Flexible Database-Driven Opacity and Spectrum Calculations

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Abstract

The integration of computational atomic physics and information technology can provide flexible, convenient tools for high energy density physicists both computational and experimental. In this work, a flexible atomic database is applied to plasma opacity and spectrum calculations. Multiple atomic data models, such as screened hydrogenic, non-relativistic (ATBASE) and jj split relativistic (RSSUTA), are seamlessly incorporated into the software architecture. High performance parallel programming is applied to accelerate the computation of both the atomic data and the opacity calculations. The user interface is graphical and provided as an easy to use and convenient method to access the data and diagnose the calculations. We present opacity and spectrum results for Kr and Nb plasmas as examples of this new capability.

Keywords

ICF, opacity, EOS, database, atomic

1. Introduction

Modeling of the energy transport in hot dense plasmas relies on radiative opacities. To calculate opacities, three fundamental aspects need to be addressed, that is, plasma population, atomic data, and the line broadening mechanism. Plasma population describes the state dynamics which reflects the effect of plasma environment characterized by thermodynamic properties such as plasma temperature and density. Atomic data provide the radiative level transition structure, collision cross sections and other recombination process rates. Line broadening determines the line shape which is sensitive to the field around the emitting ions. For atomic data, three kinds of models are often applied, that is, the detailed term accounting (DTA) method [1], the unresolved transition array (UTA) method [2] and average-atom models [3]. Because hydrodynamic simulations and experimental spectrum analysis depend on the spectrum data, many groups are developing models. In the Fusion Technology Institute at University of Wisconsin, the development of an opacity model has evolved in several stages. The first model MIXERG/IONMIX provides multigroup Rosseland and Planck absorption and emission opacities for both local thermal equilibrium (LTE) and non-LTE plasma conditions. MIXERG/IONMIX fulfills all needs by hydro simulations while using the screen hydrogenic atomic data. The second model ATBASE goes beyond the average atom model by using atomic data from the Hartree-Fock non-relativistic atomic theory. ATBASE uses the detailed term accounting method for light elements ($Z \leq 18$) and the non-relativistic unresolved transition array (UTA) method for heavy elements ($Z > 18$) assuming the LTE approximation. It has been successfully used to analyze data from light ion fusion, laser-driven inertial confinement fusion and other dense plasma experiments [4]. However, it is not sufficiently accurate to apply to the analysis of high-Z spectra. RSSUTA uses the relativistic jj coupling method and provides more accurate atomic data for high-Z elements. This model also adopts the UTA method to account for the enormous numbers of transition lines but unlike ATBASE it uses the SOSA (spin-orbit split arrays) model to consider the spin-orbit split. Using empirical formulas for various rate coefficients, this model can also calculate non-LTE opacities for high Z plasmas. Furthermore, this model is implemented for parallel computation using Message Passing Interfaces (MPIs). To facilitate and simplify the use of these models, we also have provided a graphic tool (JATBASE), which integrates an object-oriented database management system for users to access the data.

The three components in the opacity calculations can be separated, and thus can be dealt with, from the point of view of the user, with one interface independent of the data. That is, we could provide a common interface between the atomic data and the plasma model so that the plasma opacity calculations are independent of the choice of underlying atomic data models. To achieve this goal, we modularize the code architecture and employ a flexible atomic database. In this paper, we describe the code structure that supports the atomic data from the software point of view (Section 2). Then we emphasize the RSSUTA atomic data model and the non-LTE opacity calculation process in Section 3. A brief description of parallel programming implementation is also given. Finally, we discuss and present results for Nb and Kr plasmas to demonstrate the capability of the code.

2. Computer code structure

Our goal is to provide a flexible, convenient tool to calculate the opacity and spectrum. To store and retrieve the data efficiently, a database management system is used, which already includes many algorithms such as sorting and selecting. These algorithms provide fast data manipulation. The development is much easier than self-writing these algorithms by using a flat file. A graphical user interface is also used for parameter inputs. This code arrangement is similar to the multi-tier structure that often consists of three layers, that is, database, applications and graphical interface. Figure 1 shows the code structure that supports the multi-tier architecture.

For clarity, we give a brief description of the components in the code structure. The bottom layer is the computing engine, which includes the original ATBASE model and the RSSUTA model based on the jj coupling UTA method. The RSSUTA model is implemented in the parallel computing MPI to speed up the calculation since an enormous number of transitions are involved. The database provides a central management of atomic data including energy level structures, line transition properties, collisional and recombination rate coefficients. Previous results of EOS and opacities for common elements needed by ICF applications can also be stored in the database ready for use. The application contains modules that solve the LTE and non-LTE equations to calculate opacities and equation-of-states using the database The user can be a web browser connected by hypertext protocol or a standalone application connected by interobject protocol. Hardware consists of one 700 MHz computer running Oracle database management system and one 1 GHz computer running Apache web server and applications.

