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Transition from LEDCOP to ATOMIC

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Abstract. This paper discusses the development of the ATOMIC code, a new low to mid Z opacity code, which will replace the current Los Alamos low Z opacity code LEDCOP. The ATOMIC code is based on the FINE code, long used by the Los Alamos group for spectral comparisons in local thermodynamic equilibrium (LTE) and for non-LTE calculations, both utilizing the extensive databases from the atomic physics suite of codes based on the work of R. D. Cowan. Many of the plasma physics packages in LEDCOP, such as line broadening and free-free absorption, are being transferred to the new ATOMIC code. A new equation of state (EOS) model is being developed to allow higher density calculations than were possible with either the FINE or LEDCOP codes. Extensive modernization for both ATOMIC and the atomic physics code suites, including conversion to Fortran 90 and parallelization, are underway to speed up the calculations and to allow the use of expanded databases for both the LTE opacity tables and the non-LTE calculations. Future plans for the code will be outlined, including considerations for new generation opacity tables.

INTRODUCTION

Several years ago, it became apparent that the data needs of Los Alamos were such that a new series of low Z opacity tables were required. These tables needed to cover a larger range of temperatures and densities, contain better atomic physics data and plasma physics models, and be extended to higher Z elements. There were two suites of codes and databases that could be used in the new calculations and this paper reports on the development and merging of these two suites into a new Los Alamos opacity code.

The Light Element Detailed Configuration OPacity (LEDCOP) code has been used at Los Alamos to calculate low Z (< 31) opacities for the last 20 years. It is based on early opacity codes developed by Cox [1] in the 1960's and refined and expanded over the years by Huebner *et al* [2] and Magee *et al* [3]. The basic layout of the code and its databases is shown in Fig. 1a. LEDCOP takes the level information and finds the equation-of-state (EOS) by solving the Saha equation for an ideal gas, with plasma corrections. It inputs the cross sections for the bound-bound line transitions and photo-ionization, and uses them, along with the in-code free-free absorption and scattering packages, to calculate the absorption coefficients and integrated gray opacities. The output is formatted into files that can be accessed by users through the Los Alamos T-4 Opacity Web Page [4].

The basic structure of the LINES/FINE codes and their atomic physics code suite is shown in Fig. 1b. Here, on the left, are shown the codes used to calculate the basic atomic physics data, based largely of the early work of Cowan [5] during the 1960's and 1970's.

These have been greatly expanded [6,7,8] and now produce the atomic physics input for all of the codes shown in Fig. 1b, as well as the LEDCOP databases shown in Fig. 1a. The LINES and FINE codes have been used for many years to do highly detailed spectral comparisons and non-LTE calculations for a variety of users. These two codes have now been combined into ATOMIC (Another Theoretical Opacity Modeling Integration Code). The TAPS code has long been used to examine the atomic physics output and was recently bundled with the atomic physics codes to allow users to calculate atomic physics data over the web [9], as reported in this meeting.

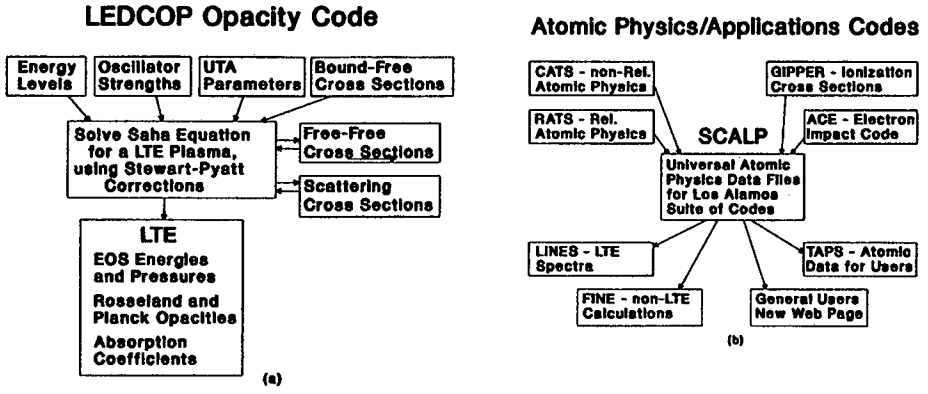

FIGURE 1. Block diagrams of the input and output structure of the two suites of Los Alamos opacity codes.

