu/2mass/

facilities and operates the survey, and the Infrared Processing and Analysis Center (Caltech), which is responsible for all data processing and archive issues. The survey began in the spring of 1997, completed survey quality observations in 2000, and is expected to publish the final catalog sometime in 2002.

The 2MASS survey utilized two new, highly automated 1.3m telescopes, one at Mt. Hopkins, AZ and one at CTIO, Chile. Each telescope was equipped with a three channel camera, which uses HgCdTe detectors, and was capable of observing the sky simultaneously at J,H, and K_S . The survey includes over twelve Terabytes of imaging data, and the final catalog is expected to contain more than one million resolved galaxies, and more than three hundred million stars and other unresolved sources to a 10σ limiting magnitude of $K_S < 14.3$.

The 2MASS program is leading the way in demonstrating the power of public archives to the astronomical community. All twelve Terabytes of imaging data are available on near-online tape storage, and the actual catalogs are stored in an Informix backed archive (see Figure 1.9 for the public access to the 2MASS data). When complete, the survey will produce the following data products:

- a digital atlas of the sky comprising more than 1 million 8'x16' images having about 4" spatial resolution in each of the three wavelength bands,
- a point source catalog containing accurate (better than 0.5") positions and fluxes (less than 5% for $K_S > 13$) for approximately 300, 000, 000 stars.
- an extended source catalog containing positions and total magnitudes for more than 500,000 galaxies and other nebulae.
- **NVSS** The National Radio Astronomical Observatory (NRAO), Very Large Array (VLA), Sky Survey (NVSS) is a publicly available, radio continuum survey³⁰ covering the sky north of -40 degrees declination. The survey catalog contains over 1.8 millions discrete sources with total intensity and linear polarization image measurements (Stokes I, Q, and U) with a resolution of 45", and a completeness limit of about 2.5 mJy. The NVSS survey is now complete, containing over two hundred thousand snapshot fields. The NVSS survey was performed as a community service, with the principal data products being released to the public by anonymous FTP as soon as they were produced and verified. The

³⁰http://www.cv.nrao.edu/~jcondon/nvss.html

primary means of accessing the NVSS data products remains the original anonymous FTP service, however, other archive sites have begun to provide limited data browsing and access to this important dataset.

The principal NVSS data products are a set of 2326 continuum map "cubes," each covering an area of 4 degrees by 4 degrees with three planes containing the Stokes I, Q, and U images, and a catalog of discrete sources on these images (over 1.8 million sources are in the entire survey). Every large image was constructed from more than one hundred of the smaller, original snapshot images.

FIRST The Faint Images of the Radio Sky at Twenty-cm (FIRST) survey³¹ is an ongoing, publicly available, radio snapshot survey that is scheduled to cover approximately ten thousand square degrees of the North and South Galactic Caps in 1.8" pixels (currently, approximately eight thousand square degrees have been released). The survey catalog, when complete should contain around one million sources with a resolution of better than 1". The FIRST survey is being performed at the NRAO VLA facility in a configuration that provides higher spatial resolution than the NVSS, at the expense of a smaller field of view.

A final atlas of radio image maps with 1.8" pixels is produced by coadding the twelve images adjacent to each pointing center. A source catalog including peak and integrated flux densities and sizes derived from fitting a two-dimensional Gaussian to each source is generated from the atlas. Approximately 15% of the sources have optical counterparts at the limit of the POSS I plates ($E \sim 20$); unambiguous optical identifications (< 5% false rates) are achievable to $V \sim 24$. The survey area has been chosen to coincide with that of the Sloan Digital Sky Survey (SDSS). It is expected that at the magnitude limit of the SDSS, approximately 50% of the optical counterparts to FIRST sources will be detected. Both the images and the catalogs constructed from the FIRST observations are being made available to the astronomical community via the project web-site (see Figure 1.7 for the public web-site) as soon as sufficient quality-control tests have been completed.

3.2 GROUND-BASED OBSERVATORY ARCHIVES

Traditional ground-based observatories have been saving data, mainly as emergency back-ups for the users, for a significant time, accumulating impressive quantities of highly valuable, but heterogeneous data. Unfortunately, with some notable exceptions, the heterogeneity and a lack of adequate funding have

³¹http://sundog.stsci.edu/top.html

FIRST Catalog Search - Microsoft Internet Explorer	
FIRST Catalog Search	
RA and Dec: 10 50 07.270 +30 40 37.52 Equinox: J2000 ▼	
Search Radius: 30 arcsec	
Search the Catalog Reset Form Help	
Dibos Hund What New Description States of Observation	
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Figure 1.7 The FIRST survey web search engine. Both images and catalog entries can be retrieved.

limited the efforts to properly archive this wealth of information and make it easily available to the broad astronomical community. We see the development of good archives for major ground-based observatories as one of the most pressing needs in this field, and a necessary step in the development of the National Virtual Observatory.

In this section, we discuss three specific ground-based observatories: the National Optical Astronomical Observatories (NOAO), the National Radio Astronomical Observatory (NRAO), and the European Southern Observatory (ESO), focusing on their archival efforts. In addition to these three, many other observatories have extensive archives, including the Canada-France-Hawaii telescope³² (CHFT), the James Clerk Maxwell Telescope³³ (JCMT), the Isaac Newton Group of telescopes at La Palma³⁴ (ING), the Anglo-Australian Observatory³⁵ (AAT), the United Kingdom Infrared Telescope³⁶ (UKIRT), and the Australia National Telescope Facility³⁷ (ATNF).

³²http://www.cfht.hawaii.edu/

³³http://www.jach.hawaii.edu/JACpublic/JCMT/home.html

³⁴http://www.ing.iac.es/

³⁵http://site.aao.gov.au/AAO/

³⁶http://www.jach.hawaii.edu/JACpublic/UKIRT/home.html

³⁷http://www.atnf.csiro.au/

NOAO The National Optical Astronomy Observatory³⁸ (NOAO) is a US organization that manages ground-based, national astronomical observatories, including the Kitt Peak National Observatory, Cerro Tololo Inter-American Observatory, and the National Solar Observatory. NOAO also represents the US astronomical community in the International Gemini Project. As a national facility, NOAO telescopes are open to all astronomers regardless of institutional affiliation, and has provided important scientific opportunities to astronomers throughout the world, who would otherwise had little or no opportunity to obtain astronomical observations.

