

NLTE analysis of spectra: FG stars

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FG stars

$$5000 < T_{\text{eff,Sun}} < 7000 \text{ K}$$

$$3 < \log g_{\text{Sun}} < 4.5$$

$$\dots -5 < [\text{Fe}/\text{H}] < -0.3$$

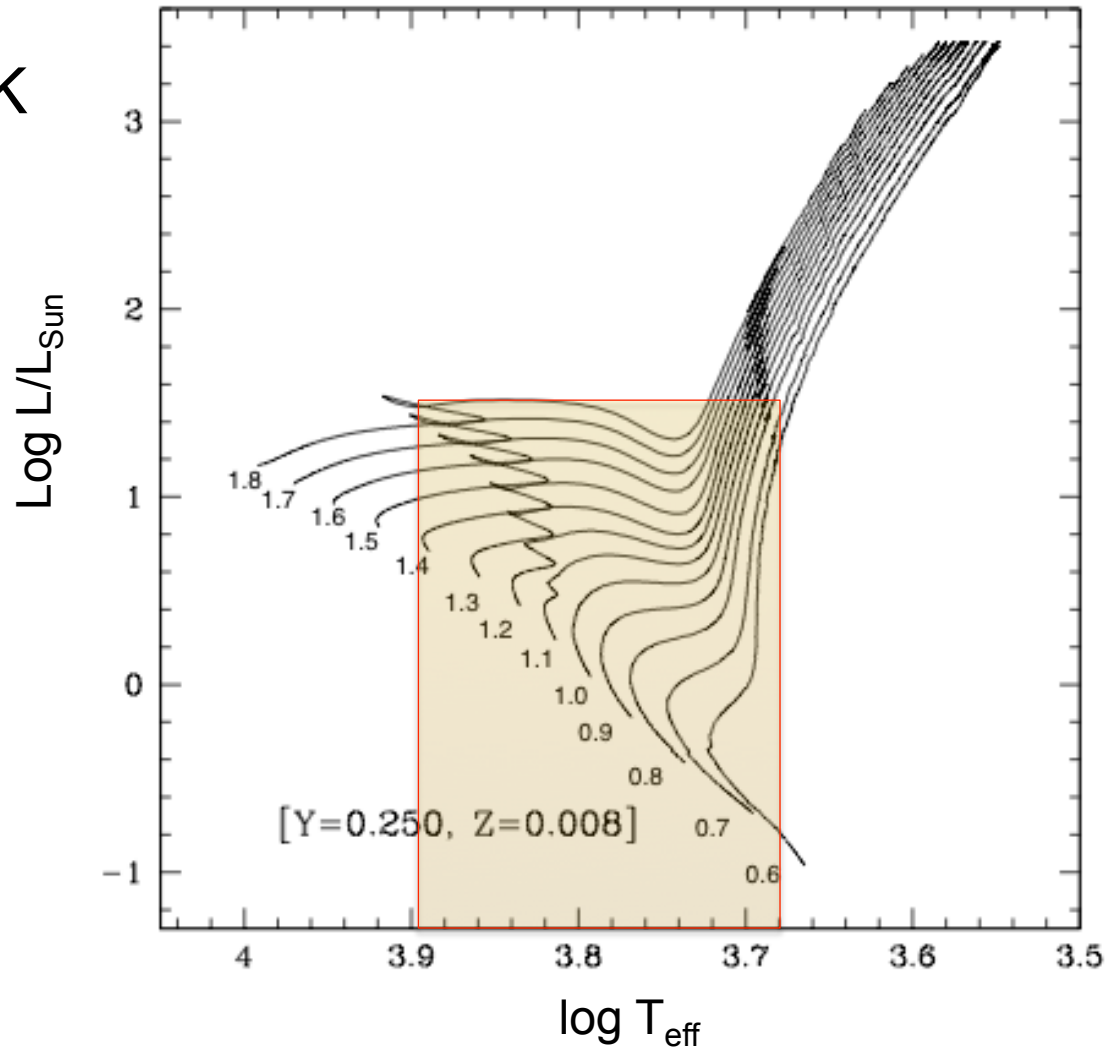


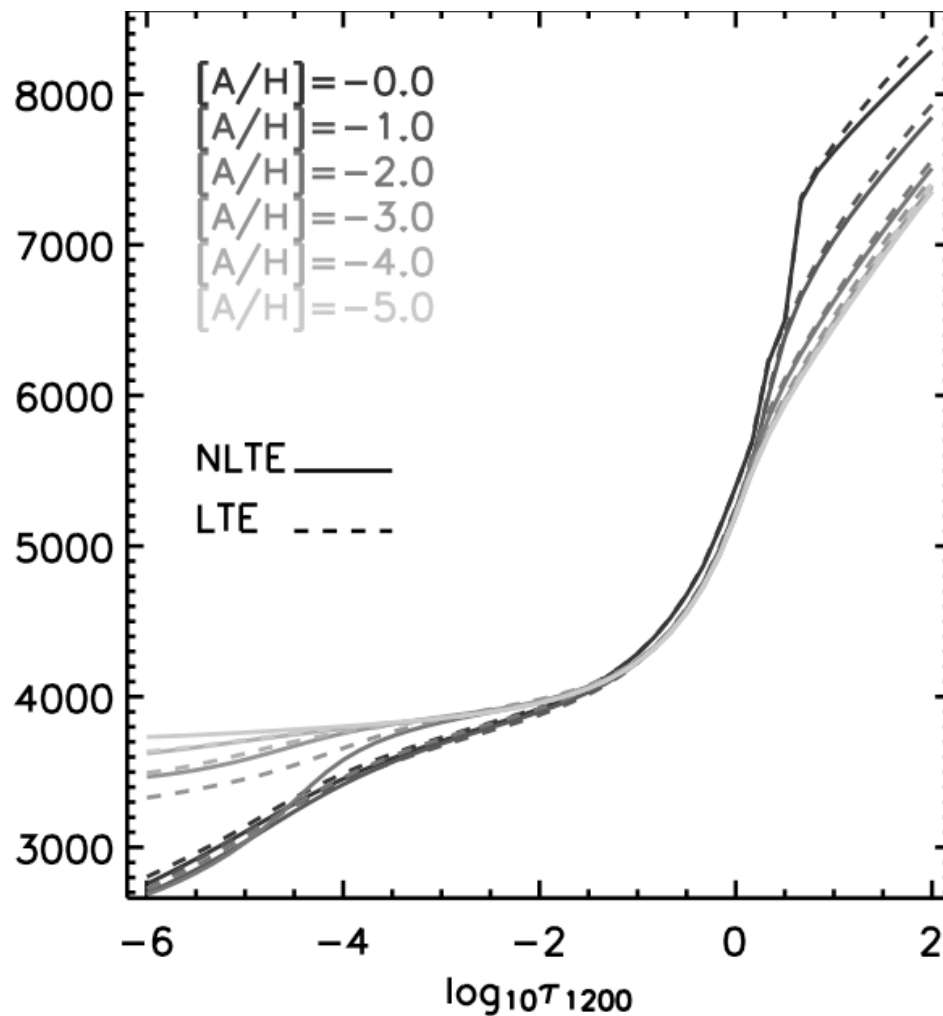
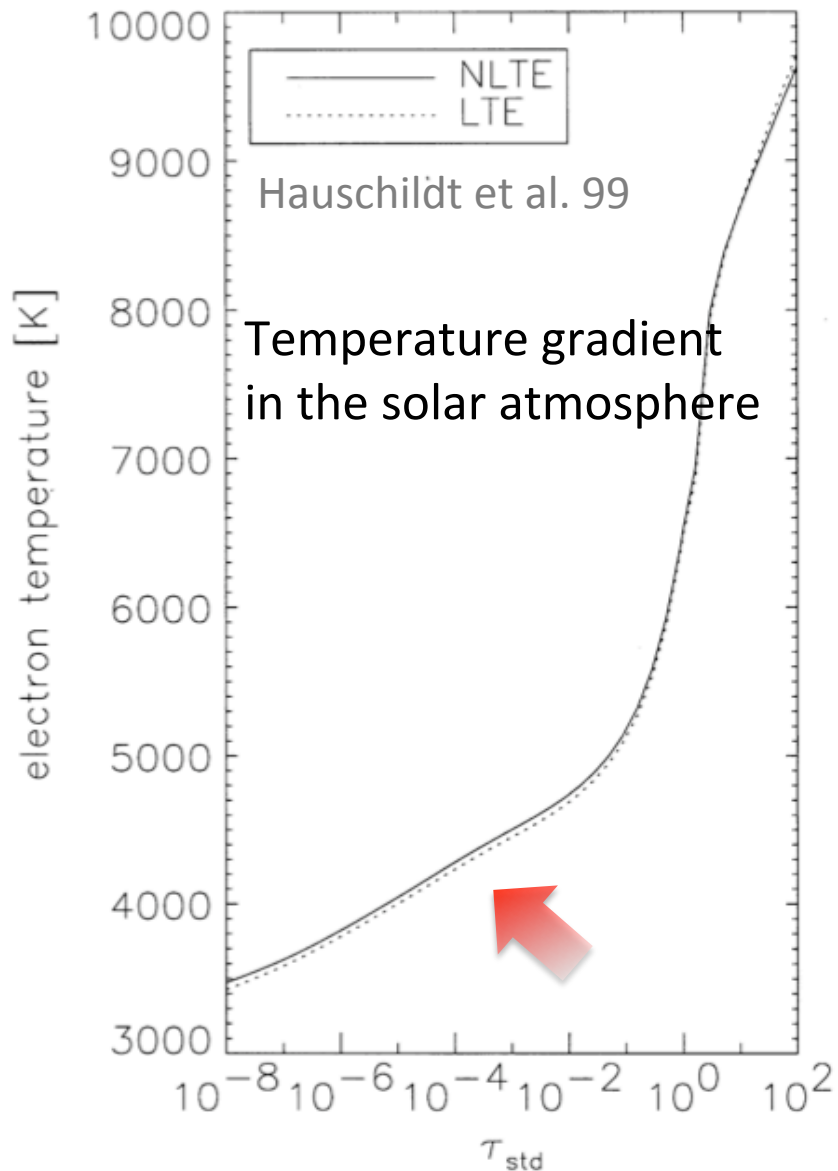
Fig. 5. Evolutionary tracks (same composition as Fig. 4) for low-mass models up to the RGB-tip.

NLTE in FG stellar atmospheres

The key questions to address

- What **atoms/molecules** are sensitive to NLTE conditions?
- Are these **species** important for the atmospheric structure (i.e. opacity, donors of electrons)?