CODE SELECTION

Each of the code suites had strengths and weaknesses that had to be evaluated before choosing which opacity code or combination of codes would be the new Los Alamos opacity code. These are summarized in Table 1.

The major points from this table are that the ATOMIC code had better atomic physics input, had internal bookkeeping to handle the data, and could do both LTE and non-LTE calculations. LEDCOP was set up to do large opacity tables and had better plasma physics packages, such as free–free absorption models and line broadening models. Based on the analysis, it was decided to use the basic structure of the ATOMIC code and to place the LEDCOP plasma physics packages in modules and add them to ATOMIC to replace its less sophisticated packages. This procedure accomplished two goals. First, it facilitated the comparisons between LEDCOP and ATOMIC, that were used to monitor the changes in ATOMIC during the transition period. Second, putting these physics packages in modules will make it easier to upgrade to better packages in the future.

The major remaining obstacles for ATOMIC were mainly computational run times and memory and diskspace limitations. These concerns were also addressed and will be discussed in a later section. The main operating philosophy from this point on was to do very rigorous comparisons with LEDCOP and try to keep the ATOMIC output as similar as possible to the LEDCOP output during the code development period.

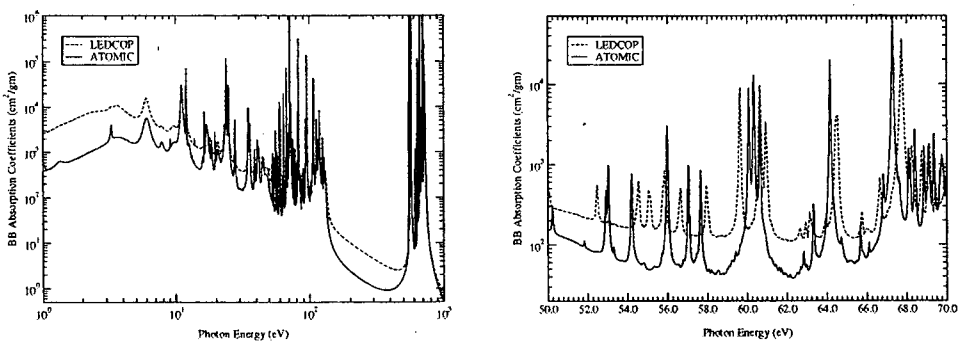

FIGURE 2. Initial spectral comparisons between the LEDCOP and ATOMIC opacity codes.

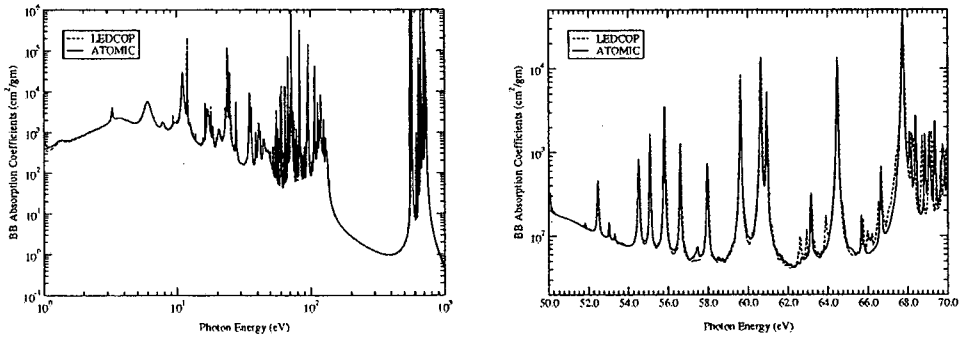

FIGURE 3. Final spectral comparisons between the LEDCOP and ATOMIC opacity codes.

a mixed SC/CI database for ATOMIC, but for our baseline comparison, the CI effects were removed from the LEDCOP database.

