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Atomic Collision Databases and Data Services - A Survey

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Abstract. Atomic collision databases and data services constitute an important resource for scientific and engineering applications such as astrophysics, lighting, materials processing, and fusion energy, as well as an important knowledge base for current developments in atomic collision physics. Data centers and research groups provide these resources through a chain of efforts that include producing and collecting primary data, performing evaluation of the existing data, deducing scaling laws and semiempirical formulas to compactly describe and extend the data, producing recommended sets of data, and providing convenient means of maintaining, updating, and disseminating the results of this process. The latest efforts have utilized modern database, storage, and distribution technologies including the Internet and World Wide Web. Given here is an informal survey of how these resources have developed, how they are currently characterized, and what their likely evolution will lead them to become in the future.

INTRODUCTION

Around the world, data centers and other more loosely defined organizations of data producers and users are participating in a revolutionary transformation in the manner in which data is exchanged. In particular, the advent of the widespread use and great utility of the World Wide Web has given birth to efforts in which data sets and databases are being converted to, and specifically created for, on-line usage. Benefits of this trend are the great ease that contemporary electronic storage and retrieval technology affords for disseminating data and the potential it holds for improving the ability to intercompare and otherwise manipulate data from central repositories.

Indeed, at present many such sites through which data can be retrieved exist. However, the Web's ubiquity and democracy (rooted in the ability of any interested party to post or download data), drives not only the beneficial increase of readily available data, but can also suffer from the pitfalls associated with the lack of

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authoritative evaluation of data. Whereas pure research may thrive on data which can be treated as informed opinion, applications require data which has an assessed reliability.

Providers of atomic collision data have certainly been active participants in all aspects of this movement and surveyed here will be some of the databases and data services presently available. Also, critical issues such as the role of data centers in collecting, evaluating, and disseminating data, standardization of data formats to facilitate exchange, integration of dispersed and fragmentary data resources, and development of convenient systems for searching and retrieving data, will be emphasized (see also Ref. [1]). However, to begin with, it will be helpful to briefly outline the rationale behind the establishment of atomic collision databases and data services, to attempt to define their role in scientific and engineering endeavors, and to generally describe the evolutionary track they have followed.

Perhaps most evident is their reason for being: the collection and preservation of data which are of use both in atomic physics and in applications of atomic physics. That is, progress is facilitated if needs arising for particular atomic collision data, or, in fact, sets of atomic collision data, can be satisfied without the concomitant need to produce and evaluate the data anew. Furthermore, the collection and organization of pre-existing data facilitates the evaluation of newly created information and can be used to identify the needs for new or improved data. Beyond only collecting data, data centers and individuals or groups participating in these activities seek to provide guidance to non-expert users of data through evaluation and recommendation.

Evaluation is the assigning of a degree of expected reliability to the available data based on expert opinion and derived from consideration of a set of criteria such as the robustness of the theoretical method or soundness of experimental method through which the data were obtained and their consistency with well established physical behavior or asymptotic limits. By recommendation, one means a further level of expert evaluation, usually involving the intercomparison of all the relevant available data, resulting in data or data sets which can be utilized by the research and application communities with a high level of confidence. Often these activities result in the construction of fitted forms for tabulated reaction cross sections, scaling laws, or other useful semiempirical formulas which can be valuable to fill in gaps in the required, but not existing, data. It should also be recognized that some applications require huge amounts of atomic data which could not feasibly be individually determined by the state-of-the-art theoretical or experimental methodologies, but rather must be produced by large-scale production computer codes. In this case, it is crucial to know the expected limits of applicability and reliability of the data generated through comparison with other theory and experiment for particular benchmark tests.