NLTE and atmospheric structure



NLTE and line formation

NLTE is crucial for **modelling spectral lines** with the goal to determine **abundances**:

Li, C, N, O (Asplund et al. 05)

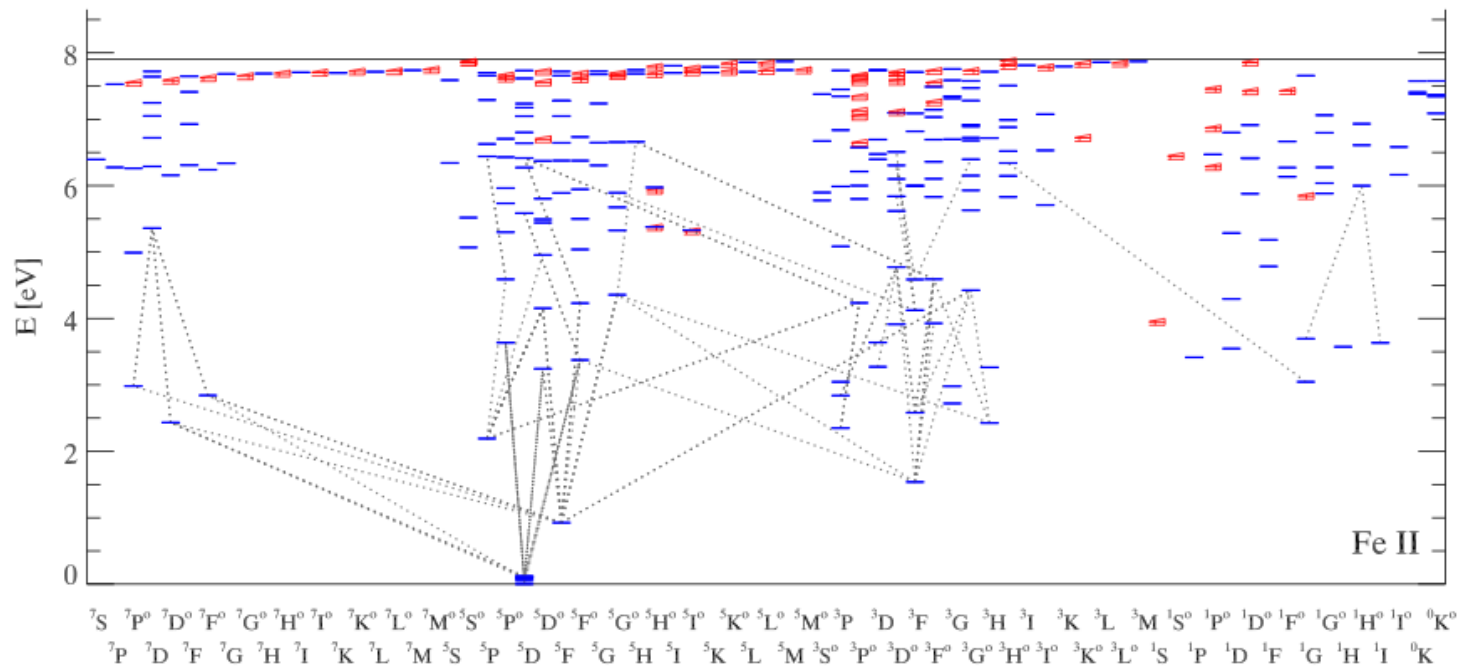
K, Na, Mg, Al, Si (Gehren et al. 06)

Mn, Fe, Co, Ni (Korn et al. 03, Bruls et al. 93, Bergemann 08,
Bergemann et al. 2011, Bergemann et al. 2012)

Sr, Ba, Eu, Sr, Pr (Bergemann et al. 2012, Mashonkina et al. 08)

Iron - a key element in astrophysics

- a proxy of stellar metallicity [Fe/H]
- used to derive effective temperature and surface gravity
 - the method of **excitation-ionization balance** (S. Sousa's talk)
- Fe I and Fe II have, by far, the largest number of lines in a spectrum of a typical F-type star, thus enabling rigorous tests of the models



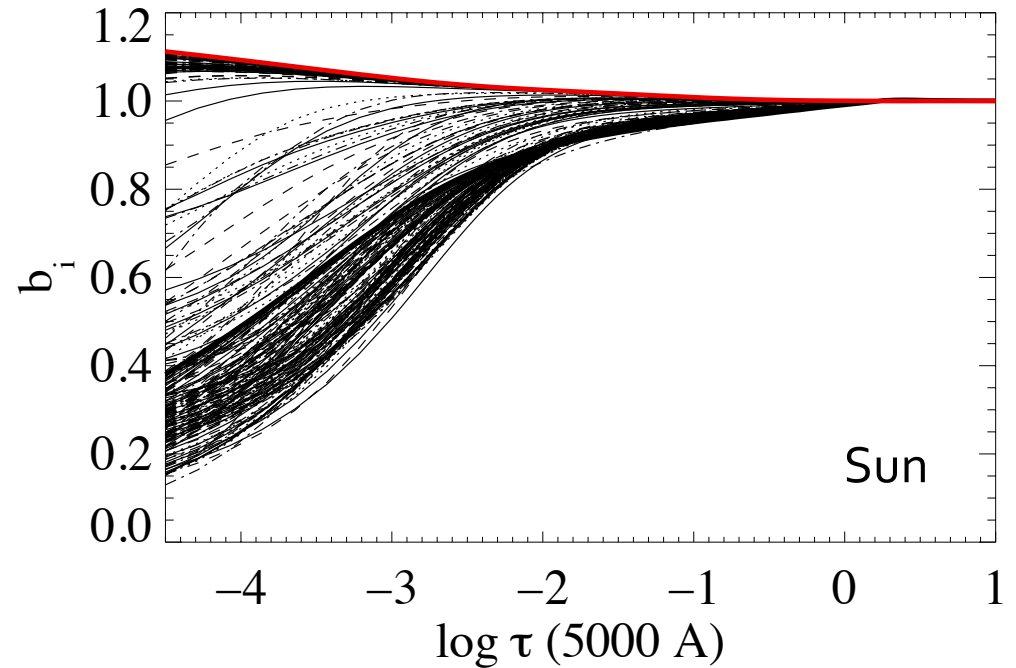
NLTE: excitation balance of Fe

$$b_i = N^{\text{NLTE}} / N_{\text{LTE}}$$

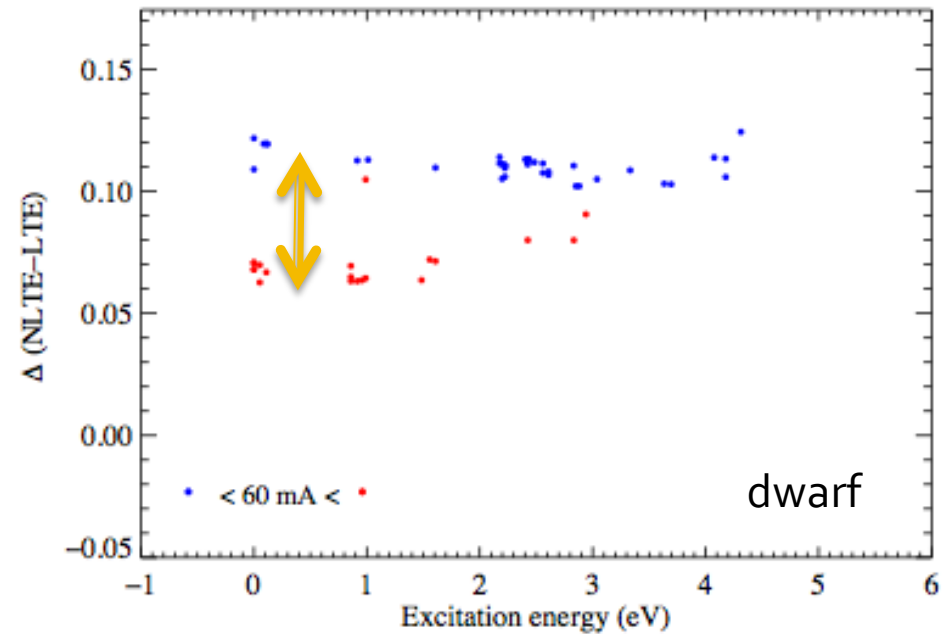
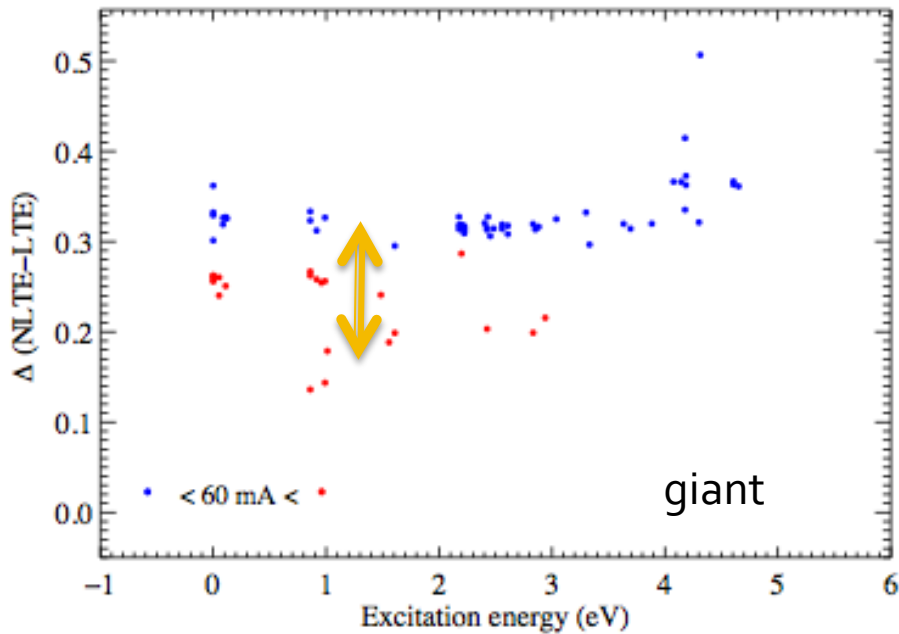
Level departure coefficients

Fe I is very sensitive to NLTE effects in FGK atmospheres:

- overionization due to strong non-local UV radiation field
- IR over-recombination



NLTE: excitation balance of Fe

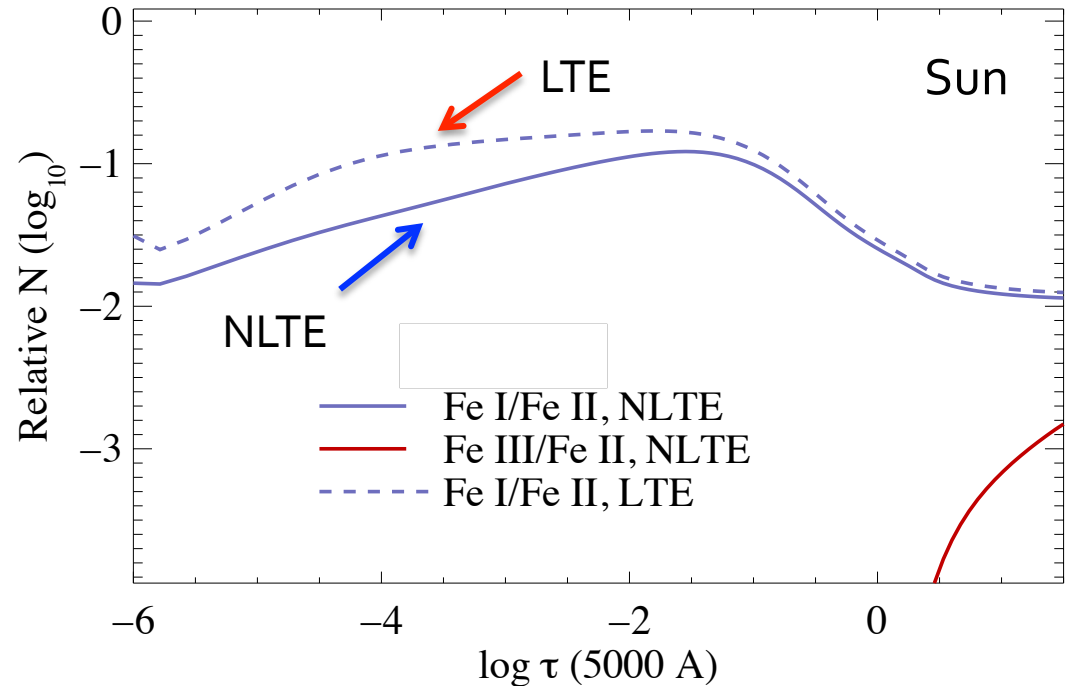


Excitation balance of Fe I is not given by the Saha-Boltzmann statistics \rightarrow wrong T_{eff} in LTE

NLTE: ionization balance of Fe

LTE overestimates
ionization fraction of Fe I/
Fe II → major impact on
[Fe/H] and $\log g$

- [Fe/H], determined either from Fe I or Fe II
- $\log g$, since [Fe II/Fe I] – indicator of surface gravity



