Stellar/Planetary Atmospheres

Part 09: NLTE rate equations

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Topics

- NLTE
  - full rate equations
  - general form of the rates
  - numerical solution

full rate equations

$$
\begin{aligned}
&\sum_{j<i} n_j \left(R_{ji} + C_{ji}\right) \\
&\quad - n_i \left\{ \sum_{j<i} \left(R_{ij} + C_{ij}\right) + \sum_{j>i} \left(\frac{n_j^*}{n_i^*}\right) \left(R_{ij} + C_{ij}\right) \right\} \\
&\quad + \sum_{j>i} n_j \left(\frac{n_j^*}{n_i^*}\right) \left(R_{ji} + C_{ji}\right) = 0.
\end{aligned}
$$

rate equations

- n_i: non-LTE population density of a level i
- n_i^*: LTE population density of the level i

$$n_i^* = \frac{g_i}{g_\kappa} n_\kappa \frac{2h^3 n_e}{(2\pi m)^{3/2}(kT)^{3/2}} \exp\left(-\frac{E_i - E_\kappa}{kT}\right).$$

- n_κ: *actual*, i.e., non-LTE, population density of the ground state of the next higher ionization stage of the same element
- E_i: excitation energy of the level i
- E_κ: ionization energy from the ground state to the corresponding ground state of the next higher ionization stage

rate equations

- system of rate equations is closed by
  - conservation equations for the nuclei
  - charge conservation equation

rate equations

- upward (absorption) radiative rates R_{ij} $(i < j)$

$$R_{ij} = \frac{4\pi}{hc} \int_0^\infty \alpha_{ij}(\lambda) J_\lambda(\lambda)\, \lambda d\lambda,$$

- downward (emission) radiative rates R_{ji} $(i < j)$

$$R_{ji} = \frac{4\pi}{hc} \int_0^\infty \alpha_{ji}(\lambda) \left(\frac{2hc^2}{\lambda^5} + J_\lambda(\lambda) \right) \exp\left(-\frac{hc}{k\lambda T} \right) \lambda d\lambda.$$

rate equations

- cross section $\alpha_{ij}(\lambda)$ of the transition $i \to j$ at the wavelength λ for bound-bound transitions

$$\alpha_{ij}(\lambda) = \hat{\sigma}_{ij}\varphi_{\lambda}(\lambda) = \frac{hc}{4\pi}\frac{\lambda_{ij}}{c}B_{ij}\varphi_{\lambda}(\lambda),$$

and

$$\alpha_{ji}(\lambda) = \hat{\sigma}_{ij}\phi_{\lambda}(\lambda) = \frac{hc}{4\pi}\frac{\lambda_{ij}}{c}B_{ij}\phi_{\lambda}(\lambda),$$

rate equations

- $\varphi_\lambda(\lambda)$: normalized absorption profile
- $\phi_\lambda(\lambda)$ is the normalized emission profile
- complete redistribution (CRD) $\rightarrow$

$$\varphi_\lambda(\lambda) = \phi_\lambda(\lambda)$$

and therefore

$$\alpha_{ij}(\lambda) = \alpha_{ji}(\lambda)$$

rate equations

- emission coefficient $\eta_{ij}(\lambda)$ for a bound-bound transition

$$\eta_{ij}(\lambda) = \frac{2hc^2}{\lambda^5}\frac{g_i}{g_j}\alpha_{ji}(\lambda)n_j$$

- absorption coefficient:

$$\kappa_{ij}(\lambda) = \alpha_{ij}(\lambda)n_i - \alpha_{ji}(\lambda)\frac{g_i}{g_j}n_j$$

rate equations

- photo ionization and photo recombination transitions, the corresponding coefficients are

$$\eta_{i\kappa}(\lambda) = \frac{2hc^2}{\lambda^5}\alpha_{i\kappa}(\lambda) n_\kappa^* \exp\left(-\frac{hc}{k\lambda T}\right)$$

and

$$\kappa_{i\kappa}(\lambda) = \left[n_i - n_\kappa^* \exp\left(-\frac{hc}{k\lambda T}\right)\right]\alpha_{i\kappa}(\lambda)$$

rate equations

- total absorption $\chi(\lambda)$ and emission $\eta(\lambda)$ coefficients:

$$\eta(\lambda) = \sum_{i<j} \eta_{ij}(\lambda) + \tilde{\eta}(\lambda)$$

and

$$\chi(\lambda) = \sum_{i<j} \kappa_{ij}(\lambda) + \tilde{\kappa}(\lambda) + \tilde{\sigma}(\lambda),$$

where $\tilde{\eta}(\lambda)$, $\tilde{\kappa}(\lambda)$ and $\tilde{\sigma}(\lambda)$ summarize background emissivities, absorption and scattering coefficients

rate equations

- line and continuum scattering
- Λ-iteration does not work!
- must use fancier method

Operator Splitting method

- define a "rate operator" in analogy to the Λ-operator:

$$R_{ij} = [R_{ij}][n]$$

- $[n]$: 'population density operator', which can be considered as the vector of the population densities of all levels at all points in the medium under consideration
- radiative rates are (linear) functions of the mean intensity J

$$J(\lambda) = \Lambda(\lambda) S(\lambda)$$

Operator Splitting method

- using the Λ-operator write $[R_{ij}][n]$ as:

$$[R_{ij}][n] = \frac{4\pi}{hc} \int \alpha_{ij}(\lambda)\Lambda(\lambda)S(\lambda)\,\lambda d\lambda.$$

- rewrite the Λ-operator as

$$\Psi(\lambda) = \Lambda(\lambda)[1/\chi(\lambda)],$$

  where we have introduced the Ψ-operator
- $[1/\chi(\lambda)]$ is the diagonal operator of multiplying by $1/\chi(\lambda)$

Operator Splitting method

- using the Ψ-operator write $[R_{ij}]$ as

$$[R_{ij}][n] = \frac{4\pi}{hc} \int \alpha_{ij}(\lambda)\Psi(\lambda)\eta(\lambda)\,\lambda d\lambda$$

  where $\eta(\lambda)$ is a function of the population densities and the background emissivities
- write $\eta(\lambda)$ as

$$\eta(\lambda) = \sum_{i<j} \eta_{ij}(\lambda) + \tilde{\eta}(\lambda) \equiv [E(\lambda)][n]$$

  where we have defined the linear and diagonal operator $[E(\lambda)]$

Operator Splitting method

- write the total contribution of a particular level k to the emissivity as

$$
\begin{aligned}
\eta_k(\lambda) = {} & \\
& \frac{2hc^2}{\lambda^5}\left\{ \sum_l \frac{g_l}{g_k}\alpha_{kl}(\lambda) \right. \\
+ & \sum_l \left[\alpha_{kl}(\lambda) \exp\left(-\frac{hc}{k\lambda T}\right) \right. \\
& \left.\left. \frac{g_l}{g_k}\frac{2h^3 n_e}{(2\pi m)^{3/2}(kT)^{3/2}} \exp\left(-\frac{E_l - E_k}{kT}\right) \right] \right\} n_k \\
\equiv {} & E_k(\lambda) n_k
\end{aligned}
$$