The NOAO has been archiving all data from their telescopes in a program called save-the-bits, which, prior to the introduction of survey-grade instrumentation, generated around half a Terabyte and over 250,000 images a year. With the introduction of survey instruments and related programs, the rate of data accumulation has increased, and NOAO now manages over 10 Terabytes of data.

- **NRAO** The National Radio Astronomy Observatory³⁹ (NRAO) is a US research facility that provides access to radio telescope facilities for use by the scientific community, in analogy to the primarily optical mission of the NOAO. Founded in 1956, the NRAO has its headquarters in Charlottesville, VA, and operates major radio telescope facilities at Green Bank, WV, Socorro, NM, and Tucson, AZ. The NRAO has been archiving their routine observations and has accumulated over ten Terabytes of data. They also have provided numerous opportunities for surveys, including the previously discussed NVSS and FIRST radio surveys as well as the Green Bank surveys.
- **ESO** The European Southern Observatory⁴⁰ (ESO), operates a number of telescopes (including the four 8m class VLT telescopes) at two observatories in the southern hemisphere: the La Silla Observatory, and the Paranal observatory. ESO is currently supported by a consortium of countries, with Headquarters in Garching, near Munich, Germany.

As with many of the other ground-based observatories, ESO has been archiving data for some time, with two important differences. First, they were one of the earliest observatories to appreciate the importance of community service survey programs (these programs generally probe to fainter flux limits over a significantly smaller area than the previously

³⁸http://www.noao.edu/

³⁹http://www.nrao.edu/

⁴⁰http://www.eso.org/

discussed surveys), which are made accessible to the international astronomical community in a relatively short timescale. Second, appreciating the legacy aspects of the four 8 meter Very Large Telescopes, ESO intentionally decided to break with tradition, and imposed an automatic operation of the telescopes that provides a uniform mechanism for data acquisition and archiving, comparable to what has routinely been done for space-based observatories (see the next section). Currently, the ESO data archive is starting to approach a steady state rate of approximately 20 Terabytes of data per year from all of their telescopes. This number will eventually increase to several hundred Terabytes with the completion of the rest of the planned facilities, including the VST, a dedicated survey telescope similar in nature to the telescope that was built for the SDSS project.

3.3 NASA SPACE-BASED OBSERVATORY ARCHIVES

With the continual advancement of technology, ground-based observations continue to make important discoveries. Our atmosphere, however, absorbs radiation from the majority of the electromagnetic spectrum, which, while important to the survival of life, is a major hindrance when trying to untangle the mysteries of the cosmos. Thus space-based observations are critical, yet they are extremely expensive. The resulting data is extremely valuable, and all of the generated data is archived. While there have been (and continue to be) a large number of satellite missions, we will focus on three major NASA archival centers: MAST, IRSA, and HEASARC (officially designated as NASA's distributed Space Science Data Services), the Chandra X-ray Observatory archive (CXO), and the National Space Science Data Center (NSSDC).

MAST The Multimission Archive at the Space Telescope Science Institute⁴¹ (MAST) archives a variety of astronomical data, with the primary emphasis on the optical, ultraviolet, and near-infrared parts of the spectrum. MAST provides a cross correlation tool that allows users to search all archived data for all observations which contain sources from either archived or user supplied catalog data. In addition, MAST provides individual mission query capabilities. Preview images or spectra can often be obtained, which provides useful feedback to archive users. The dominant holding for MAST is the data archive from the Hubble Space Telescope (see Figure 1.8 for the HST archive web-site). This archive

⁴¹http://archive.stsci.edu/mast.html

has been replicated at mirror sites in Canada⁴², Europe⁴³ and Japan⁴⁴, and has often taken a lead in astronomical archive developments.

HST Archive Search - Microsoft Int	ernet Explorer		_0
<u>File E</u> dit <u>V</u> iew F <u>a</u> vorites <u>T</u> ools	Help		No.
HST Archive			
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Archive Status	hst iue euve	UIT HUT FIRST MD	S DSS Starcast
Object N	° SI ○ SI	Resolver MBAD © NED Res Don't resolve	olve
RA	Dec	Radius (arcmin)	<u>Equinox</u> J2000 ▼
Observation Date	Exp Time (sec)	<u>Observer</u>	Program ID
Target I	Description	Datase	t Name
SEARCH	lear form	Reset to defaults	Help
<u>8</u>) Internet

Figure 1.8 The Hubble Space Telescope (HST) archive (part of the MAST holdings) interface.

Based on the archival nature of the requested data, MAST provides data access in a variety of different ways, including intermediate disk staging and FTP retrieval and direct web-based downloads. MAST holdings currently exceed ten Terabytes, including or providing links to archival data for the following missions or projects:

- the Hubble Space Telescope (HST),
- the International Ultraviolet Explorer (IUE),
- Copernicus UV Satellite (OAO-3),
- the Extreme Ultraviolet Explorer (EUVE),
- the two space shuttle ASTRO Missions:
 - the Ultraviolet Imaging Telescope (UIT),

⁴²http://cadcwww.dao.nrc.ca/hst/

⁴³http://www.stecf.org/

⁴⁴http://hst.nao.ac.jp/

- the Wisconsin Ultraviolet Photo Polarimetry Experiment (WUPPE),
- the Hopkins Ultraviolet Telescope (HUT),
- the FIRST (VLA radio data) survey,
- the Digitized Sky Survey,
- the Roentgen Satellite (ROSAT) archive,
- the Far Ultraviolet Spectroscopic Explorer (FUSE),
- Orbiting and Retrieval Far and Extreme Ultraviolet Spectrograph (ORFEUS) missions,
- the Interstellar Medium Absorption Profile Spectrograph(IMAPS) (first flight),
- the Berkeley Extreme and Far-UV Spectrometer (BEFS) (first flight).

The Hubble Space Telescope (HST) is the first of NASA's great observatories, and provides high-resolution imaging and spectrographic observations from the near-ultraviolet to the near-infrared parts of the electro-magnetic spectrum (0.1 - 2.5 microns). It is operated by the Space Telescope Science Institute (STScI) is located on the campus of the Johns Hopkins University and is operated for NASA by the Association of Universities for Research in Astronomy (AURA).

