Some thoughts on Uncertainties and Error Propagation in Collisional-Radiative Models

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Question to ask

What is the effect of uncertainties in atomic data on the uncertainties of the derived plasma kinetic parameters?

- Line intensities and level populations
- Ionization distribution characteristics
- Radiative power losses
- ...
Plan

• Collisional-radiative modeling in 30 seconds
• History
• Monte Carlo simulations for Steady-State CR
• Non-LTE Code Comparison Workshops
• Conclusions
Collisional-Radiative Models

• Solve rate equations to determine atomic state populations and all relevant parameters
  ▫ Ionization balance
    • Mean ion charge $\bar{Z}$
    • Central moments
  ▫ Spectral emission
  ▫ Power losses
• CRMs can be very different!

\[
\frac{d\hat{N}(t)}{dt} = \hat{A}(t) \cdot \hat{N}(t)
\]
Benchmarks for plasmas?.. 

A. Plasma must have
- No gradients
- No temporal behavior
- No space effects (opacity)
- Thermal EEDF (mono!)

B. Independent measurements
- Particle temperature
- Particle density
- Spectral characteristics and/or plasma population kinetics parameters

It is extraordinarily difficult to satisfy both A and B in laboratory plasmas
What data?..

- **Energy levels** (different nature, e.g., m-sublevels, levels, terms, configurations, superconfigurations)
- **Radiative rates** (Einstein coefficients or oscillator strengths)
- **Autoionization rates**
- Collisional cross sections or rate coefficients
  - Electron-impact (de)excitation and ionization
  - Photoexcitation, photoionization, photorecombination
  - Three-body recombination
  - Dielectronic capture or dielectronic recombination
  - Heavy-particle collisions
  - ...

Density limits

• **High density**
  ▫ Different for different ion charges
  ▫ LTE/Saha equilibrium
    • Collisions are much stronger than non-collisional processes
    • \( N_i = N_0 \frac{g_i}{g_0} e^{-\Delta E_{i0}/T_e} \)
    • Populations only depend on energies, degeneracies, and (electron) temperature
    • BUT: need radiative rates for spectral emission

• **Low density (corona)**
  ▫ All data are (generally) important
  ▫ Line intensities (mostly) do NOT depend on radiative rates, only on collisional rates
History + recent work

- D. Salzmann (SNRC)
  - PRA, 1980
  - \( \frac{N_{i+1}}{N_i} = f_i \)
  - \( \frac{\Delta N_Z}{N_Z} = \alpha (Z - \bar{Z}) \)
  - Most abundant changes the least

- Modern efforts
  - Auburn + NASA + Harvard + Strathclyde
    - Within one ion
    - G and R ratios in He-like ions
    - Baseline uncertainties
      - Difference between different theoretical approaches
    - Method sensitivity
      - Same method but different model sizes

“It is our opinion that a systematic approach to error is overdue in this area”
Summers et al, 2002
History (cont’d)

- Workshop “Uncertainties in atomic data and how they propagate in chemical abundances”, Tenerife, Spain, 2010
  - ~25 participants
  - MC approach
  - Analytical approach does not give a good estimate of the true statistical uncertainties
  - Importance of analysis of systematic uncertainties
Definitions

- **Ion populations**
  - $i = 0..Z_N$, $N_i$ is the total population of the ion $i$
  - $\sum_{i=0}^{Z_N} N_i = 1$

- **Mean ion charge and central moments**

\[
\bar{Z} = \sum_{i=0}^{Z_N} i \cdot N_i
\]

variance

\[
\sigma_2 = \sum_{i=0}^{Z_N} (i - \bar{Z})^2 \cdot N_i
\]

Third moment

\[
\sigma_3 = \sum_{i=0}^{Z_N} (i - \bar{Z})^3 \cdot N_i
\]
Monte Carlo vs Analytical (WSS)

- **Monte Carlo**
  - Inherently simple
  - Any distribution of uncertainties can be propagated at any stage
  - Does not require relative uncertainties to be small

- **Analytical**
  - Can become extremely complex
  - Implicitly assumes normal distribution for all input/output uncertainties
  - The Taylor expansion requires that the uncertainties be small relative to the quantities

\[
H = h(f, g, \ldots)
\]

\[
\sigma^2_H = \left( \frac{\partial h}{\partial f} \sigma_f \right)^2 + \left( \frac{\partial h}{\partial g} \sigma_g \right)^2 + \ldots
\]
Monte Carlo analysis

- Generate a (pseudo-)random number between 0 and 1
- Using Marsaglia polar method, generate a normal distribution
- Randomly multiply every rate by the generated number(s)
- To preserve physics, **direct and reverse** rates (e.g. electron-impact ionization and three-body recombination) are multiplied by the same number
- Ionization distribution is calculated for steady-state approximation
We think in logarithms...

- Sample probability distribution
  - Normal distribution with the standard deviation $\sigma$
    \[ f(x) = \frac{1}{\sigma \sqrt{2\pi}} e^{-(x-\mu)^2/2\sigma^2} \]
  - Normal distribution is applied to log(Rate)
    - log-normal distribution
Ne: fixed I&R rates

$N_e = 10^8 \text{ cm}^{-3}$

$T_e = 1-100 \text{ eV}$

Ionization stages:
Ne I-IX

**ONLY**
ground states

MC: $10^6$ runs

NOMAD code
(Ralchenko & Maron, 2001)
Ne: + stdev=0.05
Ne: + stdev=0.30
Ne: + stddev=2
Ne: + stdev=10

Structures appear!

Yu. Ralchenko, to be published
Lines: two ions populated

\[ \bar{Z} = Z + n \cdot (1 - \alpha) \]
\[ \sigma^2 = (\bar{Z} - Z) \cdot (Z + n - \bar{Z}) \]

\[ n = 1, 2, >2 \]
Standard deviation: 10

\[ \sigma_3 = f(\bar{Z}, \sigma_2) \]

Standard deviation: 2
Deviation for Z

Yu. Ralchenko, to be published

Fixed $T_e = 20$ eV
C: $10^6$ cm$^{-3}$, ground states only
C: g.s. and full model
C: full model
C: $10^6$ and $10^{17}$
C: $10^6$, $10^{17}$ and $10^{19}$
C: $10^6$, $10^{17}$, $10^{19}$, and $10^{21}$

Yu. Ralchenko, to be published
C: $10^6$, g.s.
Non-LTE Code Comparison Workshops

- Goal: to benchmark CR models against ideal cases
- Models may differ in various parameters, e.g., atomic structure, number of states, nature of states, quality of atomic data, etc.
- 15-20 codes, 20-25 participants
- Last: NLTE-7, Vienna, 2011
- Next: NLTE-8, Santa Fe, 2013
NLTE-7: Kr comparisons

S. Hansen et al, to be published in HEDP
Conclusions

• We are witnessing the beginning of the systematic analysis of uncertainty propagation in CR models
• Both analytical and MC methods are being applied
• First efforts produced a number of interesting results
• More to follow soon...