SAND2010-4282C

Collisional-radiative hybrid-structure atomic models for HED laboratory plasma diagnostics and simulations

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41st Annual Meeting of DAMOP
Houston, TX
May 25-29, 2010

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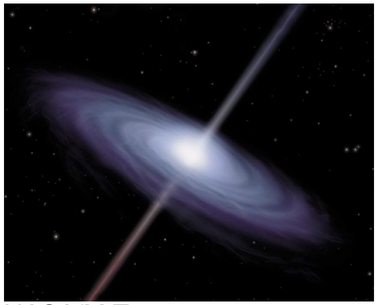
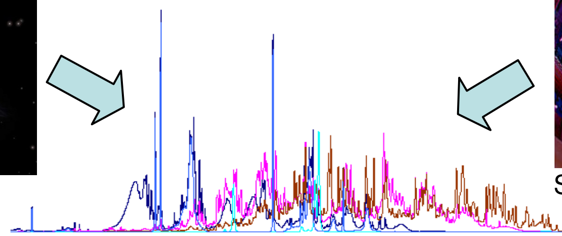
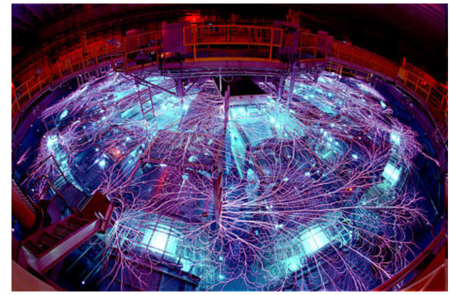
Introduction: spectroscopy provides detailed information about many plasma sources

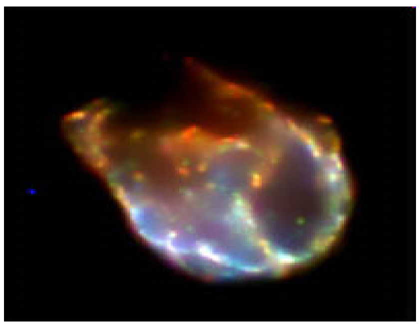


NASA/MIT
black hole accretion disk



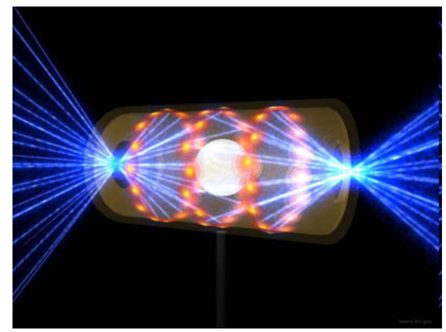


Sandia's Z machine

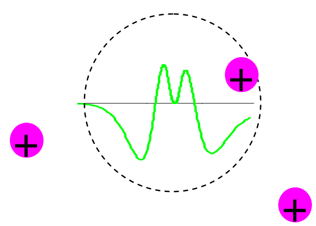


NASA/Chandra
supernova remnant

Collisional-radiative (non-LTE) models



Livermore's NIF



Atomic physics: the foundation

Outline

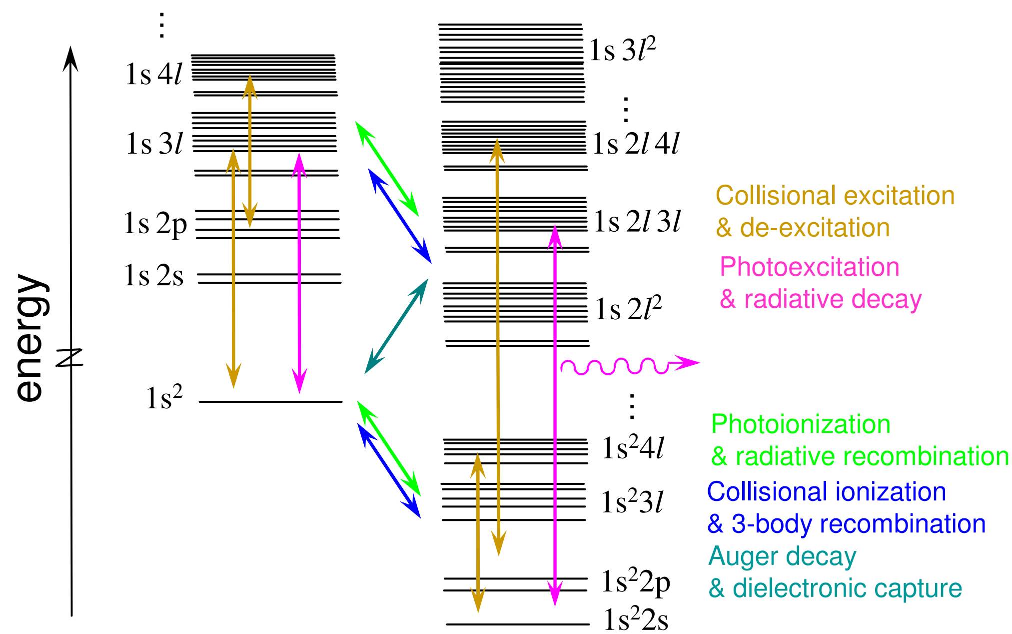
- **Introduction to collisional-radiative atomic models**
  - states & rates → synthetic spectra
  - low-density "coronal" models
  - general requirements for reliable collisional-radiative models

- **Hybrid-structure atomic models**
  - computationally tractable models that balance accuracy and completeness

- **Applications of reliable non-LTE atomic models**
  - spectroscopic plasma diagnostics
  - radiation transport
  - radiation hydrodynamics

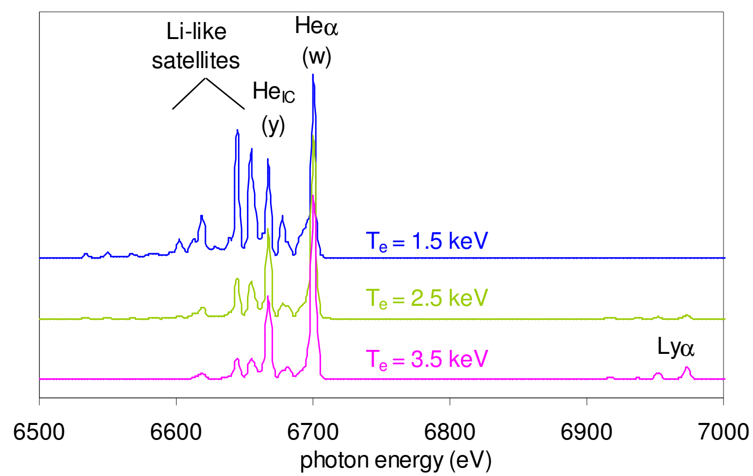
Collisional-radiative models: atomic levels (states) coupled by atomic processes (rates)

Example: He- and Li-like ions



Collisional and spontaneous rates form a rate matrix that is inverted to determine level populations.