Thus, the chain of activities which leads from fundamental data to those maintained by data centers or other providers begins with the collection of relevant literature references often through bibliographies, manual or electronic digitization of pertinent data, storage and organization of the data, efforts to evaluate and de-

termine recommendations, and dissemination and periodic updating of the results. Data is distributed through a wide range of media including peer review journals, internal reports, published books, internal databases, and Internet and World Wide Web (WWW or Web) resources. As already noted, the modern tools of information technology have had a significant and growing impact on these activities. For example, bibliographies are now often on-line, electronic mail and file transfer protocol (ftp) facilitate obtaining electronic files containing data directly from authors, scanners and digitizers greatly speed up data entry, modern databases and graphical tools help in storage, manipulation, and display of data aiding evaluation efforts, and the Internet and WWW provide a practically universal method for dissemination. This trend represents not simply a change in the medium of distribution, but, moreover, the ability to implement new capabilities such as ready means for updating and interlinking data resources.

These observations may be more fully illustrated and amplified upon by considering the history, present status and organization, and expected future regarding atomic collision bibliographic services and numerical data resources.

THE EVOLUTION OF ATOMIC COLLISION BIBLIOGRAPHIC SERVICES

The starting point for many projects seeking to provide required atomic collision data, or seeking to assess or update the present status of the data available, is the primary scientific literature. Guides to this literature, annotated and categorized bibliographies, have for a long time provided the means to find the relevant publications. For example, beginning in the early 1960's the Controlled Fusion Atomic Data Center (CFADC) at Oak Ridge National Laboratory began publishing a series of reports containing bibliographic data organized into various collision reaction categories [2]. The bibliographic entries have been gathered by groups of experts who search a range of technical journals numbering up to more than one hundred and have been stored on mainframe computers as data files to facilitate the printing of the bibliographic publications. The original series was followed by several others until 1986 [3-6], merged with efforts of other data centers, and is presently extended through an on-line database.

In particular, subsequent to 1977, this data was organized into a formal relational database accessible over a local area network and was contributed to the efforts initiated at the International Atomic Energy Agency (IAEA) to publish the "International Bulletin on Atomic and Molecular Data for Fusion" [7], a series which continues to the present. The "Bulletin" also contains entries contributed through an international network of atomic data centers and has been used to compile convenient cumulative indices [8] for articles dating up to 1980, and from 1980 to 1987. In addition to these publications, the databases maintained at the CFADC and at the IAEA Atomic and Molecular Data Unit were searchable over local networks and requests for bibliographic data were answered by mailing or

FAXing results of searches to interested users. The advent during the 1990's of high speed, reliable national and international computer networks (the Internet) led to projects to allow access directly to users.

The result has been the development of a search engine, accessible through the CFADC's WWW link [9], by which the bibliography can be searched covering entries dating from 1978 to present. Archival entries from c. 1950 to 1977 are presently being converted to the appropriate contemporary data format and edited, and will be added to the on-line database in the future. IAEA provides an interface to their complete database through the telnet protocol [10] and an independent but similar on-line database covering primarily the years 1970 to present is maintained by a European group organized through the Université Paris-Sud, Orsay called GAPHYOR [11].

The obvious advantage of this type of interface is that rather than having a user contact a data center to make a search request and then waiting for the results to arrive by postal mail or facsimile, a number of searches refining the user's needs can be made remotely with no time delay. This leverages not only the user's time, but also that of the data center's staff who can therefore concentrate on improving the overall atomic database rather than being occupied by answering bibliographic requests. The user can then download the results of successful searches directly to his/her own computer for storage or printing. Furthermore, the computerized databases have advantages over the paper documents in that they are more convenient in use, cover many years cumulatively, and can be frequently updated.

Future versions of the Web-based bibliographic search engines will also have greatly expanded capabilities not possible with bibliographies printed on paper. For example, the traditional bibliographic searches by reaction category and reactants can be supplemented by flexible searches on any keyword within article titles, or by boolean searches combining these and other tokens in any combination. Perhaps even more significantly, they may be directly linked to other resources such as numerical data tabulations, applicable scaling laws or semiempirical formulas, sets of recommended data, and even resources such as these physically located elsewhere but linked over the WWW. Such linked resources might also include primary data in Web versions of research and archival journals. As an example of one such presently developing linkage, the CFADC bibliographic engine allows searching of the ALADDIN database (described below) of recommended collision cross sections and rates.