IRSA The NASA Infrared Processing and Analysis Center (IPAC) Infrared Science Archive⁴⁵ (IRSA) provides archival access to a variety of data, with a primary focus on data in the infrared portion of the spectrum (see Figure 1.9 for the IRSA archive web-site). IRSA has taken a strong leadership position in developing software and Internet services to facilitate access to astronomical data products. IRSA provides a cross-correlation tool allowing users to extract specific data on candidate targets from a variety of sources. IRSA provides primarily browser based query mechanisms, including access to both catalog and image holdings.

IRSA contains over fifteen Terabytes of data, mostly related to the 2MASS survey, and currently maintains the archives for the following datasets at IPAC:

- the Two Micron All-Sky Survey (2MASS),
- the Space Infrared Telescope Facility (SIRTF),
- the European Infrared Space Observatory (ISO),
- the Midcourse Space Experiment (MSX),

⁴⁵http://irsa.ipac.caltech.edu

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Figure 1.9 The IRSA Public access site. From this web-site, an archive user can query the contents of the publicly available 2MASS data, as well as other datasets that have been ingested into the IRSA Informix database server.

• the Infrared Astronomical Satellite (IRAS).

The Space Infrared Telescope (SIRTF) observatory will be the fourth and final of NASA's great observatories, and will provide imaging and spectrographic observations in the infrared part of the electro-magnetic spectrum (3 – 180 microns). SIRTF is expected to be launched in 2002. The SIRTF science center (SSC) is located on the campus of the California Institute of Technology and is operated for NASA by the Jet propulsion Laboratory.

The Infrared Space Observatory (ISO) operated at wavelengths from 2.5 - 240 microns, obtaining both imaging and spectroscopic data are available over a large area of the sky. The Midcourse Space Experiment (MSX) operated from 4.2 - 26 microns, and mapped the Galactic Plane, the gaps in the IRAS data, the zodiacal background, confused regions away from the Galactic Plane, deep surveys of selected fields at high galactic latitudes, large galaxies, asteroids and comets. The Infrared Astronomical Satellite (IRAS) performed an unbiased all sky survey at 12, 25, 60 and 100 microns, detecting approximately 350, 000 high signal-tonoise infrared sources split between the faint and point source catalogs.

A significantly larger number of sources (> 500,000) are included in the faint source reject file, which were below the flux threshold required for the faint source catalog.

HEASARC The High Energy Astrophysics Science Archive Research Center⁴⁶ (HEASARC) is a multi-mission astronomy archive with primary emphasis on the extreme ultra-violet, X-ray, and Gamma ray spectral regions. HEASARC currently holds data from 20 observatories covering 30 years of X-ray and gamma-ray astronomy. HEASARC provides data access via FTP and the Web (see Figure 1.10), including the Skyview interface, which allows multiple images and catalogs to be compared.



Figure 1.10 The HEASARC public access site, where data from the x-ray and gamma-ray space missions are archived.

The HEASARC archive currently includes over five Terabytes of data, and will experience significant increases with the large number of highenergy satellite missions that are either currently or soon will be in operation. HEASARC currently provides archival access to the following missions:

• the Roentgen Satellite (ROSAT),

⁴⁶http://heasarc.gsfc.nasa.gov

- the Advanced Satellite for Cosmology (ASCA),
- BeppoSAX,
- the Compton Gamma Ray Observatory (CGRO), the second of NASA's great observatories,
- the Extreme Ultraviolet Explorer (EUVE),
- the High Energy Astrophysics Observatory (HEAO 1),
- the Einstein Observatory (HEAO 2),
- the European Space Agency's X-ray Observatory (EXOSAT),
- the Rossi X-ray Timing Explorer (Rossi XTE),
- the Advanced Satellite for X-ray Astronomy (Chandra),
- the X-ray Multiple Mirror Satellite (XMM-Newton),
- the High Energy Transient Explorer (HETE-2),

Several of these missions elicit further discussion. First, the Einstein Observatory⁴⁷ was the first fully imaging X-ray telescope put into space, with an angular resolution of a few arcseconds and was sensitive over the energy range 0.2 - 3.5 keV. The ROSAT⁴⁸ satellite was an X-ray observatory that performed an all sky survey in the 0.1 - 2.4 keV range as well as numerous pointed observations. The full sky survey data has been publicly released, and there are catalogs of both the full sky survey (Voges et al., 1999) as well as serendipitous detections from the pointed observations (White et al., 1994). The ASCA⁴⁹ satellite operated in the energy range 0.4 - 10 keV, that performed several small area surveys and obtained valuable spectral data on a variety of astrophysical sources. Finally, the Chandra (also see the next section) and XMM-Newton⁵⁰ satellites are currently providing revolutionary new views on the cosmos, due to their increased sensitivity, spatial resolution and collecting area.

Skyview⁵¹ is a web-site operated from HEASARC which is billed as a "Virtual Observatory on the Net" (see Figure 1.11). Using public-domain data, Skyview allows astronomers to generate images of any portion of the sky at wavelengths in all regimes from radio to gamma-ray. Perhaps the most powerful feature of the Skyview site is its ability to handle the geometric and coordinate transformations required for presenting the requested data to the user in the specified format.

⁴⁷ http://heasarc.gsfc.nasa.gov/docs/einstein/heao2.html

⁴⁸http://wave.xray.mpe.mpg.de/rosat/

⁴⁹http://www.astro.isas.ac.jp/asca/index-e.html

⁵⁰http://xmm.vilspa.esa.es/



Figure 1.11 The Skyview virtual telescope site, which provides access to a large number of digital imagery and catalog information.

CDA The Chandra X-ray observatory⁵² is third of NASA's great observatories, and provides high-resolution imaging and spectrographic observations in the X-ray part of the electro-magnetic spectrum. Chandra was launched by the Space Shuttle Columbia during July, 1999. Unlike the Hubble data archive, which is part of MAST, and the SIRTF data archive, which will be part of IRSA, the Chandra Data Archive (CDA) is part of the Chandra X-Ray Observatory Science Center (CXC) which is operated for NASA by the Smithsonian Astrophysical Observatory. The data is also archived at HEASARC, which is the relevant wavelength space mission archive.