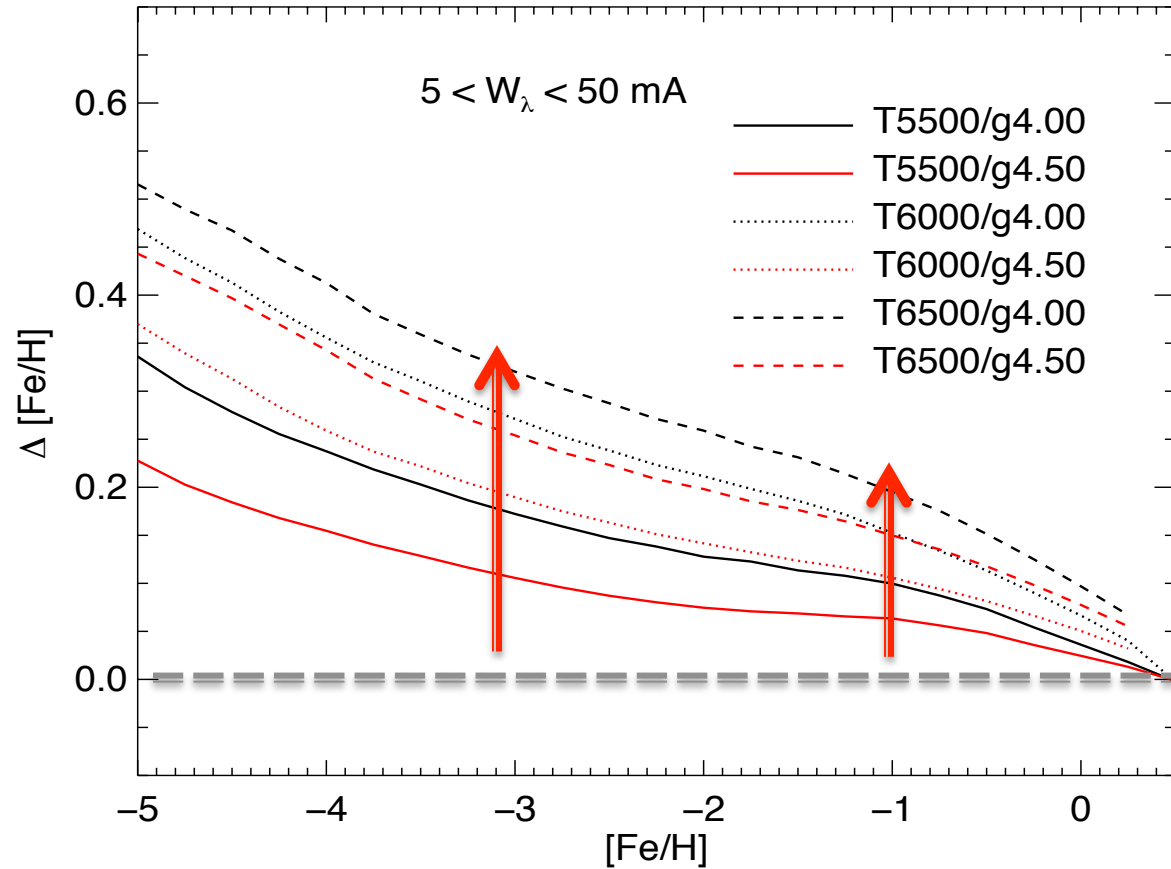
NLTE: abundances

$$\Delta = \log A (\text{non-LTE}) - \log A (\text{LTE})$$

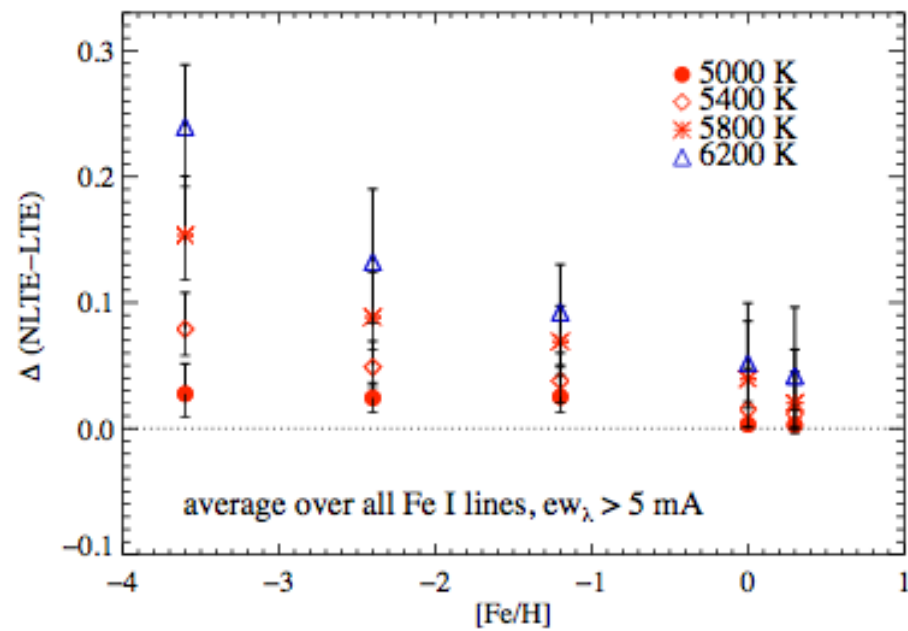
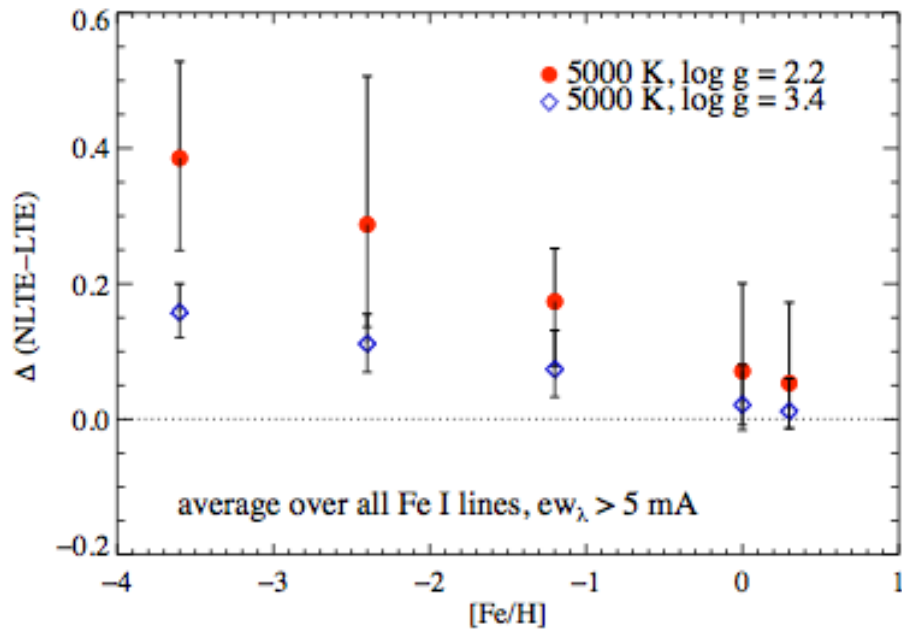
NLTE abundance correction Δ