Operator Splitting method

- first sum is the contribution of the level k to all bound-bound transitions
- second sum is the contribution to all bound-free transitions
- $\rightarrow [E(\lambda)][n]$ has the form

$$[E(\lambda)][n] = \sum_k E_k(\lambda) n_k + \tilde{\eta}(\lambda)$$

- using the $[E(\lambda)]$-operator write $[R_{ij}][n]$ as

$$[R_{ij}][n] = \frac{4\pi}{hc} \left[\int_0^\infty \alpha_{ij}(\lambda) \Psi(\lambda) E(\lambda)\, \lambda d\lambda \right] [n].$$

Operator Splitting method

- corresponding expression for the emission rate-operator $[R_{ji}]$:

$$[R_{ji}][n]$$

$$= \frac{4\pi}{hc} \int_0^\infty \alpha_{ji}(\lambda) \left\{ \frac{2hc^2}{\lambda^5} + \Psi(\lambda)[E(\lambda)][n] \right\} \exp\left(-\frac{hc}{k\lambda T} \right) \lambda d\lambda$$

Operator Splitting method

- with the rate operator write the rate equations in the form

$$
\begin{aligned}
\sum_{j<i} n_j \left([R_{ji}][n] + C_{ji}\right) \\
& - n_i \left\{ \sum_{j<i} \left(\frac{n_j^*}{n_i^*}\right) \left([R_{ij}][n] + C_{ij}\right) + \sum_{j>i} \left([R_{ij}][n] + C_{ij}\right) \right\} \\
& + \sum_{j>i} n_j \left(\frac{n_i^*}{n_j^*}\right) \left([R_{ji}][n] + C_{ji}\right) \\
= \quad & 0
\end{aligned}
$$

Operator Splitting method

- shows explicitly the non-linearity of the rate equations with respect to the population densities
- in addition, the rate equations are non-linear with respect to the electron density via the collisional rates and the charge conservation constraint condition
- split the rate operator, in analogy to the splitting of the Λ-operator, by

$$[R_{ij}] = [R^*_{ij}] + ([R_{ij}] - [R^*_{ij}]) \equiv [R^*_{ij}] + [\Delta R_{ij}]$$

  (analog for the downward radiative rates)
- $[R^*_{ij}]$ is the "approximate rate-operator"

Operator Splitting method

- rewrite the rate R_{ij} as

$$R_{ij} = [R^*_{ij}][n_{\rm new}] + [\Delta R_{ji}][n_{\rm old}]$$

  and analogous for the downward radiative rates
- $[n_{\rm old}]$: current (old) population densities
- $[n_{\rm new}]$: updated population densities to be calculated

Operator Splitting method

- $[R^*_{ij}]$ and $[R^*_{ji}]$ are linear functions of the population density operator $[n_k]$ of any level k, due to the linearity of η and the usage of the Ψ-operator instead of the Λ-operator
- write the iteration scheme in the form:

$$R_{ij} = [R^*_{ij}][n_{\mathrm{new}}] + \left([R_{ij}] - [R^*_{ij}]\right)[n_{\mathrm{old}}]$$

Solution

$$
\begin{aligned}
&\sum_{j<i} n_{j,\mathrm{new}}[R^*_{ji}][n_{\mathrm{new}}] \\
&\quad - n_{i,\mathrm{new}} \left\{ \sum_{j<i} [R^*_{ij}][n_{\mathrm{new}}] + \sum_{j>i} \left(\frac{n^*_j}{n^*_i} \right) [R^*_{ij}][n_{\mathrm{new}}] \right\} \\
&\quad + \sum_{j>i} n_{j,\mathrm{new}} \left(\frac{n^*_j}{n^*_i} \right) [R^*_{ji}][n_{\mathrm{new}}] \\
&\quad + \sum_{j<i} n_{j,\mathrm{new}} \left([\Delta R_{ji}][n_{\mathrm{old}}] + C_{ji} \right) \\
&\quad - n_{i,\mathrm{new}} \left\{ \sum_{j<i} \left([\Delta R_{ij}][n_{\mathrm{old}}] + C_{ij} \right) \right. \\
&\qquad \left. + \sum_{j>i} \left(\frac{n^*_j}{n^*_i} \right) \left([\Delta R_{ij}][n_{\mathrm{old}}] + C_{ij} \right) \right\} \\
&\quad + \sum_{j>i} n_{j,\mathrm{new}} \left(\frac{n^*_j}{n^*_i} \right) \left([\Delta R_{ji}][n_{\mathrm{old}}] + C_{ji} \right) = 0
\end{aligned}
$$

solution

- $[R^*_{ij}]$-operator contains information about the influence of a particular level on *all* transitions
- $\rightarrow$ treat the complete multi-level non-LTE radiative transfer problem including active continua and overlapping lines
- $[E(\lambda)]$-operator $\rightarrow$ information about the strength of the coupling of a radiative transition to all considered levels
- $\rightarrow$ include or neglect certain couplings *dynamically* during the iterative solution

solution

- have not yet specified either a method for the FS of the RTE or a method for the construction of the approximate Λ-operator
- $\rightarrow$ can use any method!
- above equation for $[n_{\mathrm{new}}]$ is non-linear with respect to the $n_{i,\mathrm{new}}$ and n_e:
  - coefficients of the $[R^*_{ij}]$ and $[R^*_{ji}]$-operators are quadratic in $n_{i,\mathrm{new}}$
  - dependence of the Saha-Boltzmann factors and the collisional rates from the electron density

solution

- simplify the iteration scheme $\rightarrow$
  - use a linearized and splitted iteration scheme for the solution
  - replace terms of the form $n_{j,\mathrm{new}}[R^*_{ji}][n_{\mathrm{new}}]$ by $n_{j,\mathrm{old}}[R^*_{ji}][n_{\mathrm{new}}]$:

Solution

$$
\begin{aligned}
&\sum_{j<i} n_{j,\mathrm{old}}[R^*_{ji}][n_{\mathrm{new}}] \\
&\qquad -n_{i,\mathrm{old}}\left\{\sum_{j<i}[R^*_{ij}][n_{\mathrm{new}}]+\sum_{j>i}\left(\frac{n^*_j}{n^*_i}\right)[R^*_{ij}][n_{\mathrm{new}}]\right\} \\
&\qquad +\sum_{j>i} n_{j,\mathrm{old}}\left(\frac{n^*_j}{n^*_i}\right)[R^*_{ji}][n_{\mathrm{new}}] \\
&\qquad +\sum_{j<i} n_{j,\mathrm{new}}\left([\Delta R_{ji}][n_{\mathrm{old}}]+C_{ji}\right) \\
&\qquad -n_{i,\mathrm{new}}\left\{\sum_{j<i}\left([\Delta R_{ij}][n_{\mathrm{old}}]+C_{ij}\right)\right. \\
&\qquad\qquad\qquad \left.+\sum_{j>i}\left(\frac{n^*_j}{n^*_i}\right)\left([\Delta R_{ij}][n_{\mathrm{old}}]+C_{ij}\right)\right\} \\
&\qquad +\sum_{j>i} n_{j,\mathrm{new}}\left(\frac{n^*_j}{n^*_i}\right)\left([\Delta R_{ji}][n_{\mathrm{old}}]+C_{ji}\right)=0
\end{aligned}
$$

nested iterations

- nested iteration:
- keep n_e fixed at rate equation solution step
- treat every ion independently (assumes $N_{\kappa,\mathrm{old}} \approx N_{\kappa,\mathrm{new}}$)
- all collisional rates are evaluated using the current value of n_e