The Chandra data products can be roughly divided into science-related and engineering data. The engineering data products include all data relating to the spacecraft subsystems: including such quantities as spacecraft temperature and operating voltages. The scientific data products are divided into three categories: primary, secondary, and supporting products. Primary products are generally the most desired, but the secondary products can provide important information required for more sophisti-

⁵²http://chandra.harvard.edu/

cated analysis and, possibly, limited reprocessing and fine-tuning. The actual data can be retrieved via several different mechanisms or media, including web-based downloads, staged anonymous FTP retrieval, or mailed delivery of 8 mm Exabyte, 4 mm DAT, or CDROMs.

- **NSSDC** The National Space Science Data Center⁵³ (NSSDC) provides networkbased and offline access to a wide variety of data from NASA missions, including the Cosmic Background Explorer⁵⁴ (COBE), accruing data at the rate of several Terabytes per year. NSSDC was first established at the Goddard Space Flight Center in 1966, and continues to archive mission data, including both independently and not independently (*i.e.* data that requires other data to gain utility) useful data. Currently, the majority of network-based data dissemination is via WWW and FTP, and most offline data dissemination is via CD-ROM. NSSDC is generally regarded as the final repository of all NASA space mission data.
- **PDS** In this chapter, we do not discuss in detail the great wealth of data available on solar system objects. The site for the archival access to scientific data from NASA planetary missions, astronomical observations, and laboratory measurements is the Planetary Data System⁵⁵ (PDS). The homepage for the PDS is displayed in Figure 1.12, and provides access to data from the Pioneer, Voyager, Mariner, Magellan, NEAR spacecraft missions, as well as other data on asteroids, comets, and the Planets including Earth.

4. THE FUTURE OF OBSERVATIONAL ASTRONOMY: VIRTUAL OBSERVATORIES

Raw data, no matter how expensively obtained, are no good without an effective ability to process them quickly and thoroughly, and to refine the essence of scientific knowledge from them. This problem has suddenly increased by orders of magnitude, and it keeps growing.

A prime example is the efficient scientific exploration of the new multi-Terabyte digital sky surveys and archives. How can one make efficiently discoveries in a database of billions of objects or data vectors? What good are the vast new data sets if we cannot fully exploit them?

In order to cope with this data flood, the astronomical community started a grassroots initiative, the National (and ultimately Global) Virtual Observatory (see, *e.g.*, Brunner et al., 2001, for a virtual observatory conference

⁵³http://nssdc.gsfc.nasa.gov/

⁵⁴http://space.gsfc.nasa.gov/astro.cobe

⁵⁵http://pds.jpl.nasa.gov



Figure 1.12 The Planetary Data System web-site. From this web-site, users can query and extract archived the enormous quantity of data that has been obtained on the Solar system objects.

proceedings). Recognizing the urgent need, the National Academy of Science Astronomy and Astrophysics Survey Committee, in its new decadal survey entitled *Astronomy and Astrophysics in the New Millennium*, recommends, as a first priority, the establishment of a National Virtual Observatory. The NVO will likely grow into a Global Virtual Observatory, serving as the fundamental information infrastructure for astronomy and astrophysics in the next century. We envision productive international cooperation in this rapidly developing new field.

The NVO would federate numerous large digital sky archives, provide the information infrastructure and standards for ingestion of new data and surveys, and develop the computational and analysis tools with which to explore these vast data volumes. It would provide new opportunities for scientific discovery that were unimaginable just a few years ago. Entirely new and unexpected scientific results of major significance will emerge from the combined use of the resulting datasets, science that would not be possible from such sets used singly. The NVO will serve as *an engine of discovery for astronomy* (NVO Informal Steering Committee, 2001).

Implementation of the NVO involves significant technical challenges on many fronts: How to manage, combine, analyze and explore these vast amounts

of information, and to do it quickly and efficiently? We know how to collect many bits of information, but can we effectively refine the essence of knowledge from this mass of bits? Many individual digital sky survey archives, servers, and digital libraries already exist, and represent essential tools of modern astronomy. However, in order to join or federate these valuable resources, and to enable a smooth inclusion of even greater data sets to come, a more powerful infrastructure and a set of tools are needed.

The rest of this review focuses on the two core challenges that must be tackled to enable the new, virtual astronomy:

- 1. Effective federation of large, geographically distributed data sets and digital sky archives, their matching, their structuring in new ways so as to optimize the use of data-mining algorithms, and fast data extraction from them.
- 2. Data mining and "knowledge discovery in databases" (KDD) algorithms and techniques for the exploration and scientific utilization of large digital sky surveys, including combined, multi-wavelength data sets.

These services would carry significant relevance beyond Astronomy as many aspects of society are struggling with information overload. This development can only be done by a wide collaboration, that involves not only astronomers, but computer scientists, statisticians and even participants from the IT industry.

4.1 ARCHITECTING THE VIRTUAL OBSERVATORY

The foundation and structure of the National Virtual Observatory (NVO) are not yet clearly defined, and are currently the subject of many vigorous development efforts. One framework for many of the basic architectural concepts and associated components of a virtual observatory, however, has become popular. First is the requirement that, if at all possible, all data must be maintained and curated by the respective groups who know it best — the survey originators. This requires a fully distributed system, as each survey must provide the storage, documentation, and services that are required to participate in a virtual observatory.

The interconnection of the different archive sites will need to utilize the planned high-speed networks, of which there are several testbed programs already available or in development. A significant fraction of the technology for the future Internet backbone is already available, the problem is finding real-world applications which can provide a sufficient load. A Virtual Observatory, would, of course, provide heavy network traffic and is, therefore, a prime candidate for early testing of any future high-speed networks.

The distributed approach advocated by this framework (see Figure 1.13 for a demonstration) relies heavily on an the ability of different archives to participate



Figure 1.13 One straw-man layout for a virtual observatory prototype, demonstrating the highly distributed nature of the system. Of particular importance are the high speed network interconnections, extremely large storage systems, and high performance compute servers. Image Credit: Dave Curkendall and the ALPHA group, (JPL).

in "collaborative querying". This tight integration requires that everything must be built using appropriately developed standards, detailing everything from how archives are "discovered" and "join" the virtual observatory, to how queries are expressed and data is transferred. Once these standards have been developed, implementation (or retrofitting as the case may be) of tools, interfaces, and protocols that operate within the virtual observatory can begin.