Thus, the collection and dissemination of bibliographic data has evolved from periodic publications, to computer data file storage on internal networks, to WWW and Internet resources. Along the way, advantages introduced through the coordination of efforts of contributing data centers and increased accessibility and flexibility of electronic interfaces have leveraged the available human resources devoted to these efforts and are leading to even greater utility for users.

THE EVOLUTION OF ATOMIC COLLISION DATA RESOURCES AND DATABASES

As one might readily expect, the evolution of numerical data collections and databases has followed a similar path to that of the bibliographies. That is, groups or individuals have gathered the available data from the primary literature, possibly also generating new theoretical or experimental data, and synthesized this information to form internal reports or publications containing graphical and numerical data and, often, fitting formulas and coefficients. Envisioning the capabilities that may soon be made possible by the integrated data resources mentioned above, methodologies used in this process could be significantly enhanced in the future. For example, Web resources might eventually facilitate locating, generating, gathering, displaying, and intercomparing data and scaling formulas, entirely electronically. Even if such new and remarkable systems are eventually realized, however, they will owe much to the conversion of previous data collections and databases to contemporary storage and retrieval systems.

For example, since its inception in the late 1950's, the CFADC has produced compilations of recommended atomic collision data in addition to its bibliographic collections. Named for their red bindings, these "Redbook" series [12-16] have been produced as internal ORNL reports and distributed to on the order of a few hundred researchers. In light of the present data needs of applications and the present capabilities of electronic data systems, several shortcomings of this method of distributing recommended data are apparent. First, internal reports, even though distributed externally, have only a limited audience of users. Secondly, printed volumes of data are not readily updated. For example, when new data becomes available, revised or additional recommendations must be circulated using the same distribution as the original document. Third, while printed bibliographies may not be the most flexible and convenient format for potential users, volumes of recommended data have the additional deficiency that they must be scanned or retyped in order to be interfaced to application codes. A number of advances have been made that in one way or another address these shortcomings also inherent in the valuable works of other data centers and groups.

In order to facilitate and standardize the exchange of atomic, molecular, and particle-surface interaction data among international data centers, data users, and data producers, the IAEA Data Center Network adopted the ALADDIN (A Labeled Atomic Data INterface) format and database code in 1989. ALADDIN was originally developed by Russell Hulse [17,18] of Princeton Plasma Physics Laboratory using ANSI FORTRAN/77 and relying on ASCII-formatted data files. Presently, the ALADDIN standard is being reviewed by an *ad hoc* committee of the IAEA Data Center Network to determine how best to improve it, principally to provide greater flexibility in the data formats that it can accommodate, and to update the user interface. The present versions of the program suite, evaluation functions used to compute results from the stored fitting formulas, dictionary files, and data sets

are available from the IAEA telnet site [10] or from the CFADC Web site [9]. Plans exist to set up three geographically dispersed mirror sites to maintain the official distributions of these and future files. A list of the recommended and evaluated data files is given in the accompanying table. Thus, with an accepted standard through which to exchange data, the "Redbooks" and certain other volumes of recommended data from several groups have been placed into the ALADDIN format. These files have been widely disseminated and form a backbone of recommended data used especially in significant portions of the international fusion energy research community.

