Building Tools for Atomic Data Calculations

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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 – 100keV)
- Rosseland and Planck opacities computed in tabulated form
- Spectral analysis of measured and computed spectra

Tasks

- Harden atomic physics modeling software
- Create database of requested data
- Complete processing tools to generate data, access data, and visualize data
- Complete analysis tools to compare data to experiment

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:

$$\sigma_{icc'}^{bb}(\hbar\omega) = \frac{\pi h e^2}{mc} f_{icc'} \gamma(\hbar\omega), \qquad f_{icc'} = q_\alpha (1 - \frac{q_\beta}{g_\beta}) f_{\alpha\beta}, \qquad f_{\alpha\beta} = \frac{2m}{\hbar\omega g_\alpha} \frac{1}{2k+1} |<\alpha \| T \| \beta>|^2,$$

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

Photoionization:

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

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

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

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

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

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

N by N matrix, N can be greater than 1000

Non-LTE Model

Assumptions:

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

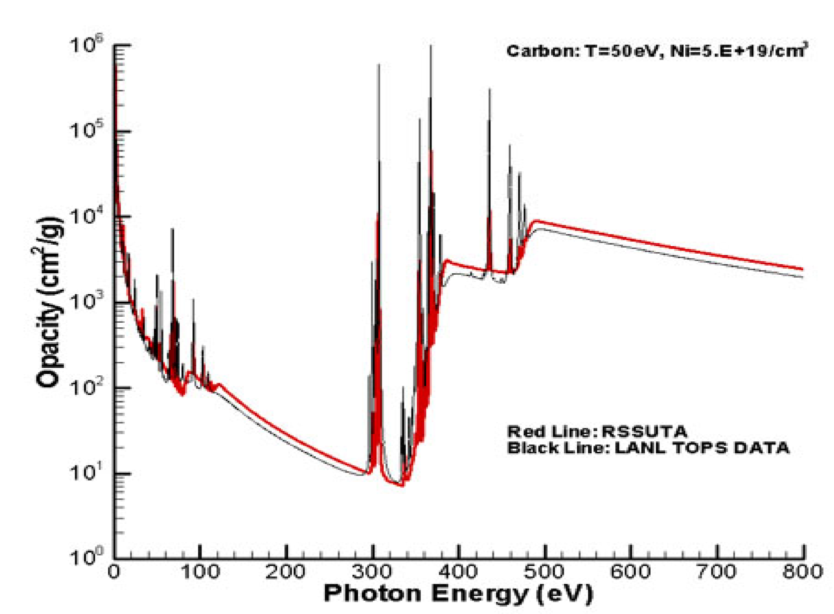
$$\frac{N_{q+1}}{N_q} = \frac{I(q \to q+1)}{R^r(q+1 \to q) + R^d(q+1 \to q) + n_e R^3(q+1 \to q)}$$

- 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.