The second major discrepancy was the factor of 3 to 10 difference in the valleys between the line peaks. This occured because of limitations in the LEDCOP database, which considers all levels with principal quantum number n, but lumps the $l > 4$ states together for the EOS and does not allow high n, high l transitions for states with $n > 5$ and $l > 4$. ATOMIC includes these transitions, with energies from 1 eV to 6 eV, and all of them are broad, with large oscillator strengths. Since it was not possible to put these transitions into LEDCOP, they were removed from the ATOMIC database for this comparison. The modified results from the two codes are shown in Fig. 3a and Fig. 3b, where agreement is now very good except for some lines at 63 eV and above 68 eV.

The remaining minor differences illustrate two of the reasons why the opacity calculations are being shifted from LEDCOP to ATOMIC. The LEDCOP lines above 68 eV are slightly shifted from the ATOMIC values due to the quantum defect fits used in LEDCOP to reduce the size of the database. The shift is not important for gray opacities, but it does impact spectral comparisons. The missing lines at 63 eV were more serious. A considerable amount of hand work was needed to build the LEDCOP databases and these transitions were inadvertently omitted. The ATOMIC databases are much more automated, reducing these types of errors.

TABLE 1. Strengths and weaknesses of ATOMIC and LEDCOP.

Code	Strength	Weakness
ATOMIC	Intermediate coupling	Extremely large data files, often only able to use a few ion stages at a time
	Accepts standard input files from many codes	Very long computational times for atomic data and opacities
	Runs both LTE and non-LTE calculations	Only had rudimentary plasma physics packages
LEDCOP	Organized for Opacity production	Input data was nonstandard and difficult to recompile or extend to higher Z elements
	Data files could contain full element data	Input data based on LS coupling and fitted energy levels
	Better plasma physics packages	Limited to LTE calculations

SPECTRAL COMPARISONS

Hydrogen and oxygen were selected for the test elements during the transition period. Hydrogen was used mainly for EOS tests. Oxygen was chosen for the spectral benchmarks for several reasons. First, it was complex enough to have a non–trival spectra, without having an excessively large database. Second, the differences between the LS coupling of LEDCOP and the ATOMIC jj coupling were minimal for this low Z. Finally, the run times for each code were short enough to allow extensive testing.

Since the atomic physics input for both codes came from the same code, CATS, the spectra should be almost exactly the same, except for differences due to the different coupling schemes and the fitting of the LEDCOP data by quantum defect fits [10]. This needed to be verified, so the first comparison between the two codes was the bound-bound spectra. In order to do this, two conditions had to be satisfied. First, since the EOS models were different, a density had to be chosen such that the occupancies of the initial configurations were the same to a few percent. Second, the Lorentz profiles were forced for both spectra, but in order to have the same halfwidths, the first of the plasma physics packages, the collisional halfwidth model, had to be transferred to ATOMIC from LEDCOP. Fig. 2a shows the spectral comparison from 1 eV to 1000 eV, while Fig. 2b shows a more detailed comparison from 50 eV to 70 eV.

As can be seen, the comparison was not very close. The major differences were traced to differences in the atomic physics data sets, one expected and one quite surprising. First, for the initial tests, the ATOMIC oxygen database was calculated in single configuration (SC) mode, with no configuration interaction (CI). The LEDCOP database was mostly SC, but had been modified for CI effects. The effect of CI can be seen most clearly in the line positions in Fig. 2b. The CI effects are very important and need to be included, in fact the SCALP code shown in Fig. 1b has been modified to produce

