

Report of the Invitational NSF Workshop on  
Scientific Database Management  
Charlottesville, VA  
March 1990

Anita K. Jones, Chairperson

## **Scientific Database Management**

**(Final Report)**

edited by  
James C. French, Anita K. Jones, and John L. Pfaltz

Supported by grant IRI-8917544 from  
the National Science Foundation

Any opinions, findings, conclusions, or recommendations expressed in this report are those of the workshop participants and do not necessarily reflect the views of the National Science Foundation.

Technical Report 90-21  
August 1990  
Department of Computer Science  
University of Virginia  
Charlottesville, VA 22903

## **Abstract**

On March 12-13, 1990, the National Science Foundation sponsored a two day workshop, hosted by the University of Virginia, at which representatives from the earth, life, and space sciences gathered together with computer scientists to discuss the problems facing the scientific community in the area of database management. This report summarizes the discussion which took place at that meeting. The report concludes that initiatives by the National Science Foundation and specific discipline professional societies are urgently needed to address the problems facing scientists with respect to data management. Although the report is addressed to the National Science Foundation, the conclusions are more widely applicable to other federal funding agencies.

Supporting materials used in the preparation of this report, including the individual panel reports and position papers, are available as a separate technical report (TR 90-22) from the Department of Computer Science at the University of Virginia.

**Program Committee:**

Hector Garcia-Molina, Princeton University  
Anita K. Jones, University of Virginia  
Steve Murray, Harvard-Smithsonian Astrophysical Observatory  
Arie Shoshani, Lawrence Berkeley Laboratory  
Ferris Webster, University of Delaware - Lewes

**Workshop Attendees:**

Don Batory, University of Texas - Austin  
Joseph Bredekamp, NASA Headquarters  
Francis Bretherton, University of Wisconsin - Madison  
Michael J. Carey, University of Wisconsin - Madison  
Vernon E. Derr, National Oceanic and Atmospheric Administration  
Glenn Flierl, Massachusetts Institute of Technology  
Nancy Flournoy, American University  
Edward A. Fox, Virginia Polytechnic Institute and State University  
James C. French, University of Virginia  
Hector Garcia-Molina, Princeton University  
Greg Hamm, Rutgers University  
Roy Jenne, National Center for Atmospheric Research  
Anita K. Jones, University of Virginia  
David Kingsbury, George Washington University Medical Center  
Thomas Kitchens, Department of Energy  
Barry Madore, California Institute of Technology  
Thomas G. Marr, Cold Spring Harbor Laboratory  
Robert McPherron, University of California - Los Angeles  
Steve Murray, Harvard-Smithsonian Astrophysical Observatory  
Frank Olken, Lawrence Berkeley Laboratory  
Gary Olsen, University of Illinois - Urbana  
John L. Pfaltz, University of Virginia  
Peter Shames, Space Telescope Science Institute  
Arie Shoshani, Lawrence Berkeley Laboratory  
Ferris Webster, University of Delaware - Lewes  
Donald C. Wells, National Radio Astronomy Observatory  
Greg Withee, National Oceanic and Atmospheric Administration

**National Science Foundation Observers:**

Y.T. Chien  
Robert Robbins  
Larry Rosenberg  
John Wooley  
Maria Zemankova

**Other Contributors:**

Umeshwar Dayal, DEC Cambridge Research Laboratory  
Nathan Goodman, Codd and Date International  
James Ostell, National Library of Medicine

# Scientific Database Management<sup>1</sup>

*“... the Earth system science initiative will founder on the rocks of indifference to data access and information management unless an aggressive and supportive new approach is taken — beginning now.”<sup>2</sup>*

## 1. Introduction and Background

This quote applies equally well to all the sciences. Over the next decade the problems posed by the exponential growth of data in a variety of scientific disciplines will become increasingly pressing. For this reason, an interdisciplinary workshop on scientific database management was organized to consider these problems and possible solutions. It brought together computer scientists and serious user/proprietors of scientific data collections in several fields of the space, earth, and life sciences. Our objective was to discuss the issues involved in establishing and maintaining large scientific data collections, and to identify opportunities for improving their management and use. More particularly, we sought to assess the current state-of-the-art, assess whether the needs of the sciences are being met, identify the pressing problems in scientific database management, and identify opportunities for improvement.

