AST5210
Stellar Atmospheres I

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- Basic concepts
- Formal solution
  - Numerical integration, scattering problem, lambda iteration, shooting, finite difference methods, Feautrier's method, accelerated lambda iteration, convergence acceleration
- MULTI non-LTE code

- Exercises
  - Na-D, Mg-b, Ca-H, Hinode BFI continua
  - getting input data - building atomic models
  - non-LTE effects for abundance determinations of stars

- non-LTE
  - Linearization, rate equations, Scharmer operator, local operator
- 3D
  - Long characteristics, short characteristics
- Energy equation
  - ODF, multi-group opacities

- Exercises (contd)
  - Na-D, Mg-b, Ca-H, Hinode BFI continua
  - getting input data - building atomic models
  - non-LTE effects for abundance determinations of stars

- contribution and response functions
- non-LTE effects for abundance determinations in stars
- other non-LTE examples
- non-equilibrium ionization

- Exercises (contd)
  - Na-D, Mg-b, Ca-H, Hinode BFI continua
  - getting input data - building atomic models
  - non-LTE effects for abundance determinations of stars

- Line formation in dynamical media
- 3D chromospheric simulations

- Exercises
  - 3D column-by-column with MULTI

Basic concepts

Basic definitions

I_ν Intensity. $\mathrm{erg\ cm^{-2}s^{-1}sr^{-1}Hz^{-1}}$

η_ν Emissivity

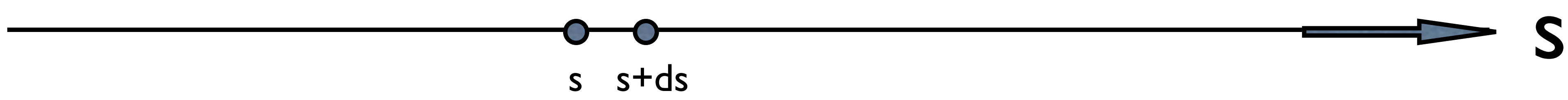
χ_ν Opacity

Intensity gives the amount of energy per unit area perpendicular to the ray in a given direction per unit time per solid angle and per frequency bin. The intensity is constant with distance in the absence of emission and absorption/scattering processes.

Emissivity gives the addition of energy to the ray through emission processes.

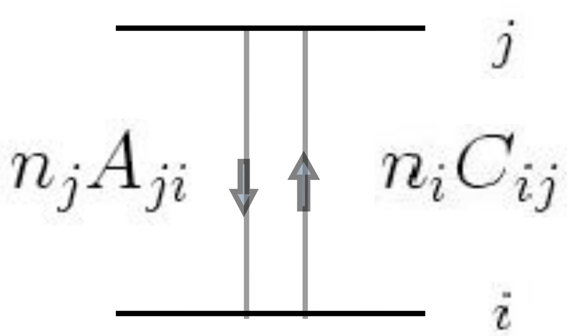
Opacity gives the removal of energy from the ray through absorption and scattering processes.

Transfer equation



$$dI_\nu = -\chi_\nu I_\nu ds + \eta_\nu ds$$

Coronal approximation: $\chi_\nu = 0$

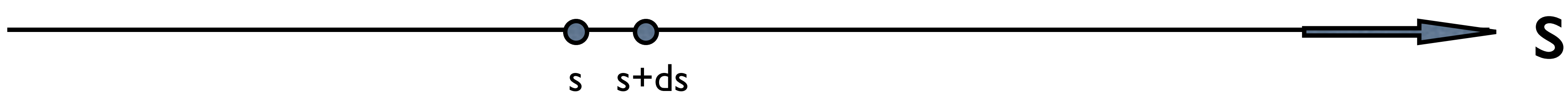


$$\eta_\nu = \frac{h\nu}{4\pi} n_j A_{ji}$$

$$n_j A_{ji} = n_i C_{ij}$$

Emissivity and rates set by local conditions.

Transfer equation



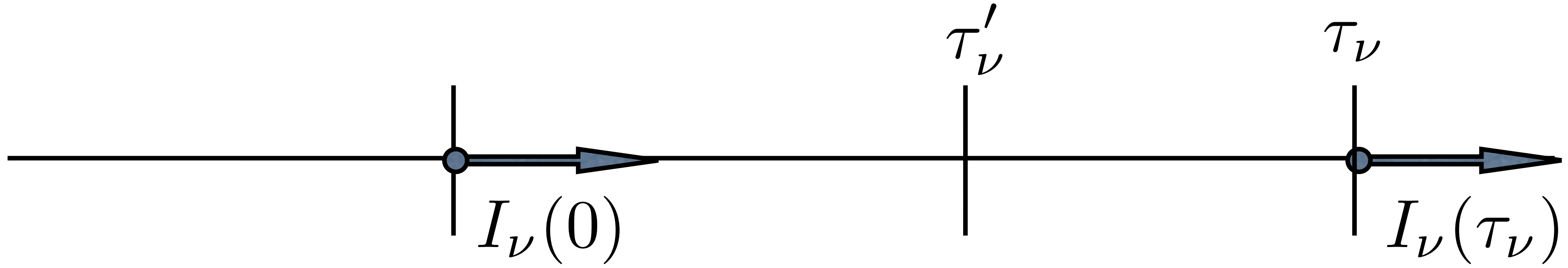
$$dI_\nu = -\chi_\nu I_\nu ds + \eta_\nu ds$$