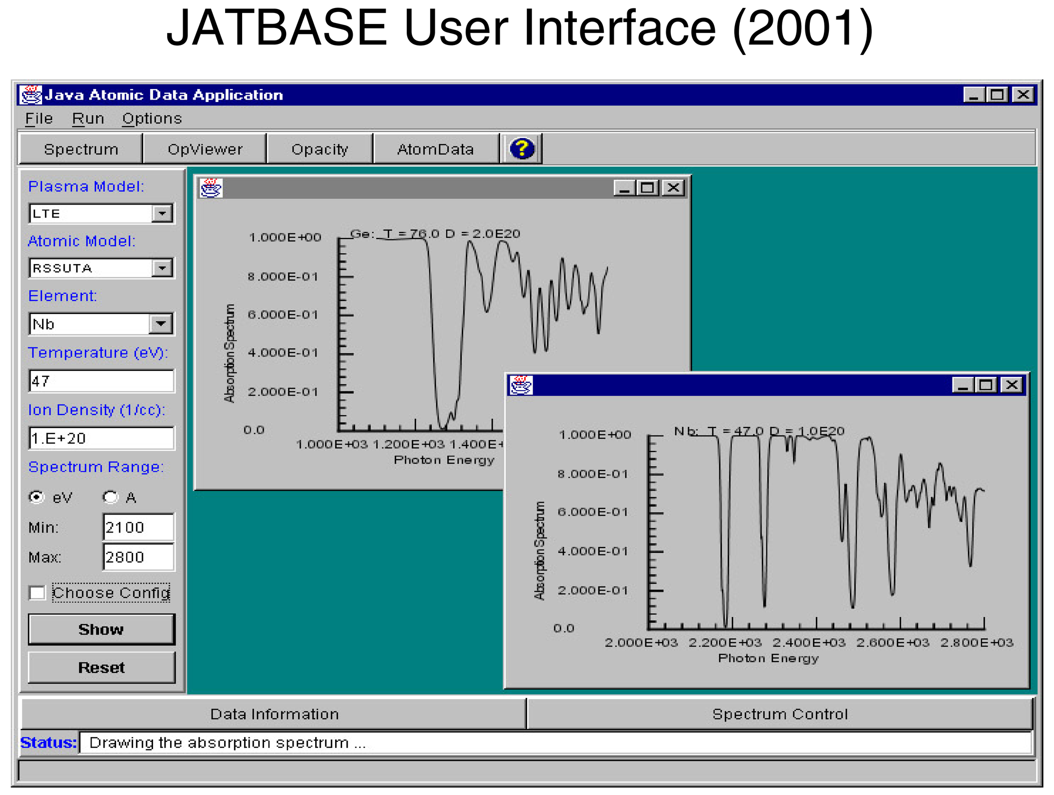
RSSUTA compares favorably to TOPS



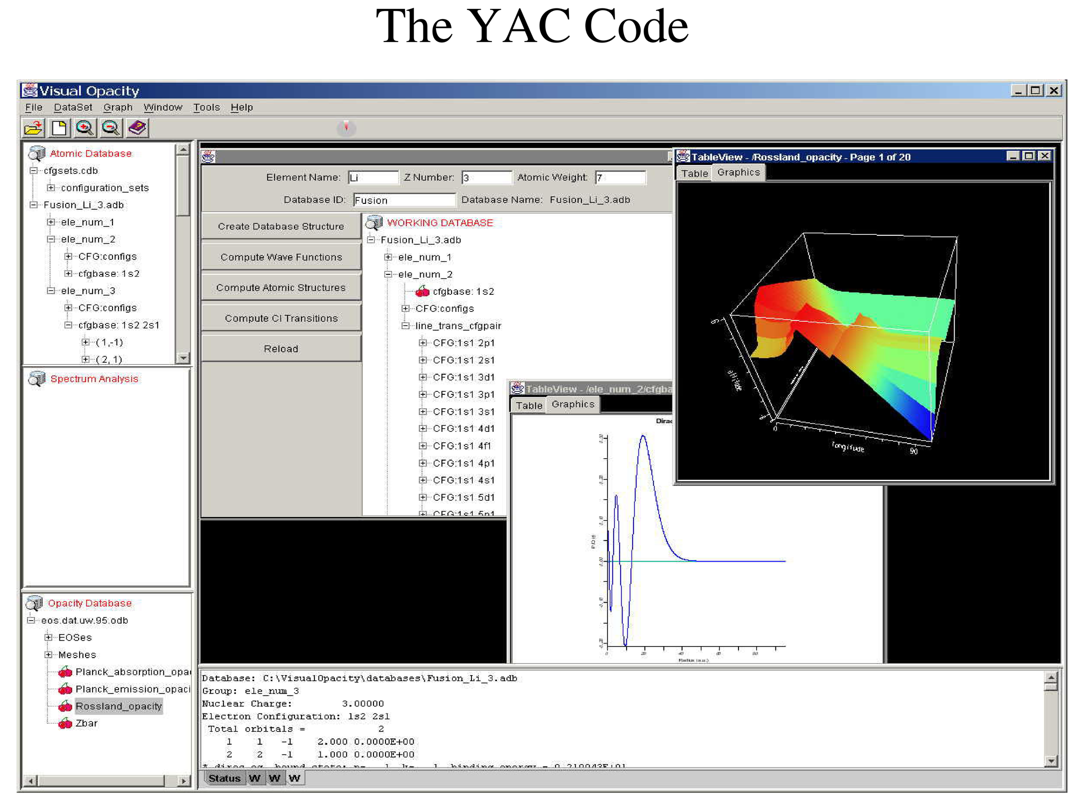
Atomic data processing tools

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

JATBASE User Interface (2001)



The YAC Code



Features of computer codes

JATBASE

- Detailed LSJ, LS coupling radiative atomic data (E, gf) for Z=1-18
- Large scale EOS and opacity calculations
- Format compatible with hydro codes
- Non-relativistic unresolved transition array method
- Storage in text data format

YAC

- Implement all physics already in JATBASE
- Relativistic unresolved transition array method (RSSUTA)
- More detailed drill-down information
- Better user interface
- 3D graphics visualization
- Universal Hierarchical Data Format (HDF)

Atomic Data Package Framework