nested iterations

- compute departure coefficients

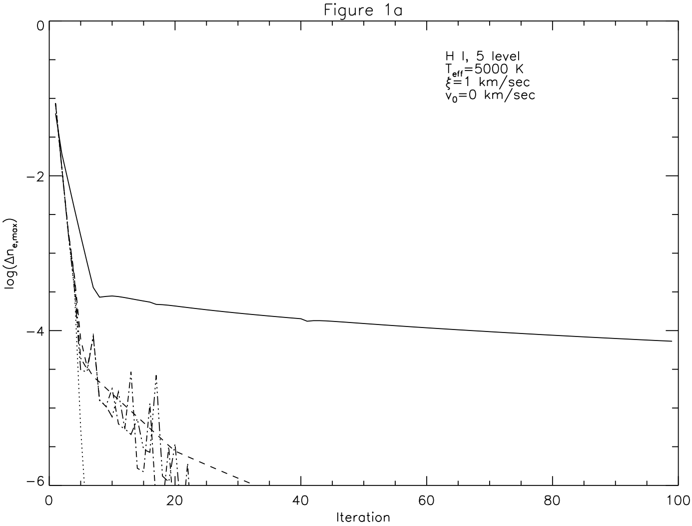
$$b_i = n_i / n_i^*$$

- n_i: new NLTE population density
- n_i^*: new 'LTE' population density computed with new n_κ
- use b_i to compute modified Q_{NLTE}

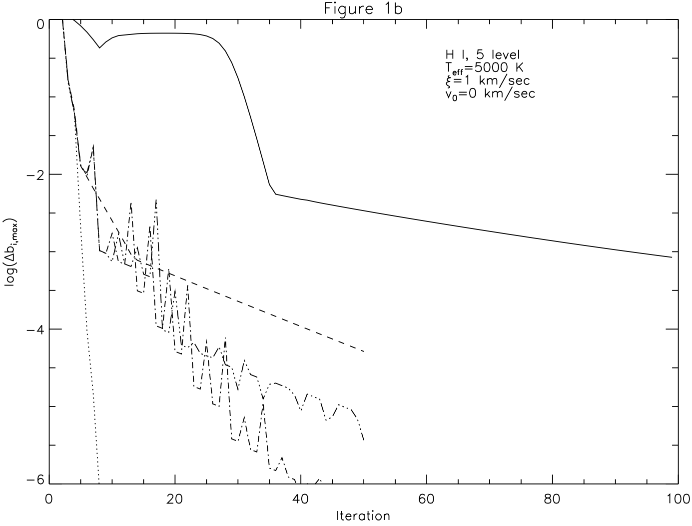
$$Q_{\mathrm{NLTE}} = \sum b_i g_i \exp\left(-\frac{\chi_i}{kT}\right)$$

- clean-up step by solving EOS with new Q_{NLTE}
- will first slow the iteration process
- in the convergence limit it will be very accurate