With populations and radiative rates, synthetic spectra can be constructed and used for plasma diagnostics or radiation-hydrodynamic simulations



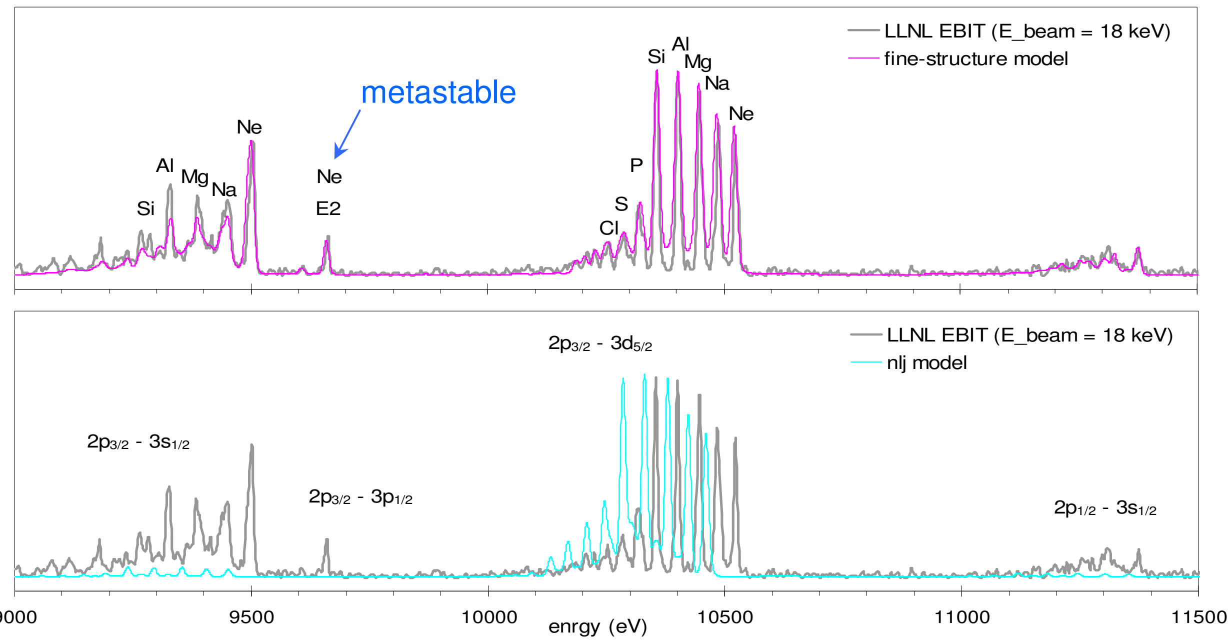
Example: K-shell Fe emission spectra

A variety of codes, (HULLAC, FAC, Cowan…) databases, (NIST, ATOMDB…), and approximations (screened hydrogenic, Lotz…) provide energy level structure and rate data – with varied accuracy.

Low-density "coronal" models generally use high-accuracy atomic data

Coronal atomic models are widely used for EBIT, tokamak, and astrophysical sources, where low densities ensure that population is concentrated in ground states

Example:
L-shell Au emission from LLNL EBIT [1]



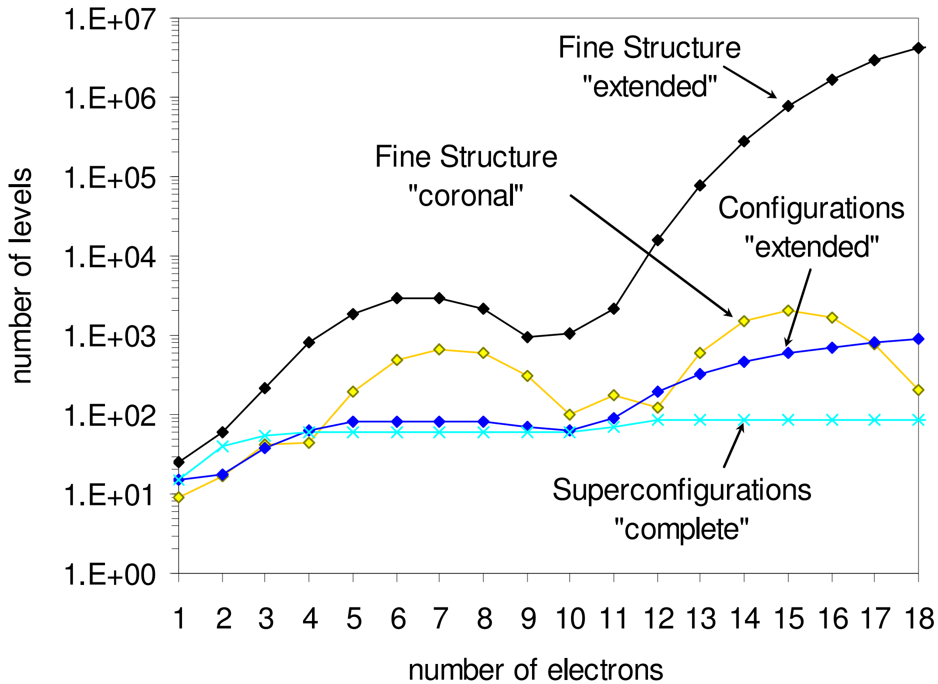
Low-density emission spectra are well-modeled by fine-structure collisional-radiative models. Less accurate models generally do not capture the effects of metastable levels or configuration interaction.