The architecture of a virtual observatory is not only dependent on the participating data centers, but also on the users it must support. For example, it is quite likely that the general astronomy public (*e.g.*, amateur astronomers, K-12 classrooms, *etc.*) would use a virtual observatory in a casual lookup manner (*i.e.* the web model). On the other hand, a typical researcher would require more complex services, such as large data retrieval (*e.g.*, images) or crossarchive joins. Finally, there will also be the "power users" who would require heavy post-processing of query results using super-computing resources (*e.g.*, clustering analysis).

From these user models we can derive "use cases", which detail how a virtual observatory might be utilized. Initially, one would expect a large number of distinct "exploratory" queries as astronomers explore the multi-dimensional

nature of the data. Eventually the queries will become more complex and employ a larger scope or more powerful services. This model requires the support of several methods for data interaction: manual browsing, where a researcher explores the properties of an interesting class of objects; crossidentification queries, where a user wants to find all known information for a given set of sources; sweeping queries, where large amounts of data (*e.g.*, large areal extents, rare object searches) are processed with complex relationships; and the creation of new "personal" subsets or "official" data products. This approach leads, by necessity, to allowing the user to perform customizable, complex analysis (*i.e.* data-mining) on the extracted data stream.

4.2 CONNECTING DISTRIBUTED ARCHIVES

As can be seen from Section 3., a considerable amount of effort has been expended within the astronomical community on archiving and processing astronomical data. On the other hand, very little has been accomplished in enabling collaborative, cross-archive data manipulation (see Figure 1.14). This has been due, in part, to the previous dearth of large, homogeneous, multi-wavelength surveys; in other words, the payoff for federating the disparate datasets has previously been too small to make the effort worthwhile. Here we briefly outline some of the key problem areas (*cf.* Szalay and Brunner, 1999) for a more detailed discussion), that must be addressed in order to properly build the foundation for the future virtual observatories.

4.2.1 Communication Fundamentals. The first requirement for connecting highly distributed datasets is that they must be able to communicate with each other. This communication takes multiple roles, including the initiation of communication, discovering the holdings and capabilities of each archive, the actual process of querying, the streaming of data, and an overall control structure. None of these ideas are entirely new, the general Information Technology field has been confronting similar issues and solutions, such as Grid frameworks (Foster and Kesselman, 2001), JINI⁵⁶ and the Web services model (see, *e.g.*, the IBM Web Service web-site⁵⁷) for more information) are equally applicable.

Clearly, the language for communicating will be the extensible markup language (XML), using a community defined standard schema. This will allow for control of the inter-archive communication and processing (*e.g.*, the ability to perform basic checkpoint operations on a query: stop, pause, restart, abort, and provide feedback to the end-user). A promising, and simple mechanism

⁵⁶A registered trademark of the SUN Microsystems corporation.

⁵⁷http://www.ibm.com/developerworks/webservices/



Figure 1.14 A prototype blueprint for the system architecture of a virtual observatory. The key concept throughout our approach is the plug—and—play model where different archives, compute services and user tools all interact seamlessly. This system model is predicated on the universal adoption of standards dictating everything from how archives communicate with each other to how data is transferred between archives, services and users.

for providing the archive communication endpoints is through web services, which would be built using the Simple Object Access Protocol⁵⁸ (SOAP), Web Services Description Language⁵⁹ (WSDL), and a common Universal Description, Discovery, and Integration⁶⁰ (UDDI) registry. An additional benefit of this approach is that pre-existing or legacy archival services can be retrofitted (by mapping a new service onto existing services) in order to participate in collaborative querying.

This model also allows for certain optimizations to be performed depending on the status of the archival connections (*e.g.*, network weather). Eventually, a learning mechanism can be applied to analyze queries, and using the accumulated knowledge gained from past observations (*i.e.* artificial intelligence), queries can be rearranged in order to provide further performance enhancements.

⁵⁸http://www.w3.org/TR/2000/NOTE-SOAP-20000508/

⁵⁹http://xml.coverpages.org/wsdl.html

⁶⁰http://www.uddi.org/

4.2.2 Archival Metadata. In order for the discovery process to be successful, the archives must communicate using shared semantics. Not only must this semantic format allow for the transfer of data contents and formats between archives, but it also should clearly describe the specific services that an archive can support (such as cross-identification or image registration) and the expected format of the input and output data. Using the web service model, our services would be registered in a well known UDDI registry, and communicate their capabilities using WSDL. Depending on the need of the consumer, different amounts (or levels) of detailed information might be required, leading to the need for a hierarchical representation. Once again, the combination of XML and a standardized XML Schema language provides an extremely powerful solution, as is easily generated, and can be parsed by machines and read by humans with equal ease. By adopting a standardized schema, metadata can be easily archived and accessed by any conforming application.

4.2.3 High Performance Data Streaming. Traditionally, astronomers have communicated data either in ASCII text (either straight or compressed), or by using the community standard Flexible Image Transport Standard (FITS). The true efficacy of the FITS format as a streaming format, however, is not clear, due to the difficulty of randomly extracting desired data or shutting off the stream. The ideal solution would pass different types of data (*i.e.* tabular, spectral, or imaging data) in a streaming fashion (similar to MPI—Message Passing Interface), so that analysis of the data does not need to wait for the entire dataset before proceeding. In the web services model, this would allow different services to cooperate in a head-to-tail fashion (*i.e.* the UNIX pipe scenario). This is still a potential concern, as the ability to handle XML encoded binary data is not known.

4.2.4 Astronomical Data Federation. Separate from the concerns of the physical federation of astronomical data via a virtual observatory paradigm is the issue of actually correlating the catalog information from the diverse array of multiwavelength data (see the skyserver project ⁶¹ for more information). While seemingly simple, the problem is complicated by the several factors.

First is the sheer size of the problem, as the cross-identification of billions of sources in both a static and dynamic state over thousands of square degrees in a multi-wavelength domain (Radio to X-Ray) is clearly a computationally challenging problem, even for a consolidated archive. The problem is further complicated by the fact that observational data is always limited by the available technology, which varies greatly in sensitivity and angular resolution as a

⁶¹http://www.skyserver.org/

function of wavelength (*e.g.*, optical-infrared resolution is generally superior to high energy resolution).

