Propagation of uncertainties in atomic data through collisional-radiative models

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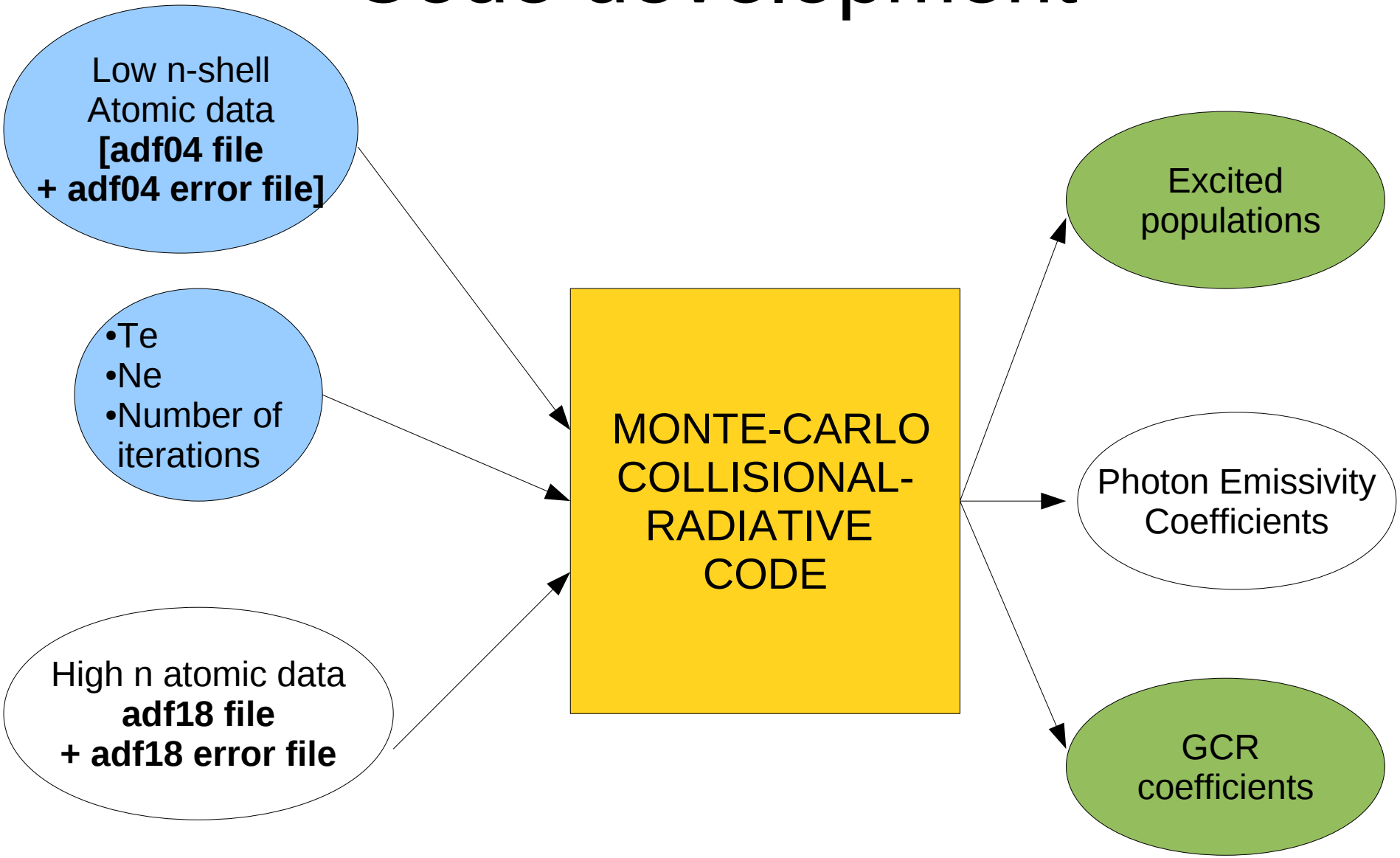
Motivation

- With error bars on atomic data:
  - One could evaluate uncertainties in derived coefficients such as *line intensities, line ratios, or effective ionization/recombination rate coefficients, and the associated diagnostics.*
  - One could determine whether discrepancies between theory and plasma measurements are due to inaccurate atomic data, missing physics in the models, or if there is in fact agreement within the uncertainties in the measurements and theory.