Opacity non-zero case

$$d\tau_\nu \equiv \chi_\nu ds \quad S_\nu \equiv \frac{\eta_\nu}{\chi_\nu}$$

$$\frac{dI_\nu}{d\tau_\nu} = S_\nu - I_\nu$$

Transfer equation



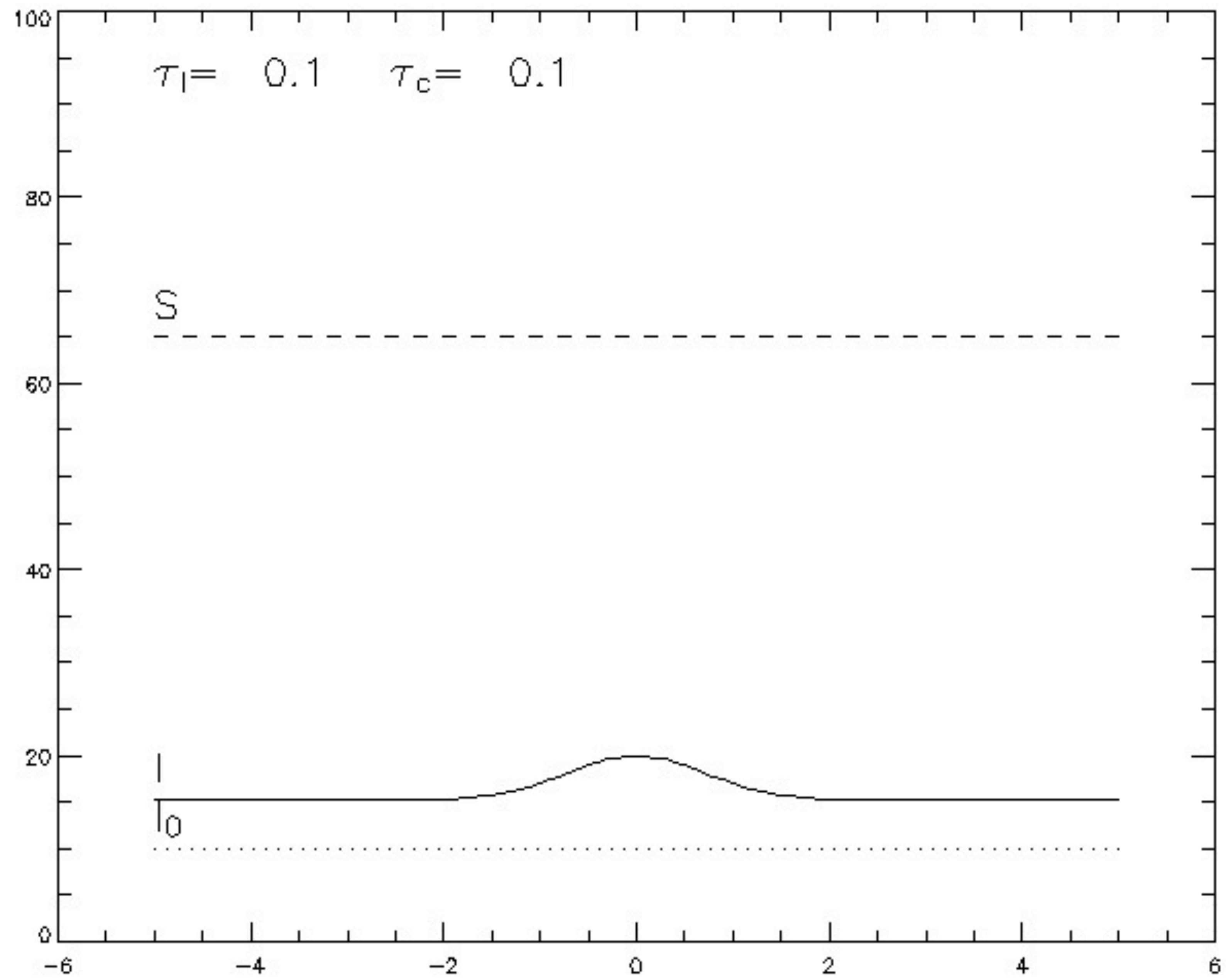
$$I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau_\nu} S_\nu(\tau'_\nu)e^{-(\tau_\nu - \tau'_\nu)}d\tau'_\nu$$

Homogeneous slab, small optical depth:

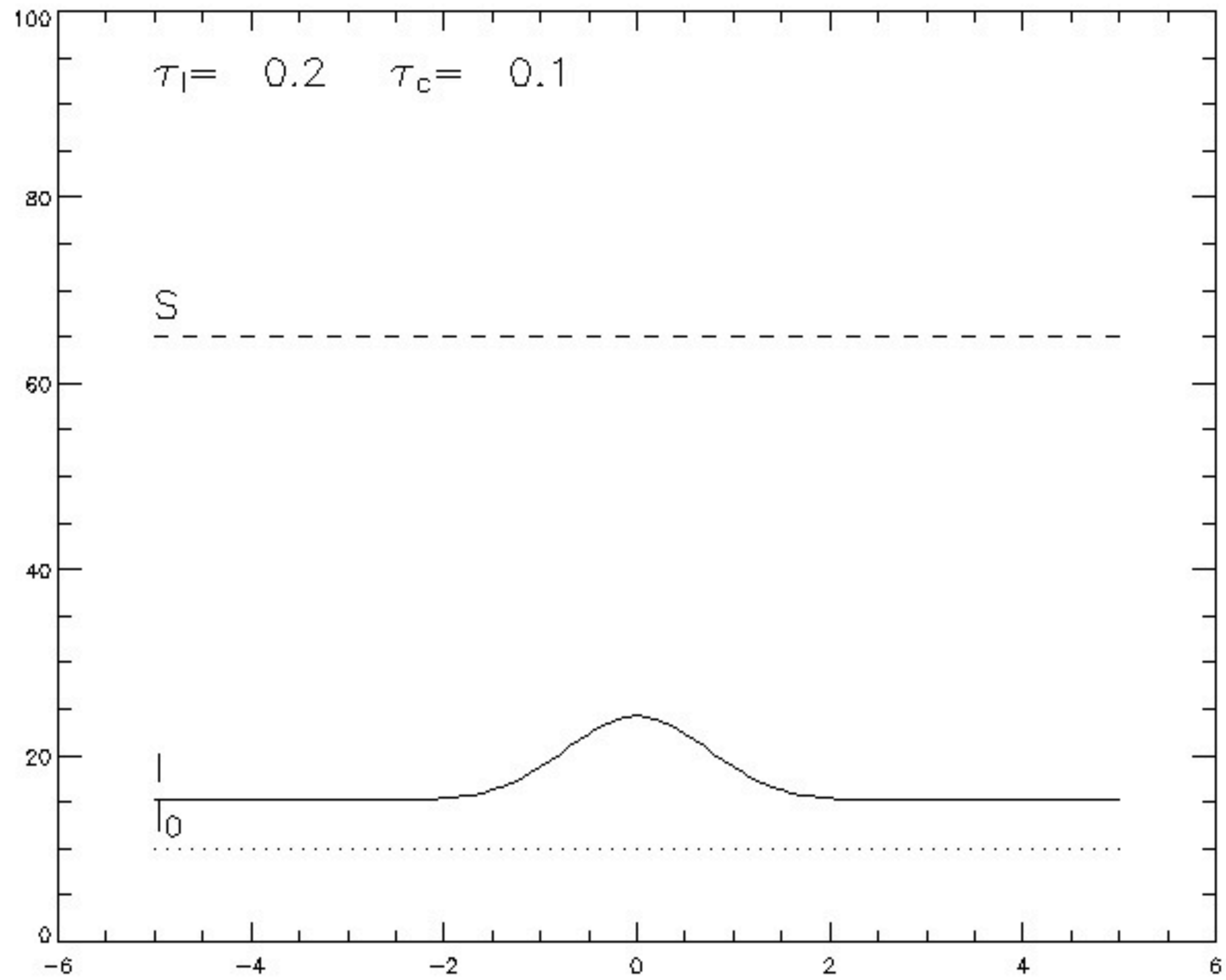
$$I_\nu(\tau_\nu) = I_\nu(0) + \tau_\nu(S_\nu - I_\nu(0))$$

Intensity (wavelength dependent!) is then an interpolation between the incoming intensity and the source function and thus always between the two. For I(0)>S we get an absorption line, for I(0)<S we get an emission line.