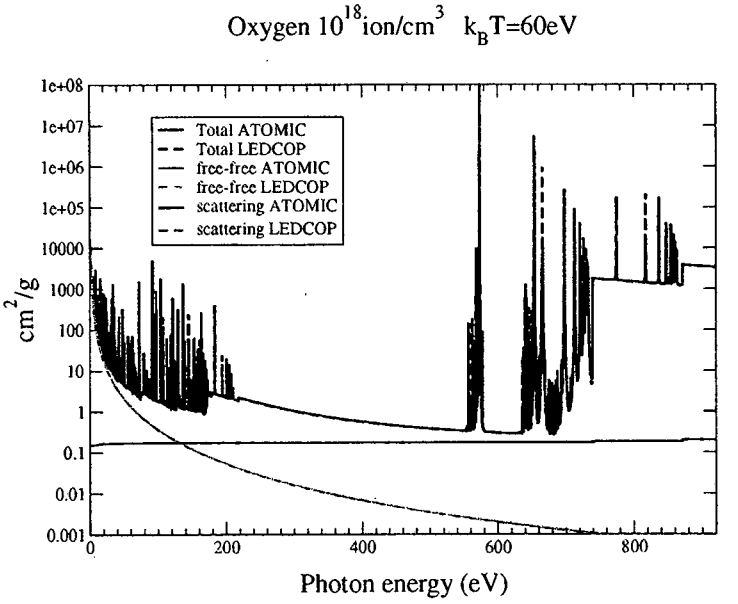

FIGURE 4. Detailed comparisons of the LEDCOP and ATOMIC opacity codes, showing the contributions from the different plasma physics packages.

PLASMA PHYSICS PACKAGE TRANSFERS

The spectral comparison showed that the atomic physics, with well understood modifications to both codes, was equivalent for both codes, which allowed meaningful comparisons of the plasma physics modules as they were transferred to ATOMIC. In addition to the collisional halfwidth model [11], the LEDCOP modules for the free-free absorption [12], scattering, and Stark profiles [13,14] were incorporated into ATOMIC. The bound-free cross sections, calculated with the GIPPER code for both LEDCOP and ATOMIC, were also found to be equivalent for both opacity codes. Fig. 4 shows the comparison between the two codes for all of the processes discussed up to this point.

Again, the temperature and density were chosen carefully to minimize the effect of the different EOS models. As can be seen, the absorption coefficients for the different proccesses agree very well, showing that all of the previously discussed plasma physics packages have been successfully transferred to ATOMIC. The only package that has not been transferred from LEDCOP is the edge broadening and/or continuum lowering model, as shown by the deep valleys between the last line of the Rydberg series and the bound-free edges. The reasons for this will be discussed in a later section.

EQUATION OF STATE MODEL

Up to now, a major consideration in the development of the ATOMIC code was to transfer physics packages from LEDCOP to ATOMIC, so that they could be verified directly against LEDCOP. New physics packages would then be added to ATOMIC when the code was more mature. There were two exceptions to this procedure, the new

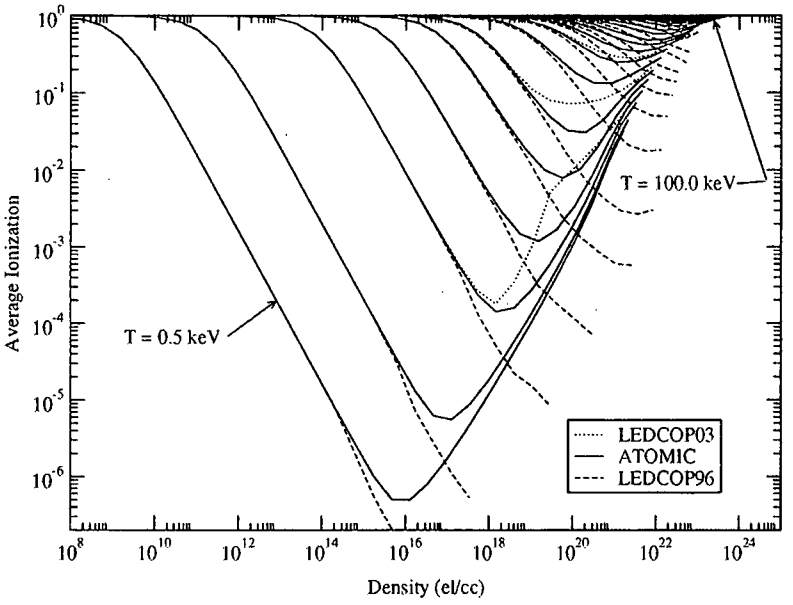

FIGURE 5. Plots of the hydrogen average ionization versus electron density for individual isotherms. The current LEDCOP is compared to ATOMIC for all isotherms, the 1996 version is only plotted for the 0.0008, 0.0015 and 0.0025 keV isotherms.