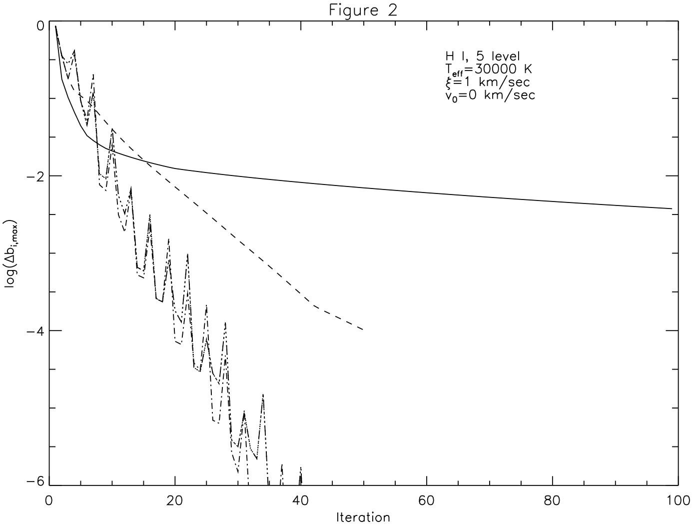
Convergence



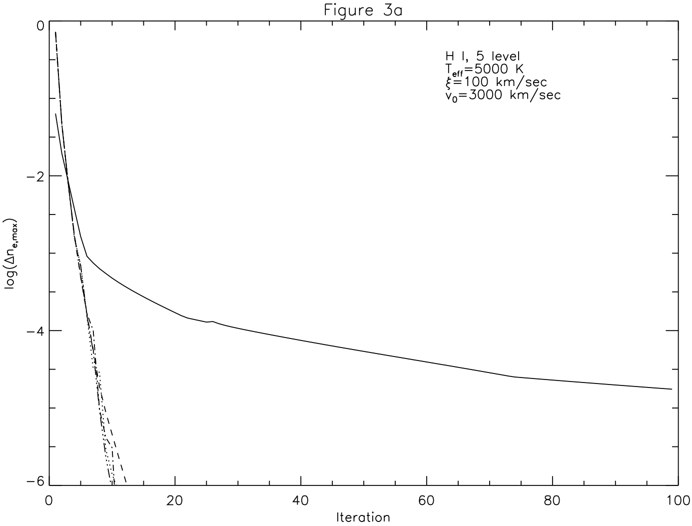
Convergence



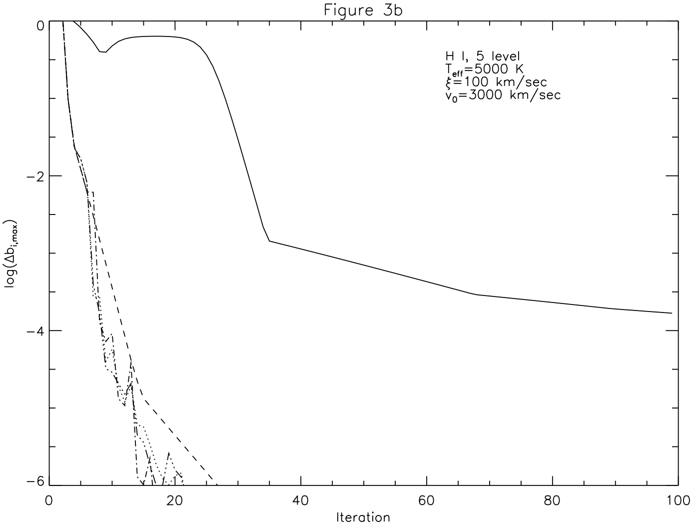
Convergence



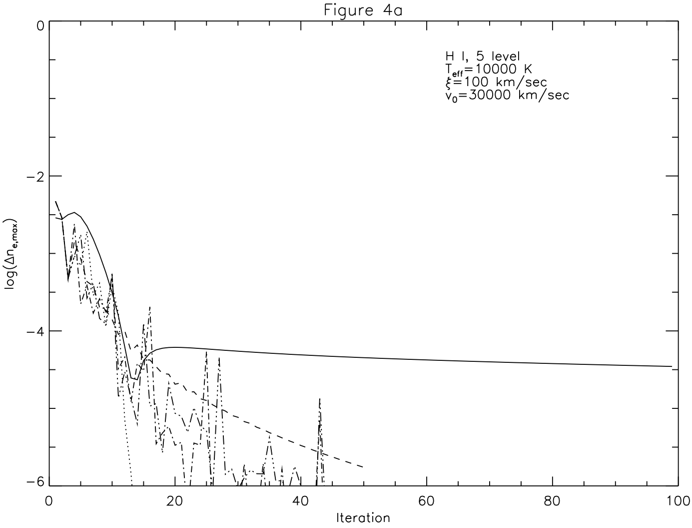
Convergence



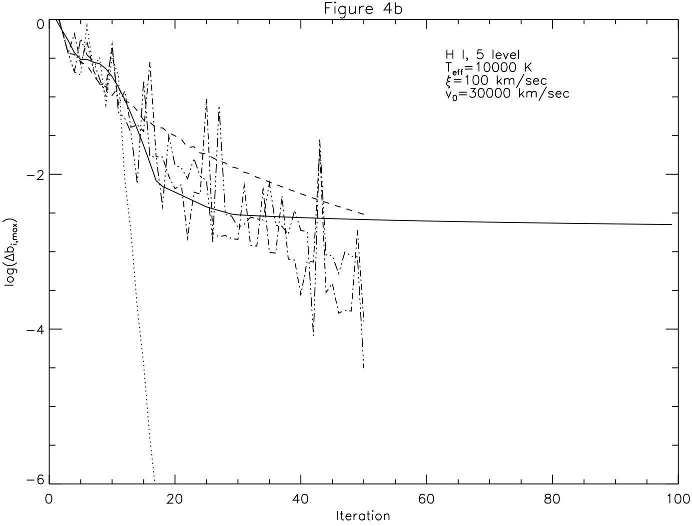
Convergence



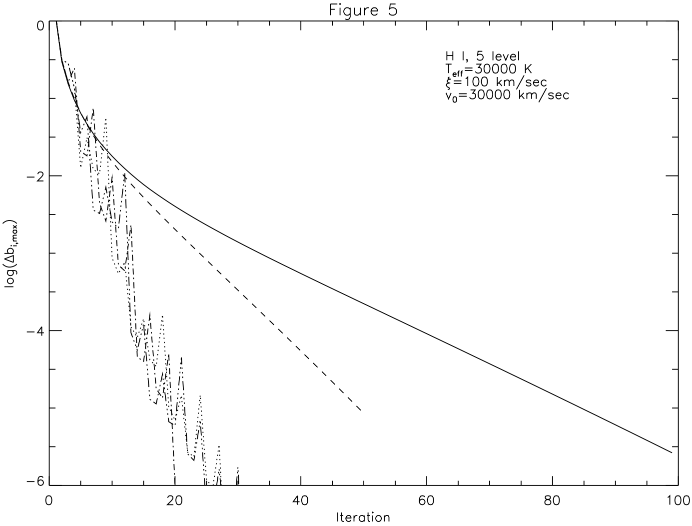
Convergence



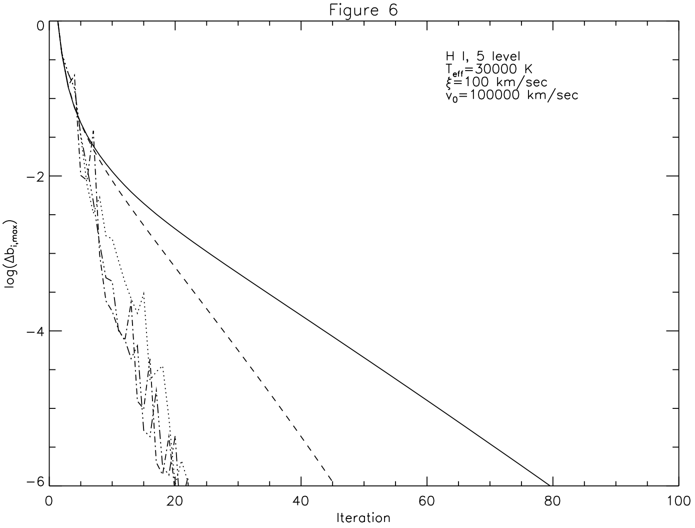
Convergence



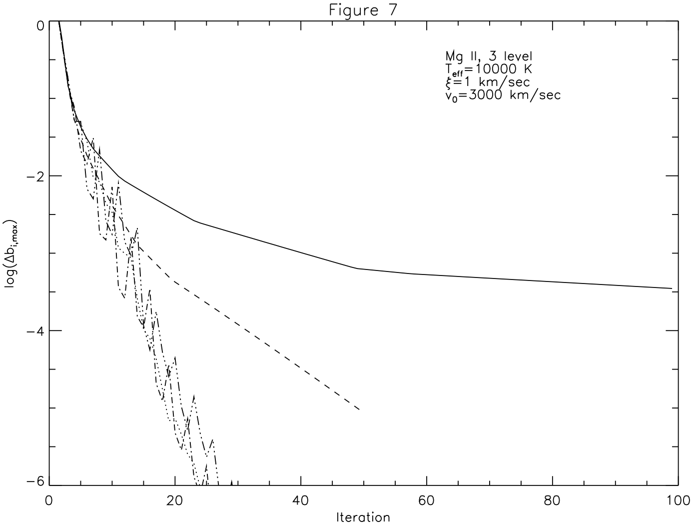
Convergence



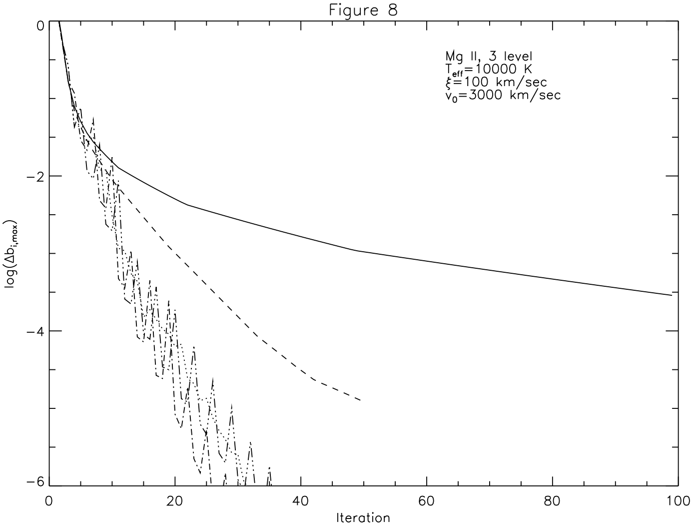
Convergence



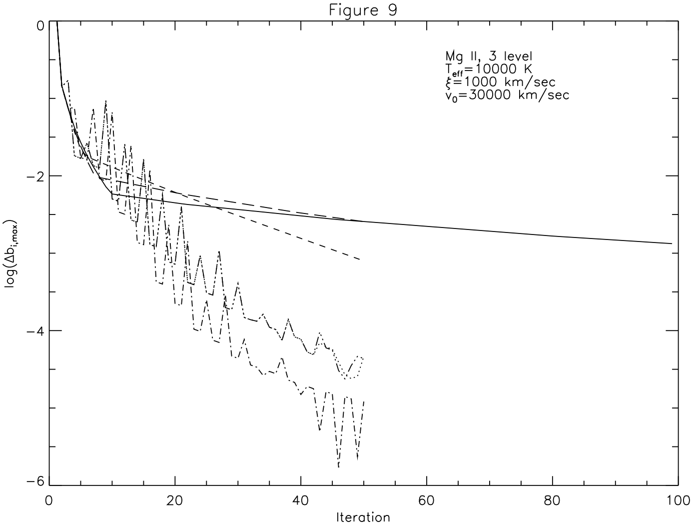
Convergence



Convergence



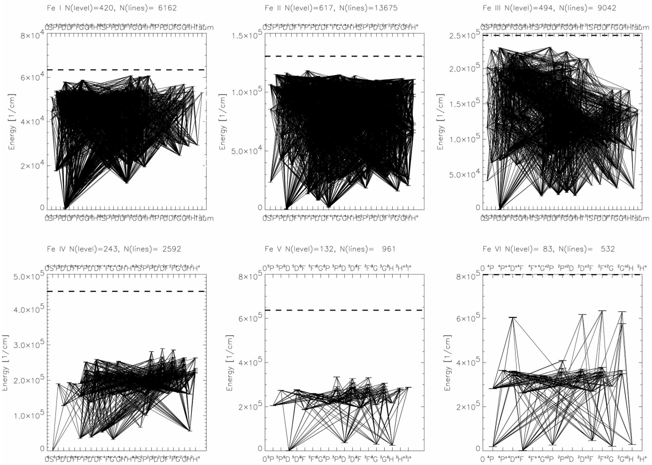
Convergence



larger problems

- so far: small problems
- could be solved by other methods, e.g.,
  - classical complete linearization
  - equivalent two-level atom (ETLA)
- but these methods do not scale to large problems
- badly conditioned rate matrix!
- significantly limit the number of individual levels
- why large problems? realism!

Fe NLTE model atoms



larger problems

- possible approximation:
- lumping entire multiplets together in a single 'super-level'
- reducing the model atom to a manageable 30 to 50 levels
- energy spread within a multiplet can correspond to a wavelength spread as large as 200 Å
- opacity will not appear at the correct wavelength
- $\rightarrow$ correction required, e.g., ODF
- $\rightarrow$ problems in moving media etc.