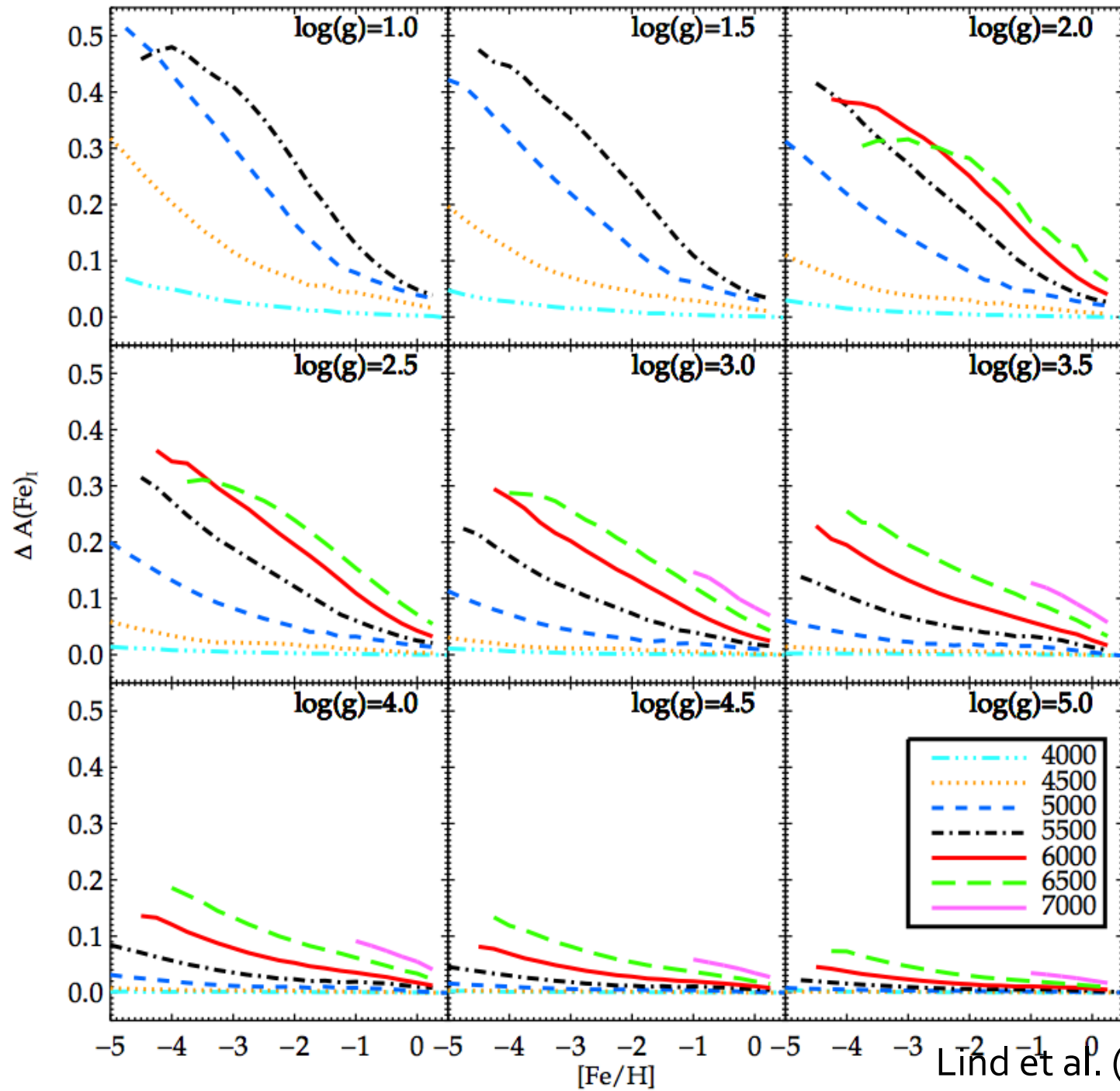
•  with  [Fe/H], log g

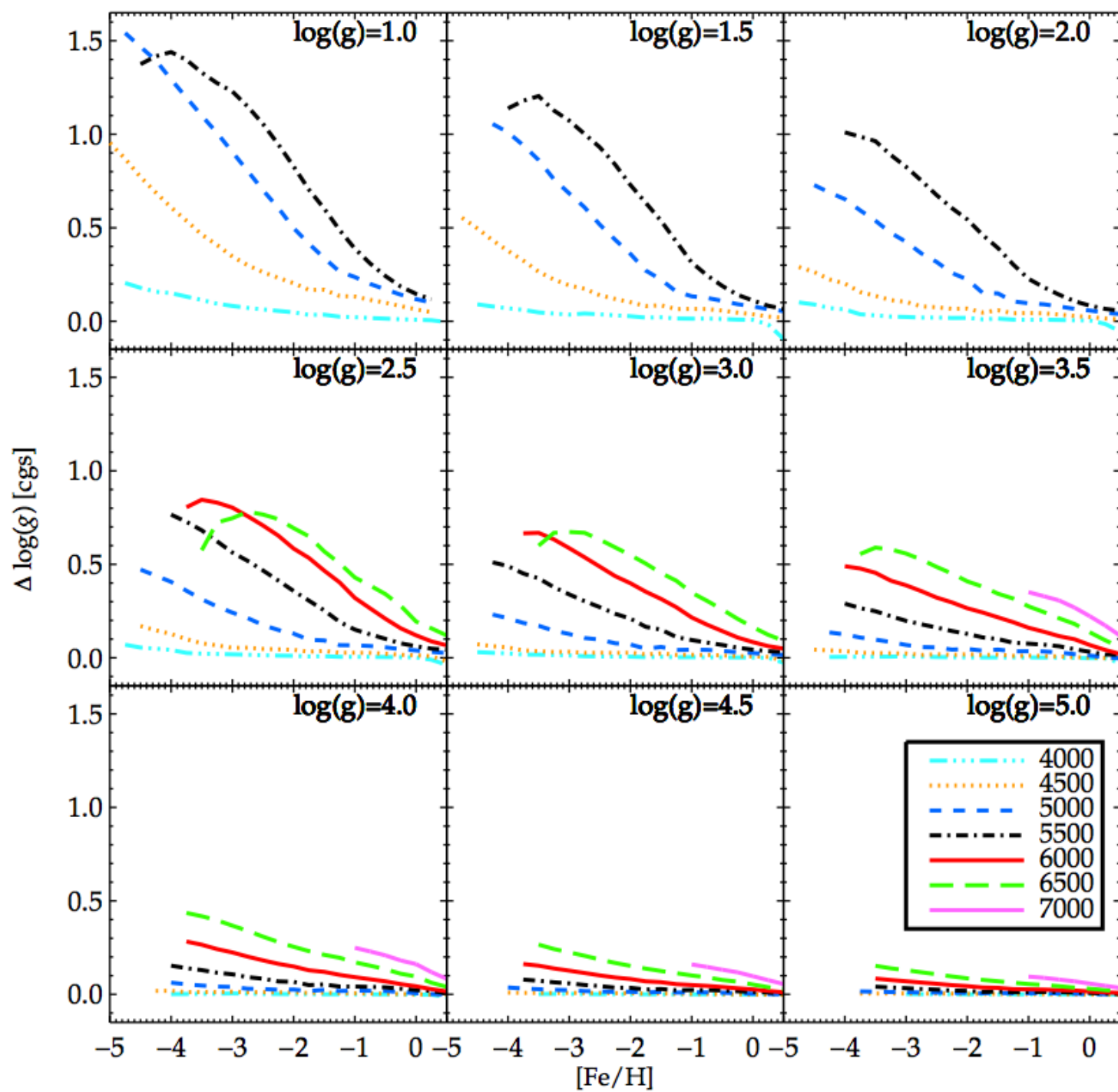
•  with  T_{eff}

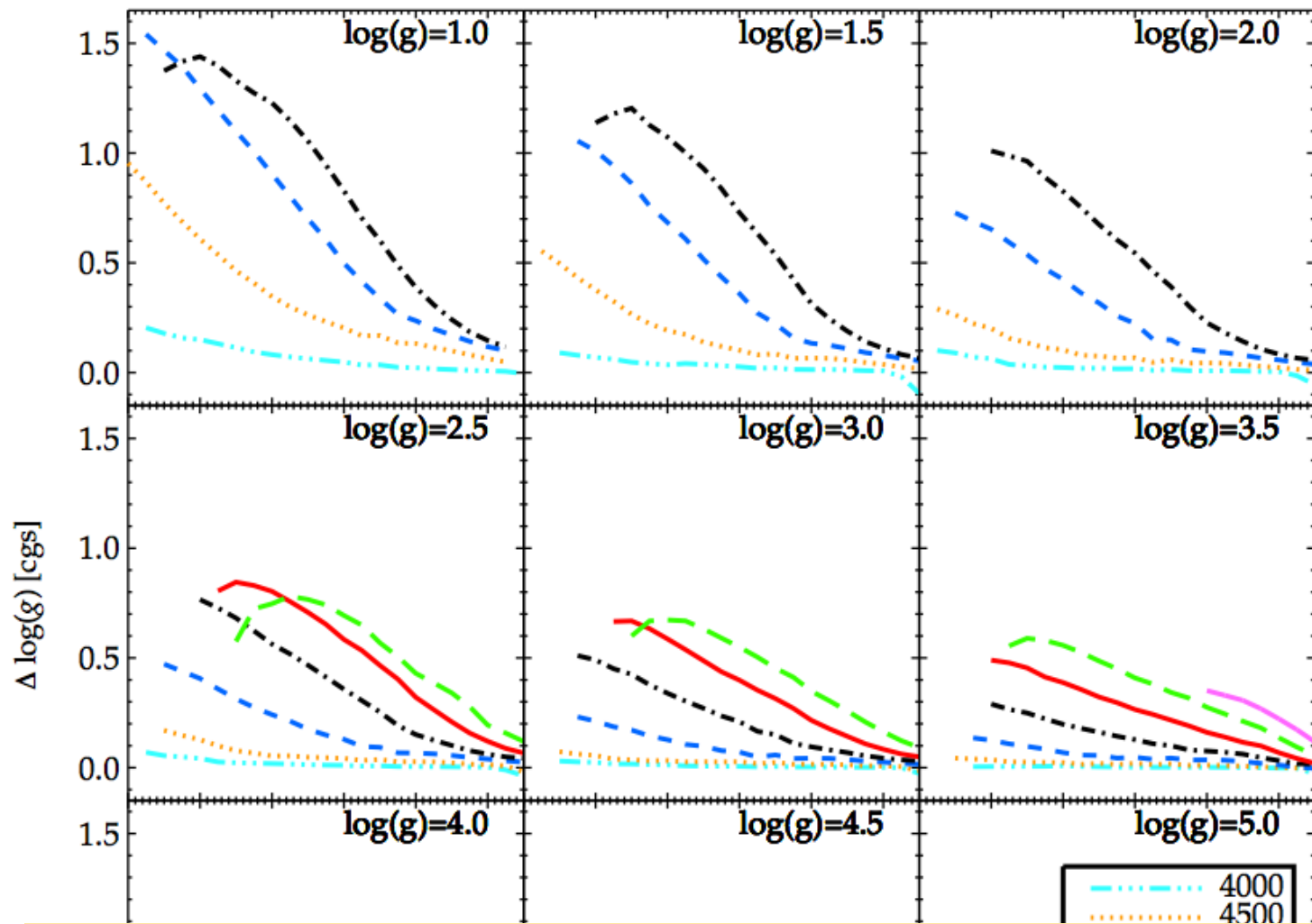


$$\Delta = \log A (\text{non-LTE}) - \log A (\text{LTE})$$

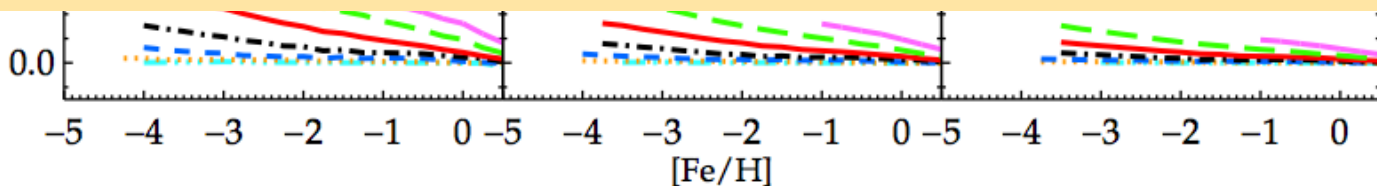








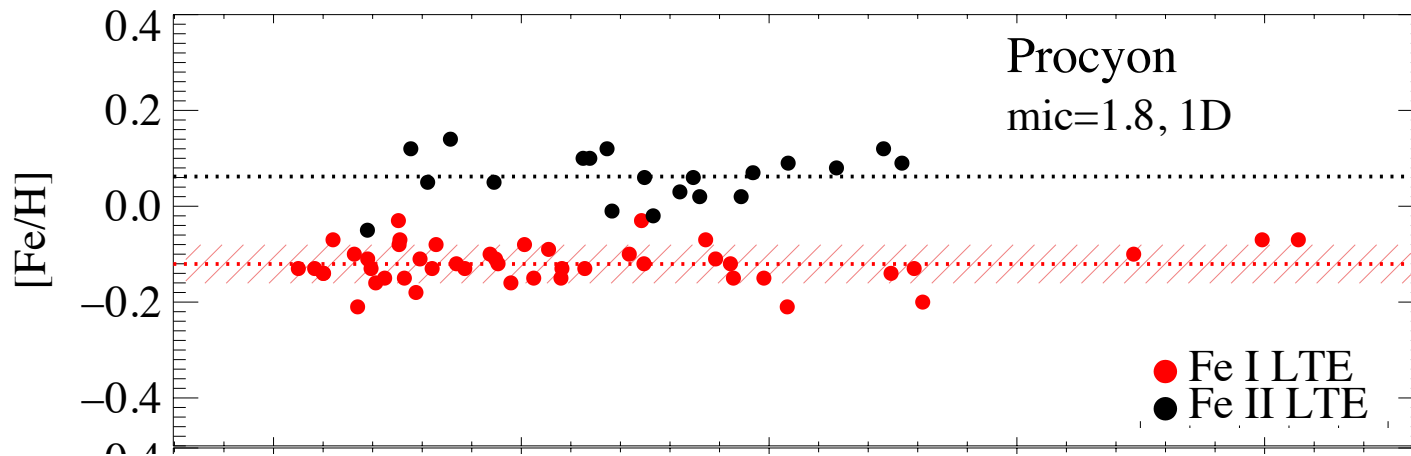
Ionization balance achieved assuming LTE leads to progressively *underestimated* gravities (up to **0.5 dex** at $[\text{Fe}/\text{H}] = -1$) and metallicities (**0.2 dex** at $[\text{Fe}/\text{H}] = -1$)



Metallicity = Fe abundance

Procyon: visual binary, astrometric mass + interferometric ang. diameter

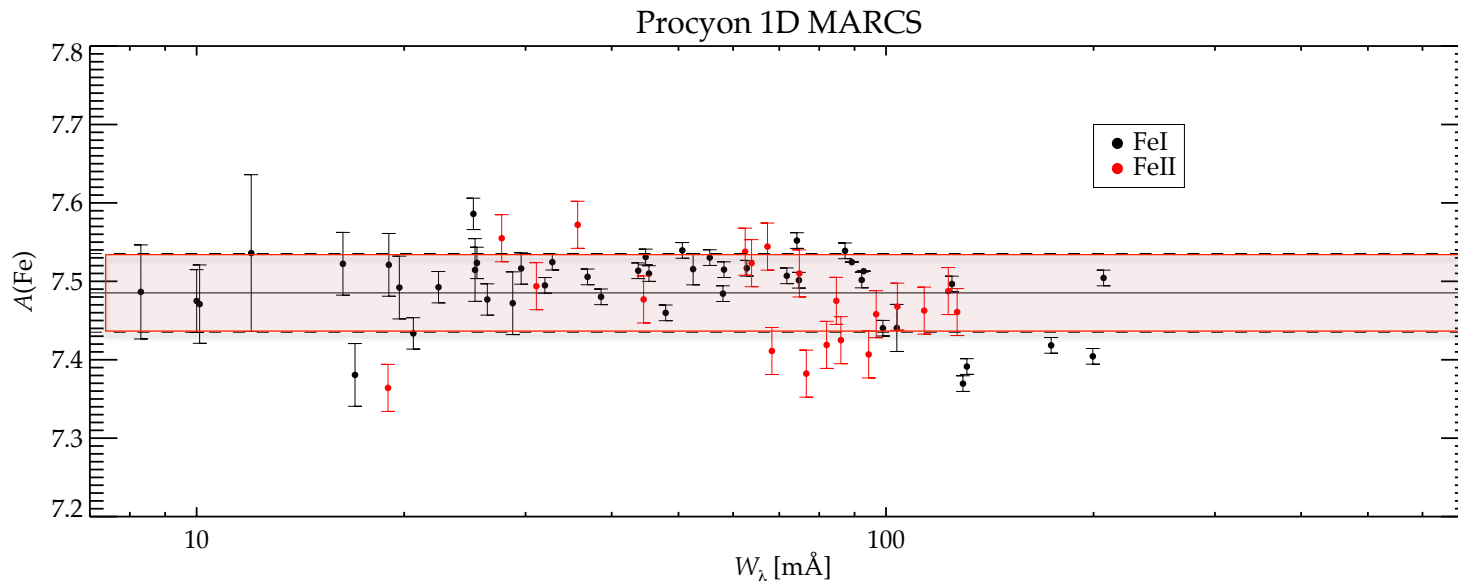
- super-solar metallicity (if LTE & Fe II) $[\text{Fe}/\text{H}] = +0.08 \dots +0.12$
- sub-solar metallicity (if LTE & Fe I) $[\text{Fe}/\text{H}] = -0.12 \dots -0.03$