ATOMIC EOS model and the blending of the Rydberg series lines into the continuum.

The LEDCOP EOS model is an ideal gas with Stewart-Pyatt corrections for higher densities. An example for hydrogen, from the 1990's, is shown as the dashed lines in Fig. 5. The average ionization is plotted along isotherms from 0.5 eV to 100 keV, and over 17 orders of magnitude in density. The model was able to handle most of the temperature-density points until it reached densities where the electronic recombination was at its maximum and pressure ionization became important. The original ATOMIC EOS model, not shown, was even more limited. The LEDCOP EOS was modified from the mid 90's onward to extend the model into the pressure ionization region, shown as the dotted lines in Fig. 5 for selected isotherms. An example of pressures for higher densities, compared to results from Quantum Molecular Dynamics (QMD) methods, is shown in Fig. 6. The pressure agreement was reasonable, even for the 2.692 eV curve, but the behavior of the average ionization curves in Fig. 5 for the lower temperatures was not physical, so it was decided to abandon this EOS model. First, many of the corrections were purely mathematical, meant just to bridge the pressure ionization region. Second, because of these changes, the model was no longer thermodynamically consistent. Finally, the model had been modified over a 20 year period and was so embedded in the LEDCOP code, it could not be easily transferred to ATOMIC.

The new EOS model for ATOMIC is an expansion and elaboration of the models of Däppen *et al* [15], Saumon and Chabrier [16], and Chabrier and Potekhin [17]. This model is based on the chemical picture, where the plasma is modeled as a collection of distinct species (all ion stages, free electrons and negative ions). It uses the minimization of the Helmholtz free energy, along with the highly accurate atomic structure data from the CATS code, to derive the LTE level populations and other thermodynamic

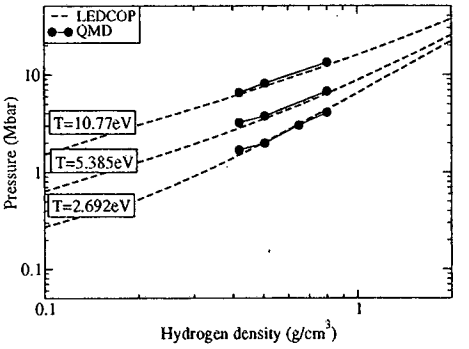

FIGURE 6. Comparison of the current LEDCOP pressures to QMD calculations.

TABLE 2. Explanation of the contributions in Eq. 1.

F_1:	Translational ion energy (classical ideal gas)
F_2:	Internal ion energy (ionization stage and excited states)
F_3:	Electron energy (ideal nonrelativistic Fermi gas)
F_4:	Coulomb interaction plasma term (strong coupling included beyond the Debye-Hückel model)
F_5:	Finite atom size effects (pressure ionization)

quantities. Within this chemical picture framework, the total plasma canonical partition function factorizes and, therefore, the total free energy becomes a sum of contributions representing various effects, as shown in Eq. 1:

$$F = F_1 + F_2 + F_3 + F_4 + F_5 \,. \tag{1}$$

where the contributions are defined in Table 2. Thermodynamically consistent plasma and EOS quantities, such as the energy and pressure, can then be obtained as derivatives of the free energy.

This model is currently in the development stage, so this paper will not go into any more detail at this time. Interested readers are directed to the paper by Hakel *et al* [18] elsewhere in this publication, where the application of this model to a pure hydrogen system is discussed in more detail. The preliminary ATOMIC EOS average ionizations for hydrogen are plotted as the solid lines in Fig. 5. As can be seen, the isotherms are now all pressure ionizing in the high density regions, at a slightly higher density than the current LEDCOP curves. The convergence of the low temperature isotherms around 1×10^{21} el/cm^3 is due to the fact that the neutral atom and ion sphere models are still being developed. Comparisons to the QMD model and experiment will continue during the EOS development.