larger problems

- example Fe II
- several 1000 bound energy levels
- $> 10^6$ spectral lines
- majority of the levels are 'predicted'
- majority of lines are semi-empirical and/or very weak
- $\rightarrow$ distinguish between
  - well-known, strong lines and levels
  - predicted lines and levels

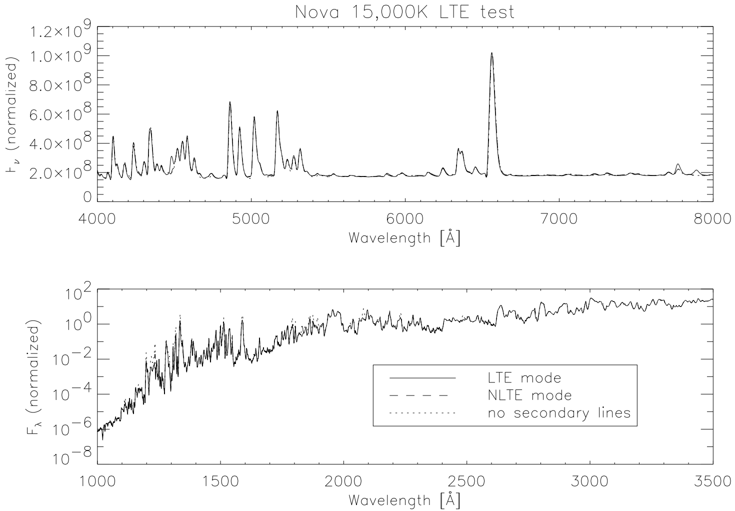
larger problems

- separate 'primary' lines from 'secondary' lines
- $\rightarrow$ defining a threshold in $\log(gf)$
- primary lines with gf-values larger than the threshold are treated in detail $\rightarrow$
  - included as transitions in the rate equations
  - include special wavelength points within the profile
- secondary lines
  - included as background NLTE opacity sources
  - not explicitly included in the rate equations
  - treated by opacity sampling

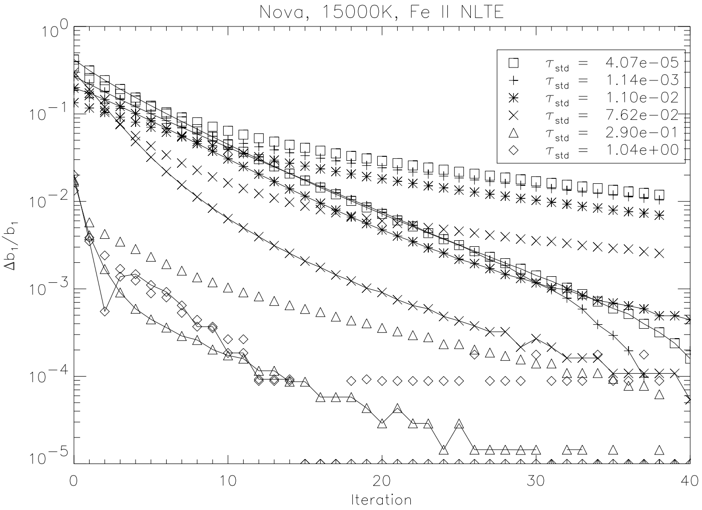
larger problems

- distinction between primary and secondary transitions is just a matter of convenience and technical feasibility
- example Fe II
  - threshold $\log(gf) = -3$
  - selection considers only observed lines between observed levels
  - include only lines with well known gf-values
  - 617 levels included in NLTE
  - 13675 primary NLTE lines

test models

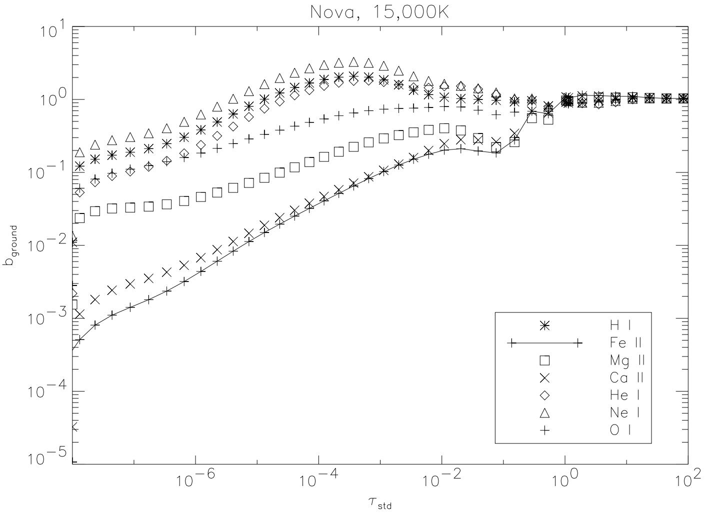

Nova 15,000K LTE test
F_ν (normalized)
Wavelength [Å]
F_λ (normalized)
Wavelength [Å]
LTE mode
NLTE mode
no secondary lines

