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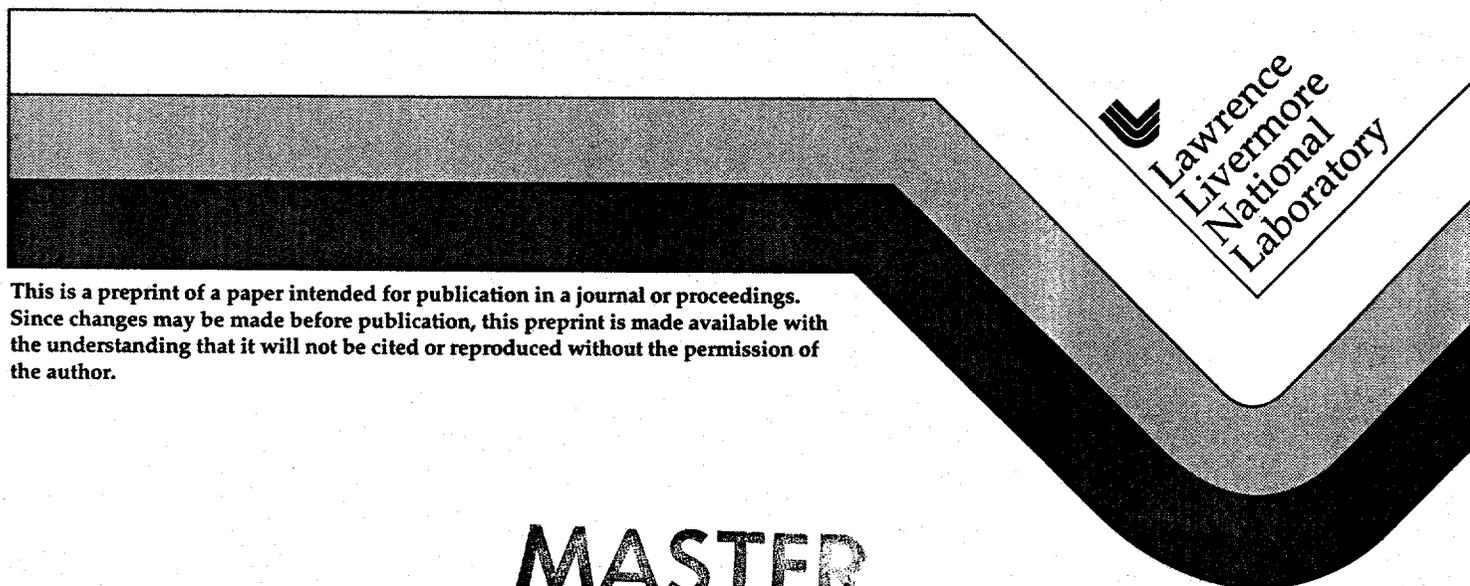
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A DISTRIBUTED ATOMIC PHYSICS DATABASE AND MODELING SYSTEM FOR PLASMA SPECTROSCOPY

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The convenient access and effective use of atomic physics data has long been a goal for workers in the field of x-ray spectroscopy. This information is required at all levels of spectroscopic analysis and it can be a major effort to locate all the information required for a study. Moreover, in recent years we have seen an increase in the need for high quality atomic data. The primary factor leading to this increased use has been the development of evermore sophisticated spectroscopic instruments on a wide range of radiation sources, both in and out of the laboratory. Additionally, the very considerable advances in computing technology now allow the use of extensive radiative models. Unfortunately, the goal of convenient access and effective use of atomic data remains elusive. Although the proliferation of computing capabilities has made it increasingly easy to carry out large-scale atomic rate calculations, these advances have been offset by difficulties in managing and evaluating the data. For the purposes of understanding it is important that the data which goes into the model atoms be readily examined, compared and otherwise manipulated.

We are undertaking to develop a set of computational capabilities which will facilitate the access, manipulation, and understanding of atomic data in calculations of x-ray spectral modeling. In this present limited description we will emphasize the objectives for this work, the design philosophy, and aspects of the atomic database, as a more complete description of this work is available.¹

The project is referred to as the Plasma Spectroscopy Initiative; the computing environment is called PSI, or the "PSI shell" since the primary interface resembles a UNIX shell window. The working group consists of researchers in the fields of x-ray plasma spectroscopy, atomic physics, plasma diagnostics, line shape theory, astrophysics, and computer science. To date, our focus has been to develop the software foundations, including the atomic physics database, and to apply the existing capabilities to a range of working problems. These problems have been chosen in part to exercise the overall design and implementation of the shell. For successful implementation the final design must have great flexibility since our goal is not simply to satisfy our interests but to provide a tool of general use to the community.