Furthermore, the quality of the data calibration (either spectral, temporal, or spatial) can also vary greatly, making it extremely difficult to to unambiguously match sources between different wavelength surveys. Finally, the sky looks different at different wavelengths (see, *e.g.*, Figure 1.1), which can produce one-to-one, many-to-one, one-to-one, many-to-many, and even one/many-to-none scenarios when federating multiwavelength datasets. As a result, sometimes the source associations must be made using probabilistic methods (Lonsdale et al., 1998; Rutledge et al., 2000).

4.3 DATA MINING AND KNOWLEDGE DISCOVERY

Key to maximizing the knowledge extracted from the ever-growing quantities of astronomical (or any other type of) data is the successful application of datamining and knowledge discovery techniques. This effort as a step towards the development of the next generation of science analysis tools that redefine the way scientists interact and extract information from large data sets, here specifically the large new digital sky survey archives, which are driving the need for a virtual observatory (see, *e.g.*, Figure 1.15 for an illustration).

Such techniques are rather general, and should find numerous applications outside astronomy and space science. In fact, these techniques can find application in virtually every data-intensive field. Here we briefly outline some of the applications of these technologies on massive datasets, namely, unsupervised clustering, other Bayesian inference and cluster analysis tools, as well as novel multidimensional image and catalog visualization techniques. Examples of particular studies may include:

- 1. Various classification techniques, including decision tree ensembles and nearest-neighbor classifiers to categorize objects or clusters of objects of interest. Do the objectively found groupings of data vectors correspond to physically meaningful, distinct types of objects? Are the known types recovered, and are there new ones? Can we refine astronomical classifications of object types (*e.g.*, the Hubble sequence, the stellar spectral types) in an objective manner?
- 2. Clustering techniques, such as the expectation maximization (EM) algorithm with mixture models to find groups of interest, to come up with descriptive summaries, and to build density estimates for large data sets. How many distinct types of objects are present in the data, in some statistical and objective sense? This would also be an effective way to group the data for specific studies, *e.g.*, some users would want only stars, others only galaxies, or only objects with an IR excess, *etc.*



Figure 1.15 A demonstration of a generic machine-assisted discovery problem—data mapping and a search for outliers. This schematic illustration is of the clustering problem in a parameter space given by three object attributes: P1, P2, and P3. In this example, most of the data points are assumed to be contained in three, dominant clusters (DC1, DC2, and DC3). However, one may want to discover less populated clusters (*e.g.*, small groups or even isolated points), some of which may be too sparsely populated, or lie too close to one of the major data clouds. All of them present challenges of establishing statistical significance, as well as establishing membership. In some cases, negative clusters (holes), may exist in one of the major data clusters.

- 3. Use of genetic algorithms to devise improved detection and supervised classification methods. This would be especially interesting in the context of interaction between the image (pixel) and catalog (attribute) domains.
- 4. Clustering techniques to detect rare, anomalous, or somehow unusual objects, *e.g.*, as outliers in the parameter space, to be selected for further

investigation. This would include both known but rare classes of objects, *e.g.*, brown dwarfs, high-redshift quasars, and also possibly new and previously unrecognized types of objects and phenomena.

- 5. Use of semi-autonomous AI or software agents to explore the large data parameter spaces and report on the occurrences of unusual instances or classes of objects. How can the data be structured to allow for an optimal exploration of the parameter spaces in this manner?
- 6. Effective new data visualization and presentation techniques, which can convey most of the multidimensional information in a way more easily grasped by a human user. We could use three graphical dimensions, plus object shapes and coloring to encode a variety of parameters, and to cross-link the image (or pixel) and catalog domains.

Notice that the above examples are moving beyond merely providing assistance with handling of huge data sets: these software tools may become capable of *independent or cooperative discoveries*, and their application may greatly enhance the productivity of practicing scientists.

It is quite likely that many of the advanced tools needed for these tasks already exist or be under development in the various fields of computer science and statistics. In creating a virtual observatory, one of the most important requirements is to bridge the gap between the disciplines, and introduce modern data management and analysis software technologies into astronomy and astrophysics.

4.3.1 Applied Unsupervised Classification. Some preliminary and illusory experiments using Bayesian clustering algorithms were designed to classify objects present in the DPOSS catalogs (de Carvalho et al., 1995) using the AutoClass software (Cheeseman et al., 1988). The program was able separate the data into four recognizable and astronomically meaningful classes: stars, galaxies with bright central cores, galaxies without bright cores, and stars with a visible "fuzz" around them. Thus, the object classes found by AutoClass are astronomically meaningful—even though the program itself does not know about stars, galaxies and such! Moreover, the two morphologically distinct classes of galaxies populate different regions of the data space, and have systematically different colors and concentration indices, even though AutoClass was not given the color information. Thus, *the program has found astrophysically meaningful distinction between these classes of objects, which is then confirmed by independent data*.

One critical point in constructing scientifically useful object catalogs from sky surveys is the classification of astronomical sources into either stars or galaxies. Various supervised classification schemes can be used for this task,

including decision trees (see, *e.g.*, Weir et al., 1995) or neural nets (Odewahn et al., 1992). A more difficult problem is to provide at least rough morphological types for the galaxies detected, in a systematic and objective way, without visual inspection of the images, which is obviously impractical. This actually provides an interesting opportunity—the application of new clustering analysis and unsupervised classification techniques may divide the parent galaxy population into astronomically meaningful morphological types on the basis of the data themselves, rather than some preconceived, human-imposed scheme.

Another demonstration of the utility of these techniques can be seen in Figure 1.16. In this experiment, the Expectation Maximization technique was applied on a star-galaxy training data set of approximately 11,300 objects with 15 parameters each. This is an unsupervised classification method which fits a number of multivariate Gaussians to the data, and decides on the optimal number of clusters needed to describe the data. Monte-Carlo cross validation was used to decide on the optimal number of clusters (see, *e.g.*, Smyth, 2000). The program found that there are indeed two dominant classes of objects, *viz.*, stars and galaxies, containing about 90% of all objects, but that there are also a half-dozen other significant clusters, most of which correspond to legitimate subclasses such as saturated stars, *etc.* Again, this illustrates the potential of unsupervised classification techniques for objective partitioning of data, identification of artifacts, and possibly even discovery of new classes of objects.