Aim of this project

- To develop the codes/framework to take uncertainties on fundamental atomic data through to derived coefficients such as
  - Excited populations.
  - Line intensities/Line ratios.
  - Generalized collisional-radiative coefficients.
- To explore the main issues associated with propagating atomic data through collisional-radiative codes.

Code development



First test case: Lithium

- We chose Li as our test case because
  - We have high quality atomic data in ADAS already.
  - We can look at the metastable resolved case for Li^{+}.
- We considered each ion of Li in the Coronal, Collisional-radiative and LTE regimes, at their temperatures of peak abundance.
- We had the following questions.
  - Do Gaussian distributions in the input data give Gaussian distributions in the derived coefficients?
  - How do the uncertainties in the fundamental data carry through to uncertainties in the derived coefficients?
  - What is the role of correlation in the atomic data?

Sample results
Li^{2+}, $Ne=1x10^{6}$ cm^{-3}, $Te=20eV$
10% error-bars on all atomic data

Excited populations

Error bar in population

Effective ionization and recombination rate coefficients.

```
== OUTPUT - Log-Normal Distribution ==

Population Vectors

   nexc  nmeta       avg            err          skew (sample)    skew (expect)
     1      1    8.411180E-16   1.152153E-16     4.224767E-01    4.154781E-01
     2      1    4.398438E-16   5.016842E-17     3.524778E-01    3.447932E-01
     3      1    4.321843E-16   4.675154E-17     3.392028E-01    3.267537E-01
     4      1    4.866534E-16   5.463937E-17     3.346749E-01    3.393203E-01
   nexc nmetap       avg            err          skew (sample)    skew (expect)
     1      2    4.622569E-18   5.726833E-19     3.828608E-01    3.750198E-01
     2      2    1.029562E-17   1.107742E-18     3.381028E-01    3.249733E-01
     3      2    1.836483E-17   1.951267E-18     3.301158E-01    3.208620E-01
     4      2    2.721534E-17   3.058918E-18     3.381415E-01    3.396918E-01

GCR Vectors

s: nmetap nmeta       avg            err          skew (sample)    skew (expect)
     1      1    1.319927E-06   1.316562E-07     3.052232E-01    3.009808E-01
r: nmeta  nmetap      avg            err          skew (sample)    skew (expect)
     1      1    5.291160E-07   3.142586E-08     2.335400E-01    1.785468E-01

CPU TIME:    3.930 MIN
```

Distribution functions of derived coefficients.