1. Objectives and Constraints

In brief our objective is to provide to the community a comprehensive capability to carry out the design and analysis of plasma spectroscopy experiments and observations in a user-oriented computational environment. The concept is to provide a complete set of computational tools that work within the framework of a modest workstation environment. However, it is realized that to be truly "user-oriented" demands a high degree of intuitiveness and simplicity.

Since research programs differ in their needs the PSI shell provides flexible capabilities at several levels of sophistication. Thus, by design, we do not force a solution onto the problem. It is important to note that we are not providing a limited set of computer programs – we are providing a set of capabilities with which individuals may satisfy their own problems, in an unconstrained way. The higher-level capabilities we undertake will be made available as example or template applications.

The PSI shell and its associated programs must be freely available. Aside from facilitating use, we hope to encourage this so that all may benefit from the contributions of others. Our work has benefited from this principle since we have gained much through the use of portable, public-

domain "middleware" for many of the underlying software tasks. In particular we refer to the means by which we provide plots, network communications, graphical user interfaces, and related tasks.

We also state what we are trying *not* to do. We are not specifically developing a vast archive of atomic physics information. While some atomic data will be provided as a consequence of our studies, we are not undertaking the major challenge of providing a critical compilation of publicly available atomic data. The capabilities we develop *are* well suited to providing researchers distributed access to a variety of data centers and archives. Establishing such a network will require that a consensus be established for on-line data retrieval. While this has not yet occurred, we hope this effort will encourage the development of a viable network.

These general objectives are realized as follows. The environment has as a principal interface a type-in window (similar to an 'xterm') which provides input to an interactive C language interpreter. This interpreter functions primarily as a vehicle for the exploratory analysis of data and modeling results. The user may interactively modify data arrays, request plots, initiate dialogs with databases, run programs, *etc.* Connectivity to databases, both remote and local, follows the client-server paradigm and is implemented via the PVM message-passing interface. A simplified graphical user interface is available for users, employing the X windowing system. Plots and spreadsheet capability are provided in the same way.

2. Design Philosophy

A modular design has been followed to allow the selective use of features. The use of UNIX library files makes these capabilities available to compiled user code. As an example, if access to atomic data is the only interest, then one may disregard the graphical or interpretive capabilities creating compiled code that interacts directly with a database. Also, the interpreter may be invoked on its own or connected to user programs via pipes for other purposes. The same applies to the graphical interface capabilities, the plotting library and other aspects of the shell.

We have placed great emphasis on the use of standards. Standards minimize code development time, take advantage of existing familiar conventions, allow the use of widely available reference materials, and simplify coupling to a user's existing methods. A different interface, IDL for example, could be used since standard UNIX features are employed.

We have attempted to obtain maximum flexibility and utility by designing at a level *below* that which is required to accomplish our tasks. This helps ensure that problems which differ from our own may be dealt with at the more primitive level of capabilities. For example, while we are providing an extensive code capability to construct atomic kinetics models, that code is constructed of more fundamental data manipulation routines and may be modified by users for their purposes.

Code development efforts too frequently fail as a consequence of drifting from the intended purposes. What appears obvious to a code developer may be extremely obscure to a physicist intent on solving a specific problem. Equally seriously, a crippling design flaw may persist simply because only a narrow range of problems were considered. We have therefore attempted, as a fundamental development policy, to address a variety of problems and to modify our work as required for generality. Thus far we have considered applications in the areas of plasma temperature and density diagnostics, atomic kinetics modeling, and the calculation of resonant rate processes. While the use of the database facilities to compute resonant cross sections is of interest to an atomic physics audience, we limit this report to the atomic modeling capabilities.

3. Databases and Atomic Kinetics Models

We will discuss our databased approach to the construction of atomic kinetics models. Our focus will be on the generality of the approach, not on the details. This discussion will clarify the way

in which the database is employed in calculations and highlights additional features of this more general scheme.

The term "atomic model" refers to the overall assembly of atomic state information, rates and cross sections which compose the rate matrix in the solution of non-LTE atomic level populations. The level populations may then be used in self-consistent radiative field calculations, to compute model emission spectra, *etc.* The rates in the rate matrix may be any microscopic process of significance in the problem. Most commonly included processes are the excitation and ionization processes due to interactions with electrons and photons. In some problems heavy ion collisions are of significance. Inverse processes are generally included through the use of detailed balance.