This workshop, conducted at the University of Virginia on March 12-13, 1990, was sponsored by the National Science Foundation. NSF requested recommendations on how to stimulate progress toward the efficient management of data within the sciences.

Many issues regarding scientific databases are similar to those found in conventional business environments, but the focus is different. For example, efficient transaction processing and concurrency control are critical to high volume data processing applications and less critical to DNA sequence analysis, seismic data analysis, or computational astrophysics. Flexible, efficient query processing, however, is vital in each environment.

The relative importance of the issues associated with any data management undertaking is determined by the characteristics of the data and the anticipated operational environment. Much scientific data can be characterized by large volume, low update frequency, and indefinite retention. In the past, it has been generally safe to assume that scientific data resulting from experimental observations was never thrown away. The future volume of data will be staggering. Mapping the three billion nucleotide bases that make up the human genome will result in an enormous volume of data. The *Magellan* planetary probe will generate a trillion bytes of data over its five year life — more image data than all previous planetary probes combined. This suggests that much scientific data will not even be on-line.

A recent article describing the state of NSFNET characterized the problem of access to the net as being hampered by a diversity within the computer world that “verges on anarchy.”<sup>3</sup> This same diversity poses an equally substantial barrier to the access of scientific data by those who need it. Indeed, one of the significant problems with scientific databases is largely logistical. According to a recent NASA study of astrophysical data:

Analyses using multiple data sets from different missions, with support from ground-based observations, are becoming an increasingly important and powerful tool for the modern-day astronomer. However, lo-

---

<sup>1</sup>The report of the NSF Invitational Workshop on Scientific Database Management, March 1990. The workshop was attended by Don Batory, Joe Bredekamp, Francis Bretherton, Mike Carey, Y.T. Chien, Vernon Derr, Glenn Flierl, Nancy Flournoy, Ed Fox, Jim French, Hector Garcia-Molina, Greg Hamm, Roy Jenne, Anita Jones, David Kingsbury, Tom Kitchens, Barry Madore, Tom Marr, Bob McPherron, Steve Murray, Frank Olken, Gary Olsen, John Pfaltz, Bob Robbins, Larry Rosenberg, Peter Shames, Arie Shoshani, Ferris Webster, Don Wells, Greg Withee, John Wooley, and Maria Zemankova. The workshop was supported by NSF grant IRI-8917544. Any opinions, findings, conclusions, or recommendations expressed in this report are those of the panels and do not necessarily reflect the views of the National Science Foundation.

<sup>2</sup> *Earth System Science: A Closer View*, Report of the Earth System Sciences Committee of the NASA Advisory Council, Jan. 1988.

<sup>3</sup> “Waiting for the National Research Network,” *AAAS Observer*, March 3, 1989.

cating the required observations and accessing and analysing the multiplicity of data sets is not easy at present.<sup>4</sup>

Perhaps the greatest problem facing the scientist is the bewildering array of commercial and custom database interfaces, computer operating systems, and network protocols to be mastered in order to examine potentially relevant data.

From the point of view of the practitioner, there are some relatively simple questions that must be answered in order to enhance the scientific research environment:

What data is available to me?  
Where is it located?  
How can I get it?  
What can I do with it?

To provide the scientific community with the means to answer these and other questions, database researchers must examine the issues peculiar to scientific database management and the sharing of scientific data.

The purpose of this workshop was to examine the issues of scientific databases in more detail with the goal of producing a planning document to guide the NSF as it considered a new research initiative in this area. In addition to the computer science representation, the workshop participants were drawn from among the various disciplines of the earth (e.g., oceanography, climatology, geology), life (e.g., microbiology), and space (e.g., astronomy, astrophysics) sciences. The overall representation was approximately 40 percent computer science and 20 percent from each area of the physical sciences. Besides NSF, a number of government agencies were represented, including Department of Energy (DOE), National Oceanic and Atmospheric Administration (NOAA), National Aeronautics and Space Administration (NASA), National Radio Astronomy Observatory (NRAO), and National Center for Atmospheric Research (NCAR).

The workshop began with invited talks from each represented area with the objective of exposing both common and distinctly different data management problems. Participants then met in one of four panels to examine the relevant issues more closely. Panel representation was proportional across all disciplines. The panel topics were: (1) Multidisciplinary interfaces: standards, metadata, multimedia, etc.; (2) Emerging and New Technologies; (3) Core Tools: access methods, operators, analysis tools, etc.; and (4) Case Study: Ozone Hole. This case study was used as a vehicle for investigating data management needs, successes, and failures in a real mission environment.