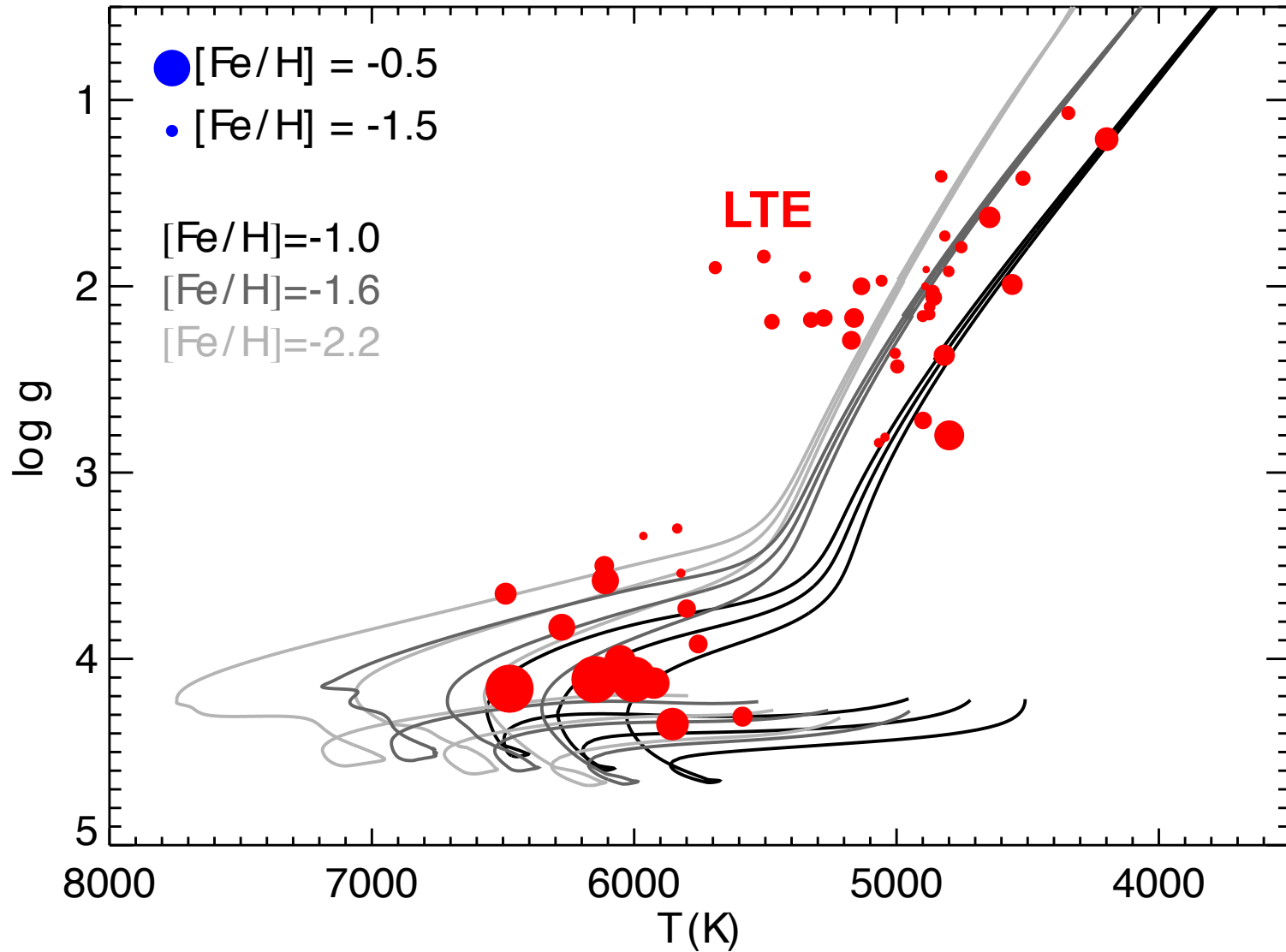
Metallicity = Fe abundance

Procyon: visual binary, astrometric mass + interferometric ang. diameter

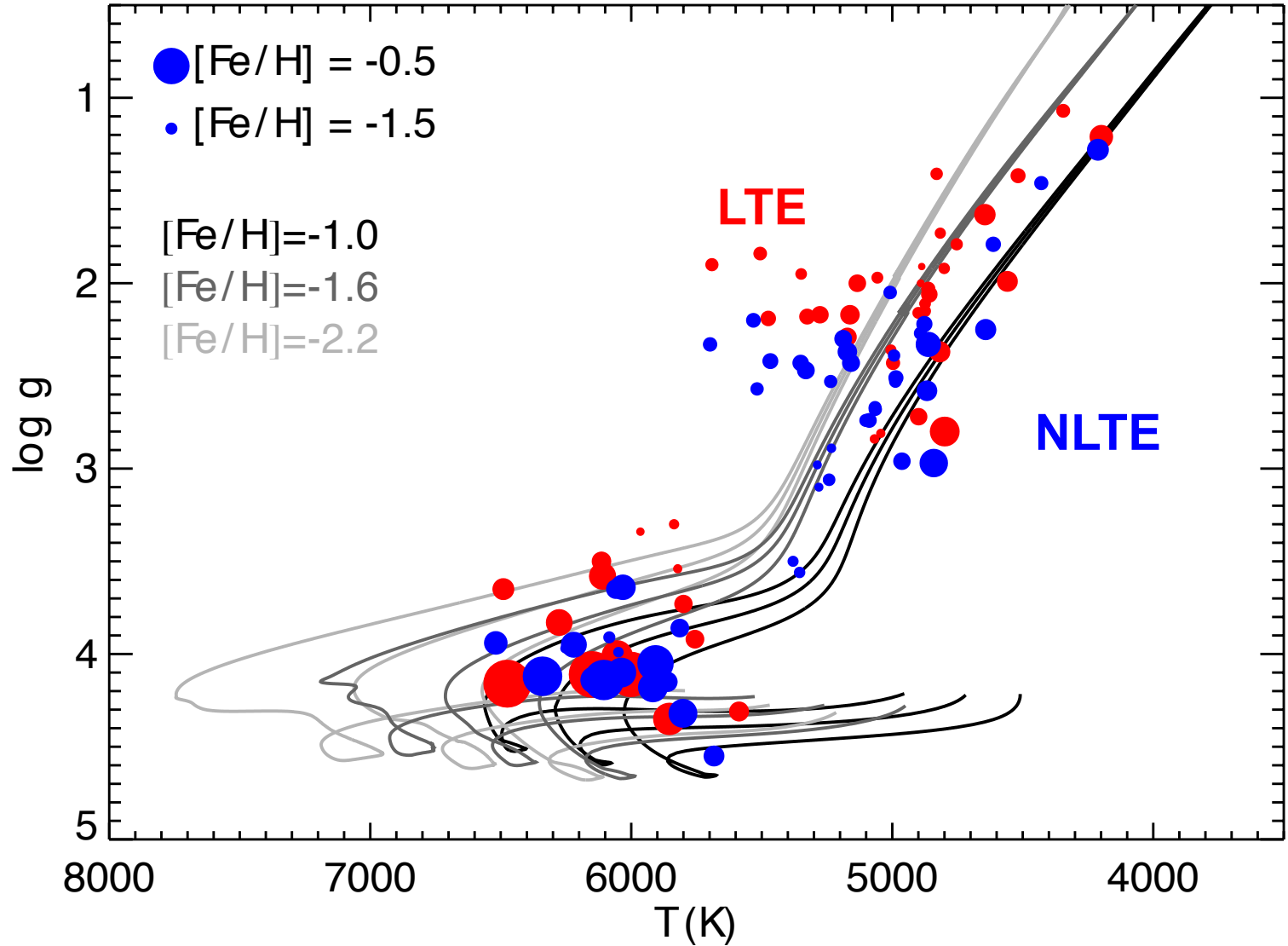
Metallicity from Fe I and Fe II lines: $[Fe/H] = -0.03$



Stellar parameters



Stellar parameters



Abundances of trace elements

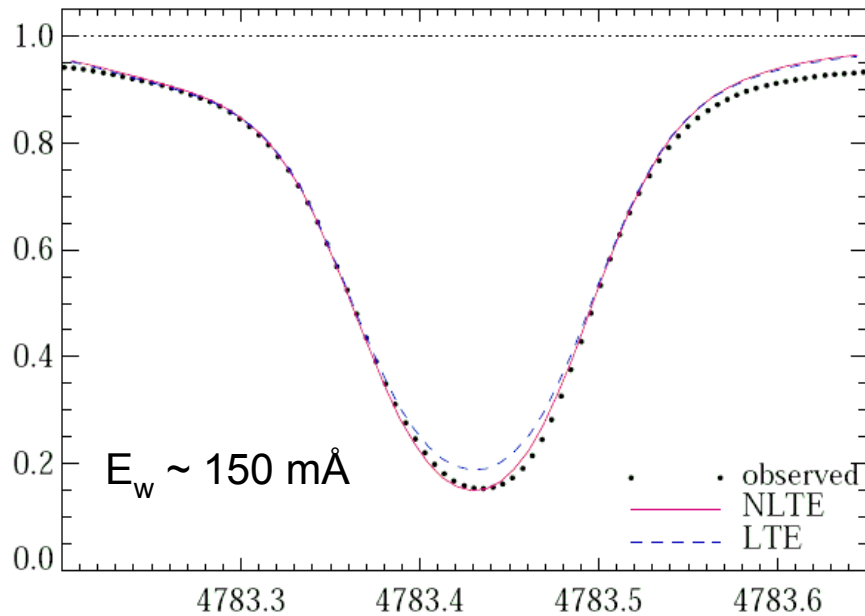
$$\Delta = \log A (\text{non-LTE}) - \log A (\text{LTE})$$

NLTE abundance corrections are a function of T_{eff} , $\log g$, and $[Z]$, but also depend on the atomic properties:

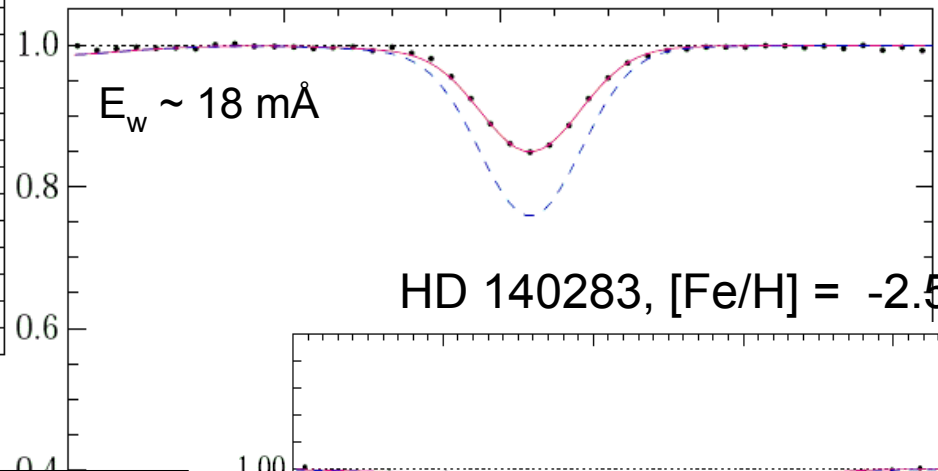
- Ti I: $-0.05 < \Delta < +0.3$
- Mn I: $-0.1 < \Delta < +0.5$
- Co I: $-0.1 < \Delta < +0.7$