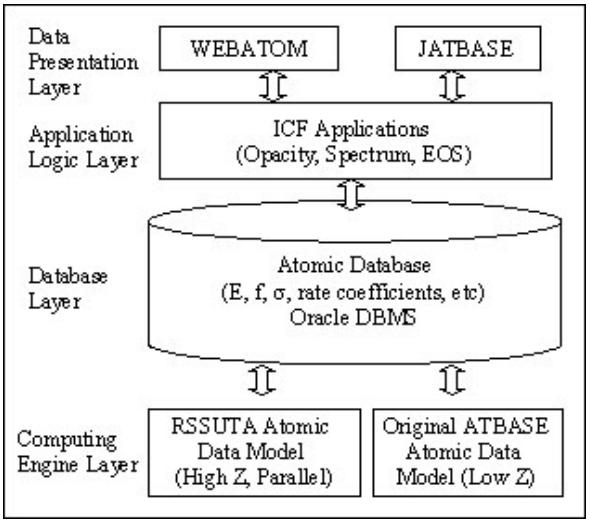

Figure 1. The code structure that includes the database, applications and graphical interface.

3. Opacity model

As discussed, the calculation of opacity involves three components. We will give a more detailed description for the atomic data model and the non-LTE plasma model. For line broadening mechanisms, we include the natural line broadening, Doppler broadening and Stark broadening for which we use simple empirical formulas. The ATBASE data model is based on Cowan's non-relativistic theory and it has been discussed in Ref. [5]. Here we emphasize the RSSUTA model [6] and the calculation of high Z non-LTE opacities.

3.1 RSSUTA atomic data model

In the RSSUTA atomic data model, the wave functions are determined by the Dirac equation:

$$[c\alpha \cdot p + (\beta - I)c^2 + V(r)]\psi = \varepsilon\psi \ , \tag{1}$$

where α and β are the usual Dirac matrices. V(r) is the potential. The wave function ψ has the form

$$\psi_{n\kappa m} = \frac{1}{r}\begin{bmatrix} P_{n\kappa m}(r)\chi_{\kappa m} \\ iQ_{n\kappa m}(r)\chi_{-\kappa m} \end{bmatrix},$$

where P(r) and Q(r) are the radial parts and χ is a function of angular and spin coordinates in the usual notation.

The Dirac equation is solved numerically to obtain the wave functions for electron orbitals and the self-consistent potential. The photoexcitation cross sections for the configuration-to-configuration transition are calculated from the single-electron transition properties. In the configuration average approximation, the cross section can be written as

$$\sigma_{icc'}^{bb}(\hbar\omega) = \frac{\pi he^2}{mc} f_{icc'}\gamma(\hbar\omega) \ , \tag{2}$$

where $f_{icc'}$ is the configuration average oscillator strength, and $\gamma(\hbar\omega)$ is the line shape function. If the transition energy is assumed to be approximately the same for all lines of the transition array, the relation of the averaged array oscillator strength $f_{icc'}$ to the single-electron transition oscillator strength $f_{\alpha\beta}$ is

$$f_{icc'} = q_\alpha(1-\frac{q_\beta}{g_\beta})f_{\alpha\beta},$$
$$f_{\alpha\beta} = \frac{2m}{\hbar\omega g_\alpha}\frac{1}{2k+1}|<\alpha \| T \| \beta>|^2 \tag{3}$$

where $\hbar\omega$ is the photon energy, q_α, q_β are the occupation numbers of orbital α, β respectively, k is the rank of electric multipoles, g_α is the statistical weight for initial orbital α and $<\alpha \| T \| \beta>$ is the bound-bound reduced transition matrix element.

The photoionization cross section for configuration c of ionic stage i can be written as

$$\sigma_{ic} = \frac{\pi he^2}{mc}\sum_\alpha q_\alpha \frac{df_\alpha}{d\varepsilon}, \tag{4}$$

where the summation runs over all subshells of the configuration. $\frac{df_\alpha}{d\varepsilon}$ is the density of oscillator strength, given by

$$\frac{df_\alpha}{d\varepsilon} = \frac{2m}{3\hbar\omega g_\alpha}|<\alpha \| T \| \varepsilon>|^2, \tag{5}$$

where $<\alpha \| T \| \varepsilon>$ is the energy-normalized transition matrix element from the initial bound orbital state α to the continuum orbital state ε.