test models

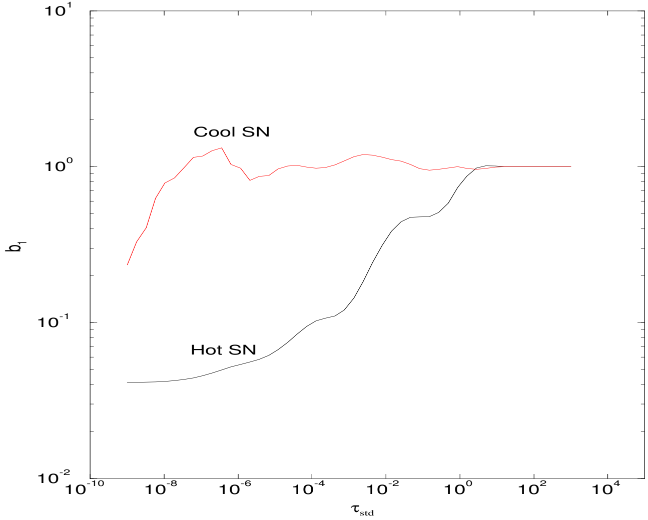


Nova, 15000K, Fe II NLTE
τ_{std} = 4.07e−05
τ_{std} = 1.14e−03
τ_{std} = 1.10e−02
τ_{std} = 7.62e−02
τ_{std} = 2.90e−01
τ_{std} = 1.04e+00
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
$\Delta b_1/b_1$
0
10
20
30
40
Iteration

test models

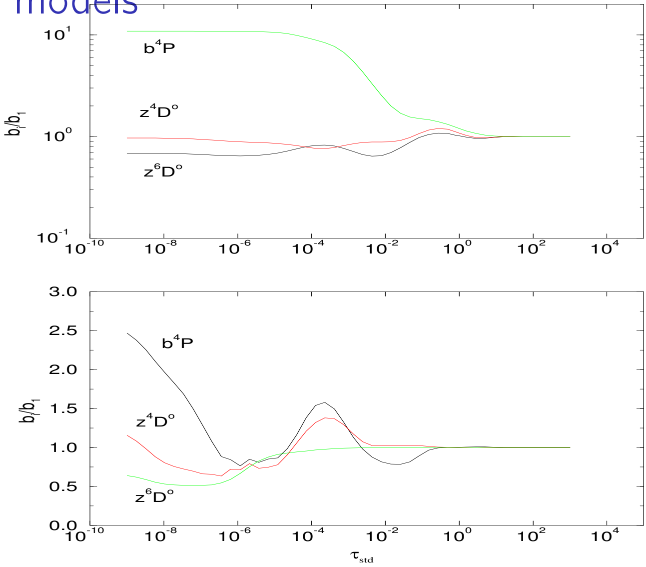

Nova, 15,000K
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
b_{ground}
10^{-6}
10^{-4}
10^{-2}
10^0
10^2
τ_{std}
H I
Fe II
Mg II
Ca II
He I
Ne I
O I

test models

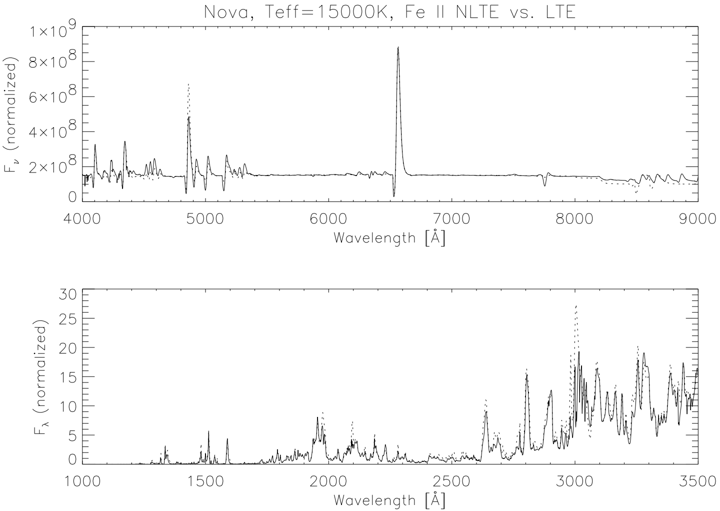


Cool SN
Hot SN
10^{1}
10^{0}
10^{-1}
10^{-2}
b_1
10^{-10}
10^{-8}
10^{-6}
10^{-4}
10^{-2}
10^{0}
10^{2}
10^{4}
τ_{std}

test models

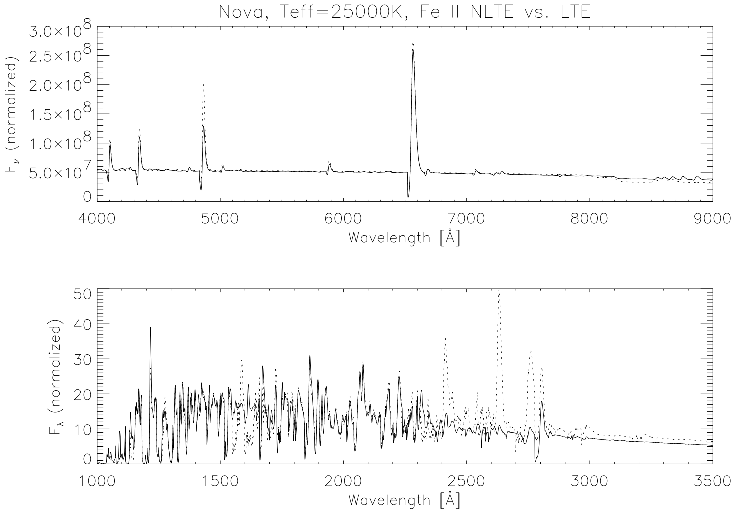

b4P
z4Do
z6Do
bi/b1
10-10 10-8 10-6 10-4 10-2 100 102 104
3.0 2.5 2.0 1.5 1.0 0.5 0.0
τstd

test models

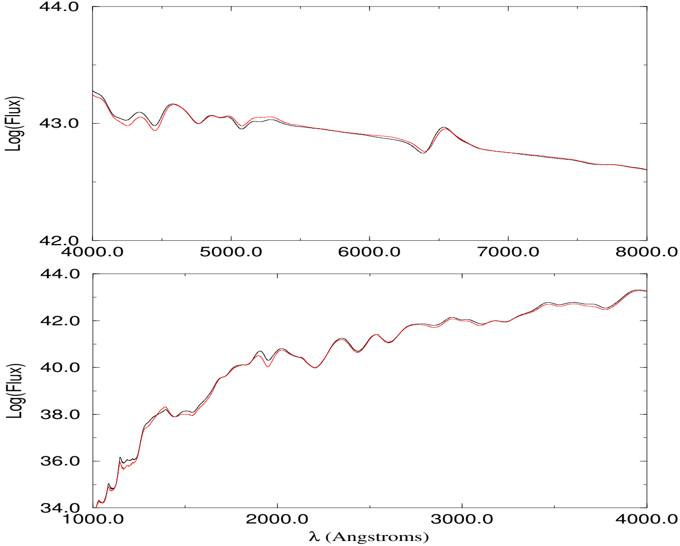


Nova, Teff=15000K, Fe II NLTE vs. LTE
F_ν (normalized)
1×10^9
8×10^8
6×10^8
4×10^8
2×10^8
0
4000
5000
6000
7000
8000
9000
Wavelength [Å]
F_λ (normalized)
30
25
20
15
10
5
0
1000
1500
2000
2500
3000
3500
Wavelength [Å]