[1] Brown, Hansen *et al.* PRE **77**, 066406 (2008)

For complex ions, extensive fine structure models become intractable

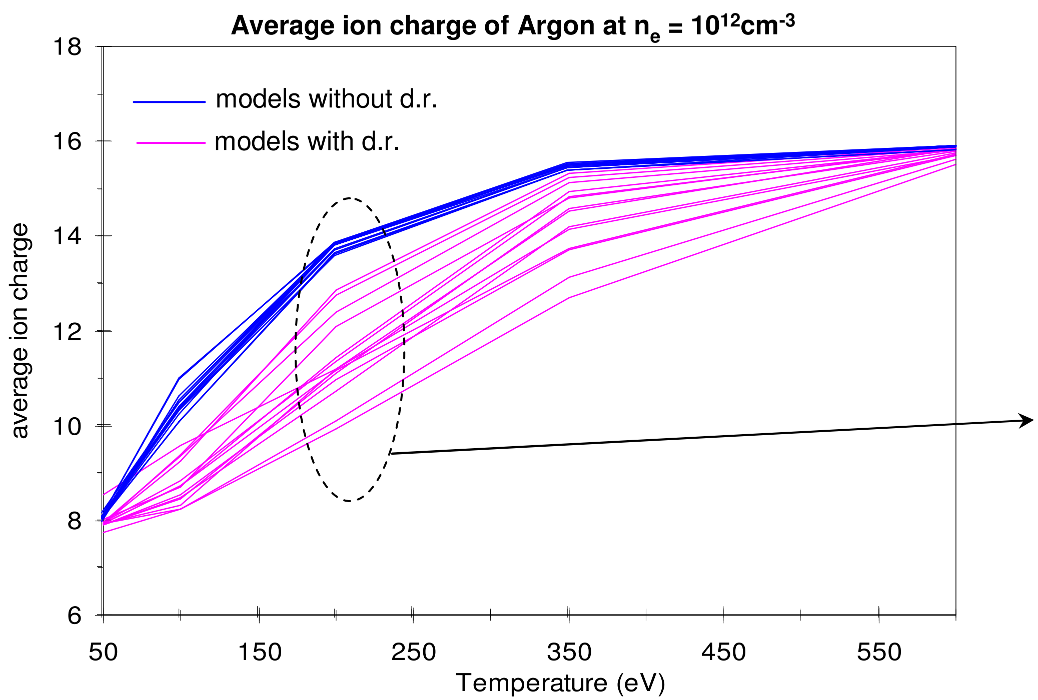
While the number of singly-excited, “coronal” levels remains reasonable with increasing ion complexity, the number of levels required for an extensive model grows exponentially.

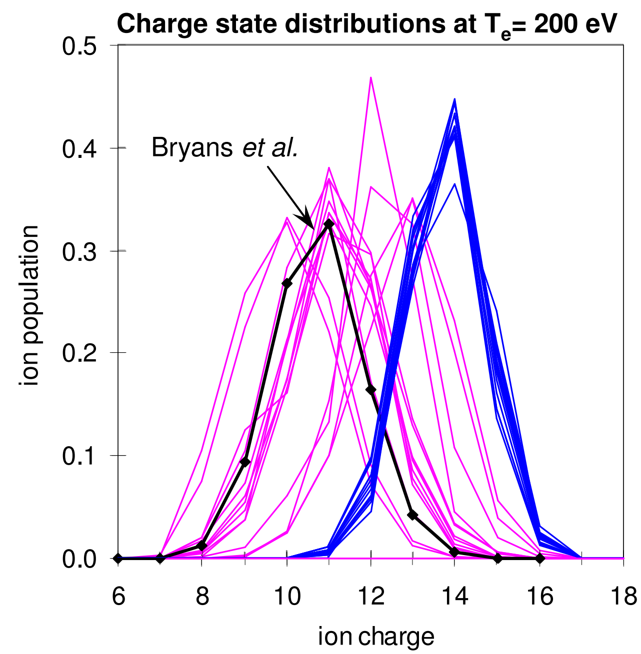
However, only “complete” models with extensive multiply-excited structure can accurately account for dielectronic recombination and satellite emission.



Dielectronic recombination is critical for accurate collisional-radiative modeling

Recent non-LTE workshop results illustrate the importance of d.r.
– and the challenge of getting it right.





For coronal plasmas, global d.r. rates can be used (e.g. Mazotta [2], Bryans [3]), but these do not guarantee accurate satellite emission and are not valid at high densities.

[2] Mazotta *et al.*, Astron. Astrophys. Supp **133**, 403 (1998)
[3] Bryans *et al.* Ap J Supp **167**, 343 (2006)