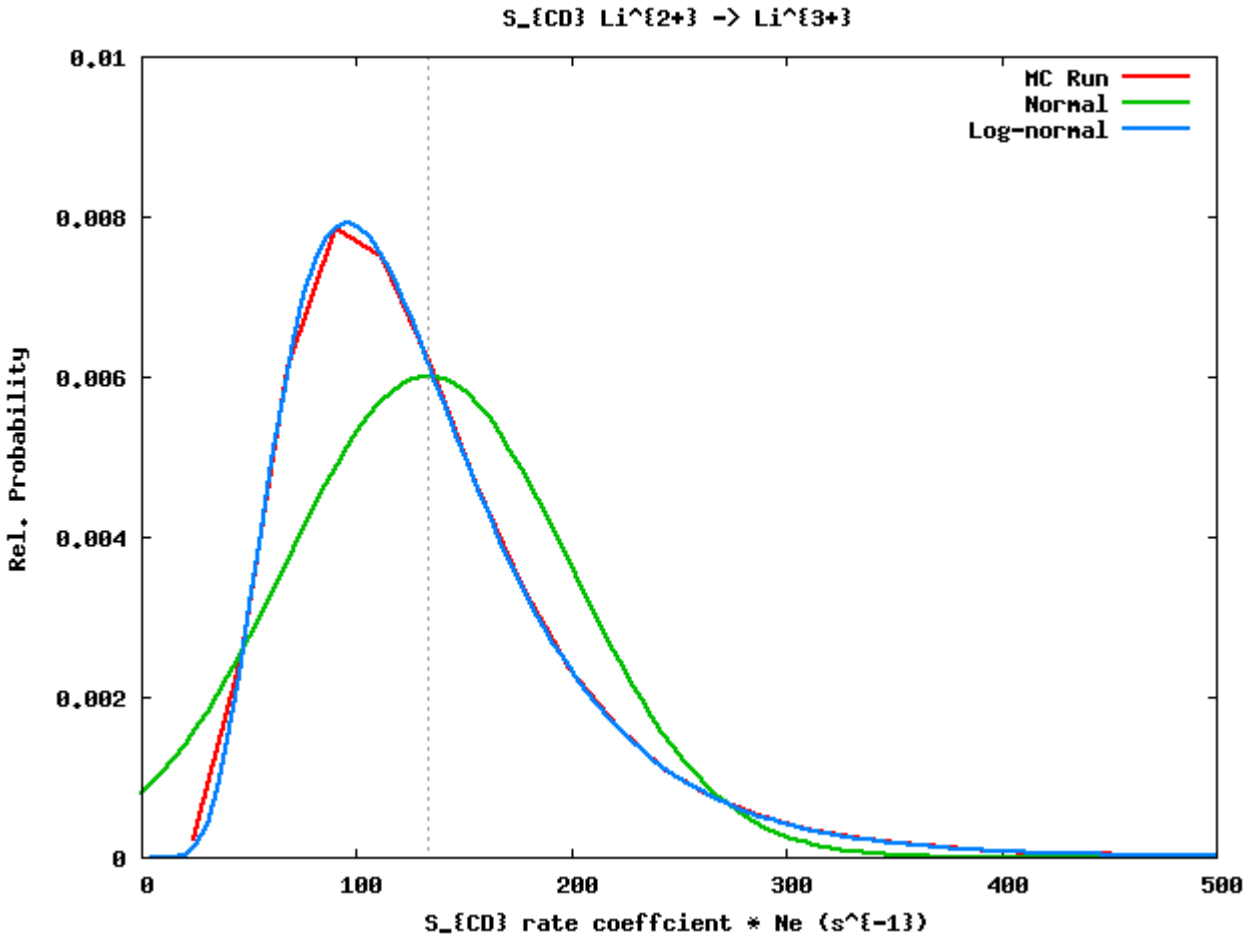
- For most cases Gaussian distribution of uncertainties in the input atomic data leads to Gaussian distribution of the derived coefficients.
- However, all of the output coefficients are bounded by zero, leading to ***log-normal distributions.***

$$f(x_i) = \frac{1}{\sqrt{2\pi s_i^2 x_i^2}} e^{\frac{(\ln(x_i) - m_i)^2}{2s_i^2}}$$

- When one gets close to the LTE regimes, the low-n populations are also bounded by the thermodynamic limit.
- This means that the results using zero error won't always correspond to the peak of the distribution function.

Li^{2+} Effective ionization rate coefficient.

