Next Generation of Graphical User Interface for Calculations of Radiative Properties

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Abstract

Based on the previous code JATBASE, we are developing an improved suite of atomic physics codes (YAC). New features include the three-dimensional presentation of opacity data and the Hierarchical Data Format (HDF) for data storage. Physics models include screen hydrogenic model, non-relativistic atomic structure model and jj split relativistic UTA model. Non-LTE opacities for high Z elements are calculated using a hybrid model which employs the semi-empirical rate coefficients and the detailed configuration accounting method. Parallel with this standalone program, a web application (WEBATOM) is currently under development, aiming at web accessibility to our atomic database system with graphical user interface.

Outline

1. Current UW-FTI atomic physics capabilities
2. Theoretical atomic models for calculations of radiative properties
3. Various atomic data processing tools
4. Future work

UW-FTI atomic physics capability

- Atomic properties computed using state-of-the-art models (Z=1-92)
- Plasma state computed using state-of-the-art equilibrium and non-equilibrium models (1 eV – 100 keV)
- Rosseland and Planck opacities computed in tabulated form
- Spectral analysis of measured and computed spectra

Theoretical Atomic Models

❖ Hydrogen-like model
Radiative and collisional properties are calculated by assuming only one electron (nl or nlj) in the system that has an effective charge state.

❖ Average Atom model – self-consistent potential, TFD
Assuming only one pseudo-atom in the plasma.

❖ Unresolved Transition Array method (UTA)
A single profile is used to represent a cluster of transition arrays.

❖ Detailed Configuration Accounting (DCA)
The radiative and collisional properties are done on the configuration level.

❖ Detailed Term Accounting (DTA)
The most complex method that explicitly calculates the radiative and collisional properties under LS or JJ or intermediate coupling scheme.

Relativistic Single-Configuration UTA method

Wave functions are solved from the Dirac equation:

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

Cross sections are calculated under the configuration average approximation :

Photoexcitation:

$$\sigma_{\kappa\kappa'}^{bb}(\hbar\omega)=\frac{\pi he^2}{mc}f_{\kappa\kappa'}\gamma(\hbar\omega),\qquad f_{\kappa\kappa'}=q_\alpha(1-\frac{q_\beta}{g_\beta})f_{\alpha\beta},$$

$$f_{\alpha\beta}=\frac{2m}{\hbar\omega g_\alpha}\frac{1}{2k+1}|<\alpha\|T\|\beta>|^2.$$

Voigt line shape, natural, Doppler, Stark and UTA broadening

Photoionization:

$$\sigma_{i\kappa}=\frac{\pi he^2}{mc}\sum_\alpha q_\alpha\frac{df_\alpha}{d\varepsilon},\qquad \frac{df_\alpha}{d\varepsilon}=\frac{2m}{3\hbar\omega g_\alpha}|<\alpha\|T\|\varepsilon>|^2,$$

Plasma Models to Obtain Atomic State Populations

❖ LTE Model (Local Thermal Equilibrium) -- Collisional ionization and three-body recombination

❖ Corona Model -- Collisional ionization and radiative recombination

❖ Collisional Radiative Equilibrium(CRE) Model

$$N_i\sum_{j\neq i}^{N}W_{ij}-\sum_{j\neq i}^{N}N_jW_{ji}=0\quad,$$

$$W_{ij}=B_{ij}J_{ij}+n_eC_{ij}+\beta_{ij}+n_e\gamma_{ij},$$

$$W_{ji}=A_{ji}+B_{ji}J_{ji}+n_eD_{ji}+n_e(\alpha_{ji}^{RR}+\alpha_{ji}^{DR})+n_e^2\delta_{ji},$$

(i , j = 1,N ; N: total atomic states)

N by N matrix, N can be greater than 1000

Hybrid Non-LTE Model

Assumptions:

- Consider collisional and radiative atomic processes at the ion stage level

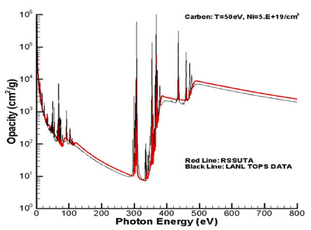
$$\frac{N_{q+1}}{N_q}=\frac{I(q\to q+1)}{R^r(q+1\to q)+R^d(q+1\to q)+n_eR^3(q+1\to q)}$$

- Rate coefficients use semi-classical formulas, such as Lotz's for electron ionization, Kramer's for radiative recombination.
- Screened hydrogen-like atomic data are used for rate coefficient calculations.
- Local thermal equilibrium (LTE) approximation for energy levels in each ion stage.

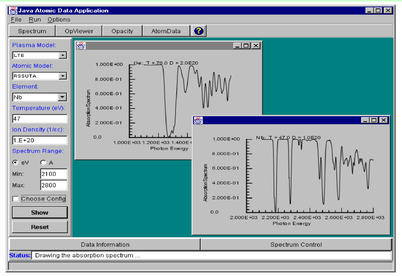
Using accurate atomic energy levels, oscillator strengths from either NRSUTA model or high-Z RSSUTA model, enables us to calculate high-Z non-LTE opacities.

Radiative rates taken into account, therefore <Z> is more accurate than LTE calculations of <Z> for high temperature low density plasmas.

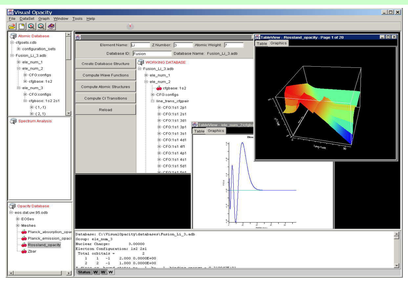
RSSUTA compares favorably to LANL's TOPS



JATBASE User Interface (2001)



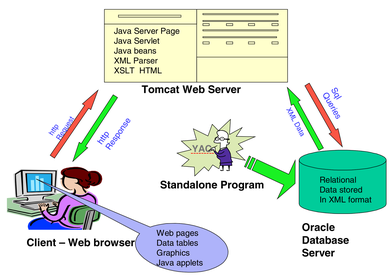
The YAC Code



Features of computer codes

JATBASE	YAC
• Detailed LSJ, LS coupling radiative atomic data (E, gf) for Z=1-18	• Implement all physics already in JATBASE
• Large scale EOS and opacity calculations	• Relativistic unresolved transition array method (RSSUTA)
• Format compatible with hydro codes	• More detailed drill-down information
• Non-relativistic unresolved transition array method	• Better user interface
• Storage in text data format	• 3D graphics visualization
	• Universal Hierarchical Data Format (HDF)

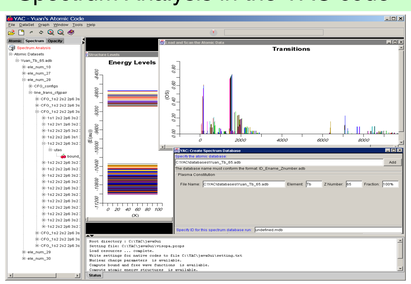
Atomic Data Package Framework



Atomic data processing tools

- JATBASE (completed)
  – Jiankui Yuan's Ph.D. thesis
- YAC (In progress)
  – Standalone application to process data
- WEBATOM (In progress)
  – Web interface to data

Spectrum Analysis in the YAC code



Future Work

Components have been done:

1. Relativistic wave functions for both bound state and free state orbitals.
2. Energy structure calculations for both the DTA model and the UTA model.
3. Bound-bound transitions for the UTA model.

Components will be done:

1. Bound-free photon-ionization cross sections.
2. Free-free bremsstrahlung.
3. LTE and non-LTE level populations.
4. Data processing in the graphical interface.