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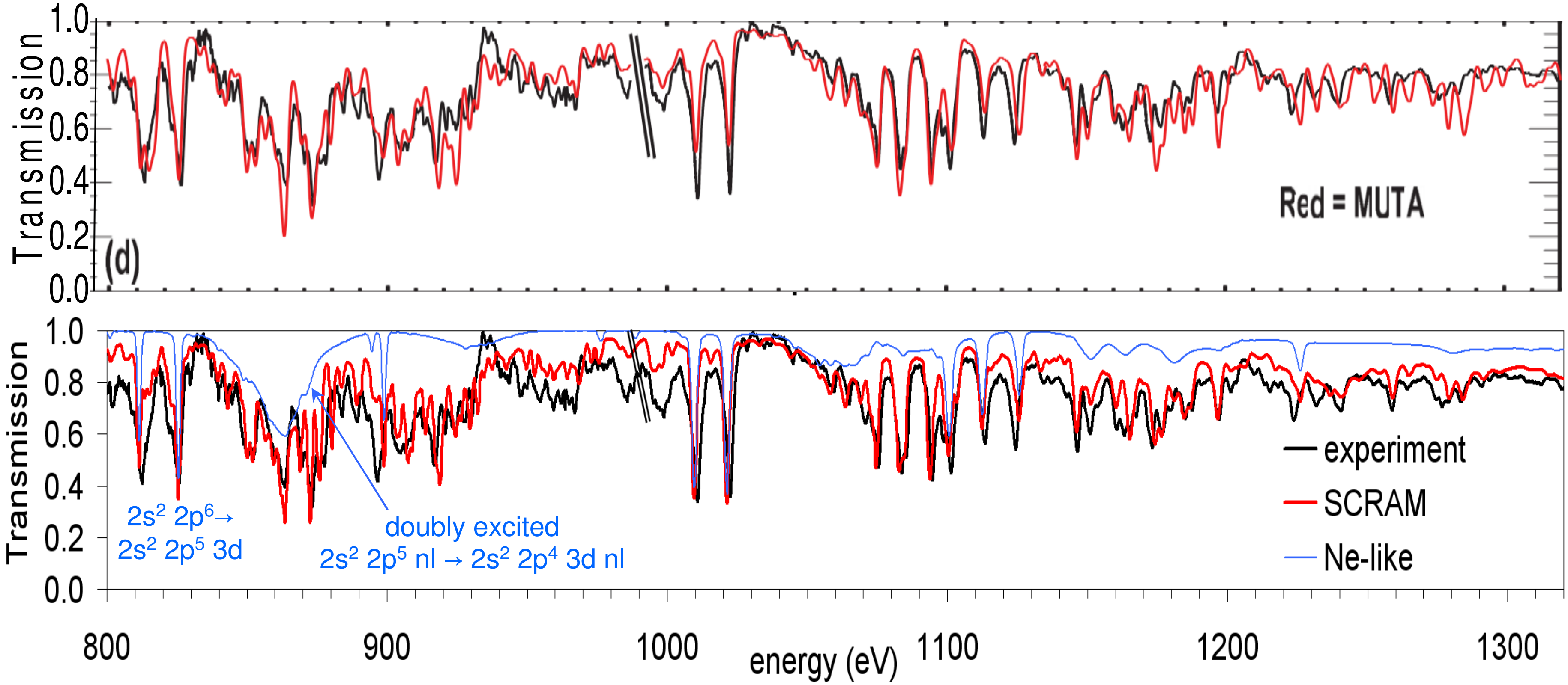
Heroic modeling efforts can give excellent agreement with high-density experimental data



LANL's MUTA [4], a huge fine-structure model with more than 10^7 transitions (some averaged) matches measured Fe L-shell transmission [5] very well, – as does a smaller hybrid-structure model [6].

[4] Mazevet and Abdallah, J. Phys. B **39**, 3419 (2006)
[5] Bailey *et al.* PRL **99**, 265002 (2007)
[6] Hansen *et al.*, HEDP **3**, 109 (2007)

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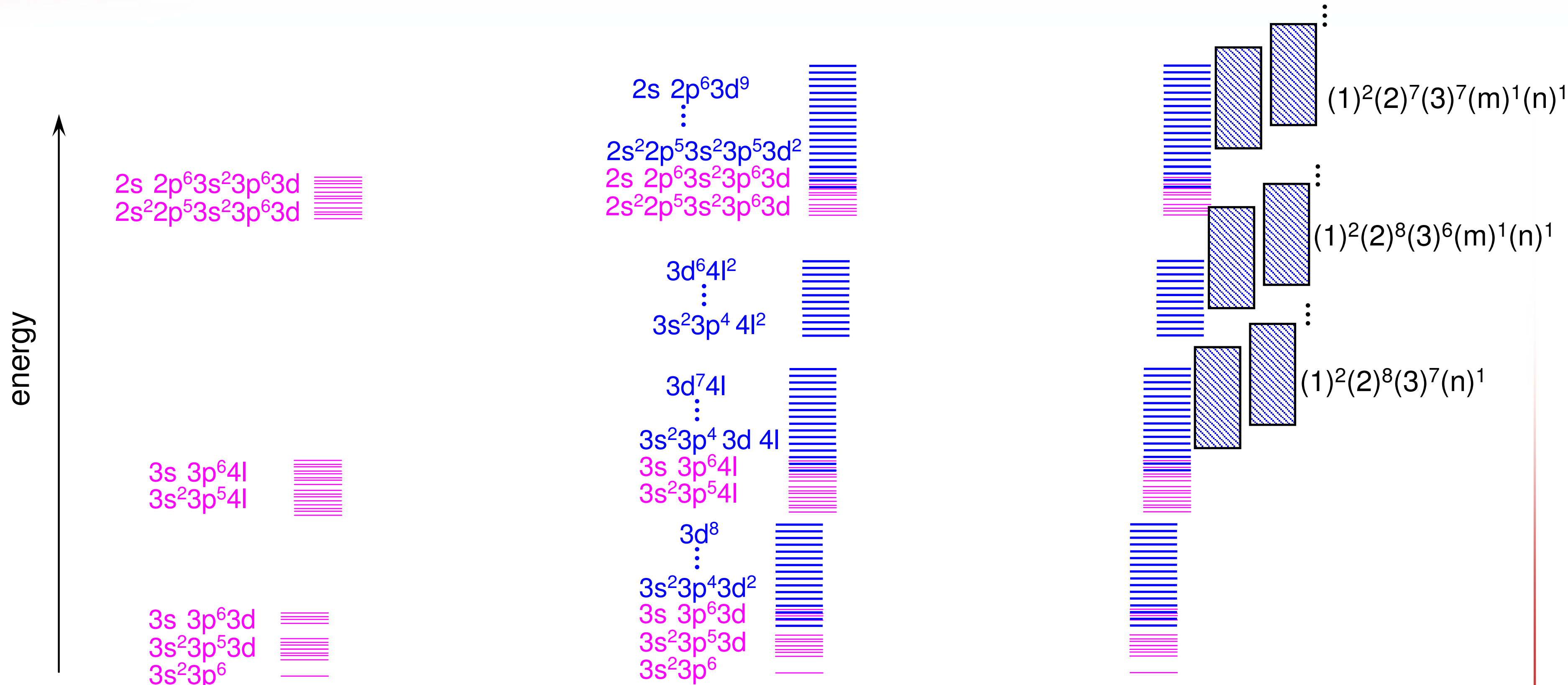
A hybrid-structure approach to collisional-radiative modeling has many advantages



Fine structure (FAC) treatment of "coronal" levels ensures good results at low densities: N ~ 200

Supplemental configs (FAC) with configuration-interaction shifts provide continuity at moderate densities: N ~ 14,000 (800 non-rel)

Supplemental superconfigurations (screened hydrogenic) ensure statistical completeness and exhaustive d.r. channels: N ~ 80

Hybrid-structure models are computationally tractable even for complex ions.