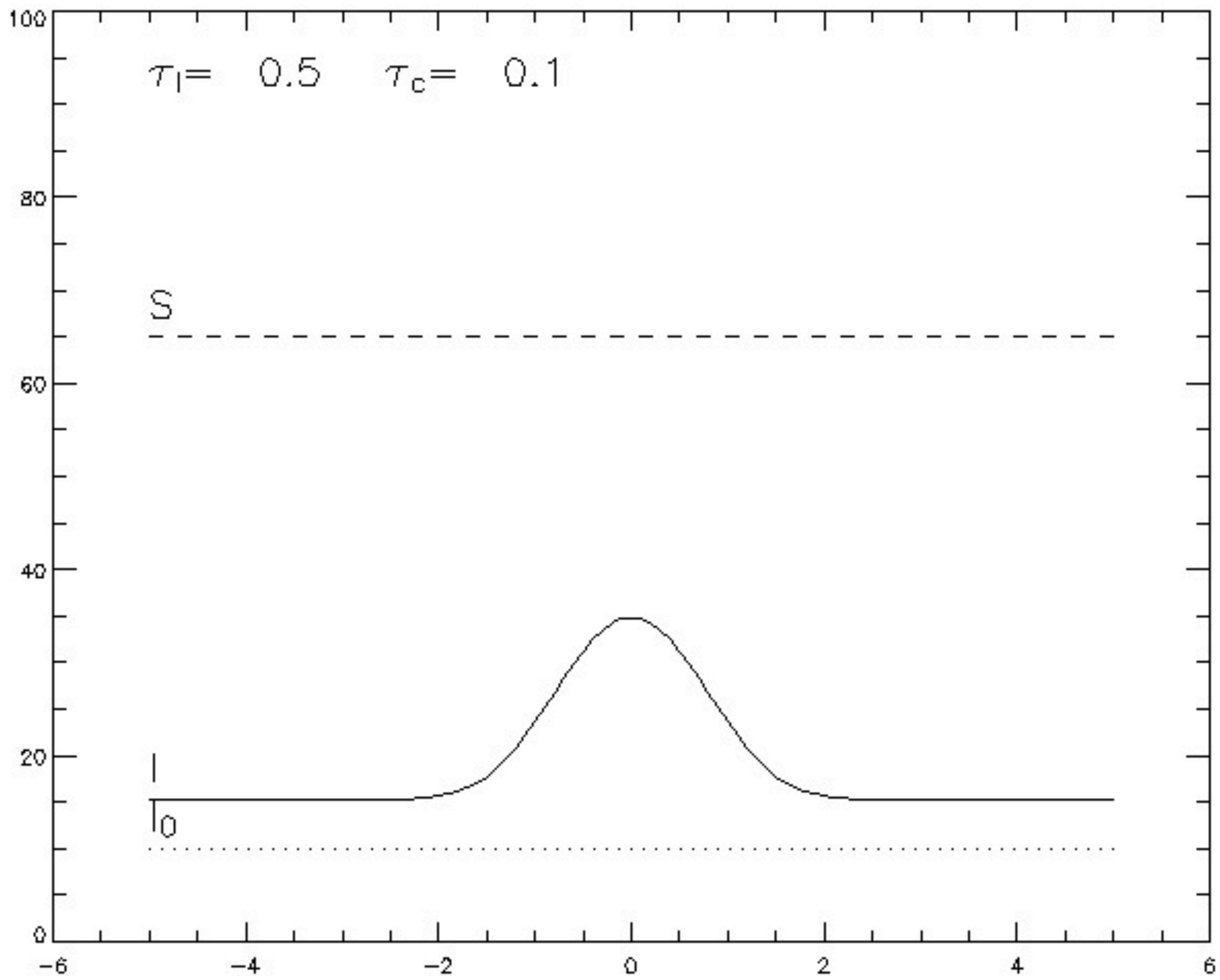
Homogeneous slab



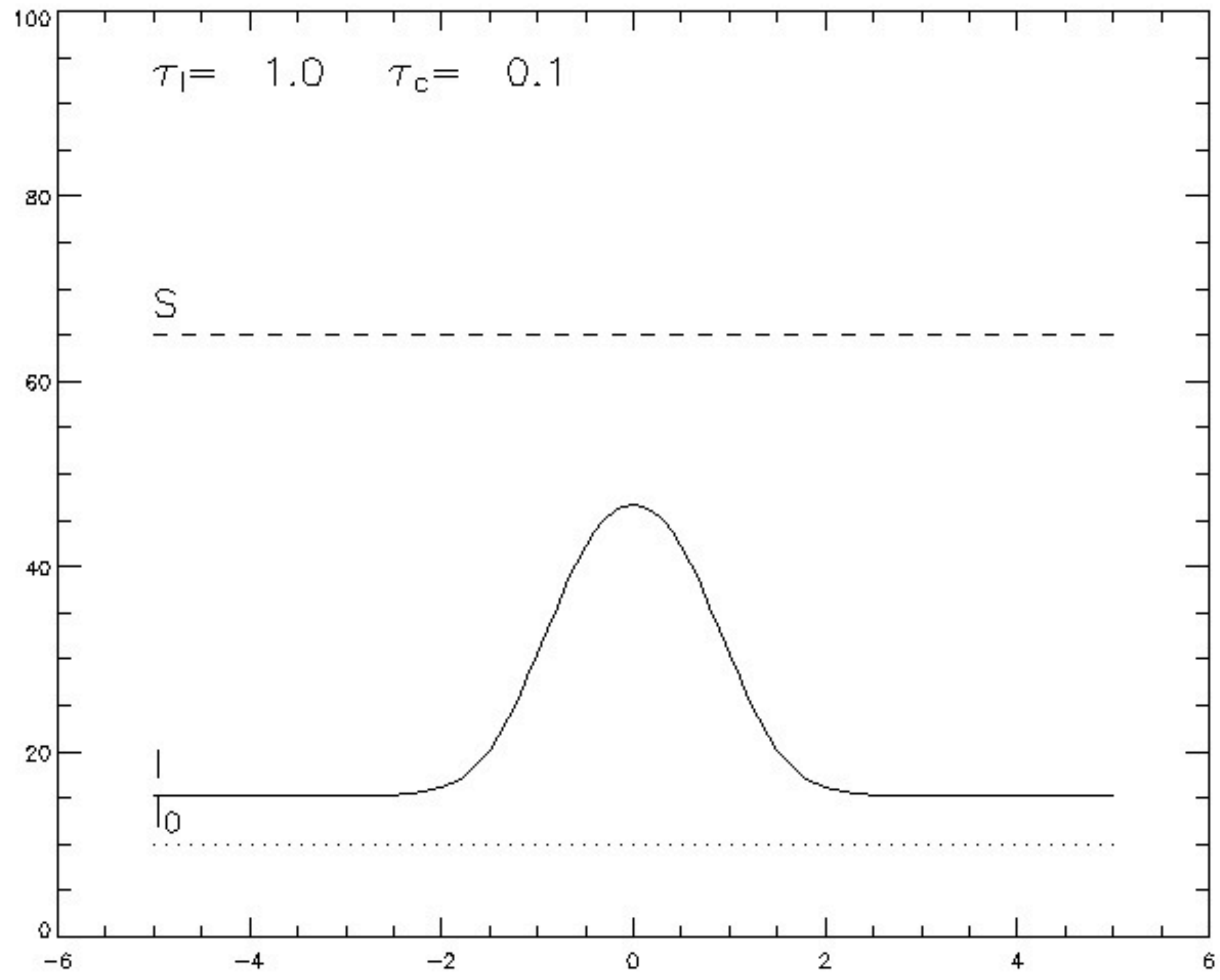
Homogeneous slab



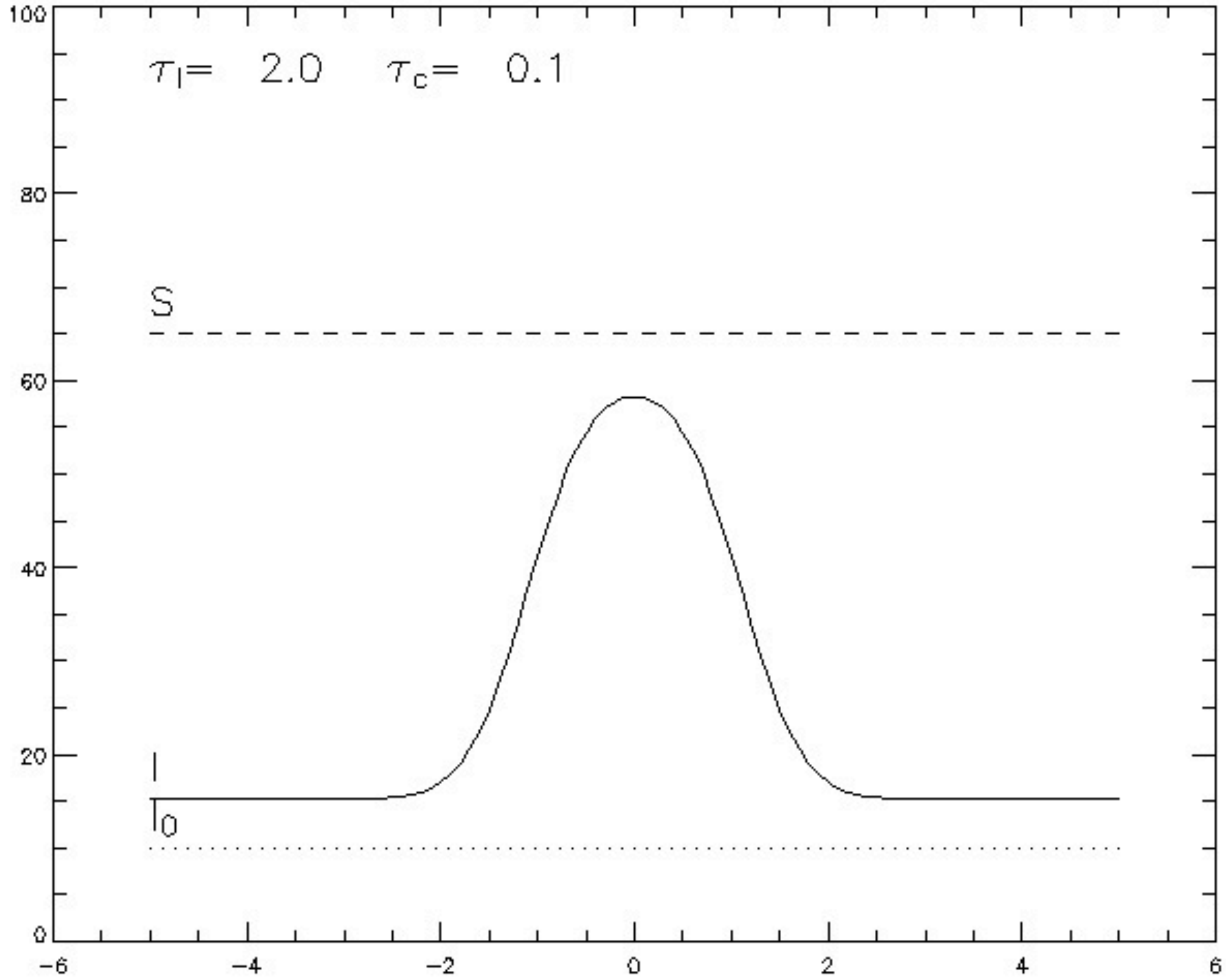
Homogeneous slab