This document is a digest of the workshop proceedings summarizing the panel discussions and highlighting the workshop recommendations. The individual panel reports are given in a companion document<sup>5</sup> along with other supporting material used in the preparation of this report.

## **2. Dimensions of Scientific Database Systems**

The workshop observed that databases can be characterized in terms of at least three dimensions (which need not be independent). The three we identified are:

level of interpretation,  
intended analysis, and  
source.

---

<sup>4</sup> *Astrophysics Data System Study*, Final Report, NASA, March 1988.

<sup>5</sup> Available as Technical Report 90-22 from the Department of Computer Science, University of Virginia, Charlottesville, VA 22901. This document includes the separate panel reports so that the interested reader will have the opportunity to form his/her own opinions. Self-describing data formats received much attention in the workshop so we have included an example of one international standard format (FITS) as an appendix. Because of the thoughtful issues raised by the participants in their position papers, we have included those also as an appendix.

Characterizing data of interest along these dimensions helps to clarify salient aspects so that data management issues can be more clearly enunciated and explored.

In the discussion that follows we use the terms “data set” and “database.” By data set we mean data related to a single experiment or mission. We use the term database more generally to denote any aggregate of data.

**2.1. Level of interpretation:** A scientific database may be a simple collection of raw data, or real world observations, or it may be a collection of highly processed interpretations. At least two of the panels observed that this dimension manifestly affects what one expects of the data set, and how one employs it. One proposed subdivision of this axis is

*raw/sensor data:* (seldom saved) raw values obtained directly from the measurement device;

*calibrated data:* (normally preserved) raw physical values, corrected with calibration operators;

*validated data:* calibrated data that has been filtered through quality assurance procedures, (most commonly used data for scientific purposes);

*derived data:* frequently aggregated data, such as gridded or averaged data;

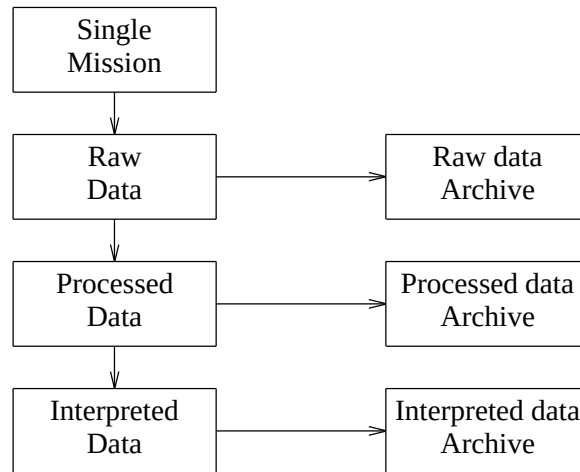
*interpreted data:* derived data that is related to other data sets, or to the literature of the field.

This sequence of successively greater interpretation need not be precisely correct. But it does indicate that the type of data in a data set can be highly dependent on its level of processing. Moreover, information about the processing must also be retained and distributed with any data set; this ancillary descriptive data and information is vital to fully understanding and using a data set.

**2.2. Intended Scientific Analysis:** Our assumption is that all scientific data sets are subject to further analysis, otherwise there is little reason to retain them. The nature of such subsequent analysis frequently determines what particular representational format is most desirable. Much earth science data is analyzed statistically; time sequenced, multidimensional tables are common. A predominant activity in biological genome databases is elaborate pattern matching over linear, character data. Multi-spectral analysis in the space sciences apply transformations (e.g. Fourier) to very large two and three dimensional arrays. For each type of analytic processing, a database with different characteristics is most appropriate.