Mn in NLTE

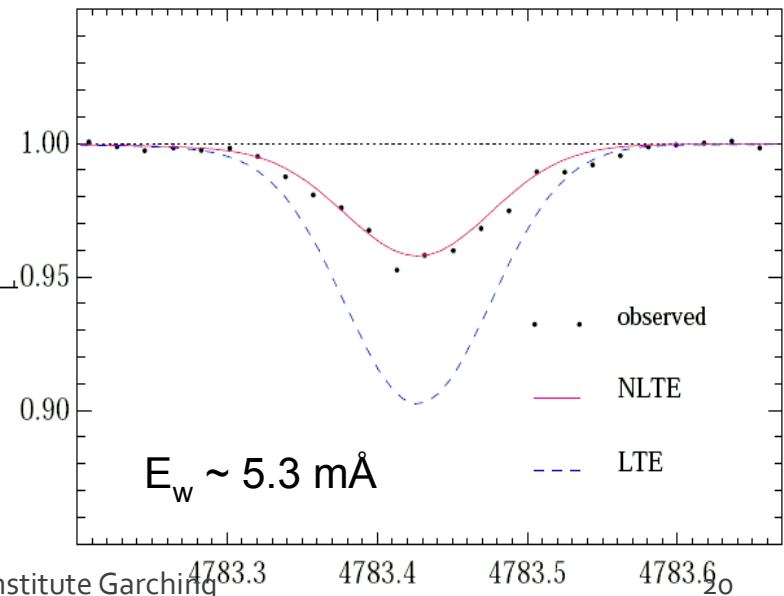
The Sun



HD 34328, $[\text{Fe}/\text{H}] = -1.5$



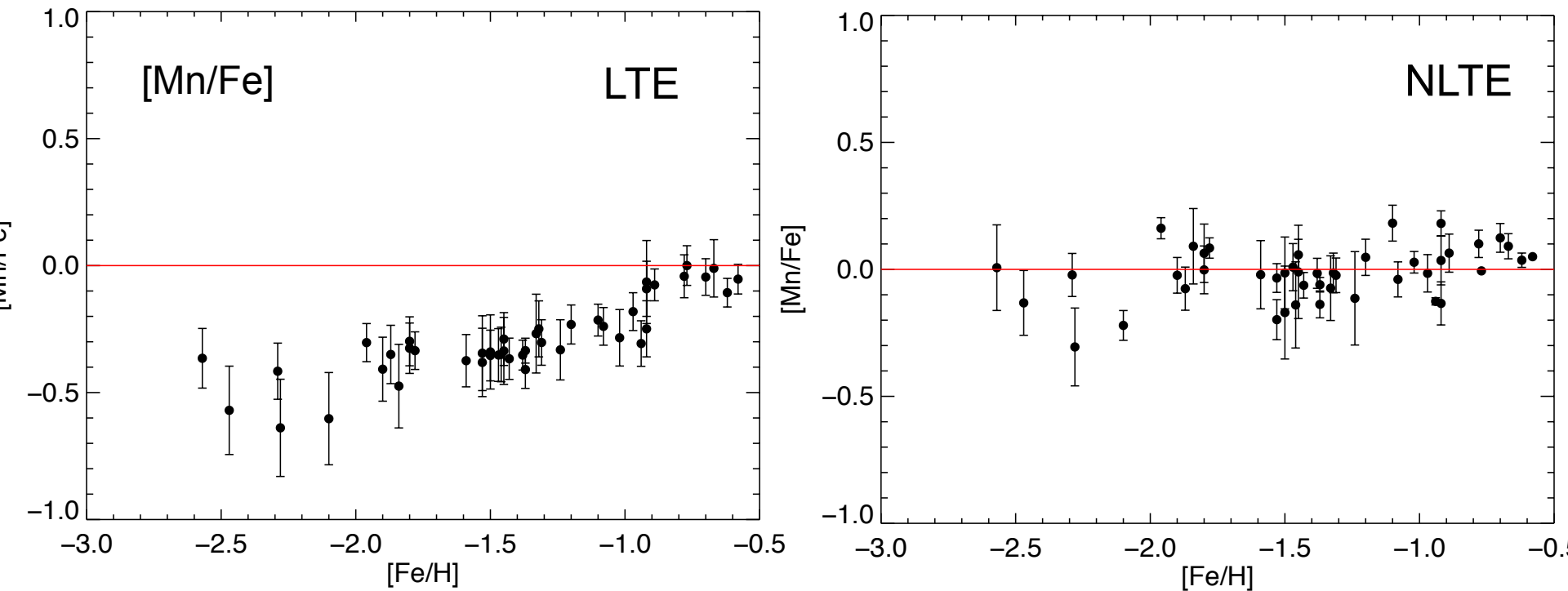
HD 140283, $[\text{Fe}/\text{H}] = -2.5$



Metal-poor stars: inter-atomic collisions are sparse and radiation field is much stronger due to the absence of line blanketing, thus NLTE effects are extreme.

Applications: Galactic Archaeology

Chemical evolution of Mn: $[\text{Mn}/\text{Fe}]$ with $[\text{Fe}/\text{H}]$



NLTE online database



<http://www.inspect-stars.net/>

Welcome to the INSPECT project

A database for Interactive NLTE Spectroscopy of late-type stars.

Get started by choosing your element from the periodic table.

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- [Documentation](#)
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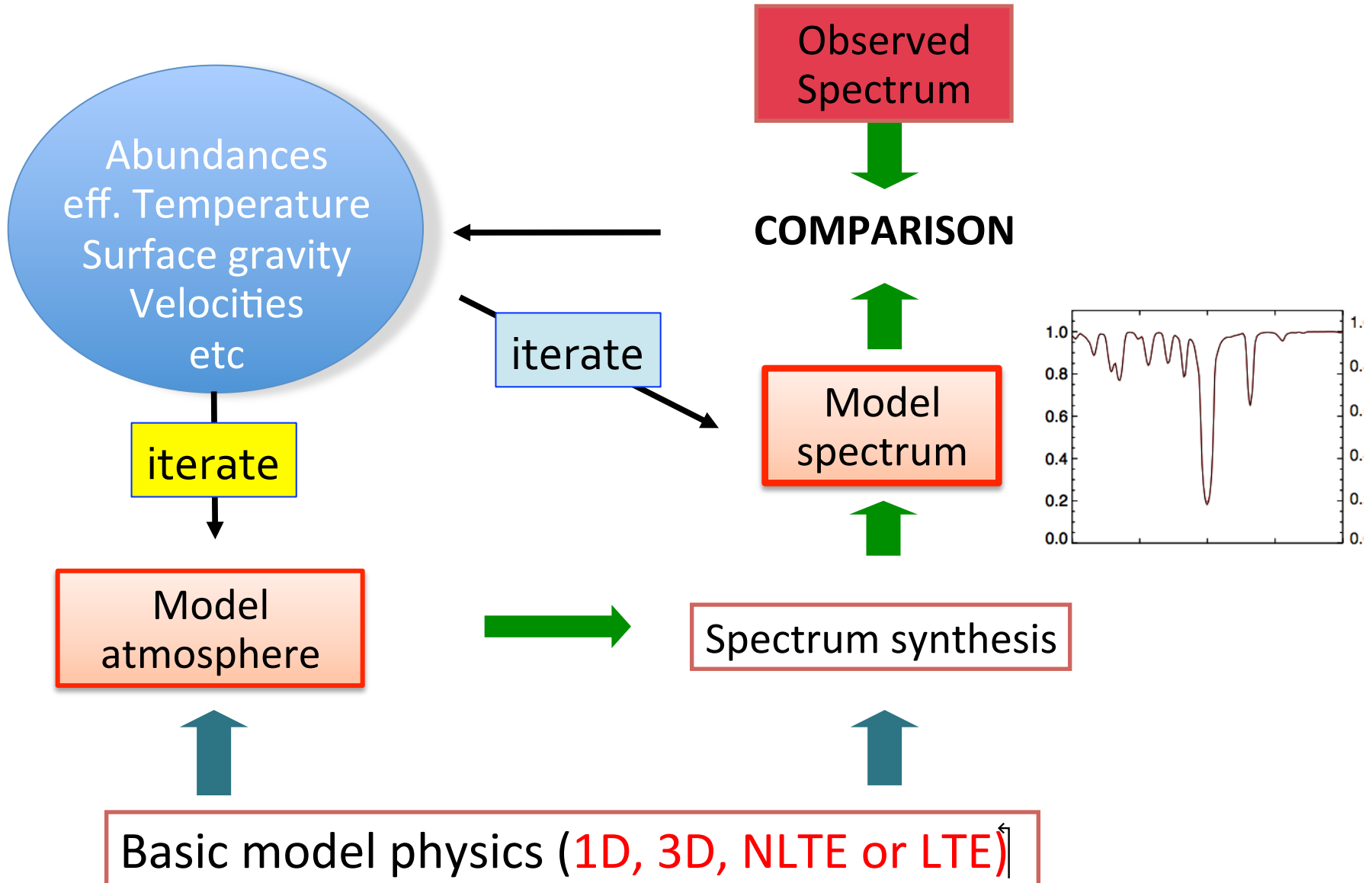
[pmwiki.org](#)

[edit SideBar](#)

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo

Introduction

The idea



Kurucz model atmospheres
(lecture by R. Kurucz)

Model
atmosphere



Basic model physics (1D, 3D, NLTE or LTE)



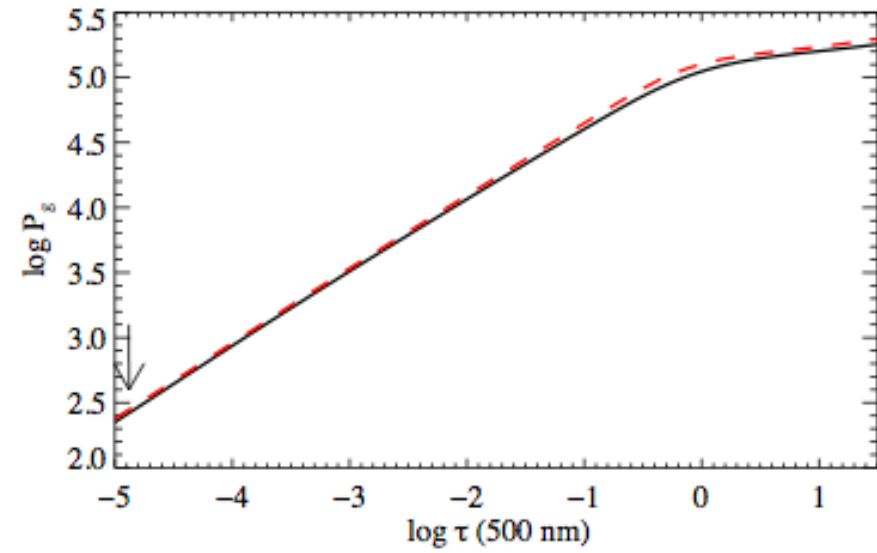
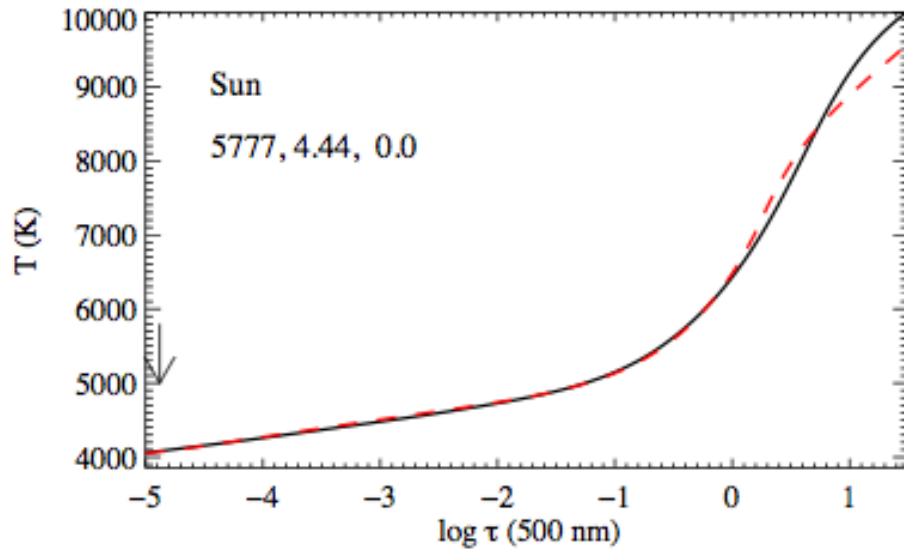
Spectrum synthesis