TABLE 1. Available recommended/evaluated data sets in ALADDIN format

<ol style="list-style-type: none"> 1. Atomic and Molecular Data for Fusion, Part I - Recommended Cross Sections and Rates for Electron Ionization of Light Atoms and Ions [19] 2. Recommended Data on Excitation of Carbon and Oxygen Ions by Electron Collisions [20] 3. Recommended Data on Atomic Collision Processes Involving Iron and its Ions [21] 4. Collisions of Carbon and Oxygen Ions with Electrons, H, H₂, and He, Atomic Data for Controlled Fusion Research, Vol. V [22] 5. Atomic and Molecular Data for Fusion, Part II - Recommended Cross Sections and Rates for Electron Ionization of Light Atoms and Ions: Fluorine to Nickel [23] 6. Recommended Data for Excitation Rate Coefficients of Helium Atoms and Helium-like Ions by Electron Impact [24] 7. Atomic and Molecular Data for Fusion, Part III - Recommended Cross Sections and Rates for Electron Ionization of Atoms and Ions: Copper to Uranium [25] 8. Elementary Processes in Hydrogen-Helium Plasmas [26] 9. Collisions of H, H₂, He, and Li Atoms and Ions with Atoms and Molecules, Atomic Data for Controlled Fusion Research, Vol. I [27] 10. Collisional Processes of Hydrocarbons in Hydrogen Plasmas [28] 11. Recommended Cross Sections for Collision Processes of Hydrogen Ground-State and Excited Atoms with Electrons, Protons, Multiply Charged Ions [29] 12. Particle Reflection from Surfaces: A Recommended Database [30] 13. Sputtering Data [31] 14. Recommended Data for Physical Sputtering [32]

In another measure, to widen the audience to which the original graphs, tables, and reference lists contained in the "Redbooks" are available, the two most requested volumes have been completely scanned into graphic file format and placed

in a hypertext linked arrangement on the CFADC Web site [9]. This organization and storage will also allow future updates of individual reaction cross sections to be made in such a way that only the master copy residing on the Web site need be modified. Thus the latest updates will be directly accessible to all users. This system will also facilitate linking the graphic files and corresponding ALADDIN entries to the bibliographic search engine and other future tools for data mining and manipulation.

A different approach to providing primary atomic data and, moreover, derived data for modeling and interpreting radiating plasmas, is embodied in the Joint European Torus (JET) - Strathclyde University Atomic Data and Analysis Structure (ADAS), developed principally by Hugh Summers. ADAS is a suite of computer codes implementing a full collisional-radiative model developed for diagnosing fusion and astrophysical (solar) plasmas. It has an accompanying collection of atomic data files gathered from the literature, contributed by collaborators, and extended through JET contracts. ADAS was originally developed as a proprietary tool for fusion research at JET but an international consortium now exists to allow the use of ADAS by a much wider community. Detailed descriptions of ADAS can be found in the on-line manuals and periodic consortium bulletins, mirrored at the Strathclyde [33] and CFADC [34] Web sites. This system has many of the attributes of a state-of-the-art tool for applications of atomic data: a relatively complete data collection, routines to provide semiempirical or otherwise estimated data when the appropriate information does not exist, and a graphical user interface for data previewing, selection of processing codes and parameters, and display of results.

Other well known data projects and data collections exist which bear mention here especially to illustrate the range of organizations and scopes of coverage among them. For example, the Opacity Project, a huge undertaking to produce atomic data such as energy levels, f -values, and photoionization cross sections for astrophysically abundant species through extensive R-matrix calculations, was carried out by a large international group of researchers over a number of years. It has yielded information required to understand, as its name rightly implies, stellar envelope opacity but has found application in a wide range of uses. Information regarding the Opacity Project can be found on its Web site [35] and tables of data can be downloaded by anonymous ftp from the project's database, TOPbase [36]. Also, to provide detailed information for the astrophysically important element iron and its ions, the Iron Project has carried out work with similar goals [37]. Not only theoretical groups have followed the path of making their data collections available through the Internet. For example, the Atomic Physics for Fusion experimental group at ORNL has for many years produced electron impact ionization data regarding ions of particular interest in fusion energy and other applications. Until recently, the data were available only through the articles published in research journals and through internal reports which sometime contained additional, unpublished data. The extensive data from this long running experiment is now available through the WWW [9], organized in a user-friendly set of hyperlinked indices, graphs, and tables which may be easily searched, viewed, and downloaded.