In developing such models it is necessary to first *define* the rate equations by choosing which atomic levels to include. This step includes determining the level of detail required, which is problem-specific. In general, low-lying excited states are quite highly resolved. Highly excited states may often be adequately described as composite levels, with the assumption that the constituent states are in relative statistical equilibrium. Each ionization stage of a multi-ion atomic model may require slightly different levels of description as we seek to balance the accuracy of our description with the computational burden of a large rate equation set.

In our approach, we use a SQL-compliant relational database to store and retrieve the atomic energy level and cross section data. This approach has a number of advantages in that we can use the sophisticated database search engine to retrieve the desired data in an effortless fashion. Each energy level is sufficiently described that we can specify the states of interest in a variety of ways – but always in terms of properties of the state, not according to an arbitrary key value. Determining the appropriate level description for an atomic model is often an iterative procedure. To simplify this activity we have developed a general approach to level deletion and consolidation. As with the database retrieval process, we make selections and determine level consolidation groupings by referring to the physical properties of the atomic states. For example, we might choose to delete all levels where the outer electron has a quantum number $n > 6$. The user can invoke this constraint in a single statement. A more complicated example of level grouping is: "combine all levels of a multi-electron atom where the outer electron has the same n value, and inner-shell electrons have similar $n\ell$ configurations, but *only* if the outer electron has $n > 4$." This is simply stated in our approach due to the use of logical combinations of physics-based constraints. The detailed process of executing these operations is of no particular interest and occurs in the background. The user never needs to write loops or learn how data is stored.

Given the atomic level definitions we must then obtain the necessary atomic rates and collision cross sections. In the database, a cross section is characterized in terms of the levels which it connects. Extracting cross sections for a particular set of levels reduces simply to referring to the levels using the same criteria as originally used to extract the level data. The database determines which cross sections match the specified criteria and returns the result. As a consequence we are assured of congruence between the levels and the transition data. This can be a significant problem when working with massive sets of data.

A further advantage of a database is that it simplifies the practice of merging calculational results. When dealing with multiple calculations for the same data one encounters the problem of establishing level identifications. In particular, this arises when we want to use rates from one calculation, but the energy levels from another. The database simplifies this problem in level identification by constructing groups based, as before, on properties of the levels. The database makes it straightforward to group energy levels by good quantum numbers, *e.g.* total momentum and parity. Once equivalent groups from different calculations are paired, then relative energy ordering can be used to assign a specific level-to-level mapping. The generality of the procedure makes it trivial to include other sets of quantum "numbers" in the pairing, including configurational information. The grouping criteria are set by the user in the same logical manner as in level consolidation. Once the level mapping is set, the rates are transparently mapped into the space of the new energy levels.

In many cases a database may contain only a subset of the data we require. Additional databases, local or remote, may then be subsequently queried for further data. Ultimately, omissions in the rate matrix must be identified and filled – if necessary by use of more approximate semi-classical or empirical methods. Many such options are provided in PSI shell. Note that the evaluation of a rate generally requires an integral over a distribution function. Since we are interested in problems where non-Maxwellian distributions could apply (either for electrons or ions) we make use of cross sections, rather than integrated rate coefficients, up to the point where the rate equations are solved. The small time spent integrating is well worth the flexibility. For the same reason, we compute and store *cross sections* for the resonant collision processes. We follow the approach of Badnell² and others^{3,4} in computing energy-averaged dielectronic capture cross sections, from which we obtain cross sections for resonant excitation and dielectronic recombination. By suitable binning of the resonance states we can include contributions from states up to quite large quantum number with a modest number of terms. For atoms ionized a few times, this approach has been shown to be accurate and avoids difficulties encountered with more comprehensive treatments.^{2,5}

Finally, we note that when states are grouped into composite levels, transitions involving these states must be scaled and possibly summed, to account for changes in the statistical weights and level energies. This tedious exercise is handled without specific action by the user. Once the energy levels are defined (including the specification of composite levels), then the averaging, summing, or deletion of rates is completely determined and executed by the model assembly code.

In practice, the tasks of retrieval, level consolidation, remapping, *etc.* are all carried out by an atomic model assembly code, based on criteria set by the user. This may also be done interactively in which case, at his convenience, the user may examine the data in a spreadsheet display, plot values, or write files. If the user's goal is simply to obtain atomic data, this is easily accomplished.

4. Summary

We have described the Plasma Spectroscopy Initiative, an on-going project in x-ray spectroscopy modeling. The description has been brief and focused on the interests of this conference. While a full atomic kinetics model may be unnecessary for many research activities, the component tasks of accessing atomic data, correlating rates and levels, merging data sets, and general data manipulation have a much broader applicability. As our goal is to develop a community resource, we are particularly interested in understanding how this work may prove useful to others.

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