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TITLE SUPERCOMPUTERS AND ATOMIC PHYSICS DATA

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SUPERCOMPUTERS AND ATOMIC PHYSICS DATA

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ABSTRACT

The advent of the supercomputer has dramatically increased the possibilities for generating and using massive amounts of detailed fine structure atomic physics data. Size, speed, and software have made calculations which were impossible just a few years ago into a reality. Further technological advances make future possibilities seem endless. The cornerstone atomic structure codes of R. D. Cowan[1] have been adapted into a single code CATS[2] for use on Los Alamos supercomputers. In section I, we provide a brief overview of the problem; in Section II, we report a sample CATS calculation using configuration interaction to calculate collision and oscillator strengths for over 300,000 transitions in neutral nitrogen; and in Section III, we report our future supercomputer needs.

KEYWORDS

Atomic physics data, atom, ion, nuclear charge, electron, energy levels, configuration, configuration interaction, oscillator strength, collision strength, plane-wave Born, distorted wave, memory management, random access files.

Presentation media requirement: transparency projector

I. Overview

A plasma consists of positively charged ions (atoms in which a number of bound electrons have been removed) in a gas of free electrons. Ions of a variety of elements and charge states may be present. Each ion can exist in an infinite number of quantum energy levels. These levels are derived by considering bound electron configurations which are different distributions of electrons in shells based on principal quantum number (n) and orbital angular momentum (ℓ). Levels are determined by vector coupling of the orbital angular momentum and spin of the electrons giving rise to many levels from one configuration. Frequently, several configurations can contribute to the description of a given level; this is called configuration interaction. In principle, there are an infinite number of configurations contributing to the levels of an ion, but, in practice, configurations are limited to those which are deemed important to a problem. Atomic physics calculations are performed in order to describe these levels and the processes which occur. Hence, a massive amount of computation and data can be required to model the ions of a plasma.

On the order of 1000 levels will result from 50 simple configurations for atoms of low-Z (Z less than 30). However, a single complex configuration may be constructed which will require far more memory than that available on current Los Alamos computers. For high-Z near neutral atoms, the configurations are more complex and result in more levels. The number of levels therefore can become gigantic depending on the number and complexity of configurations chosen. In addition, if configuration interaction is used each configuration cannot be calculated separately

When an atom (ion) collides with free electrons or photons, transitions of bound electrons occur between levels; this means that the number of transitions which need to be considered for a model of 1000 levels is of the order of $\frac{(1000)^2}{2}$ or 500,000. Most of the computer time in an atomic calculation of this type is consumed in calculating the electron-ion collision cross-sections. If a low level computational model that calculates transitions at a rate of one per second is used, the entire calculation will take approximately 150 hours of CRAY-XMP time for a single ion stage. Since most applications require more than one ion species, we must multiply 150 by the number of ion species. In addition, a supercomputer is required to process and verify the millions of words of data which are produced by such a calculation. Therefore, interactive programs which access, operate, and display portions of these large data sets are necessary.

II. Sample Calculation

In this section, we describe an actual calculation which approaches the magnitude of that discussed in Section I. CATS was used to calculate neutral nitrogen using 30 configurations, including configuration interaction between all configurations of like parity, resulting in 786 fine structure levels. Plane-wave Born (PWB) collision strengths and electric dipole oscillator strengths were computed for over 300,000 allowed transitions between levels. Collision strengths were calculated at 21 impact energies per transition. Over seven million words of atomic data were saved on disk files for later use. The job took 16.1 hours of CPU, and an insignificant amount of I/O time on the CRAY-XMP-416, or about 0.2 seconds per transition for the 21 impact

energies. A more sophisticated method (i.e. distorted wave or close-coupling) for computing collision strengths could easily increase total run time by a factor of 100. Figure 1 shows the fine structure level-to-level collision strengths corresponding to the $1s^2 2s^2 2p^3$-$1s^2 2s^2 2p^2 3s^1$ configuration change.

III. Future Needs

The major portion of the time spent for the sample calculation was dominated by performing matrix multiplications (on the order of 100 x 100 matrices) for each transition. Therefore, a speedup for this type of operation would lead to faster overall CATS run times.

The sample calculation required a modest 2-3 million octal words. The size of the problem will increase dramatically as the number and complexity of configurations increase and more levels are produced. Memory management keeps CATS at the optimum size for a given problem. Memory management is essential in CATS because it is impossible to get good estimates of array sizes until execution time. A standard memory managing package would be very desirable.

The least important factor seems to be I/O time: however, the codes which access the atomic data files should see a higher percent of I/O usage. The atomic data are stored as nonstandard variable-length-record random access files with a directory. A standard file managing package of this type would be very desirable.

In summary, computational rates need to be increased by a factor of 10 in order to make more accurate numerical models feasible, and more memory will be required to handle complex configurations and high-Z elements

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