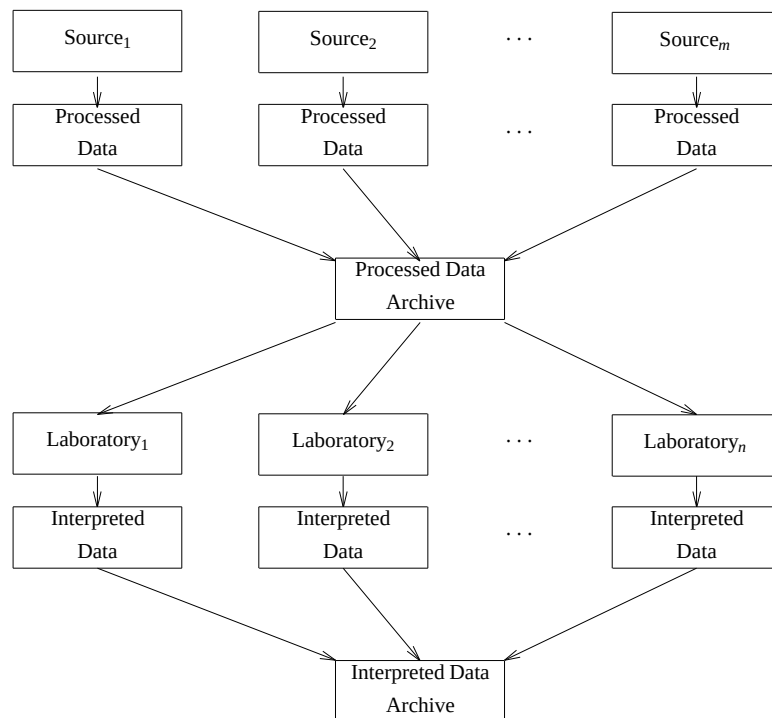
The criticism of the relational data model is largely that this model is designed for commercial applications, and seems unsuited to scientific applications. For example, much of science data represents discrete sampling of functions of several dimensions, e.g.,  $(x,y,z,t)$ . Often the results are sequences, in which order is important. The relational data model, in contrast, represents sets of values. It is, therefore, not a natural way to represent multidimensional objects. Secondly, the classes of transformations scientists wish to apply to data are larger and more complex than those within the relational model and, in some cases, such as interpolation and Fourier analysis, rely on characteristics of the data which are not part of the relational description. Thirdly, much more ancillary information is required. Fourthly, updating and correcting data sets is a very different process for scientific databases.

**2.3. Source:** This dimension, which is not generally mentioned in the database literature, may be the most fundamental. In Figure 2-1, we illustrate a familiar *single-source* database environment. Here we envision a single mission, such as the *Magellan* planetary probe, generating the data. Either raw or physical data may be retained in its original state in a raw data archive. Commonly, the raw data will be processed, by instrument calibration or by noise filtering, to generate a collection of more usable calibrated or validated data. Finally, this processed data will be interpreted in light of the original goals of the generating mission.



Single-source Data  
**Figure 2-1**

Both the syntactic complexity and the semantic complexity of the interpreted data will be much greater than any of its antecedent data. It will have different search and retrieval requirements. Possibly, only the interpreted data will be published.



Multi-source Data  
**Figure 2-2**

In contrast to such a single-mission/single-source data archive one has data archives that are derived from multiple sources employing multiple data generation protocols. Figure 2-2 illustrates a typical *multisource* collection of data. This structure would characterize the Human Genome project in which several different agencies, with independent funding, missions, and methodologies, generate processed data employing different computing systems and database management techniques. All eventually contribute their data to a common data archive, such as GENBANK, which subsequently becomes the data source for later interpretation by multiple research laboratories that also manage their local databases independently. In each of the local, multiple, and probably very dynamic, databases one would expect different retrieval and processing needs, as well as different documentation requirements.

This classification of databases in terms of level of interpretation, intended analysis, and source, however imperfect, helped clarify discussions at the workshop. In the following section, we list issues in scientific database management. The importance of an individual issue is dependent on the position of the database of interest in this multidimensional space.

### 3. Problems

All sciences have major data management problems, for example: handling increasing data volume; metadata<sup>6</sup> management; integration of database facilities with applications; finding data; access policy; ease of use; and consistent long term funding. Long term funding is a common problem. But different sciences seem to have different technical data management problems that are domain specific. In the following sections we have subdivided the problems raised at the workshop into two large categories, main issues and lesser issues, and described them more fully within each category. This subdivision has been imposed to indicate a sense of relative importance to the reader without attempting a fruitless exercise of exactly ranking the problems.

#### 3.1. Main Issues in Scientific Database Management

The issues and problems discussed in this section received most of the attention of the participants.