The spectrum structures are very complex for the M or N shell transitions. The UTA model characterizes these unresolved spectral structures using the average transition energy and a variance. In the UTA method, the average energy and the standard deviation of the energy distribution of a given electronic configuration are the first and second moments of the Hamiltonian,

$$E_{av} = \left(\langle\varphi_i \mid H \mid \varphi_i\rangle\right)_{av}, \tag{6}$$

and

$$\sigma^2 = \left(\langle\varphi_i \mid H \mid \varphi_i\rangle^2\right)_{av} - \left(\langle\varphi_i \mid H \mid \varphi_i\rangle\right)^2_{av}, \tag{7}$$

where H is the sum of the electrostatic and spin-orbit operator,

$$H = \sum_{i<j=1}^{N}\frac{e^2}{r_{ij}} + \sum_{i=1}^{N}\zeta(r_i)s_i\cdot l_i. \tag{8}$$

The numerical formulas for the UTA moments are written in a concise form in Ref. [7].

3.2 Non-LTE model

Assuming steady state and using the average rate coefficients, the non-LTE equation that determines the densities of the charge states can be written as

$$\frac{N_{q+1}}{N_q} = \frac{I(q \to q+1)}{R^r(q+1 \to q) + R^d(q+1 \to q) + n_e R^3(q+1 \to q)}, \tag{9}$$

where $I(q \to q+1)$ is the rate coefficient of the electron impact ionization and $R^{r,d,3}(q+1 \to q)$ are the rate coefficients for the radiative, dielectronic and 3-body recombination, respectively. Coronal equilibrium is the special case of this equation at low plasma density in which $n_e R^3(q+1 \to q) \ll R^{r,d}(q+1 \to q)$. On the other hand, LTE is the special case at high plasma density. It is not difficult to solve the Saha equation as long as we have the energy levels. In our opacity model, two kinds of atomic data are used: ATBASE non-relativistic data and RSSUTA relativistic data. In calculations, these two kinds of data can be used independently or mixed together. Solving the non-LTE equation is difficult for high Z elements. The SCROLL model [8], developed by A. Bar-Shalom, J. Oreg and M. Klapisch uses a sophisticated method to calculate these rate coefficients and thus more accurate data can be obtained. In our model, because of the lack of this capability, we use empirical formula for these rate coefficients which are derived mostly under the screen hydrogenic approximation. The process of computing non-LTE opacities in our opacity model is as follows: we first solve the above non-LTE equation using the empirical formulas to obtain the population of each charge state, then we assume the Boltzmann distribution in each charge state to obtain the configuration population. Finally, the opacity can be calculated using either the ATBASE data or the RSSUTA data. This method provides more accurate $\overline{Z}$ than the LTE model under high temperature and low density plasma conditions, which is important in the equation-of-state calculations.

3.3 Parallel implementation

To obtain accurate atomic data, a large number of wave function bases are needed. Therefore, a sparse interaction matrix as large as 100,000×100,000 must be solved for eigenvalues and eigenfunctions. Since the computation of each block of the sparse matrix is independent from any other, it is possible to distribute the computation of each block across processors as in Ref. [9]. In our model, we use the single configuration, single transition approximation and cope with the enormous number of relativistic configurations and transition lines for high Z elements. If we ignore the interactions between configurations, the calculation for each configuration is independent. Therefore, the communication cost can be minimized and hence we can predict the speedup should be proportional to the processor number. We have performed several runs to determine performance of the RSSUTA parallel code implemented in MPI. We use Ti-like (22 electrons) W (Z = 74) as a sample. For this ion stage, there are 262 relativistic electron configurations. The same calculations have been repeated on 1, 4, 8, 16, 32, 64, 128, 256 processors using the NPACI IBM SP machine. Wall clock time has been recorded for each processor. The calculation time is the average of all wall clock time for each run. We find that the speedup almost linearly increases with the number of processors, as we expect.

4. Sample results and discussions

We use an absorption experiment [10] of a Nb plasma at temperature 47 eV and density 1.E+20 cm^{-3} as an example. In Figure 2 we show three different calculation methods. The RSSUTA atomic data model is used for both LTE and non-LTE conditions, resulting in a $\overline{Z}$ of 12.93 and 10.69, respectively. While the NRSUTA model uses ATBASE atomic data for LTE conditions and the $\overline{Z}$ is found to be 12.53. In order to illustrate the importance of jj splitting, we compare the 3d-2p transmission spectrum using RSSUTA model and NRSUTA model with experiment as shown in the upper small graph. We can see that the jj splitting RSSUTA model agrees with experiment which has two subarray transitions while the NRSUTA model has only one transition.