SIU, SME
codes



Model
spectrum

Model atmosphere



Model atmosphere

```
'TEFF 4300. GRAVITY 1.50000 LTE '  
'TITLE [0.0] VTURB=1.0 KM/SEC L/H=1.50 MARCS-OS ASPLUND ABUNDANCES  
'OPACITY IFOP 1 1 1 1 1 1 1 1 1 1 1 1 0 1 0 0 0 0 0'  
'CONVECTION ON 1.50 TURBULENCE OFF 0.00 0.00 0.00 0.00'  
'ABUNDANCE SCALE 1.00000 ABUNDANCE CHANGE 1 0.92080 2 0.07837'  
'ABUNDANCE CHANGE 3 -10.99 4 -10.66 5 -9.34 6 -3.65 7 -4.26 8 -3.38'  
'ABUNDANCE CHANGE 9 -7.48 10 -4.20 11 -5.87 12 -4.51 13 -5.67 14 -4.53'  
'ABUNDANCE CHANGE 15 -6.68 16 -4.90 17 -6.54 18 -5.86 19 -6.96 20 -5.73'  
'ABUNDANCE CHANGE 21 -8.99 22 -7.14 23 -8.04 24 -6.40 25 -6.65 26 -4.59'  
'ABUNDANCE CHANGE 27 -7.12 28 -5.81 29 -7.83 30 -7.44 31 -9.16 32 -8.46'  
'ABUNDANCE CHANGE 33 -9.75 34 -8.71 35 -9.48 36 -8.76 37 -9.44 38 -9.12'  
'ABUNDANCE CHANGE 39 -9.83 40 -9.45 41 -10.62 42 -10.12 43 -20.00 44 -10.20'  
'ABUNDANCE CHANGE 45 -10.92 46 -10.35 47 -11.10 48 -10.27 49 -10.44 50 -10.04'  
'ABUNDANCE CHANGE 51 -11.04 52 -9.85 53 -10.53 54 -9.77 55 -10.97 56 -9.87'  
'ABUNDANCE CHANGE 57 -10.91 58 -10.46 59 -11.33 60 -10.59 61 -20.00 62 -11.03'  
'ABUNDANCE CHANGE 63 -11.52 64 -10.92 65 -11.76 66 -10.90 67 -11.53 68 -11.11'  
'ABUNDANCE CHANGE 69 -12.04 70 -10.96 71 -11.98 72 -11.16 73 -12.21 74 -10.93'  
'ABUNDANCE CHANGE 75 -11.81 76 -10.59 77 -10.66 78 -10.40 79 -11.03 80 -10.91'  
'ABUNDANCE CHANGE 81 -11.14 82 -10.04 83 -11.39 84 -20.00 85 -20.00 86 -20.00'  
'ABUNDANCE CHANGE 87 -11.14 88 -10.04 89 -11.39 90 -20.00 91 -20.00 92 -12.51'  
'ABUNDANCE CHANGE 93 -11.14 94 -10.04 95 -11.39 96 -20.00 97 -20.00 98 -20.00'  
'ABUNDANCE CHANGE 99 -11.14 100 -10.04 101 -11.39 102 -20.00 103 -20.00 104 -20.00'  
'READ DECK6 ',dep,' RHOX,T,P,XNE,ABROSS,ACCRAD,VTURB, FLXCNV,VCONV,VELSND'
```

A – abundance of an element, $A = \log N/N_H + 12$
N - total number density of an element

Model atmosphere

Column mass density $m(t)$

Gas pressure $P(t)$

Temperature $T(t)$

Electron concentration $N_e(t)$

```
READ DECK6 72 RHOX,T,P,XNE,ABROSS,ACCRAD,VTURB, FLXCNV,VCONV,VEL:
 1.11438611E-03  4303.3 1.114E+01 1.188E+09 1.197E-04 5.762E-03
 1.46933430E-03  4325.0 1.469E+01 1.499E+09 1.309E-04 5.781E-03
 1.90642161E-03  4338.1 1.906E+01 1.806E+09 1.404E-04 5.788E-03
 2.44338350E-03  4355.4 2.443E+01 2.200E+09 1.541E-04 5.798E-03
 3.09334096E-03  4372.8 3.093E+01 2.664E+09 1.704E-04 5.816E-03
 3.87393779E-03  4391.0 3.874E+01 3.217E+09 1.900E-04 5.851E-03
 4.80510076E-03  4409.4 4.805E+01 3.867E+09 2.128E-04 5.891E-03
 5.91112062E-03  4428.0 5.911E+01 4.629E+09 2.393E-04 5.939E-03
 7.22091430E-03  4446.5 7.221E+01 5.515E+09 2.698E-04 5.995E-03
 8.76903374E-03  4464.8 8.769E+01 6.544E+09 3.046E-04 6.061E-03
 1.05970558E-02  4482.7 1.060E+02 7.729E+09 3.440E-04 6.141E-03
 1.27556538E-02  4500.1 1.276E+02 9.088E+09 3.885E-04 6.240E-03
 1.53040028E-02  4517.4 1.530E+02 1.066E+10 4.389E-04 6.356E-03
 1.83113451E-02  4534.4 1.831E+02 1.246E+10 4.961E-04 6.489E-03
```

... 72 depth points - t

LTE line formation

- the profile function

$$\psi(\nu - \nu_0) = \phi(\nu - \nu_0) = \frac{H(a, \nu)}{\sqrt{\pi} \Delta \nu_D} \quad \text{with} \quad a = \frac{\gamma_R + \gamma_3 + \gamma_4 + \gamma_6}{4\pi \Delta \nu_D} \quad \nu = \frac{\nu - \nu_0}{\Delta \nu_D}$$

- line absorption coefficient

$$\kappa_\lambda^l = \frac{\pi e^2}{m_e c} \frac{\lambda}{c} b_i \frac{N_i^{\text{LTE}}}{N_{\text{El}}} N_{\text{H}} \log \varepsilon f_{ij} \frac{H(a, \nu)}{\Delta \lambda_D} \left(1 - \frac{b_j}{b_i} e^{-hc/\lambda kT} \right) \quad \kappa_\lambda = \kappa_\lambda^l + \kappa_\lambda^c$$

$$S_\nu \equiv \frac{2hc^2}{\lambda^5} \frac{1}{e^{hc/kT\lambda} - 1} = B_\nu$$

Line source function, assumed to be Planck function

$$I_\lambda(\tau_\nu = 0, \mu) = \int_0^\infty S_\lambda(\tau_\lambda) e^{-\tau_\lambda/\mu} d\tau_\lambda/\mu$$

Emergent intensity

$$F_\lambda(0) = 2\pi \int_0^\infty S_\lambda(T(\tau_\lambda)) E_2(\tau_\lambda) d\tau_\lambda$$

Surface flux

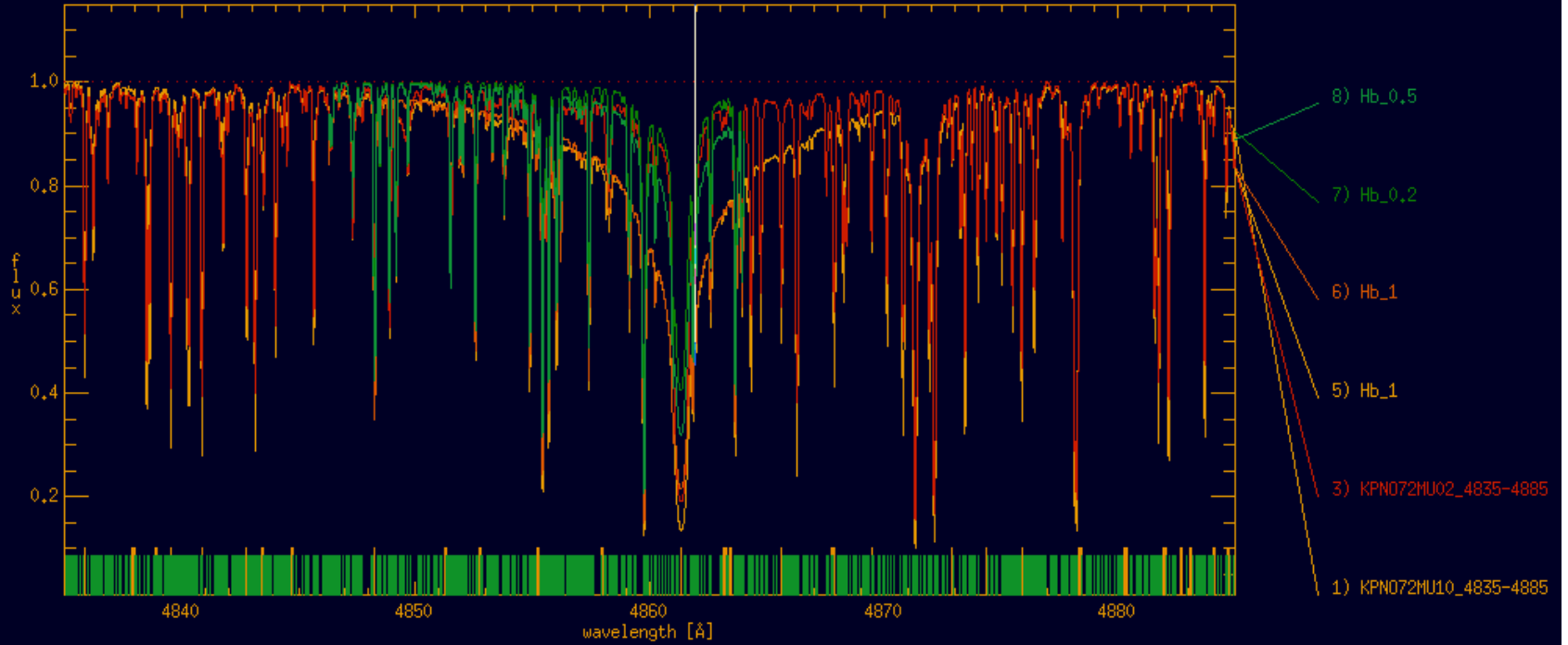
NLTE line formation

$$b_i(\tau_0) = \frac{n_i(\tau_0)}{n_i^*(\tau_0)},$$

$$\kappa_\nu^l = b_l \kappa^{*l} \frac{1 - \frac{b_u}{b_l} e^{h\nu/kT}}{1 - e^{h\nu/kT}}.$$

$$S_\lambda = \frac{2h\nu_0^3}{c^2} \frac{1}{\frac{b_l}{b_u} e^{h\nu_0/kT} - 1}.$$

SPECTRUM - COMPARISON



```

LINEFORMATION
START
CANCEL
Atmos.   : t<Teff><logg><logz>.dat OR grid interpolation
Teff     : 5777    K
log(g)   : 4.44    [cm/s^2]
[Fe/H]   : 0.00
Xi       : 0.90    km/s
CONSTANT MICROTURBULENCE
XI-file  : hm-micro.xi
LTE - LINEFORMATION
Departures:
Termdesig.:
-----
Wmin     : 4834.500  Å
Wmax     : 4885.500  Å
Stepwidth-crit.: 0.100000
Min.stepwidth : 5.  mA / 5000 Å
Max.stepwidth : 1.50  Å / 5000 Å
-----
FLUX
Cos(theta) : 1.00000
NORMALIZED
ALL EXISTING LINES
ATOMIC AND MOLECULAR LINES
IGNORE    QUADRATIC STARK EFFECT
-----
SEARCH EXACT ATMOSPHERE ON
INTEGRATION: GAUSS-QUADRATURE

```

- define a model atmosphere or provide

T_{eff}
logg

[Fe/H]