**3.1.1. Metadata:** Scientific databases hold a wide spectrum of kinds of data: *raw data* — values measured by a sensors or other instruments; *calibrated data* — normalized raw data correcting for instrument, environment, or other experimental differences; *validated data* — errors removed; *derived products* — computed values, graphs; and *interpreted data* — with respect to models. For the data to be meaningfully processed later, the *metadata* associated with the data must be preserved and accessible. This is the information required to identify data of interest based on content, validity, sources, preprocessing, or other selected properties. Metadata includes:

- Who did what and when
- Device characteristics
- Transform definitions
- Documentation and citations
- Structure and format descriptions

It is imperative that the metadata remain attached to the data for it to be meaningful.

**3.1.2. Locating Data:** Early in any scientific inquiry, the need to find data becomes critical to the successful outcome of the investigation. Hypotheses need to be corroborated, or perhaps, archived data is to be mined for possible undiscovered properties. It becomes necessary to address questions such as:

---

<sup>6</sup>The commonly used term “metadata” is highly overloaded. One panel recommended avoiding its use altogether. We use it here with some reluctance, trusting that its meaning will be clear from context.



What data exists and where is it?  
Is the data relevant to my interests?  
Do useful data items exist?

This implies the need for a rather general data browsing capability providing facilities first for locating data sets, and then for scanning them for indications of probable interest.

**3.1.3. User Interfaces:** To manipulate data and produce information, a scientist needs to access data and apply analysis tools in concert. Failure to integrate the data management and analysis environments restricts the productivity of the scientist. Typically, extant systems are not integrated. This may be due to the fact that the data management environment was created by a computer scientist and the analytic environment was created by a discipline specialist.

Lack of integration will likely be even more of a problem to a scientist crossing discipline lines to attempt to analyze data from a foreign discipline. Integration becomes more important as one adds functionality to provide an automated assistant to the scientist. Such an assistant must track interlaced data and analysis steps.

The easier a user interface is to use, the more productive a scientist can be. In addition to being intuitive and easy to use, user interfaces need to:

- be domain specific
- handle differing levels of user sophistication (novice/expert)
- browse across different, distributed database management systems (DBMS)
- provide “hooks” for special application programs
- access a hierarchy of storage in a user-transparent fashion
- support tracking of data accessed across multiple DBMS to maintain an audit trail of transformations applied to create each data set.

Achieving a system that will support multi-disciplinary research across a variety of databases will be greatly facilitated by having sophisticated user interfaces hiding the heterogeneous reality and unifying disparate environments.

**3.1.4. More Flexible Representational Structures:** Perhaps the single unifying cry of the workshop was that existing data models are inadequate for science data needs. The relational model has some advantages. Chief among them is that it is well-defined and has solid theoretical underpinnings. And, more pragmatically, it exists within successful commercial products. However, the semantic gap between the relational model and what scientists need must be addressed. We must seek alternatives such as extending the relational paradigm, object-oriented database technology, extensible tool kits, and logic databases. We must also consider alternatives to the relational model for efficiently supporting temporal, spatial, image, sequences, graph, and other more richly structured data.

**3.1.5. Appropriate Analysis Operators:** One area of concern noted by most of the participants was the lack of appropriate operators within existing DBMS for manipulating the kinds of data encountered in scientific applications. For example, more flexible comparison operators are necessary when attempting to match DNA sequences or retrieve image data. There was not universal agreement as to where these operators belong — within the DBMS as intrinsic operators or external to the DBMS as utilities or part of an analysis package. The approach used now is to have a commercial DBMS export data for use by external utilities. Often the data cannot be exported in a format compatible with the utility program so the scientist is forced to produce ASCII files that are subsequently massaged into an appropriate form. If results of the analysis are to be saved, the process must be reversed and the updated data imported back into the DBMS. Since there are no standards this is a tedious and time consuming process.

Extensible database technologies provide the mechanism for embedding custom operators into the DBMS. A philosophical question arises as to how much custom functionality is desirable within the

DBMS. Rather than embed domain specific operators in a DBMS, it may be more appropriate to create a standardized integrated analysis environment in which a DBMS can interact with a variety of useful tools.

**3.1.6. Standards:** Heterogeneity in data and operational environments is a fact of life. We must find ways to promote consistency within and across scientific disciplines. It is unreasonable to expect all disciplines to converge on some unifying standard, so heterogeneity will continue to be a force to be reckoned with. However, there are already instances of standardization within disciplines — the astrophysics community has endorsed FITS<sup>7</sup> as its data interchange standard — and this trend should continue. It was noted that the most successful standardization efforts arise when an organization creates a useful data format and associated analysis tools and then distributes them widely and also maintains them at no charge.