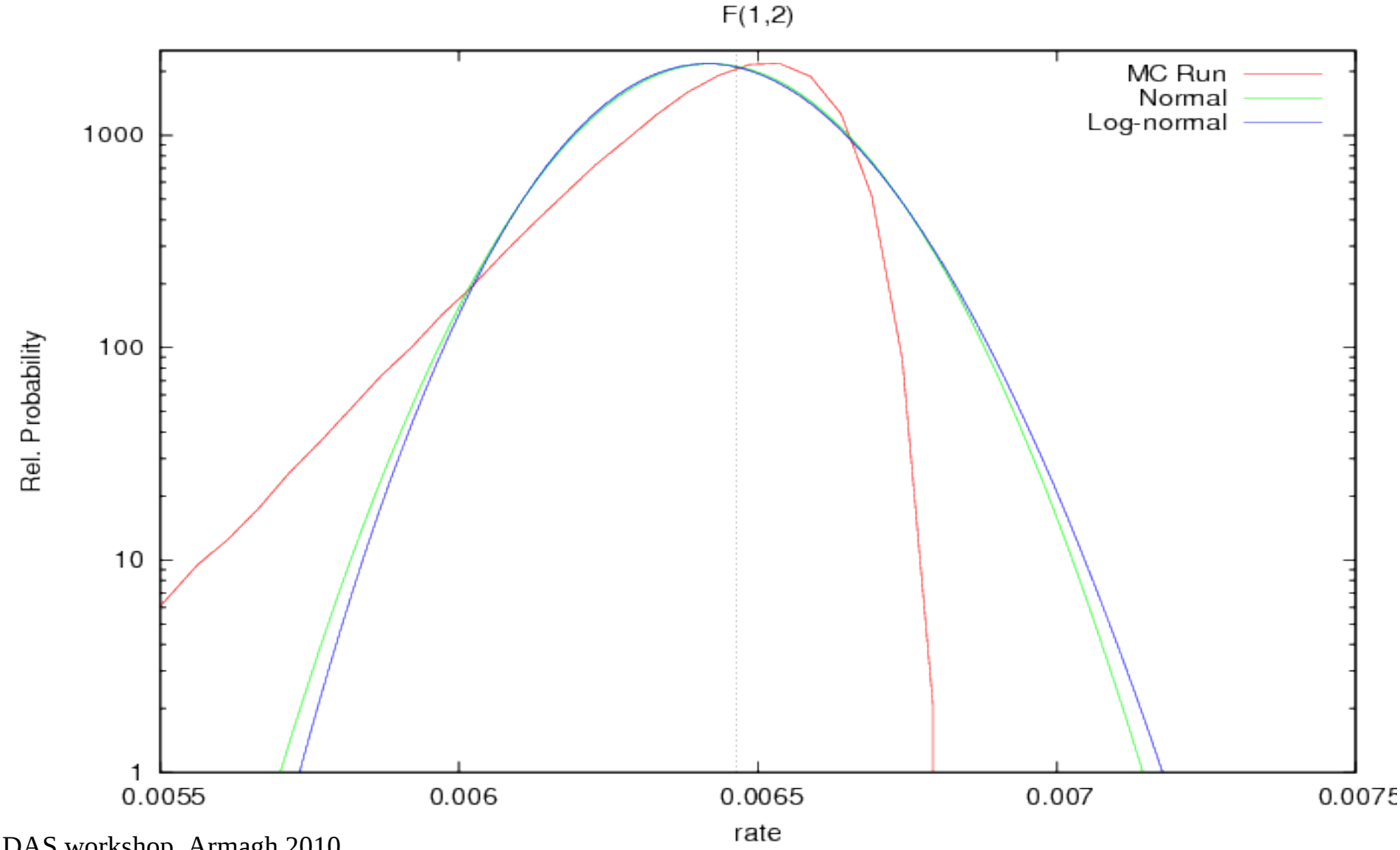
Ne = $1x10^{14}$ cm^{-3}, Te = 20eV, 50% errors.



- Log-normal distribution is appropriate for quantities bounded by zero.
- The results with zero error don't correspond to the peak of the distribution.
- The log-normal distribution is still described by two parameters.