Xi: microturbulence

- Min wavelength
- Max wavelength

- Flux or Intensity?
 $\cos\theta = ?$

- **Linelist?**

LINELIST - atomic data for each line

STAT	ION	LAMBDA	MPT	E-LOW	LABU	LABL	JU	JL	IW	GAMRAD	LOG(GF)	GF-REF	LOG(C6)	C6-REF	NEW GF	NEW C6	LOG(C4)
DEL	Mn II	4861.701					10.1813G	5G(5.0 5.0)	0.20	6.47E+08	-2.412	KUC	-31.662	KUC	0.000	0.000	-14.862
	Cr I	4861.734					3.375	5D 3P(2.0 2.0)	0.20	1.95E+08	-2.988	KUC	-31.936	KUC	0.000	0.000	-15.020
	MgH I	4861.779	24.1				0.206	B,v X,v(0.0 0.0)	0.20	9.40E+07	-3.833	KUC	-32.957	STD	-3.851	0.000	0.000
	MgH I	4861.779	24.1				0.206	B,v X,v(0.0 0.0)	0.20	9.40E+07	-3.914	KUC	-32.957	STD	-3.914	0.000	0.000
	CH I	4861.828	12.1				1.090	B,v X,v(0.0 0.0)	0.20	9.40E+07	-3.804	KUC	-32.526	STD	-4.159	0.000	0.000
	Cr I	4861.845					2.530	5F 5G(3.0 4.0)	3.50	3.61E+08	-3.959	KUC	-31.910	KUC	-0.736	0.000	-15.604
	>Fe I	4861.953					4.638	i5D 5P(2.0 1.0)	0.20	2.88E+08	-2.063	KUC	-30.358	UNS	-1.353	0.000	-13.836
DEL	SiH I	4861.964	28.1				0.51A	A,v X,v(0.0 0.0)	0.20	9.40E+07	-4.937	KUC	-32.922	STD	0.000	0.000	0.000
	CH I	4861.969	12.1				0.558	A,v X,v(0.0 0.0)	0.20	9.40E+07	-2.700	KUC	-32.608	STD	-3.050	0.000	0.000
	CH I	4862.002	12.1				0.558	A,v X,v(0.0 0.0)	0.20	9.40E+07	-4.680	KUC	-32.928	STD	-5.030	0.000	0.000
	MgH I	4862.018	24.1				0.868	B,v X,v(0.0 0.0)	0.20	9.40E+07	-2.207	KUC	-32.881	STD	-2.207	0.000	0.000
	MgH I	4862.018	24.1				0.868	B,v X,v(0.0 0.0)	0.20	9.40E+07	-2.247	KUC	-32.881	STD	-2.247	0.000	0.000
	CH I	4862.025	12.1				1.090	B,v X,v(0.0 0.0)	0.20	9.40E+07	-3.782	KUC	-32.526	STD	-4.132	0.000	0.000
DEL	SiH I	4862.043	28.1				0.51A	A,v X,v(0.0 0.0)	0.20	9.40E+07	-4.937	KUC	-32.922	STD	0.000	0.000	0.000
	Mn I	4862.050		43			3.840	4P 4P(2.5 1.5)	0.20	8.89E+06	-1.393	KUC	-32.021	KUC	0.000	0.000	-15.487
	Co I	4862.086					4.064	2D 2F(1.5 2.5)	0.20	6.27E+07	-0.901	KUC	-31.516	KUC	0.000	0.000	-14.129
DEL	Ni II	4862.152					12.475	2G(4.5 4.5)	0.20	8.65E+08	-2.413	KUC	-31.738	KUC	0.000	0.000	-14.183
DEL	V I	4862.159					2.86SH	4F(2.5 1.5)	0.20	1.82E+08	-3.619	KUC	-31.495	KUC	0.000	0.000	-12.475
	CH I	4862.178	12.1				0.558	A,v X,v(0.0 0.0)	0.20	9.40E+07	-4.780	KUC	-32.608	STD	-5.130	0.000	0.000
	CH I	4862.212	12.1				0.558	A,v X,v(0.0 0.0)	0.20	9.40E+07	-2.662	KUC	-32.608	STD	-3.012	0.000	0.000

CURSOR: (4861.934, 0.18) LINE-POS.: 4861.951 54.62%

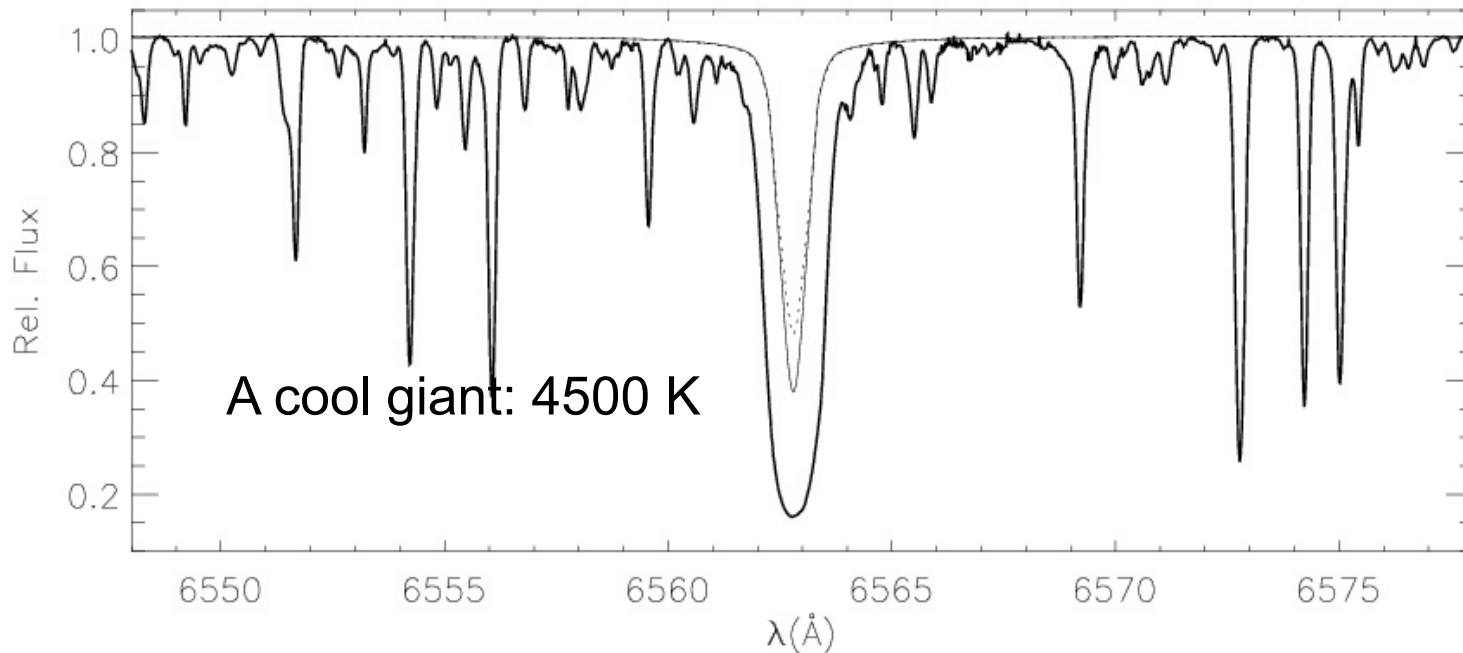
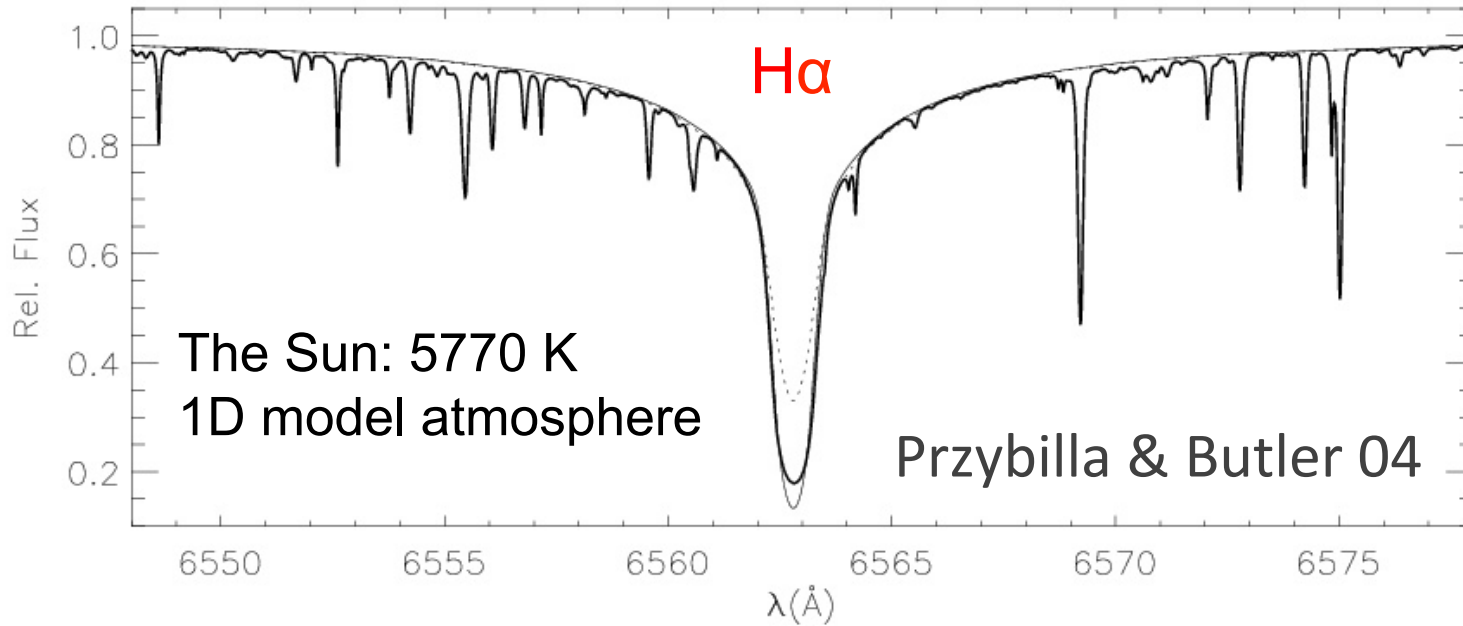
PLOT DEL UNDEL EDIT SELECT UNSELECT LINFO

STAT	ION	LAMBDA	MPT	E-LOW	LABU	LABL	JU	JL	IW	GAMRAD
DEL	Mn II	4861.701					10.1813G	5G(5.0 5.0)	0.20	6.47E+08
	Cr I	4861.734					3.375	5D 3P(2.0 2.0)	0.20	1.95E+08
	MgH I	4861.779	24.1				0.206	B,v X,v(0.0 0.0)	0.20	9.40E+07
	MgH I	4861.779	24.1				0.206	B,v X,v(0.0 0.0)	0.20	9.40E+07
	CH I	4861.828	12.1				1.090	B,v X,v(0.0 0.0)	0.20	9.40E+07
	Cr I	4861.845		31			2.530	5F 5G(3.0 4.0)	3.50	3.61E+08
	>Fe I	4861.953					4.638	i5D 5P(2.0 1.0)	0.20	2.88E+08
DEL	SiH I	4861.964	28.1				0.51A	A,v X,v(0.0 0.0)	0.20	9.40E+07
	CH I	4861.969	12.1				0.558	A,v X,v(0.0 0.0)	0.20	9.40E+07
	CH I	4862.002	12.1				0.558	A,v X,v(0.0 0.0)	0.20	9.40E+07
	MgH I	4862.018	24.1				0.868	B,v X,v(0.0 0.0)	0.20	9.40E+07
	MgH I	4862.018	24.1				0.868	B,v X,v(0.0 0.0)	0.20	9.40E+07
	CH I	4862.025	12.1				1.090	B,v X,v(0.0 0.0)	0.20	9.40E+07
DEL	SiH I	4862.043	28.1				0.51A	A,v X,v(0.0 0.0)	0.20	9.40E+07
	Mn I	4862.050		43			3.840	4P 4P(2.5 1.5)	0.20	8.89E+06
	Co I	4862.086					4.064	2D 2F(1.5 2.5)	0.20	6.27E+07
DEL	Ni II	4862.152					12.475	2G(4.5 4.5)	0.20	8.65E+08
DEL	V I	4862.159					2.86SH	4F(2.5 1.5)	0.20	1.82E+08
	CH I	4862.178	12.1				0.558	A,v X,v(0.0 0.0)	0.20	9.40E+07
	CH I	4862.212	12.1				0.558	A,v X,v(0.0 0.0)	0.20	9.40E+07

CURSOR: (4861.934, 0.18) LINE-POS.: 4861.951 54.62%

PLOT DE

Hydrogen lines – T_{eff} diagnostics



3) MRD_UVESGauss06/ 5774, 4.50, -0.21, Xi: 1.07, Gauss: 3.7, F: 1, RV: -0.3km/s, cf: 1.503e-02

