NLTE Code Comparison Workshops: an overview

Yuri Ralchenko
Atomic Spectroscopy Group
National Institute of Standards and Technology
Gaithersburg MD, USA

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IAEA, Vienna, Austria

NIST
National Institute of Standards and Technology
U.S. Department of Commerce

Non-LTE Code Comparison Workshops

- Goal: to benchmark CR models for plasma population kinetics against ideal cases (practically no “clean” experiments in (relatively dense) plasmas)
- In other words: validation and verification of CR models
- Models may differ in various parameters, e.g., atomic structure, number of states, nature of states, quality of atomic data, etc.
- Opacity codes, spectral line shapes codes
- NLTE: 15-20 codes, 20-25 participants
- Last: NLTE-9, Paris, 2015
- Next: NLTE-10, San Diego CA, Nov-Dec 2017

Codes ARE different!!!

- Atomic structure
  - Fine structure (levels)
  - Atomic terms
  - Relativistic configurations
  - Non-relativistic configurations
  - Superconfigurations
  - Average atom
  - …
- Calculation methods
  - Plane-wave Born
  - Coulomb Born
  - Distorted wave
  - Close coupling
  - …
- Plasma physics
  - Opacity effects
  - Ionization potential lowering

Parameters to compare

- **Global parameters (vs. temperature and/or density)**
- – Total number of ionization stages
- – Total number of energy levels
- – Total statistical weight over all states
- – Mean ion charge Z
- – Second central moment $\sigma 2$ (variance)
- – Difference (ΔZ,$\Delta \sigma 2$) (with regard to a reference code)
- – Third central moment (skewness)
- – Internal energy
- – Partition function
- – Maximal principal quantum number over all ion stages
- – Total, bound-bound, bound-free, and free-free radiative power losses

- **Ion charge-stage parameters (for one combination of temperature and density; vs.**
- **ion charge)**
- – Ion charge-state populations
- – Ionization potential (from the corresponding ground state)
- – Total number of levels
- – Total statistical weight
- – Maximal principal quantum number for an ion stage
- – Effective ionization rates (absolute or fractional)
- total, collisional, photoionization, or autoionization
- – Effective recombination rates (absolute or fractional)
- total, three-body, radiative, or dielectronic
- – α/S ratio (i.e., recombination to ionization ratio)
- – Net rate
- – Excitation-autoionization rate
- – Dielectronic recombination rate for $\Delta n = 0$ and $\Delta n > 0$ channels

Parameters to compare (cont'd)

- **Level population parameters (vs. energy or level number)**
- – Statistical weight
- – Level population *Ni*
- – Ratios *Ni /NSaha* and *Ni /NLT E* (explained below)
- – Shell populations
- – Occupation numbers
- – Population influx (absolute and fractional)
- total, excitation or deexcitation, radiative, ionization or three-body recombination,
- photorecombination, dielectronic recombination or dielectronic
- capture
- – Population outflux (absolute and fractional)
- total, excitation or deexcitation, radiative, ionization or three-body recombination,
- photoionization, autoionization

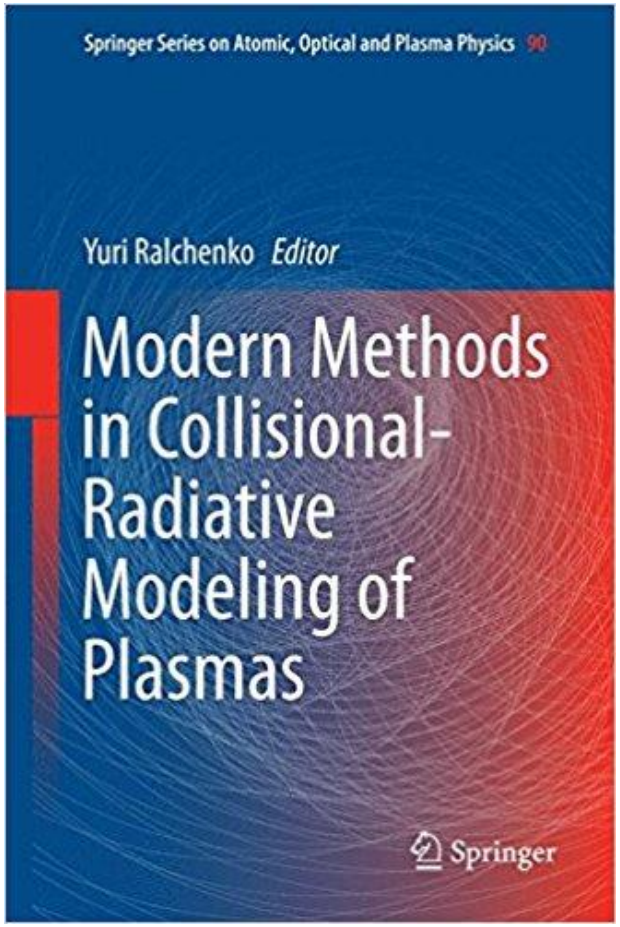
- **Spectra (vs. energy or wavelength)**
- – Total, bound-bound, bound-free and free-free emission
- – Total, bound-bound, bound-free and free-free transmission
- – Spectrum for a selected ion stage

How to compare different models?

- Find sensitive parameters!
- Compare **integral characteristics**
  - Ionization distributions
  - Radiative power losses
- Compare **effective (averaged) rates**
- Compare **deviations from equilibrium** (LTE)

- NLTE Workshops
  - Chung et al, HEDP **9**, 645 (2013)
  - Fontes et al, HEDP **5**, 15 (2009)
  - Rubiano et al, HEDP **3**, 225 (2007)
  - Bowen et al, JQSRT **99**, 102 (2006)
  - Bowen et al, JQSRT **81**, 71 (2003)
  - Lee et al, JQSRT **58**, 737 (1997)
- Typically ~**25** participants, ~**20** codes

Comprehensive overview of CR modeling methods



Chapter 8:
Validation and Verification of Collisional-Radiative Models

Critical issues

- Critical mass of participants/codes
- Variety of parameters to compare
- Good analysis of submitted data: database, interface, graphics