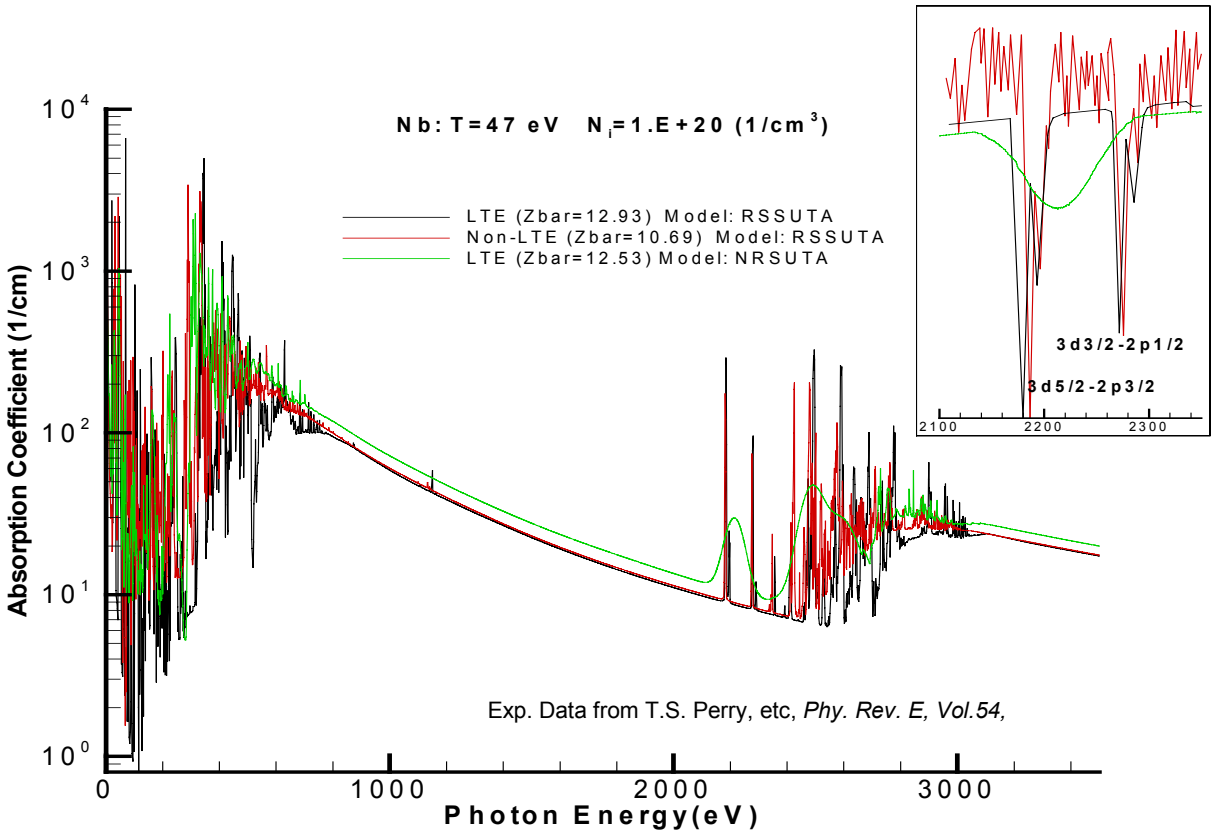

Figure 2. Absorption coefficient for Nb plasma. Comparison with experiment for transition 3p-2d is shown in the upper small graph.