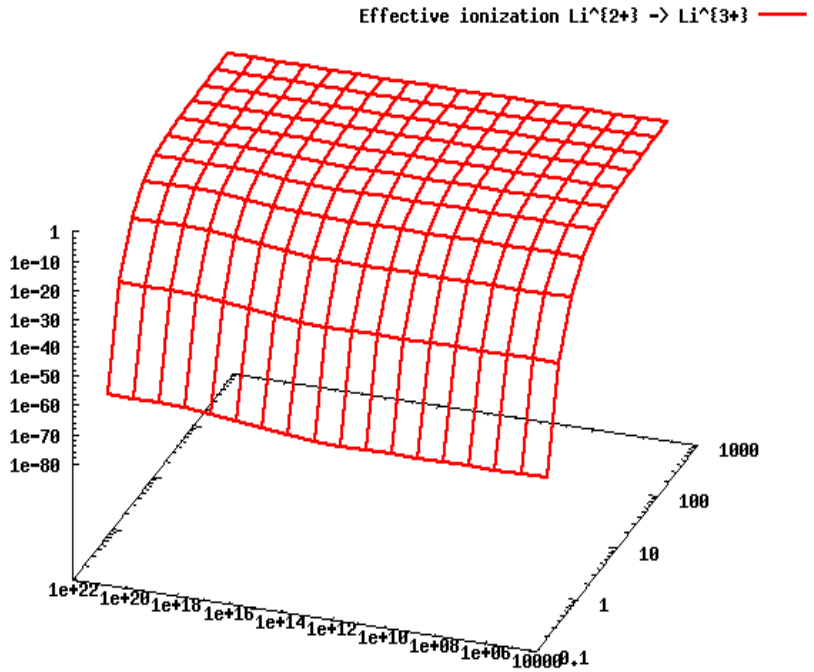
Li^{2+} F_{rec} (n=2) populations near LTE limit

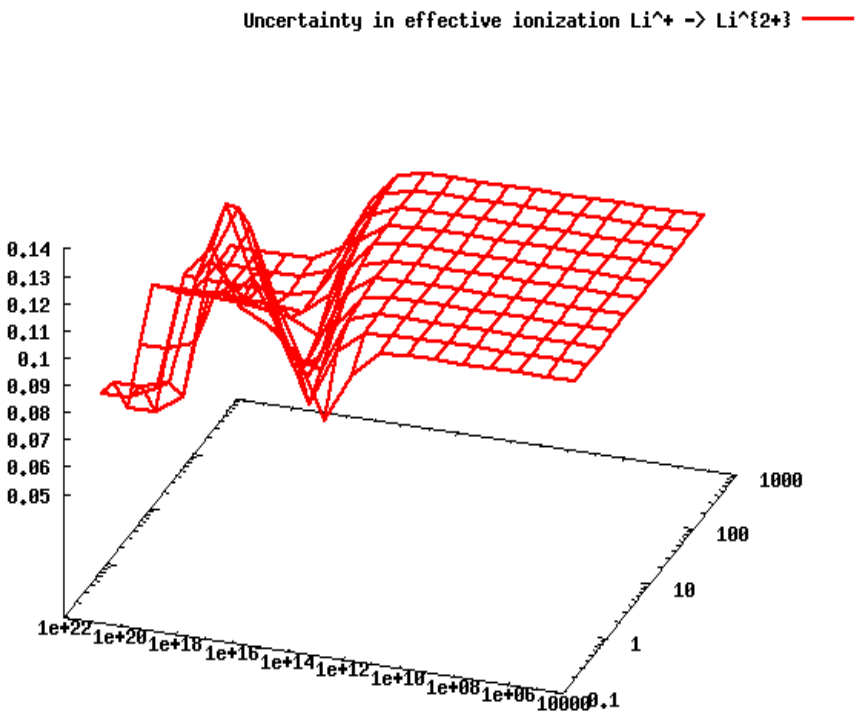
$Ne=1x10^{20}$ cm^{-3} and Te =20eV.