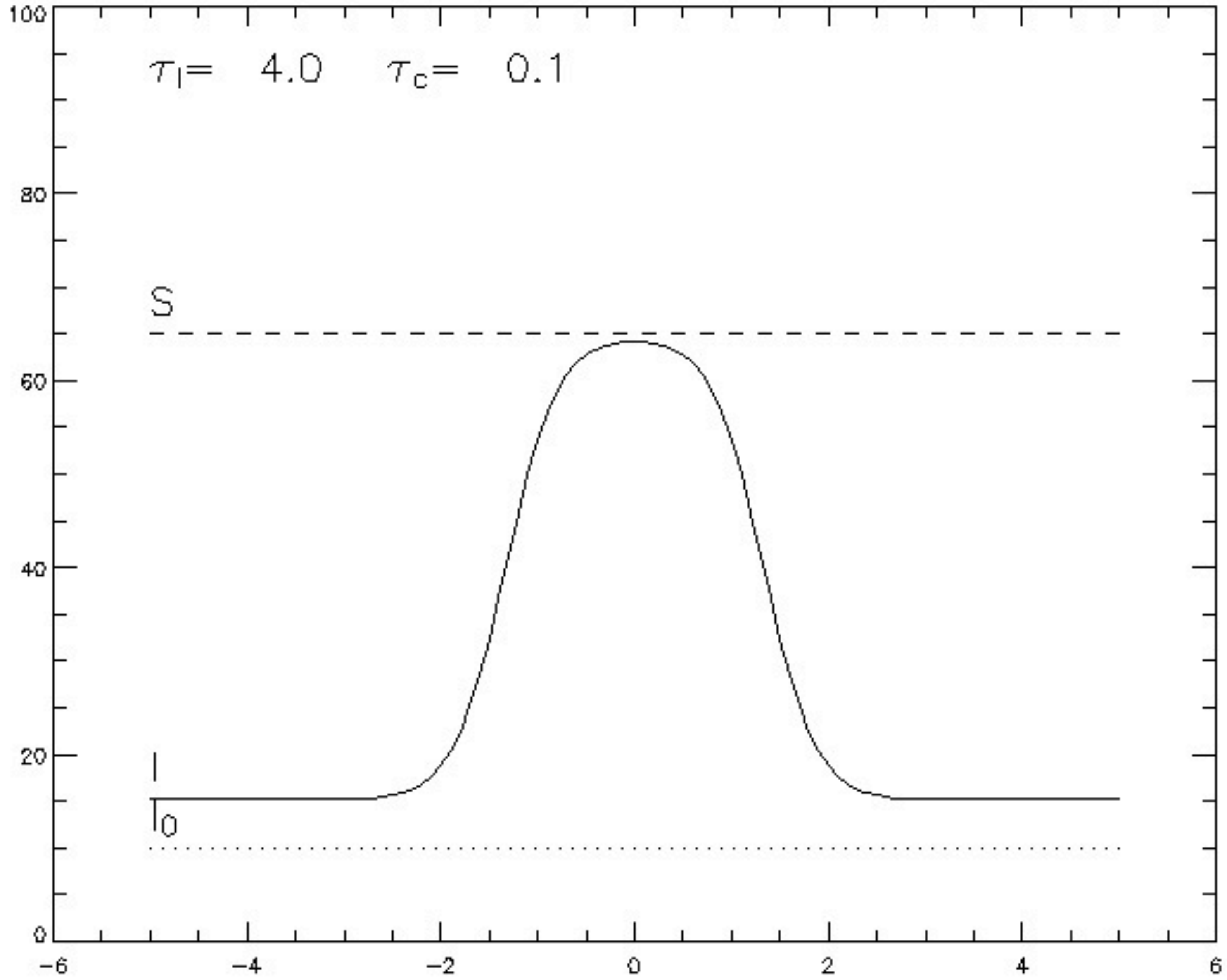
Homogeneous slab



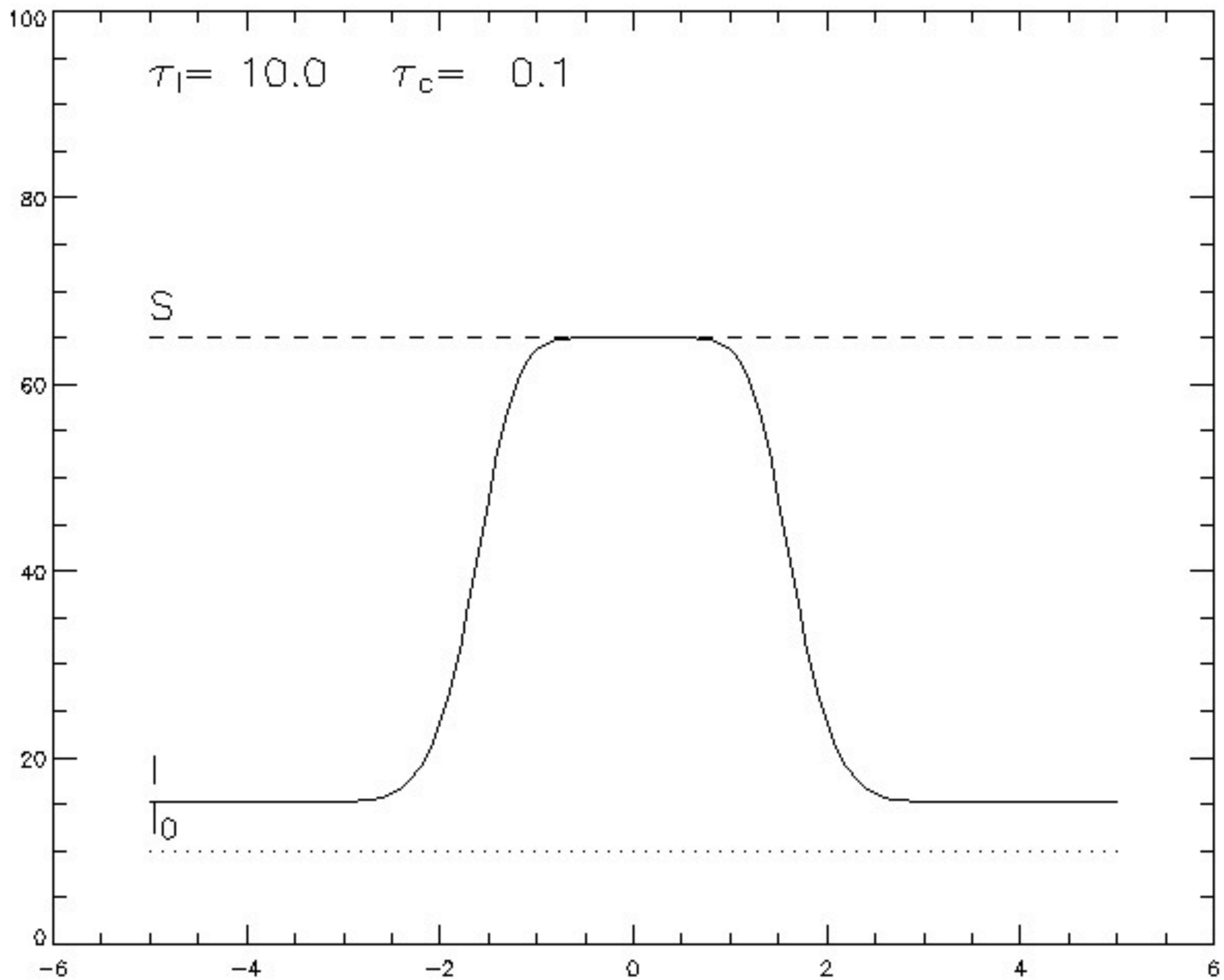
Homogeneous slab



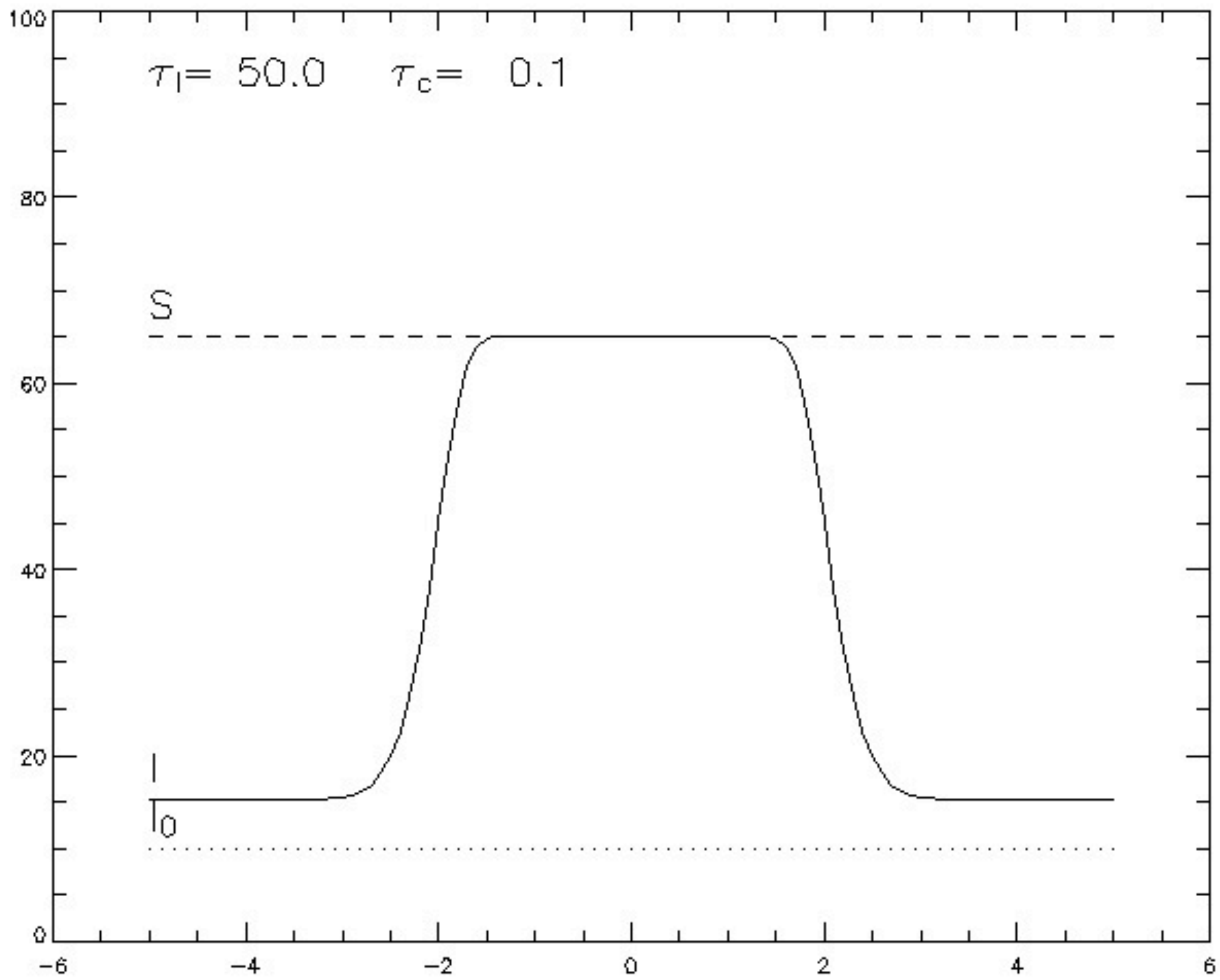
Homogeneous slab



