18-Data Bases and Communications

The Protein Data Bank operates a WAIS server permitting retrieval of abstracts by index term. The IUCr is investigating similar techniques for accessing its collections of CIF structural data files and biographical information in the World Directory of Crystallographers. The technical aspects of such a project are less daunting than the requirements for data security and cost retrieval.

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DS-18.03.03ADVANCES IN GLOBAL DATABASES AND COMMON DATA EXCHANGE FORMATS. By S.R. Hall, Crystaliography Centre, University of Western Australia, Nedlands 6009, Australia.

Crystallographers are prolific generators and users of data, and as a consequence their databases are amongst the largest and best organised in science. The rapid growth of databases has been possible because of the modularity of crystal data; the strong computational background of the discipline; and a high level of cooperation within the profession promoted by its national societies, the IUCr and its journals. These factors have enabled databases to be developed and maintained at reasonable cost.

The methods for accessing these databases have, however, changed little in the past two decades, despite rapid changes in computer technology during that time. Certainly data retrieval rates have improved; better graphical interfaces have made data interpretation easier; and remote access facilities are emerging, but the currency of data is still determined largely by the physical distribution of media. The economic and organisational reasons for this are, however, about to change.

Most scientists have access to global computer networks, though these tend to be poorly utilised (except, perhaps, for email use) because of unfamiliarity, cost and inertia. The continuing improvement of national and international network services strengthens the rationale for globally accessible single-site databases. Such facilities provide for immediate online access to the latest data at a reduced overall cost to both the distributor and the user. The IUCr CIF data archive, and the next World Directory of Crystallographers (WDC9), will be available soon as global databases directly accessible from the Chester IUCr office.

Common data exchange protocols, such as the STAR File (Hall, 1991 JCICS 31, 327-333), serve a vital role in the development and access of global databases. This talk will discuss these, and use the Molecular Information File (MIF/SMD), a recent development for exchanging general chemical data, as an example of this interaction.

DS-18.03.04 EXPERIENCE WITH THE PAN- EUROPEAN INFORMATION SERVICE CONCISE. By H.D. Flack, Laboratoire de Cristallographie, University of Geneva, 24 quai Ernest-Ansermet, CH-1211 Genève 4, Switzerland.

CONCISE is a pilot information service, a part of the COSINE project (of RARE) for electronic communications for European research. CONCISE is accessible over the European research networks, over public data networks and using the telephone network. Access is by way of email, interactive session or file transfer. At the present time (25th Feb. 1993) use of CONCISE is free of charge. From the readers' and information-providers' point of view, CONCISE may be viewed as the electronic equivalent of a newsletter structured on a (mainly) hierarchical arrangement of items. The ordinary user may read and copy these news items. However contributions must be sent to an information provider (editor) for them to be included on CONCISE. The European Crystallographic Committee has arranged to have a special interest group for crystallography on CONCISE and the secretary is currently acting as an information provider for crystallographic news in Europe to CONCISE. The news items included are announcements of national and European meetings, meeting reports, indexes of Acta Crystallographica and the Journal of Applied Crystallography, personalia, news from the International Union of Crystallography and the European Crystallographic Committee, etc. Certainly the most flexible way of consulting CONCISE is by way of an interactive session. However for those who have difficulty obtaining an interactive connection - this is particularly true for the countries of East and Central Europe - access to CONCISE by email is a satisfactory alternative. For the information provider it turns out that submission of information by way of email is the easiest option, as an item is prepared in the form of an ASCII file with a few bookeeping commands added.

DS-18.03.05 PROMISE AND PITFALLS IN ELECTRONIC INFORMATION. By E.N. Maslen*, Crystallography Centre, University of Western Australia, Nedlands, Western Australia 6009

New communications technology has the potential to provide scientists with information on the latest scientific developments rapidly, and cheaply. The dream of a desk-top supercomputer is approaching reality, and technical means for linking that device to comprehensive data banks of scientific information should be with us by the year 2000. We will soon be able to transform scientific data into the form which we find easiest to assimilate, with minimal effort. This also has the potential to drive into bankruptcy those sectors of the scientific publishing industry unwise or unfortunate enough to mis-calculate its consequences. Scientists regard many aspects of management as peripheral to the public well-being, with good reason. Nevertheless the challenges in managing electronic publishing of scientific information are as demanding as the technical challenges whose resolution brought this new age. It is not just a question of anticipating which competing technologies will survive, but timing their introduction optimally. The nature of the advances in electronic information that are expected will be outlined, and the management challenges posed by those advances will be described.

DS-18.03.06 ELECTRONIC MAIL: STIMULATING COMMUNICATION. By M.M. Teeter, Department of Chemistry, Boston College, Chestnut Hill, MA 02167. USA

The advent of electronic mail has greatly impacted scientific research worldwide. Communication has sped up so much that conversations are possible via email nearly in real time. Many forums for communication across the network now exist and these can stimulate research collaborations as well as career development.

The first ingredient for communication is an address list. For crystallographers, this is currently available both by ftp and by fileservers via both the Protein Data Bank and EMBL. The address list enables direct communication for information or research collaboration as well as providing a mailing list of email accessible crystallographers.