Uncertainties in GCR coefficients

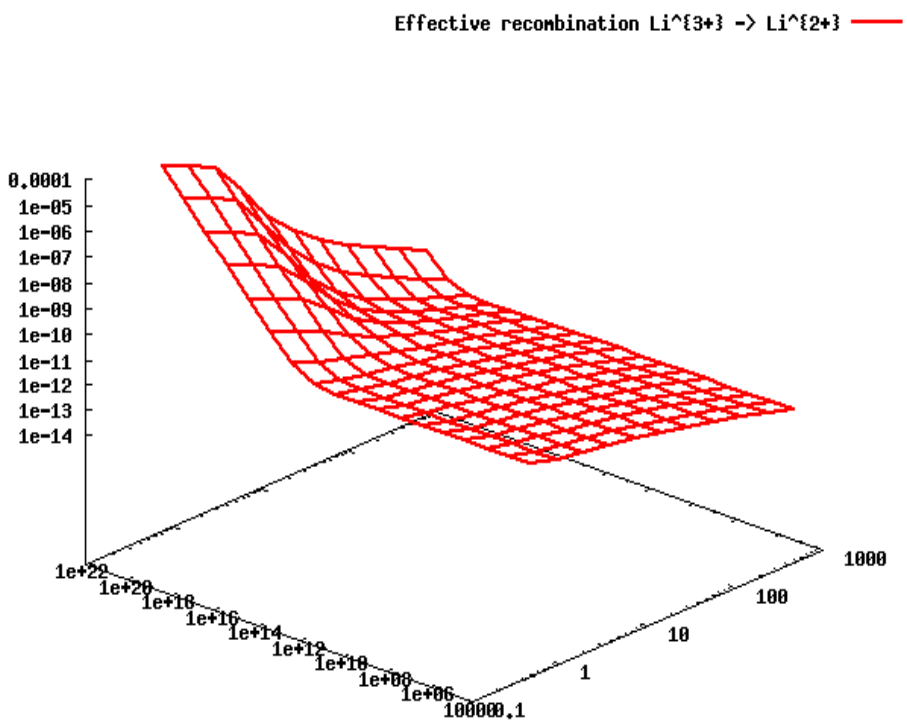
$$S_{CD,\sigma\to\upsilon} = \left(\mathcal{S}_{\upsilon\sigma} - \sum_{j=1}^{O}\mathcal{S}_{\upsilon j}\sum_{i=1}^{O}\mathcal{C}_{ji}^{-1}\mathcal{C}_{i\sigma}\right)$$