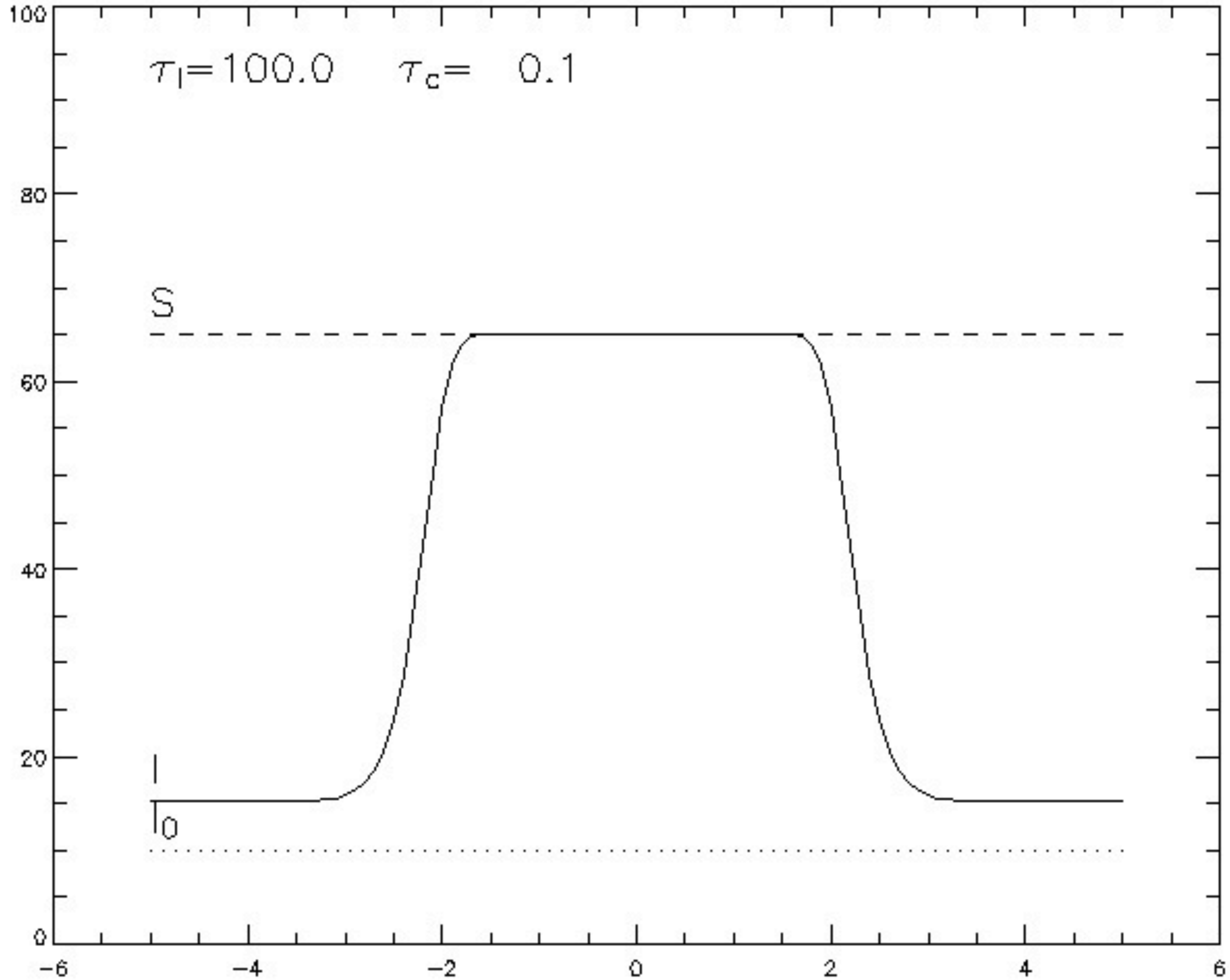
Homogeneous slab



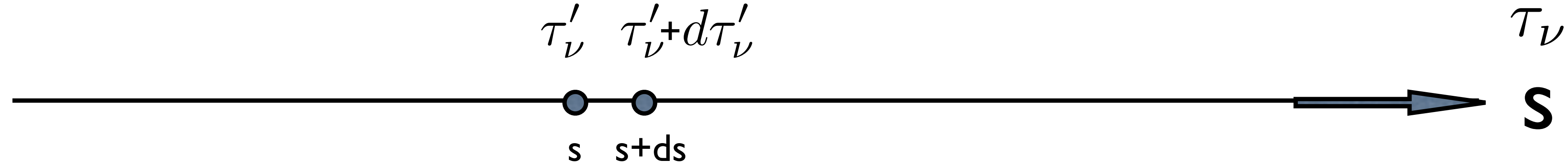
Homogeneous slab



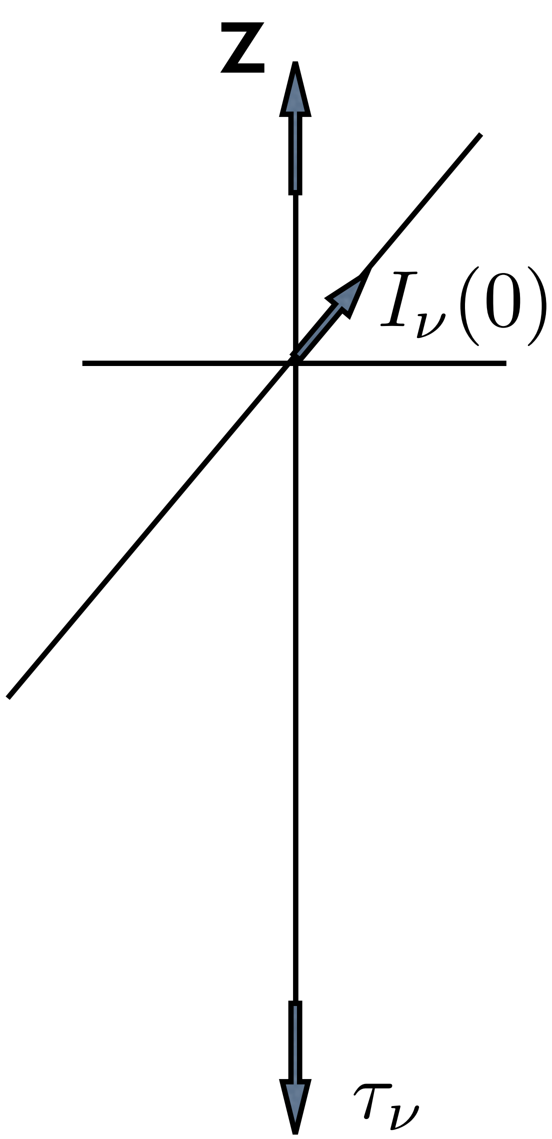
Homogeneous slab



Transfer equation



$$I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau_\nu} S_\nu(\tau'_\nu)e^{-(\tau_\nu - \tau'_\nu)}d\tau'_\nu$$



Semi-infinite atmosphere, 1D:

$$I_\nu(0) = \frac{1}{\mu}\int_0^{\infty} S_\nu(\tau'_\nu)e^{-\tau'_\nu/\mu}d\tau'_\nu$$

where mu is the cosine of the angle between the ray and the normal of the atmosphere