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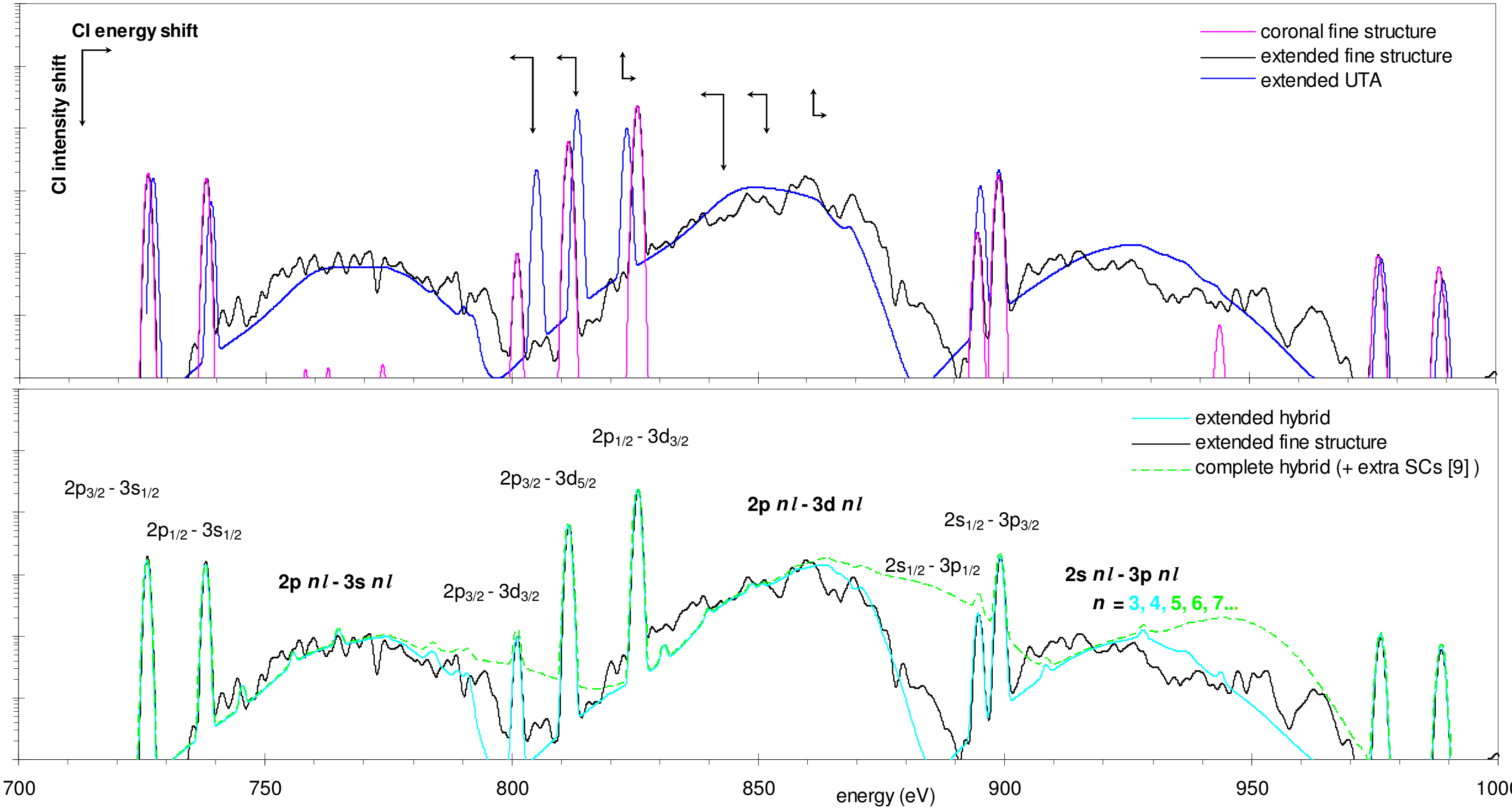
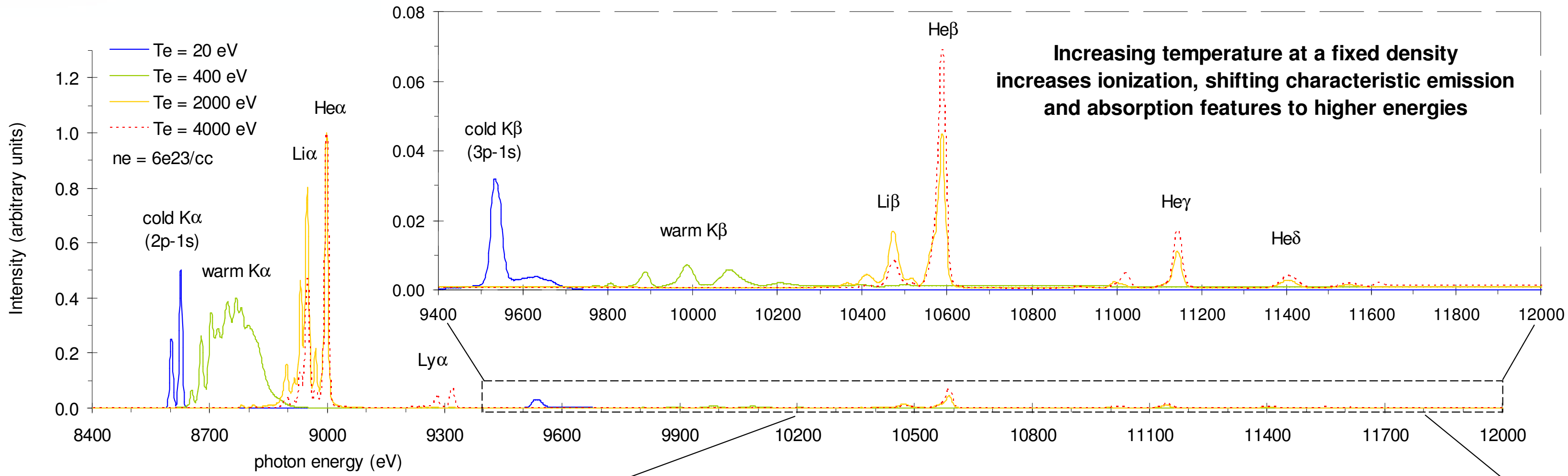
Extending configuration interaction (CI) from fine structure transitions to UTAs is key