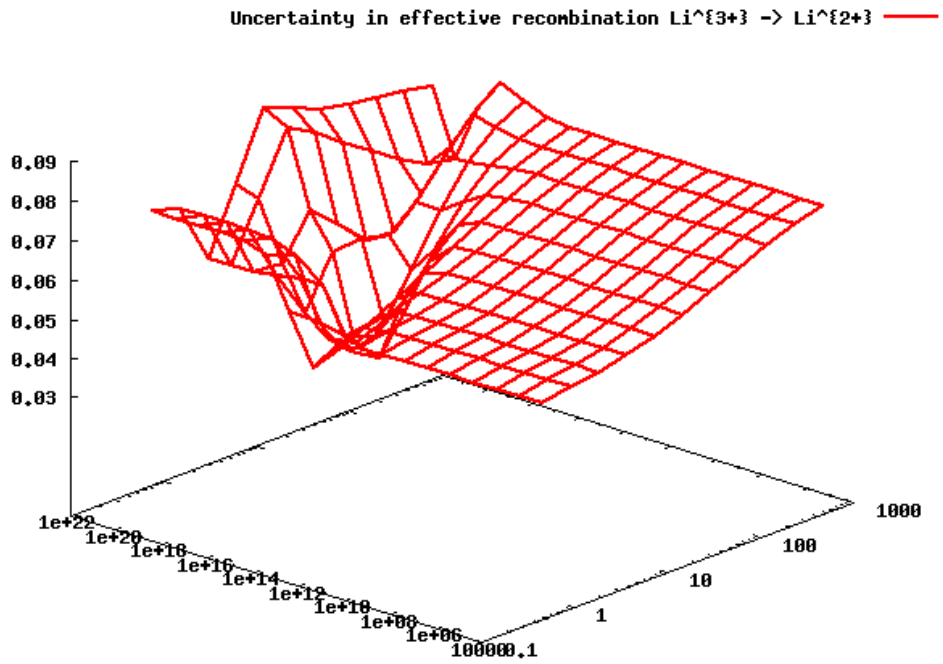




Uncertainties in GCR coefficients

$$\alpha_{CD,v'\to p} = \left(\mathcal{R}_{pv'} + \sum_{j=1}^{O}\mathcal{C}_{pj}\sum_{i=1}^{O}\mathcal{C}_{ji}^{-1}\mathcal{R}_{iv'}\right)$$