Figure 1.16 An example of unsupervised classification of objects in the star-galaxy training data set from DPOSS, from the experiment using the Expectation Maximization multivariate Gaussians mixture modeling. Two dominant clusters found are shown, encoded as circles (in reality stars) and crosses (galaxies). The plot on the left shows a typical parameter projection in which the two classes are completely blended. The plot on the right shows one of the data projections in which the two classes separate.

4.3.2 Analyzing Large, Complex Datasets. Most clustering work in the past has only been applied to small data sets. The main reasons for this

are due to memory storage and processing speed. With orders of magnitude improvement in both, we can now begin to contemplate performing clustering on the large scale. However, clustering algorithms have high computational complexity (from high polynomial, order 3 or 4, to exponential search). Hence a rewriting of these algorithms, shifting the focus from performing expensive searches over small data sets, to robust (computationally cheap) estimation over very large data sets is in order.

The reason we need to use large data sets is motivated by the fact that new classes to be discovered in the data are likely to be rare occurrences (else humans would have surely found them). For example, objects like quasars (extremely luminous, very distant sources that are believed to be powered by supermassive black holes) constitute a tiny proportion of the huge number of objects detectable in our survey, yet they are an extremely important class of objects. Unknown types (classes) of objects that may potentially be present in data are likely to be as rare. Hence, if an automated discovery algorithm is to have any hope of finding them, it must be able to process a huge amount of data, millions of objects or more.

Current clustering algorithms simply cannot run on more than a few thousand cases in less than 10–dimensional space, without requiring weeks of CPU time.

- 1. Many clustering codes (*e.g.*, AutoClass) are written to demonstrate the method, and are ill-suited for data sets containing millions or billions of data vectors in tens of dimensions. Improving the efficiency of these algorithms as the size and complexity of the datasets is increased is an important issue.
- 2. With datasets of this size and complexity, multi-resolution clustering is a must. In this regime, expensive parameters to estimate, such as the number of classes and the initial broad clustering are quickly estimated using traditional techniques like K-means clustering or other simple distance-based method (Duda and Hart, 1981). With such a clustering one would proceed to refine the model locally and globally. This involves iterating over the refinements until some objective (like a Bayesian criterion) is satisfied.
- 3. Intelligent sampling methods where one forms "prototypes" of the case vectors and thus reduces the number of cases to process. Prototypes can be determined based on nearest-neighbor type algorithms or K-means to get a rough estimate, then more sophisticated estimation techniques can refine this. A prototype can represent a large population of examples. A weighting scheme based on number of cases represented by each prototype, as well as variance parameters attached to the feature values assigned to the prototype based on values of the population it represents,

are used to describe them. A clustering algorithm can operate in prototype space. The clusters found can later refined by locally replacing each prototype by its constituent population and reanalyzing the cluster.

- 4. Techniques for dimensionality reduction, including principal component analysis and others can be used as preprocessing techniques to automatically derive the dimensions that contain most of the relevant information. See, *e.g.*, the singular-valued decomposition scheme to find the eigenvectors dominant in the data set in a related application involving finding small volcanos in Magellan images of Venus (Aubele et al., 1995).
- 5. Scientific verification and evaluation, testing, and follow-up on any of the newly discovered classes of objects, physical clusters discovered by these methods, and other astrophysical analysis of the results. This is essential in order to demonstrate the actual usefulness of these techniques for the NVO.

4.3.3 Scientific Verification. Testing of these techniques in a real-life data environment, on a set of representative science use cases, is essential to validate and improve their utility and functionality. Some of the specific scientific verification tests may include:

- 1. A novel and powerful form of the quality control for our data products, as multidimensional clustering can reveal subtle mismatch patterns between individual sky survey fields or strips, *e.g.*, due to otherwise imperceptible calibration variations. This would apply to virtually any other digital sky survey or other patch-wise collated data sets. Assured and quantified uniformity of digital sky surveys data is essential for many prospective applications, *e.g.*, studies of the large-scale structure in the universe, *etc.*
- 2. A new, objective approach to star-galaxy separation could overcome the restrictions of the current accuracies of star-galaxy classifications that effectively limits the scientific applications of any sky survey catalog. Related to this is an objective, automated, multi-wavelength approach to morphological classification of galaxies, *e.g.*, quantitative typing along the Hubble sequence, or one of the more modern, multidimensional classification schemes.
- 3. An automated search for rare, but known classes of objects, through their clustering in the parameter space. Examples include high-redshift quasars, brown dwarfs, or ultraluminous dusty galaxies.
- 4. An automated search for rare *and as yet unknown* classes of astronomical objects or phenomena, as outliers or sparse clusters in the parameter

space, not corresponding to the known types of objects. They would be found in a systematic way, with fully quantifiable selection limits.

- 5. Objective discovery of clusters of stars or galaxies in the physical space, by utilizing full information available in the surveys. This should be superior to most of the simple density-enhancement type algorithms now commonly used in individual surveys.
- 6. A general, unbiased, multiwavelength search for AGN, and specifically a search for the long-sought population of Type 2 quasars. A discovery of such a population would be a major step in our understanding of the unification models of AGN, with consequences for many astrophysical problems, *e.g.*, the origins of the cosmic x-ray background.

This clustering analysis would be performed in the (reduced) measurement space of the catalogs. But suppose the clustering algorithm picks out a persistent pattern, *e.g.*, a set of objects, that for reasons not obvious to human from the measurements, are consistently clustered separately from the data. The next step is for the astronomer to examine actual survey images to study this class further to verify discovery or explain scientifically why the statistical algorithms find these objects different.

Some enhanced tools for image processing, in particular, probabilistic methods for segmentation (region growing) that are based both on pixel value, adjacency information, and the prior expectation of the scientist will need to be used to aid in analysis and possibly overcome some loss of information incurred when global image processing was performed.