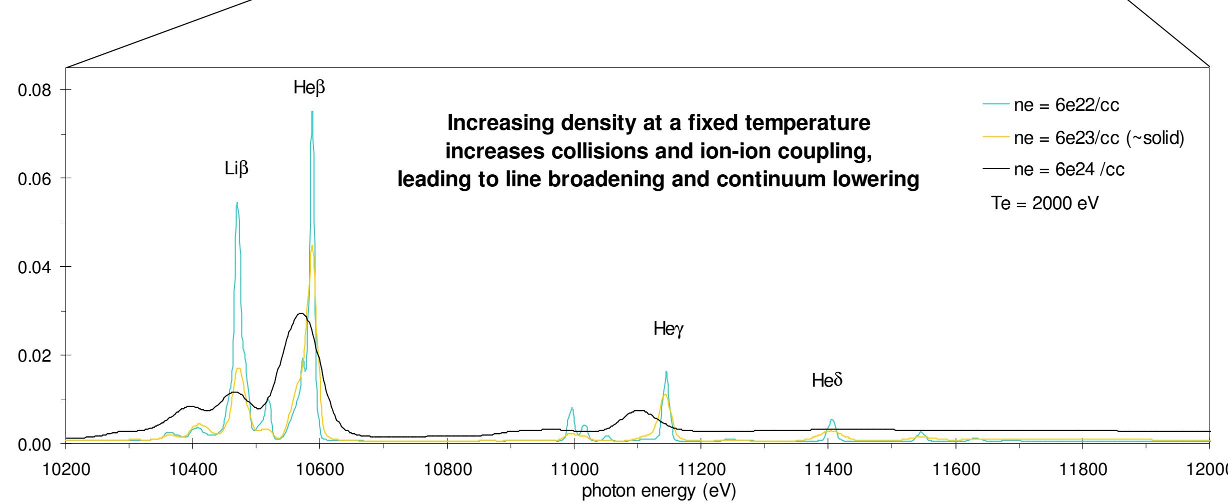


Each nlj – nlj transition in each ion has its own CI corrections obtained from the overlapping sets of fine structure transitions and UTAs [1]

[1] Brown, Hansen *et al.* PRE **77**, 066406 (2008)
[9] Scott and Hansen, HEDP **6**, 39 (2010)

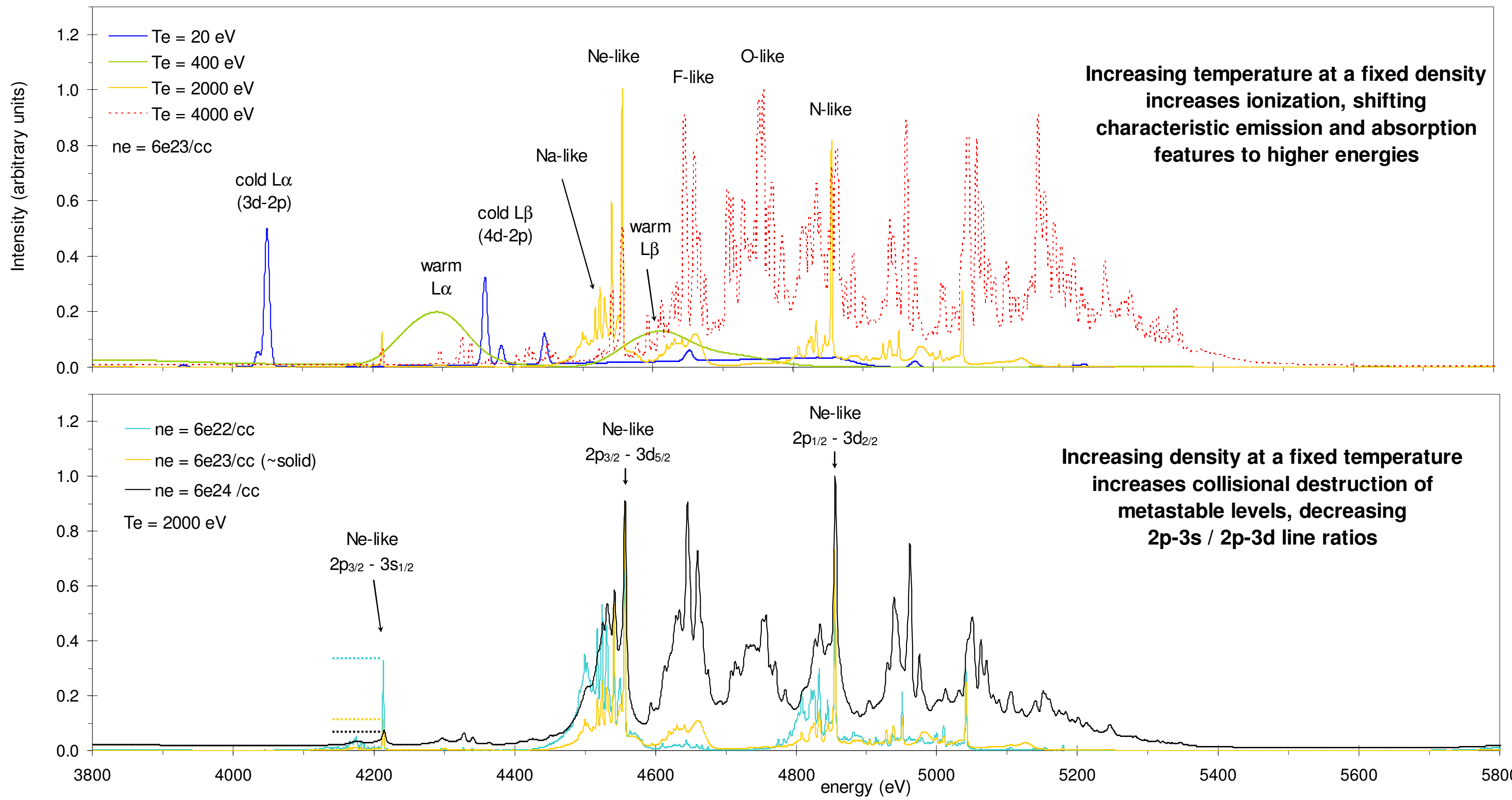
K-shell spectra are the traditional workhorses of spectroscopic plasma diagnostics