**3.1.7. Standards for Data Citation:** There was strong sentiment that data used in the conduct of an investigation should be cited prominently. A standard citation mechanism would allow other researchers to locate and examine precisely the data used in the investigation. It would also give due credit to the data collectors.

It was noted that much of the interesting metadata is actually citations into the scientific literature. These citations too should be handled in a standard way so that where possible their content may be examined as part of a search for important data or to help assess the quality of data which is being browsed.

## **3.2. Other Issues in Scientific Database Management**

The following issues and problems associated with scientific database management arose in the discussions of the workshop. We have rated them as less important issues because, either (1) there exist partial, although imperfect, solutions to the problem, (2) they seemed to be less frequently encountered, or (3) the problems are not readily amenable to a technological solution. While these may be less important from our perspective, there exist views in the scientific database management world (using the general dimensions described in section 2) in which they can be very important.

**3.2.1. Data Set Transmission:** Data sets residing at one site (usually the collecting site or a designated repository) may have to be transmitted to the site where subsequent analysis will take place. Participants observed that there exist a number of wide area networks of sufficient bandwidth and reliability to handle most reasonably sized data sets. However, transmission of very large data sets may be slow. The delay in response time may be associated with the time to access and transmit the data set at the host site, as much as network delays.

**3.2.2. Conversion of Data Sets to Local Site Format:** A data set received from a foreign site may be in a format that is incompatible with the local analysis system. Subsequent data set conversion may depend upon adequate metadata to interpret the format and structure of the data, and more generally, upon the conventions expected by the local analysis system. Some discipline specific models for data exchange already exist, such as FITS in the astronomical community.

**3.2.3. Making Multiple Data Sets Comparable:** Analysis involving multiple data sets from disparate sources can be difficult. Relations obtained from Oracle, Ingres, or other relational DBMS need not be immediately comparable. With data coming from even less rigid data models, such as object-oriented DBMS, the problem is magnified. A straightforward technical approach involves converting all data sets to a local standard as described above. At a much deeper level, this problem involves the general issue of data fusion, which must take into account the semantics (or intended meaning) of the data items in order to make meaningful comparisons.

---

<sup>7</sup> A brief description of the FITS standard can be found in Appendix A of the companion document Tech. Report 90-22.

**3.2.4. Need for Interoperability of Multivendor DBMS:** In some ways this is a subset of the preceding issue, in some ways it is a superset. The goal would be to allow analysis programs running under the aegis of one DBMS to directly query/access data stored in a different DBMS.

**3.2.5. Quality Assessment of a Data Set:** Participants repeatedly noted the difficulty in assessing the quality of a received data set. While quality assessment has always been a fundamental scientific problem, many of the technical barriers arise due to insufficient metadata to interpret the data.

**3.2.6. Volume of Scientific Data, Need for Permanent Archiving:** The expected volume of sensor generated scientific data is awesome. In the coming decade it will far outstrip the resources available to analyze it. The issue is: should (can) all of it be archived for possible later interpretation, or should (can) it be passed through some preliminary filter to determine what should be saved. The answers to these questions will be directly related to the cost-effectiveness of archival storage media.

A directly related issue — that data production is often well-funded, while data management is poorly funded, if funded at all — was a recurrent theme.

**3.2.7. Proprietary Behavior of PI's with Respect to Data Sets:** Data collecting Principal Investigators (PI's) and their funding agencies have little incentive to release verified, but uninterpreted, data sets in a timely fashion. In fact, there are a number of sociological and monetary disincentives to do so.

**3.2.8. Data Management is not Respected in Scientific Communities:** It was repeatedly noted that data management is not an attractive career path within the scientific disciplines, whose primary goal is one of discovery. There is a need to educate both domain scientists and computer scientists in each others fields. However the time investment is viewed as a distraction from the major field.

This summary should convey to the reader the variety of problems faced by scientists in the management of their data. Unless these problems are addressed now, scientists in the 90's will find data management an increasing barrier to continued progress in their fields.