CODING IMPROVEMENTS

Two of the weaknesses listed in Table 1 for ATOMIC, and its entire suite of atomic physics codes, were long computational times and large databases. While advances in disk size and processor speed will reduce these problems, an aggressive code improve-

ment program was undertaken both for ATOMIC and the entire suite of atomic physics codes. The first step for all of the codes was to remove machine dependent coding, such as CRAY pointers, and to upgrade to Fortran 90, in order to make the codes platform independent. Timing tests were then performed on different machines to guide the selection of the next generation of computers for the opacity calculations. An example of a timing test for the CATS code run on a selection of computers available at Los Alamos is shown in Fig. 7. Thus far, ATOMIC, CATS, RATS, TAPS and ACE have been converted, the others shown in Fig. 1a are in the process of conversion.

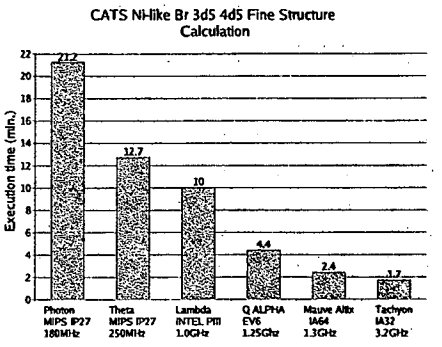

FIGURE 7. Timing comparisons of the CATS code on various platforms.

Another major effort has been to use parallelization techniques in the calculations. The ATOMIC code was altered to run individual temperature–density cases on separate nodes, monitor the status of each node for data recovery or resubmission, and assemble the final data tables. The ATOMIC EOS data for hydrogen in Fig. 5 was run with this version. Using 4 nodes on the THETA (a LANL supercomputer with SGI ORIGIN 2000 processors) machine profiled in Fig. 7, 1932 EOS points were calculated in less than 30 seconds. A similar technique is being implemented in CATS for the eigenvalue solver routines. Two other parallelization efforts are being developed in ATOMIC, one for speed and one to extend the size of the calculations. For cases where complex, highly detailed spectra are needed, the line profile calculations take over 90 % of the CPU time, so another version of ATOMIC is being developed to distribute the profile calculations to different nodes for a single temperature-density point. Finally, new parallel matrix solvers are being implemented in the non-LTE side of ATOMIC to increase the size of the rate matrices $\mathbf{Ax} = \mathbf{B}$ that ATOMIC can handle. Thus far, an increase of an order of magnitude has been achieved for non-sparse matrices and it is hoped to reach a size of 10^6 by 10^6 for sparse matrices. Ultimately, all these versions of ATOMIC will be merged together.

ATOMIC and its predecessor FINE typically only considered the ion stages of interest in spectra comparisons and calculated all possible transitions for these ion stages, regardless of the transition strength. This proved impractical for general opacity calculations because the size of the database was near the maximum of the available disk space for oxygen and caused excessively long run times searching through unnecessary data. A study was undertaken with oxygen to examine the effect on the absorption coefficients of cutting off the transitions at different strengths, which is shown in Fig. 8. It turned out that the excited transitions shown in Fig. 8a reached their terminal value around a cutoff of 10^{-3}, but the inner–shell transitions in Fig. 8b needed a cutoff closer to 10^{-6} to attain

TABLE 3. Timing run statistics

Code and Conditions	# of Lines (millions)	Run Time (hrs)
ATOMIC: Line by Line	67.0	32.00
ATOMIC: Line by Line	383.0	178.00
ATOMIC: Histogram	67.0	1.11
ATOMIC: Histogram	1200.0	2.78
LEDCOP: Line by Line	1.3	1.17

their final values. Using 10^{-6} as a lower bound on the database reduced the database size by 65 % and improved the run time by 5 %.