test models

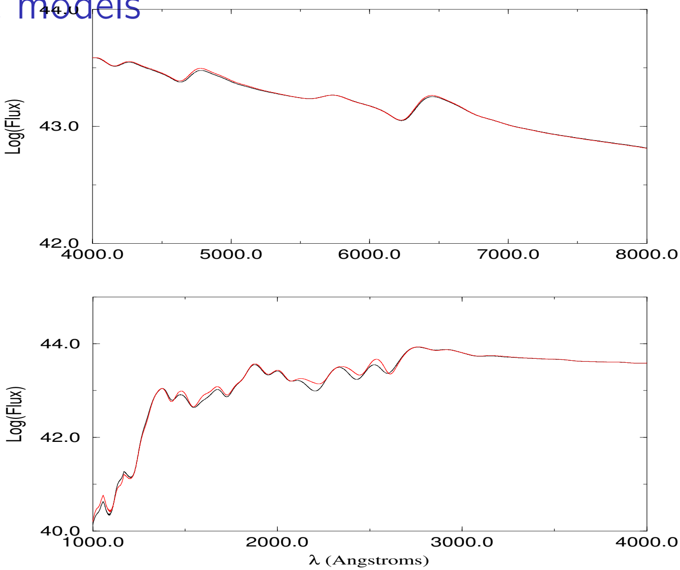

Nova, Teff=25000K, Fe II NLTE vs. LTE
F_ν (normalized)
3.0×10^8
2.5×10^8
2.0×10^8
1.5×10^8
1.0×10^8
5.0×10^7
0
4000
5000
6000
7000
8000
9000
Wavelength [Å]
F_λ (normalized)
50
40
30
20
10
0
1000
1500
2000
2500
3000
3500
Wavelength [Å]

test models



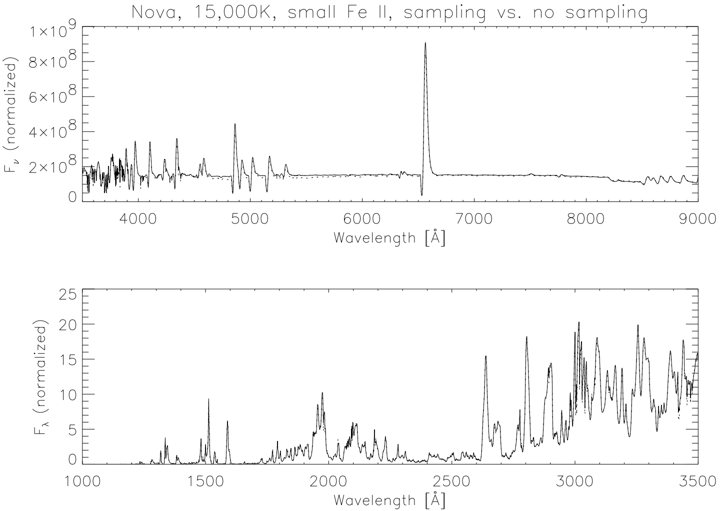
44.0
43.0
42.0
Log(Flux)
4000.0
5000.0
6000.0
7000.0
8000.0
44.0
42.0
40.0
38.0
36.0
34.0
Log(Flux)
1000.0
2000.0
3000.0
4000.0
λ (Angstroms)

test models

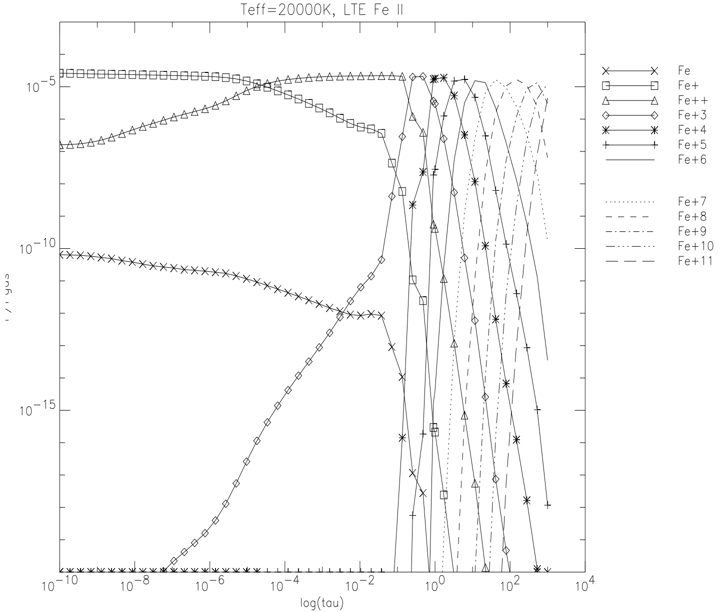


44.0
43.0
42.0
Log(Flux)
4000.0
5000.0
6000.0
7000.0
8000.0
44.0
42.0
40.0
Log(Flux)
1000.0
2000.0
3000.0
4000.0
λ (Angstroms)

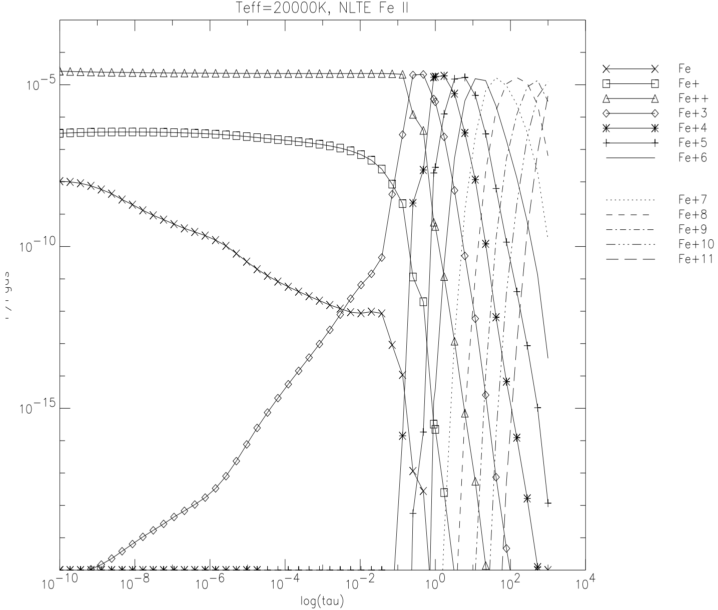
test models


Nova, 15,000K, small Fe II, sampling vs. no sampling
F_ν (normalized)
0
2×10^8
4×10^8
6×10^8
8×10^8
1×10^9
4000
5000
6000
7000
8000
9000
Wavelength [Å]
F_λ (normalized)
0
5
10
15
20
25
1000
1500
2000
2500
3000
3500
Wavelength [Å]