Other extensive collections of primary atomic data have been stored and organized, especially regarding electron-impact excitation and ionization, and heavy-particle impact charge transfer, at the Data and Planning Center of the National Institute for Fusion Science (NIFS) in Nagoya. This and other data are contained in a modern relational database and is accessible through a Web based interface [38]. Of particular interest in astrophysics, but potentially useful in other applications as well, are the astrochemistry database at the University of Manchester [39] and the atomic data for line emission modeling and diagnosis called CHIANTI [40]. An extensive survey of atomic data available on the Web has been made by Yuri Ralchenko who maintains a current list of the URLs (Uniform Resource Locators, the formal name for the WWW addresses of various types of resources) at the Weizmann Institute of Science Plasma Laboratory Web site [41]. The latter site is also being used to develop other innovative atomic data resources, such as an on-line, restricted version of the widely used ATOM code which can now be run through the Web to compute electron-impact excitation cross sections in the Coulomb-Born-Exchange approximation.

All of these resources exist at relatively well known sites and are readily located through the links listed on most data center or research lab sites. However, the individual who has an interest in providing benchmark data, or who devotes his/her time to collecting data and performing evaluations outside of one of these larger organized data projects or services has always been a significant source of useful information. In the past, one would find their work in the published literature, but now, in addition, one can find it on the Web! For example, Y.-K. Kim and M.E. Rudd have for a long time had an interest in providing evaluated electron-impact ionization data in easily parameterized forms for use in a wide range of applications including radiation effects in matter, lighting, semiconductor processing, and fusion plasmas. Recently, they have developed a theoretical method based on well established behaviors of the ionization cross section and developed a Web site through which their results can be obtained for a range of molecules [42].

SUMMARY AND OUTLOOK

Thus, individual researchers, groups, data centers, and networks of data centers have taken to heart the message that atomic data can be best preserved and exchanged by taking advantage of modern electronic storage, database, and communications technologies. The future certainly holds a continuation of this trend, and hopefully after a time, a synthesis and synergetic amalgamation of these resources. However, to assure that this goal is reached a concerted effort must be made in a number of areas.

Efforts to coordinate the production of needed data should be enhanced through improved communication among the interested parties, namely, among data producers, data users, data centers, and funding entities. Recognition of the crucial role of atomic collision data in applications makes it imperative that the atomic

physics community can responsively provide needed information, and that allowing for the necessary checks through consideration of particular data by several groups, that this be accomplished efficiently. The need for efficiency also applies to data center activities which could also be coordinated further to enhance the overall scope of existing evaluated and recommended data, and to cooperatively further the development of data collection, organization, manipulation, and dissemination technologies. These actions also call for heightened openness and fairness in sharing and citing resources and efforts made by other groups.

Data centers should also be wary to continue to provide not only raw data, but also evaluated and recommended data sets, to maintain the reliability of data for applications whenever possible. Use of production codes can also be made more reliable through comparisons and benchmarking of data produced by them in cooperation between principal users, producers, and data centers. Data centers should also seek to accelerate the trend in providing users with interfaces to integrated resources. As use of the Web becomes the paradigm of choice for users, data centers must respond by developing Web compatible tools and engines allowing access to all their data resources in a way which provides the user with the pertinent data, advises what to do to fill in gaps in the available data, and provides assessments of the expected reliability of the data found.

These efforts are particularly pertinent now since, for especially the past twenty years, reasonably accurate atomic data for a wide range of reactions has been accumulated, much of which has been evaluated or at least collected, and it would be deleterious to fail to take advantage of the current technology and preserve, organize, and synthesize it. Finally, in recognition of the importance of these efforts to applications and further development of the capabilities within the field itself, the case for greater and broader support must be made clearer for data production and the chain of activities (collection-organization-preservation-synthesis-dissemination) that leads to evaluated and recommended data.

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