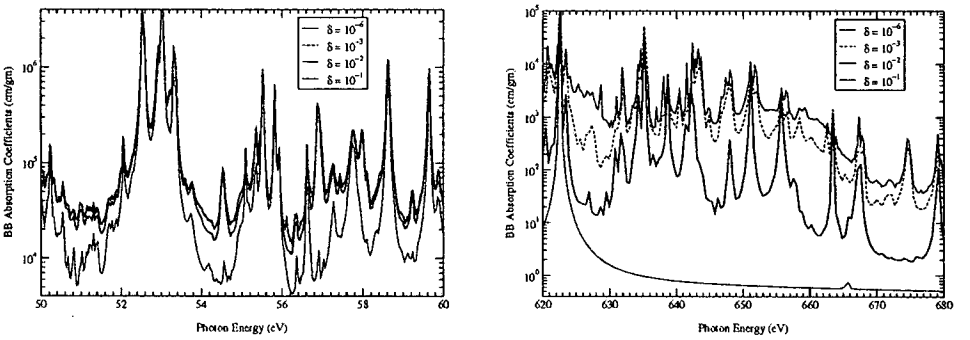

FIGURE 8. Spectral plots of the ATOMIC absorption coefficients, run with different oscillator strength cutoffs in the database.

The run reduction was relatively small because the majority of the run time is in the line profile calculation. A method is being developed to replace the line by line calculation with a histogram model [19] for cases with many millions of lines. The model uses bin widths 5 to 10 times narrower than the photon energy grid spacing to sum up the oscillator strength and reproduce the spectra. The time savings for the initial test runs are shown in Table 3 for the same oxygen case as in Fig. 8. The results for LEDCOP are also shown for comparison.

The difference in the Rosseland and Planck opacities for the two 67 million line cases was less than 2 %, and it is hoped that further refinement of this model will reduce the difference even more.

Two final examples illustrate the type of changes being made to speed up the atomic physics suite of codes. A fractional occupancy number model has been included in RATS, which speeds up large scale calculations by a factor of 10 [20]. An option has been put into GIPPER to allow interpolation to be used to fill in some relativistic photo-ionization cross section points, instead of calculating every energy point. This has resulted in a speed-up of a factor of 500 in large scale calculations [21].

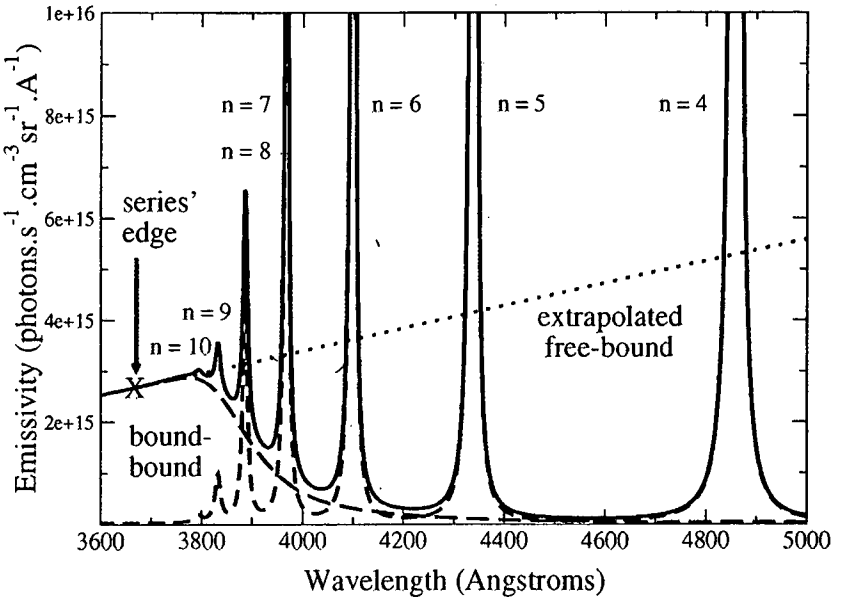

FIGURE 9. Idealized plot of the merging of the hydrogen 2*s* to *np* Rydberg sequence with the 2*s* edge, using occupation probabilities to blend the sequence with the photo-ionization edge.

FUTURE CONSIDERATIONS

As mentioned above, two new models are being incorporated into ATOMIC: the EOS model and the blending of the Rydberg series with the photo–ionization edge. This blending will replace the present continuum lowering model in LEDCOP and provide a smoother transfer of the oscillator strength from the Rydberg sequence to the photo-ionization cross section as the Rydberg sequence is truncated by the dense plasma conditions. The EOS occupation probabilities for both the upper and lower states are used to reduce the transition strength and extend the photo-ionization cross section, as shown schematically in Fig. 9. This is an enhancement of the work of Däppen *et al* [15] and Hubeny *et al* [22].