real models

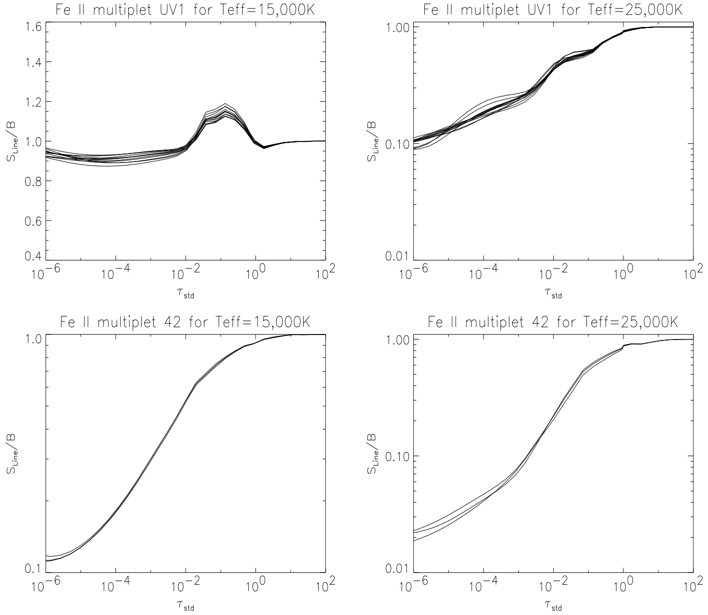

Teff=20000K, LTE Fe II
10^{-5}
10^{-10}
10^{-15}
10^{-10}
10^{-8}
10^{-6}
10^{-4}
10^{-2}
10^{0}
10^{2}
10^{4}
log(tau)
Fe
Fe+
Fe++
Fe+3
Fe+4
Fe+5
Fe+6
Fe+7
Fe+8
Fe+9
Fe+10
Fe+11

real models



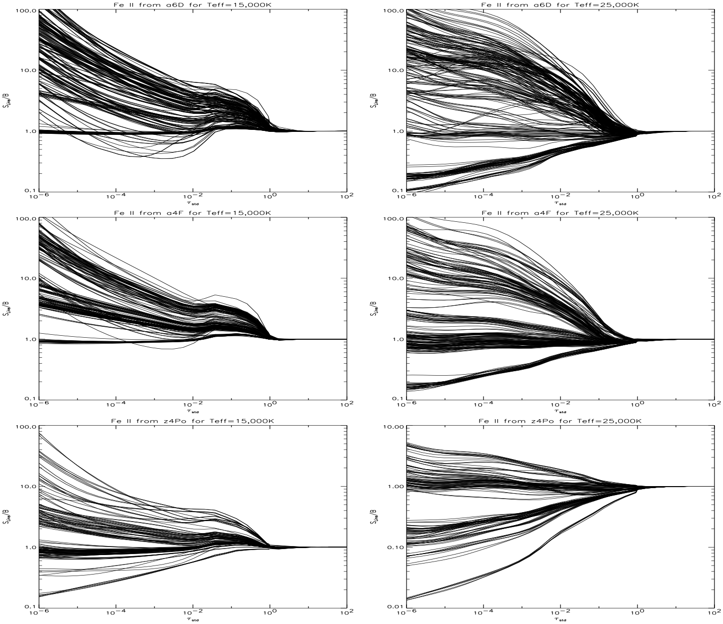
Teff=20000K, NLTE Fe II
10^{-5}
10^{-10}
10^{-15}
10^{-10} 10^{-8} 10^{-6} 10^{-4} 10^{-2} 10^{0} 10^{2} 10^{4}
log(tau)
Fe
Fe+
Fe++
Fe+3
Fe+4
Fe+5
Fe+6
Fe+7
Fe+8
Fe+9
Fe+10
Fe+11

real models



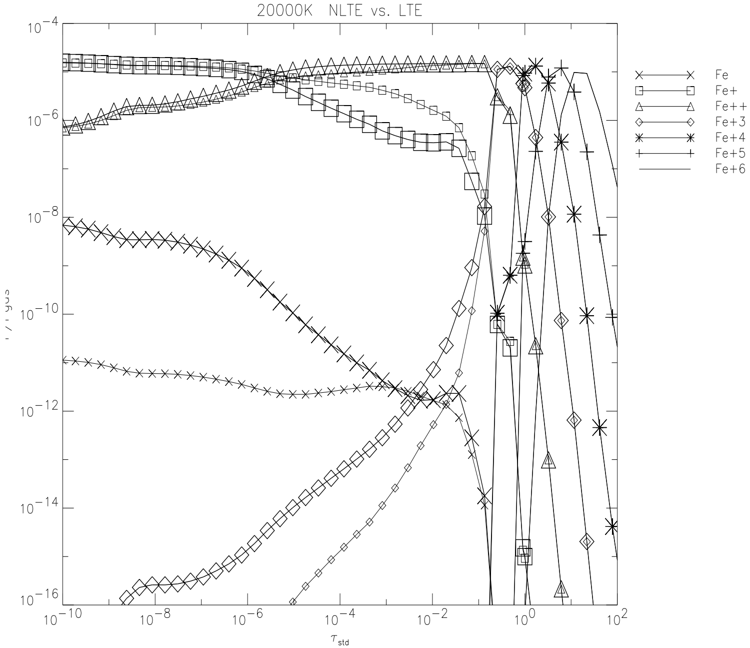
Fe II multiplet UV1 for Teff=15,000K
Fe II multiplet UV1 for Teff=25,000K
Fe II multiplet 42 for Teff=15,000K
Fe II multiplet 42 for Teff=25,000K
S_{Line}/B
τ_{std}

real models



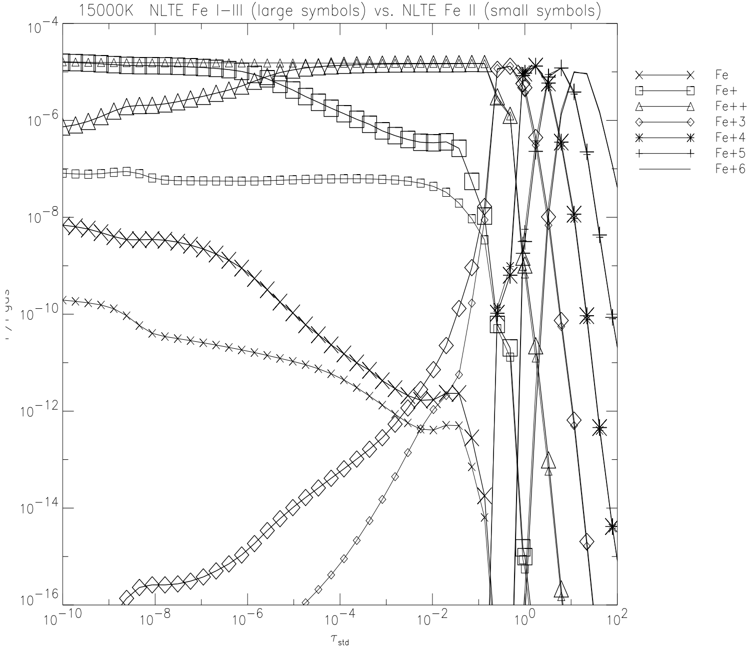
Fe II from a6D for Teff=15,000K
Fe II from a6D for Teff=25,000K
Fe II from a4F for Teff=15,000K
Fe II from a4F for Teff=25,000K
Fe II from z4Po for Teff=15,000K
Fe II from z4Po for Teff=25,000K
S_{line}/B
τ_{std}

real models



20000K NLTE vs. LTE
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{-16}
10^{-10}
10^{-8}
10^{-6}
10^{-4}
10^{-2}
10^{0}
10^{2}
τ_{std}
Fe
Fe+
Fe++
Fe+3
Fe+4
Fe+5
Fe+6

real models



15000K NLTE Fe I–III (large symbols) vs. NLTE Fe II (small symbols)
Fe
Fe+
Fe++
Fe+3
Fe+4
Fe+5
Fe+6
τ_{std}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{-16}
10^{-10}
10^{-8}
10^{-6}
10^{-4}
10^{-2}
10^{0}
10^{2}