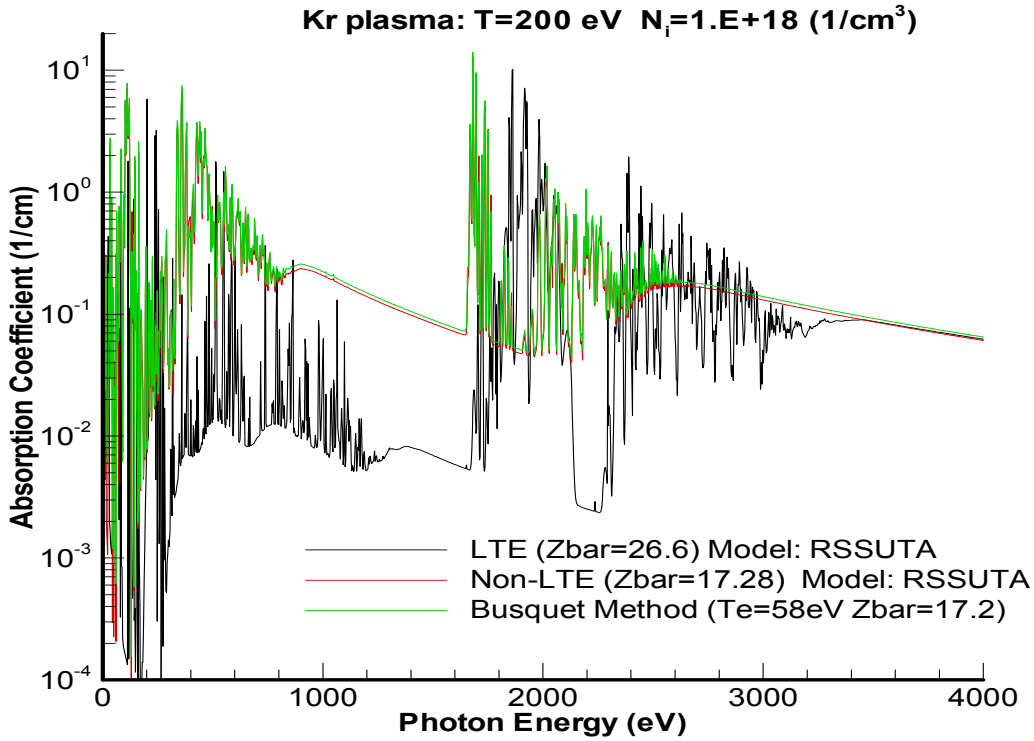

Figure 3. Absorption coefficient for a Kr plasma using three different models.

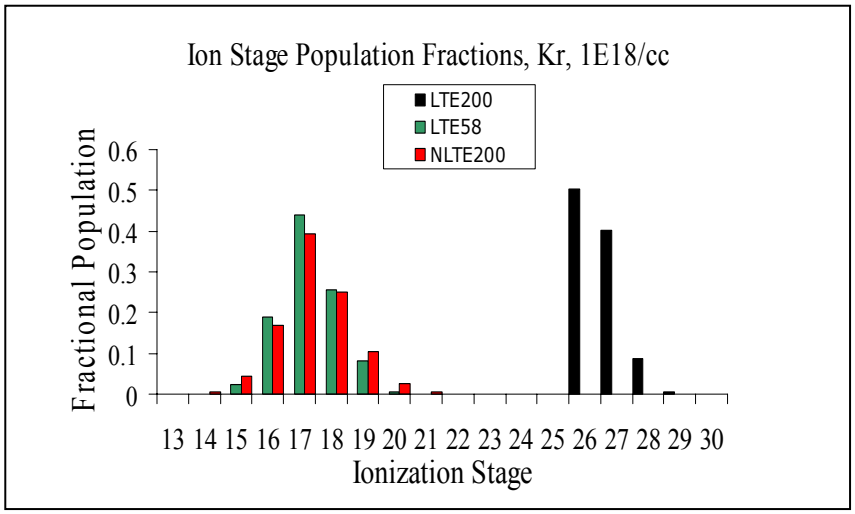

Figure 4. Ionization stage distributions.

In Figure 3, we compare the absorption coefficients using both LTE and non-LTE models for a Kr plasma at temperature 200 eV and density 1.E+18 cm^{-3} to represent a low density and high temperature case. The $\overline{Z}$ result from LTE calculation is 26.6 while the non-LTE is 17.28. So the LTE model predicts about 50% more ionization than non-LTE. We also compare the non-LTE result with the calculation by the Busquet method [11]. In the Busquet method, we find the temperature where the non-LTE ZBAR corresponds to the LTE ZBAR; here it is at a temperature of 58 eV. We then use this temperature in an LTE calculation, which is also shown in the figure. We can see the results from the non-LTE calculation at a temperature of 200 eV and the Busquet method at a temperature of 58 eV are in agreement and can understand this agreement by looking at the ionization stage distribution, which is given in Figure 4.

5. Summary

We have developed an environment that has potential to provide easy and accurate spectrum and opacity calculations for radiation transport modelers and experimentalists. It integrates modern information technology to provide spectrum and opacity that is heavily dependent on the atomic database. We have also presented our RSSUTA model that can be applied to high Z elements for both LTE and non-LTE plasma conditions. Future work includes the improvement of various rate coefficients since currently we are using the empirical hydrogenic formulas.

Acknowledgment

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