The two major themes of this paper have been the controlled transfer of the opacity models from one code to its successor and the studies to reduce the calculation times. The need for the calculation speedup can be seen in some of the numerical comparisons done by Neuforge-Verheecke *et al* [23] between the LEDCOP opacities and the Livermore OPAL opacities for their helioseismology model. This model requires very accurate opacities to match the observations, but it was discovered during the calculations that some of the opacity differences were due more to interpolation errors in the tables than to differences in the theoretical results. This is illustrated in Fig. 10, where the closest calculated opacities for plasma conditions at the bottom of the convection zone are plotted versus temperature for the two nearest R ($R = \rho/T_6^3$, $T_6 = T(^oK)/10^6$) curves from the standard opacity tables. The OPAL numbers are definitely higher, but much of the difference at a $\log T$ of 6.3 is due to the different grid spacings in the $\log T$ points. When an interpolation in $\log T$ and $\log R$ is done to get the opacity at $\log R$ of -1.7513, the difference between the two values is 6.1 %. When the LEDCOP numbers

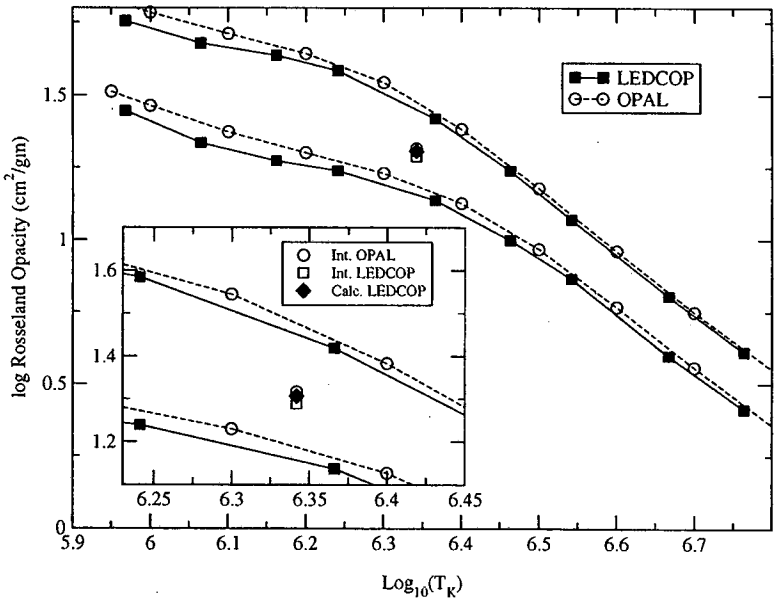

FIGURE 10. Comparisons of Rosseland opacities for a solar astrophysical mixture, showing both the differences due to models and the differences due to interpolation.

were recalculated at the exact $\log T$ and $\log R$, the difference between the OPAL and LEDCOP values dropped to 2.3 %, showing that more than half the difference was due to the interpolation.

As more and more modeling codes start requiring opacities with an uncertainty of 5% or less, these large interpolation errors are unacceptable. There will always be some interpolation errors, but they can be reduced by providing more grid points, especially at critical temperatures and densities. In the above example, at least 50 % more temperature points are needed and the number of R curves should be doubled. Therefore, not only do the opacity codes need to be speeded up to handle the expanded atomic physics data, they need to be faster to provide the expanded opacity tables that will be needed in the future.

CONCLUSIONS

The transfer from the LEDCOP code to the ATOMIC code is proceeding on schedule. Detailed comparisons of the LEDCOP and ATOMIC numbers are employed to reduce computation errors in the new ATOMIC code. Independent verification of the new EOS and Rydberg series cutoff models are being done wherever possible. All of the Los Alamos suite of codes are being modernized and speeded up to handle the new requirements for the next generation of opacity calculations.

ACKNOWLEDGMENTS

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