## **4. Recommendations**

The discussions at the workshop clearly indicated the need for two distinct initiatives in scientific database management. We recommend that the federal agencies — in particular the National Science Foundation — create a broad research initiative directed toward the solution of the technical problems facing scientific database management. There are, however, many problems which fall outside the purview of the NSF and which can most effectively be addressed by the scientific professional societies. Both roles are discussed more fully below.

### **4.1. The Role of the Professional Societies**

The professional societies, in their leadership role within disciplines, are the obvious vehicle for focusing attention on the data management problems within each discipline. They are also in the best position to represent the disciplines and to encourage cooperation in forums promoting interdisciplinary activity.

**We recommend that the professional societies aggressively implement recommendations 1 through 5. This may involve expansion of current activities and/or the creation of new initiatives.**

**4.1.1. Metadata:** The concept of metadata is fundamental to the effective use of scientific data. Many issues in the management of scientific data are, in fact, issues related to the management of the metadata. In particular, metadata must remain immutably associated with the data it describes. It is important here to distinguish two particular uses of the term metadata: (1) a low level description of the data necessary to provide a data interchange format; and (2) the description of the characteristics of the data which enable it to be interpreted properly.

While it would not be wise or even desirable to attempt to impose specific standards across the different sciences, it is essential to introduce standardization into interchange formats, the methods for describing data and metadata. A single format does not adequately support all needs and requirements even within a single discipline. Self-describing formats solve this problem. As an example, the FITS standard used internationally within the astrophysics community has proved to be very successful in promoting the interchange of data among various sites. Two international standardization efforts (ASN.1 and SGML<sup>8</sup>) are already well underway and bear careful consideration.

**Recommendation 1:** *Promote standardization of data interchange descriptions that use self-describing data formats.*

Working groups within the professional societies are the most appropriate means of investigation and standardizing the appropriate metadata that should be associated with data in the discipline.

**Recommendation 2:** *Standardize the description of data within each scientific discipline.*

One aspect of this is to promulgate control lexicons of standardized descriptive terminology that is appropriate within a discipline.

**4.1.2. Standards for Data Citation:** The scientific communities should be encouraged to develop methods to foster the publication of important databases, and to reward those involved properly. There should be an international standard for citing database collections.

**Recommendation 3:** *Require appropriate citation of data and the deposit of relevant data into the appropriate archive before permitting publication in the societies' journals.*

**4.1.3. Volume of Scientific Data, Need for Permanent Archiving:** The problem of the increasing volume of data will force some hard decisions with respect to the retention of the data. At some point it will become necessary to decide whether to discard data and if so, what data to discard. This will result in policy decisions which can only be made by specialists in the relevant sciences.

**Recommendation 4:** *Promote and fund workshops to investigate and recommend policy relative to the retention of data.*

**4.1.4. Sociological Problems:** There are many nontechnical barriers to the successful solution of scientific database management problems. These include chronic underfunding, PI's unwillingness to release data in a timely fashion, and the shortage of individuals trained to analyze the data.

**Recommendation 5:** *Promote and fund workshops directed toward resolving the sociological problems hindering the development of sound data management policy.*

## **4.2. The Role of the National Science Foundation**

Whereas the professional societies are particularly well positioned to influence the individual disciplines, the NSF can assume a more expansive leadership role in the effort to bring multiple disciplines into some state of conformance and cooperation. We recommended that the NSF launch a broad research

---

<sup>8</sup> ASN.1, Abstract Syntax Notation (ISO standards 8824 and 8825), and SGML, Standard Generalized Markup Language (ISO standard 8879), are efforts to standardize the specification of the structure of data so that it may be easily converted into any host format.

initiative to attack the technical problems impairing effective scientific database management. In some cases this will only require expansion of an existing NSF program. To be successful, this research initiative must involve multiple Directorates because the problems span all disciplines. A coordinated Foundation-wide research effort would allow all Directorates to share in the fruits of technical progress. As an effective starting point, NSF should stress exploratory implementations which produce prototypes of direct relevance to specific disciplines. This has the direct benefit of involving the domain scientists intimately and early in the design process. It is imperative to launch this research initiative now.

This workshop was chartered by NSF which asked the workshop participants what it should do to further scientific database management. While our recommendations are directed to NSF, many participants believe that other agencies, and even private funding sources, should participate in the aggressive execution of the recommendations that follow.