There are also potential applications of interest for the searches for Earthcrossing asteroids, where a substantial portion of the sky would be covered a few times per night, every night. The addition of the time dimension in surveys with repeated observations such as these, would add a novel and interesting dimension to the problem. While variable objects obviously draw attention to themselves (*e.g.*, supernovae, gamma-ray bursts, classical pulsating variables, *etc.*), the truth is that we know very little about the variability of the deep sky in general, and a systematic search for variability in large and cross-wavelength digital sky archives is practically guaranteed to bring some new discoveries.

4.4 ASTRONOMICAL DATA VISUALIZATION

Effective and powerful data visualization would be an essential part of any virtual observatory. The human eye and brain are remarkably powerful in pattern recognition, and selection of interesting features. The technical challenge here is posed by the sheer size of the datasets (both in the image and catalog domains), and the need to move through them quickly and to interact with them "on the fly".

The more traditional aspect of this is the display of various large-format survey images. One of the new challenges is in streaming of the data volume itself, now already in the multi-TB range for any given survey. A user may need to shift quickly through different spatial scales (*i.e.* zoom in or out) on the display, from the entire sky down to the resolution limit of the data, spanning up to a factor of approximately 10^{11} (!) in solid angle coverage. Combining the image data from different surveys with widely different spatial resolutions poses additional challenges. So does the co-registration of images from different surveys where small, but always present systematic distortions in astrometric solutions must be corrected before the images are overlaid.

Another set of challenges is presented by displaying the information in the parameter spaces defined in the catalog domain, where each object may be represented by a data vector in tens or even hundreds of dimensions, but only a few can be displayed at any given time (*e.g.*, 3 spatial dimensions, color, shape, and intensity for displayed objects). Each of the object attributes, or any user defined mathematical combination of object attributes (*e.g.*, colors) should be encodeable on demand as any of the displayed dimensions. This approach will also need to be extended to enable the display of data from more than one survey at a time, and to combine object attributes from matched catalogs.

However, probably the most interesting and novel aspect is the combination and interaction between the image and catalog domains. This is only becoming possible now, due to the ability to store multi-TB data sets on line, and it opens a completely new territory. In the simplest approach this would involve marking or overplotting of sources detected in one survey, or selected in some manner, *e.g.*, in clustering analysis, on displayed images.

In the next level of functionality, the user would be able to mark the individual sources or delineate areas on the display, and retrieve the catalog information for the contained sources from the catalog domain (see, *e.g.*, Figure 1.17 for a demonstration). Likewise, it may be necessary to remeasure object parameters in the pixel domain and update or create new catalog entries. An example may be measuring of low-level signals or upper limits at locations where no statistically significant source was cataloged originally, but where a source detection is made in some other survey, *e.g.*, faint optical counterparts of IR, radio, or x-ray sources. An even more sophisticated approach may involve development of new object classifiers through interaction of catalog and image domains, *e.g.*, using genetic algorithms.

Visualization of these large digital sky surveys is also a powerful education and public outreach tool. An example of this is the virtual sky project⁶² (see Figure 1.18 for the project homepage).

⁶²http://www.virtualsky.org



Figure 1.17 A prototype of the visualization services which would empower scientists to not only tackle current scientific challenges, but also to aid in the exploration of the, as yet unknown, challenges of the future. Note the intelligent combination of image and catalog visualizations to aid the scientist in exploring parameter space.Image Credit: Joe Jacob and the ALPHA group, (JPL).

5. SUMMARY

We are at the start of a new era of information-rich astronomy. Numerous ongoing sky surveys over a range of wavelengths are already generating data sets measured in the tens of Terabytes. These surveys are creating catalogs of objects (stars, galaxies, quasars, *etc.*) numbering in billions, with tens or hundreds of measured numbers for each object. Yet, this is just a foretaste of the much larger data sets to come, with multi-Petabyte data sets already on the horizon. Large digital sky surveys and data archives are thus becoming the principal sources of data in astronomy. The very style of observational astronomy is changing: systematic sky surveys are now used both to answer some well-defined questions which require large samples of objects, and to discover and select interesting targets for follow-up studies with space-based or large ground-based telescopes.

This vast amount of new information about the universe will enable and stimulate a new way of doing astronomy. We will be able to tackle some major problems with an unprecedented accuracy, *e.g.*, mapping of the large-scale structure of the universe, the structure of our Galaxy, *etc.* The unprecedented

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Figure 1.18 The Virtual Sky web-site which provides public access to several different data products, including images from the DPOSS survey.

size of the data sets will enable searches for extremely rare types of astronomical objects (*e.g.*, high-redshift quasars, brown dwarfs, *etc.*) and may well lead to surprising new discoveries of previously unknown types of objects or new astrophysical phenomena. Combining surveys done at different wavelengths, from radio and infrared, through visible light, ultraviolet, and x-rays, both from the ground-based telescopes and from space observatories, would provide a new, panchromatic picture of our universe, and lead to a better understanding of the objects in it. These are the types of scientific investigations which were not feasible with the more limited data sets of the past.

Many individual digital sky survey archives, servers, and digital libraries already exist, and represent essential tools of modern astronomy. We have reviewed some of them, and there are many others existing and still under development. However, in order to join or federate these valuable resources, and to enable a smooth inclusion of even greater data sets to come, a more powerful infrastructure and a set of tools are needed.

The concept of a virtual observatory thus emerged, including the incipient National Virtual Observatory (NVO), and its future global counterparts. A virtual observatory would be a set of federated, geographically distributed, major digital sky archives, with the software tools and infrastructure to combine them in an efficient and user-friendly manner, and to explore the resulting data sets whose sheer size and complexity are beyond the reach of traditional approaches. It would help solve the technical problems common to most large digital sky surveys, and optimize the use of our resources.

This systematic, panchromatic approach would enable new science, in addition to what can be done with individual surveys. It would enable meaningful, effective experiments within these vast data parameter spaces. It would also facilitate the inclusion of new massive data sets, and optimize the design of future surveys and space missions. Most importantly, the NVO would provide access to powerful new resources to scientists and students everywhere, who could do first-rate observational astronomy regardless of their access to large ground-based telescopes. Finally, the NVO would be a powerful educational and public outreach tool.

Technological challenges inherent in the design and implementation of the NVO are similar to those which are now being encountered in other sciences, and offer great opportunities for multi-disciplinary collaborations. This is a part of the rapidly changing, information-driven scientific landscape of the new century.

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