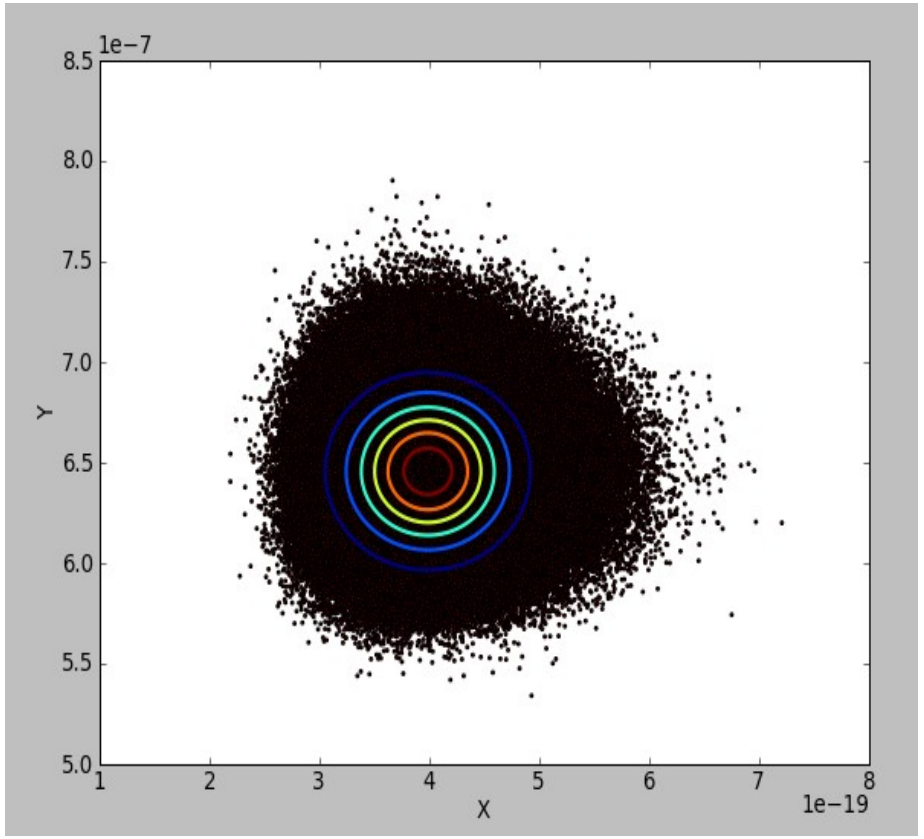




Correlation in derived coefficients

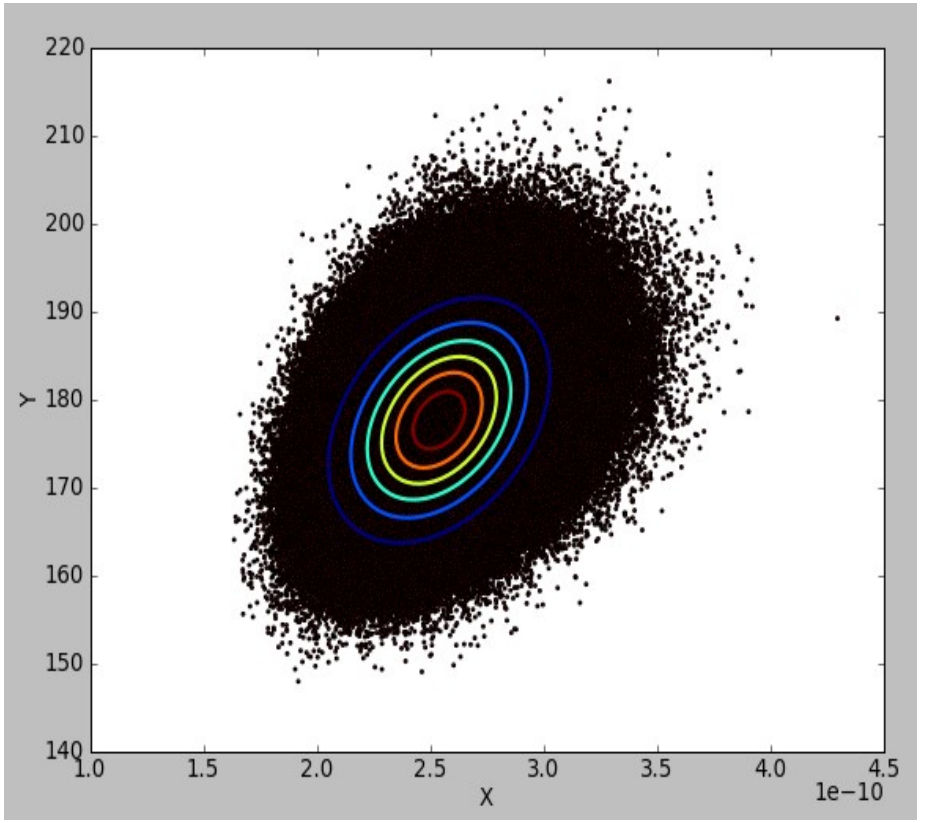
Li^{+} ionization and recombination

$Te=2eV$, $Ne=1x10^{6}$ and $1x10^{14}$ cm^{-3}



Effective ionization

Effective recombination



Effective ionization

Effective recombination

Further code developments

- We plan to
  - add photon emissivity coefficients to the output data.
  - add the projection matrix (adf18) data to the collisional-radiative matrix.
    - We could include errors in the projection matrix data.
    - A Monte-Carlo set of ADAS 204 runs could produce an error adf18 file.
  - write an equilibrium ionization balance code to use the correlated GCR coefficient data with error bars.
  - Note that any data in the adf04 file could be included in the modeling (i.e. charge exchange data, proton collisions).

The next part of the project: Error bars on the fundamental atomic data

- We plan to generate uncertainties on the fundamental atomic data for:
  - **Excitation** data via a Monte-Carlo set of R-matrix calculations where we vary the input parameters (e.g. Lambda parameters, energy mesh etc).
    - We plan to explore various schemes to evaluate the uncertainties.
    - Very open to any ideas. (e.g. different structure codes?)
    - We will use the ADAS8#3 PERL script.
  - **Ionization** data by
    - Comparing Post/Prior scattering potentials in a DW calculation.
    - Or by a Monte-Carlo set of RMPS calculations (would give correlated errors)
  - **Recombination** data (DR + RR).
    - Vary structure through lambda parameters?

Experimental benchmarking

- We would also like to do a set of comparisons with experimental measurements.
  - Line ratio diagnostics for astrophysics.
  - Impurity transport studies for fusion.
  - Could also do comparisons with EBIT line ratios/line intensities.
- If you would like to get involved, let myself or Mike Witthoeft know.