Changes in temperature and density have signature effects on K-shell emission

Reliable hybrid models offer new diagnostic opportunities with L-shell spectra



L-shell diagnostics have attractive features including unambiguous temperature dependence and resolution-independent density sensitivity

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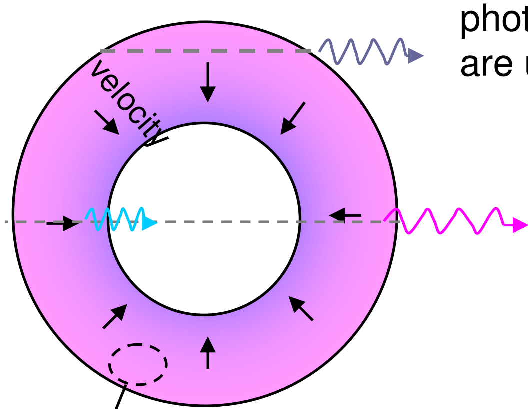
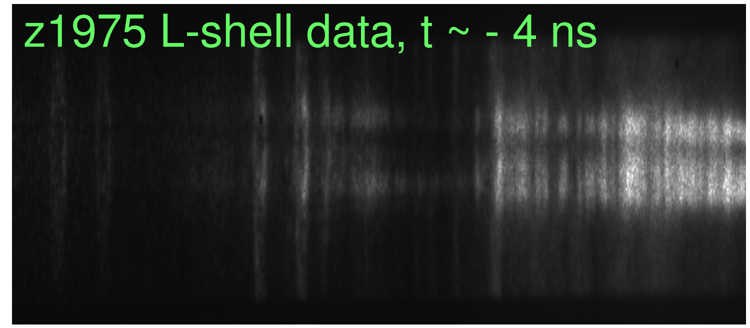
Temporally and spatially resolved spectra give information beyond temperature and density

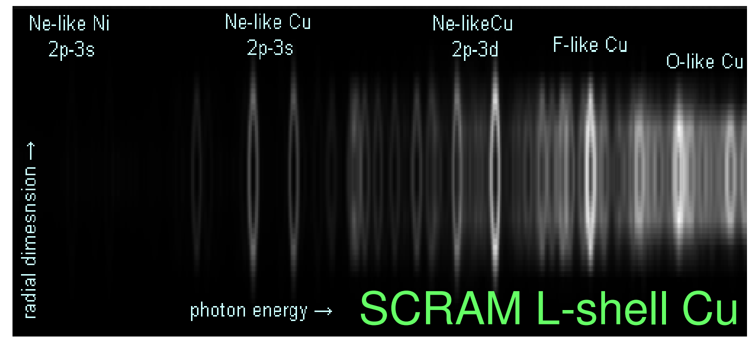


photons from shell edge are unshifted ($v_{||} = 0$)

photons from shell center are maximally shifted ($v_{||} = v$)

plasma conditions:
nion = ion density
Te = electron temperature





60 cm/μs, T_e ~ 3 keV, n_e ~$10^{21}cm^{-3}$
decreasing over ~ 5mm

Radially resolved spectra from an imploding plasma yield information about implosion velocities and gradients