**We recommend that NSF coordinate and lead in the implementation of recommendations 6 through 13.**

**4.2.1. Metadata:** The importance of metadata to the effective use of scientific data was discussed above.

**Recommendation 6:** *Perform research in methods for describing metadata and promote standardization in the management of metadata.*

It is essential to standardize the methods for describing metadata in order to gain effective access to the accumulated body of data. Emerging international standards should be considered in this regard.

**4.2.2. Standards for Data Citation:** NSF should provide leadership in seeking an international standard for data citation. As a condition of funding, NSF should require that projects creating scientific data sets provide explicitly for depositing the data into an appropriate archive. For example, ICPSR, a repository of social science data at the University of Michigan, was mandated by NSF.

**Recommendation 7:** *NSF should include the matter of cataloging and publication of databases in its planning of NSFNET and other national networks. Research proposals for projects leading to databases should be required to include plans for publishing, cataloging, and either maintaining or transferring results to national archives.*

**4.2.3. Volume of Scientific Data, Need for Permanent Archiving:** The need to generate appropriate data retention policy was discussed earlier. The importance of this issue cannot be overstated. However, no matter what policy is involved, it will always be preferable to defer the decision. That is only possible when storage capacity is increased.

**Recommendation 8:** *Perform further basic research in storage device technology and in representation techniques for better utilization of the available capacity.*

**4.2.4. Locating Data:** Locating appropriate data can be a formidable task. It must be possible to easily learn of the existence of data, assess its suitability to the task at hand, and ultimately, acquire the data. This breaks naturally into two subgoals: (1) find the relevant data sets from among all candidate data sets; and (2) once located, find relevant data from within the data sets. The discipline of “information science” has established many precepts associated with the location of relevant data. It and the information retrieval community should be considered when approaching the issue of scientific database management.

**Recommendation 9:** *Perform basic research in information science and information retrieval to improve the ability of interested researchers to locate relevant scientific data.*

**4.2.5. Data Analysis:** There are many generic analysis areas that are applicable to many scientific disciplines. Common needs include, for example, statistical analysis, time series analysis, and general linear algebra capabilities. Techniques should be developed to package these together with domain specific analysis methods and integrate them with suitable database technology. Of course, appropriate user interfaces will have to be considered as well. An appropriate analysis environment must also include audit mechanisms to record the complete set of transforms leading to the creation of a data set.

**Recommendation 10:** *Support the creation of one or more data analysis environments for science data that includes database and data archival processing. In these environments, special attention should be given to the integration of the user interface, the analysis component, and the database management system.*

A fundamental consideration here is how much of the analysis capability belongs in a database management system. Components common to multiple disciplines should be identified, but it would not be appropriate to attempt the inclusion of capabilities sufficient to handle all disciplines in a single database management system. Rather, an approach which allows selective inclusion of analysis capability is preferable.

**4.2.6. More Flexible Representational Structures:** A recurring theme is that the relational model of data is not adequate to accommodate the diverse modeling needs of the sciences. The relational model is based on set theory and does not provide adequate support for entities which rely fundamentally on order for their structure.

**Recommendation 11:** *Perform basic research in emerging database technologies such as object-oriented database systems, extensible database systems, and logic database systems. Further, explore alternatives to the relational model of data such as models directly supporting lists, sequences, and graphs.*

It is important to focus on conceptual modeling tools that can describe the various scientific applications in terms of objects, structures and operators useful to scientific information. It is not enough to have an extension to a relational model, or an object oriented DBMS. We need conceptual models that specify the constructs and operators useful for scientific data (including spatial, temporal, sequence, images, etc.) and operators over them that can be imbedded into query languages.

**4.2.7. Heterogeneity:** Despite appropriate efforts at standardization, heterogeneous data systems will remain. As more interdisciplinary investigations are mounted, there will be more pressure to analyze data drawn from disparate disciplines, resulting in the need to make multiple data sets comparable, convert data sets to local site format, and create multivendor distributed database systems.

**Recommendation 12:** *Perform research directed at solving the problems of heterogeneous data management environments.*

The professional societies can best attack the heterogeneity issue within the scientific disciplines. NSF should assume a leadership role in solving the problems across disciplines. However, this can only be successful if NSF works closely with the other funding agencies (e.g., NASA, NIH, etc.) that work more directly with particular scientific communities.

**Recommendation 13:** *The NSF should coordinate a multiagency task force charged with promoting the creation of a harmonious environment which enhances the ability of scientists to freely and easily exchange data.*