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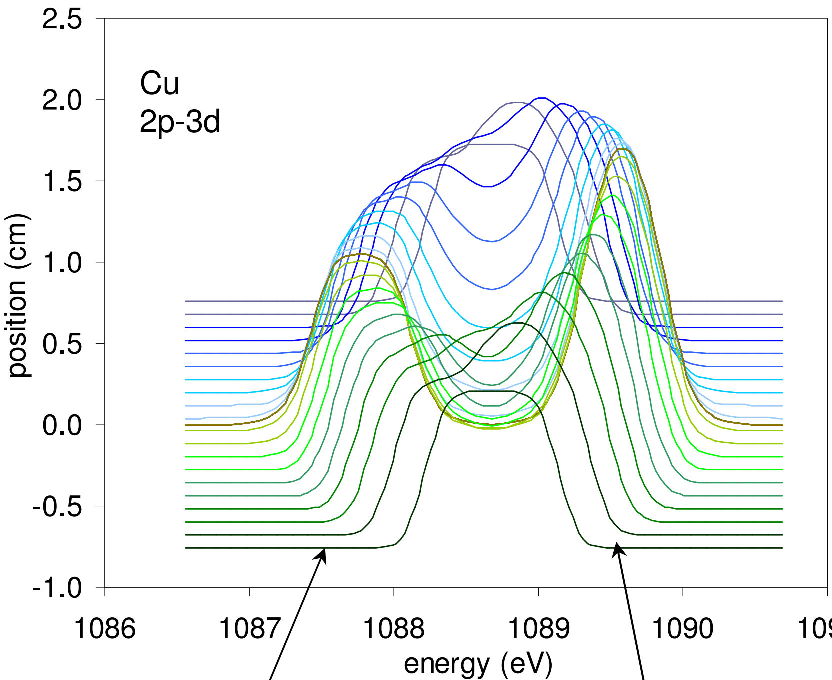
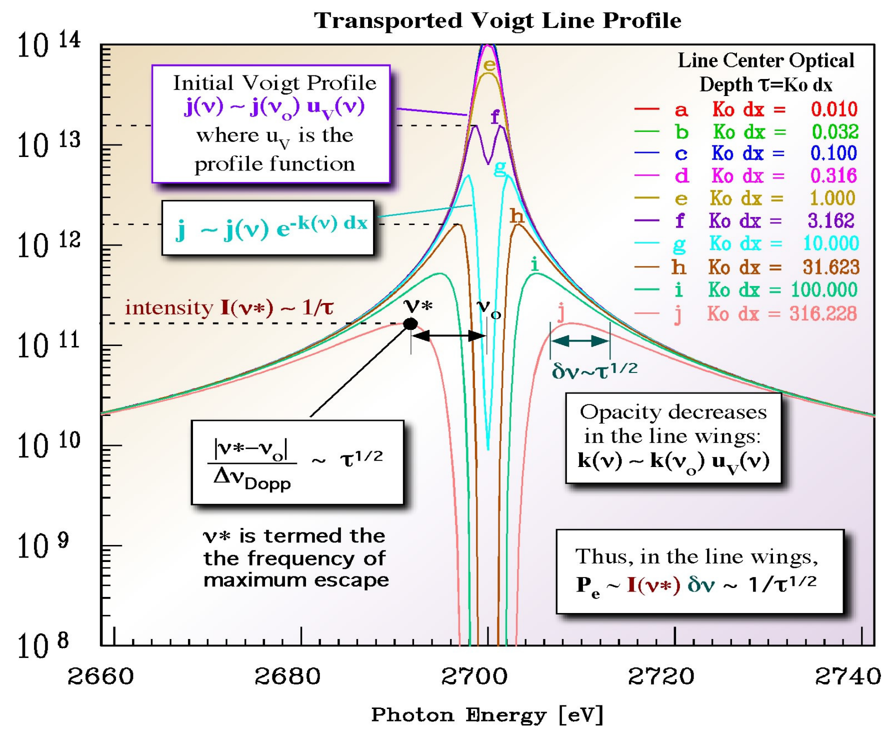
Self-consistent radiation transport is important for optically thick plasmas

Opacity effects can lead to complex signatures in radially resolved spectral lines (*c.f.* Jones, Maron, *et al.*)



red-shifted line from near-side plasma is absorbed by cool outer plasma region

blue-shifted line from far-side plasma is unattenuated

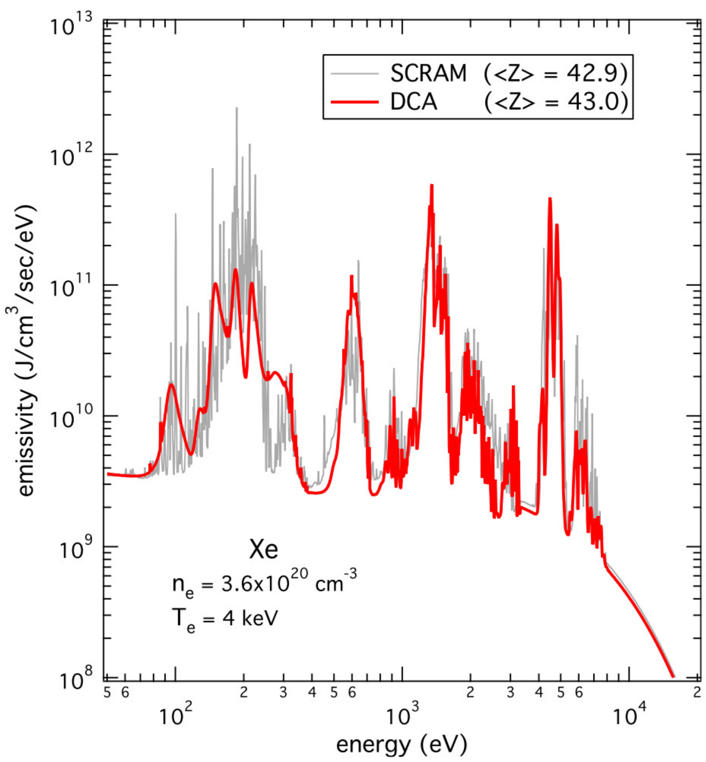


NRL C-R models with radiation transport have given excellent agreement with Z-pinch K-shell spectra (Dasgupta, Apruzese, Thornhill *et al.*)

Accurate non-LTE models benchmark the fast in-line models used in radiation-hydrodynamics simulations

Most in-line radiation transport has limited spectral resolution ("groups") so spectroscopic accuracy is not required. However, *completeness* is necessary for reliable <Z>, power losses, and opacities.

Spectroscopic-quality hybrid models with ~ 3 - 60 min runtimes can be used to benchmark the faster models (*e.g.* DCA [9]) used in radiation-hydrodynamic codes.



Computational constraints in rad-hydro require runtimes ~ 1 second!

[9] Scott and Hansen, HEDP (2010)

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Summary

- **Low-density (coronal) plasmas require models that have:**
  - highly accurate rates and wavelengths (configuration interaction)
  - complete dielectronic recombination channels
  - limited atomic structure

- **At higher densities, collisional-radiative models must include:**
  - reasonably accurate radiative decay rates and wavelengths
  - continuum lowering and line broadening
  - extensive energy level structure

- **Models for non-LTE plasmas at intermediate densities must have <u>all</u> of these qualities**
  - hybrid-structure models combine fine-structure “coronal” levels with configuration- and superconfiguration-averaged states

- **Reliable non-LTE atomic models are critical for HEDLP**
  - plasma diagnostics
  - radiation hydrodynamics

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