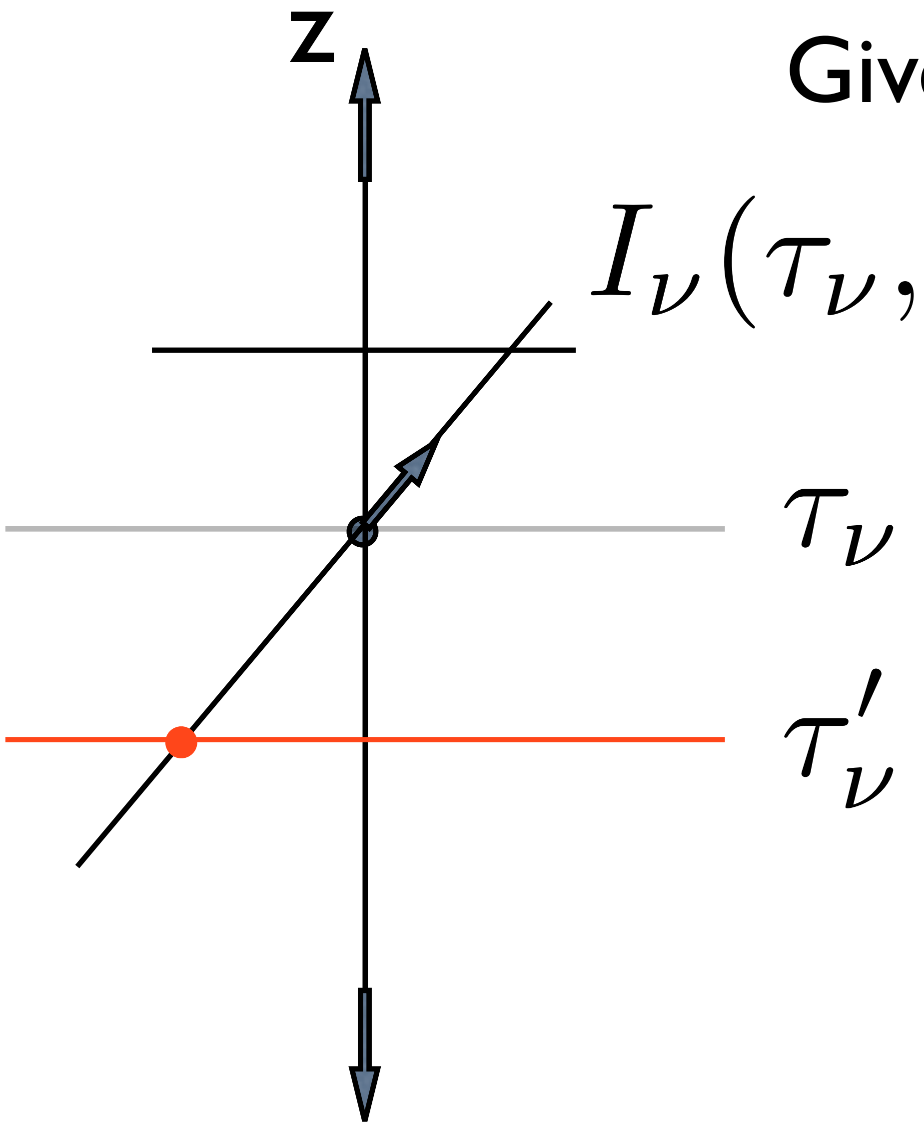
Eddington Barbier relation

Assuming a linear source function:

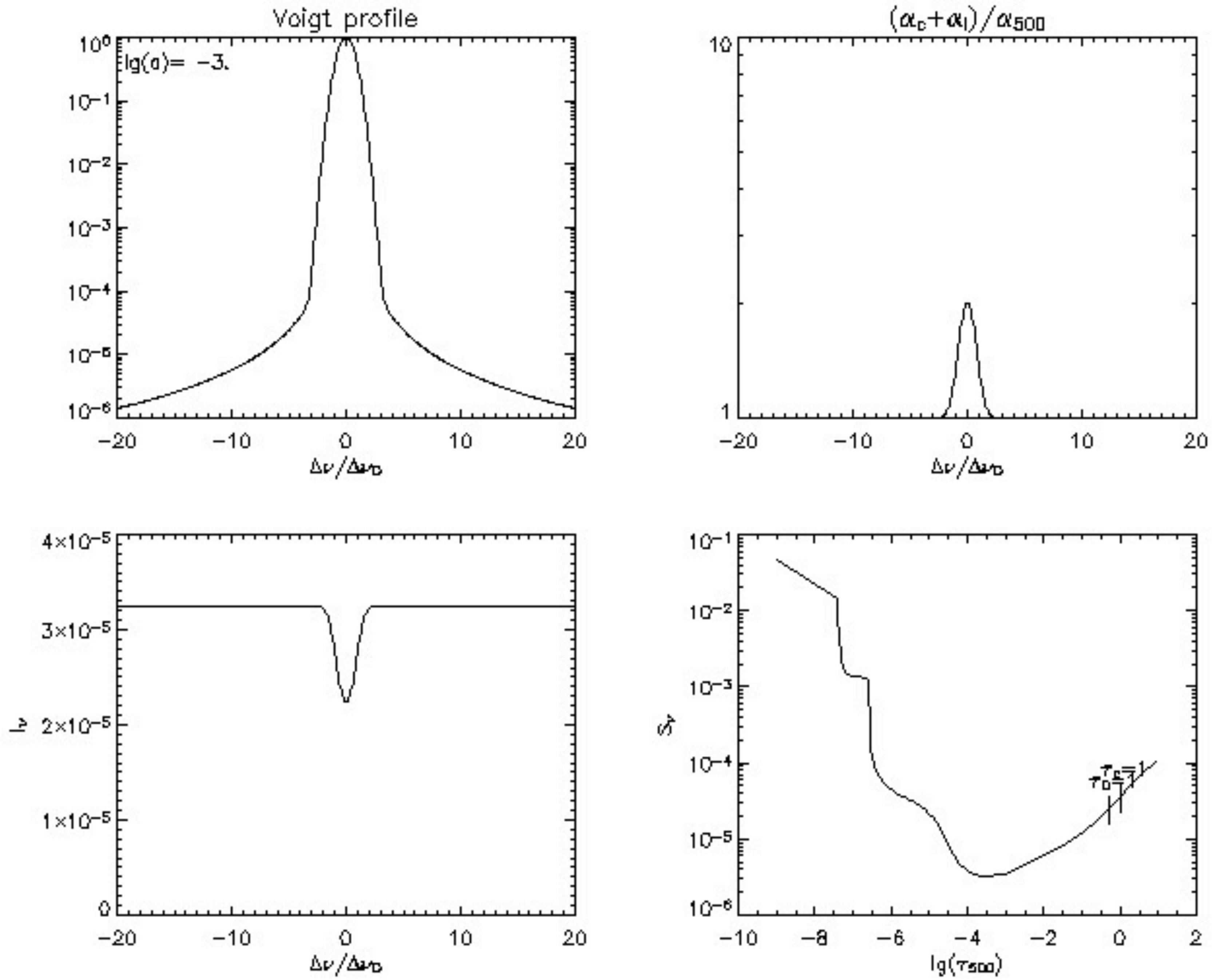
$$S_\nu(\tau'_\nu) = a + b\tau'_\nu$$

Gives a formal solution:

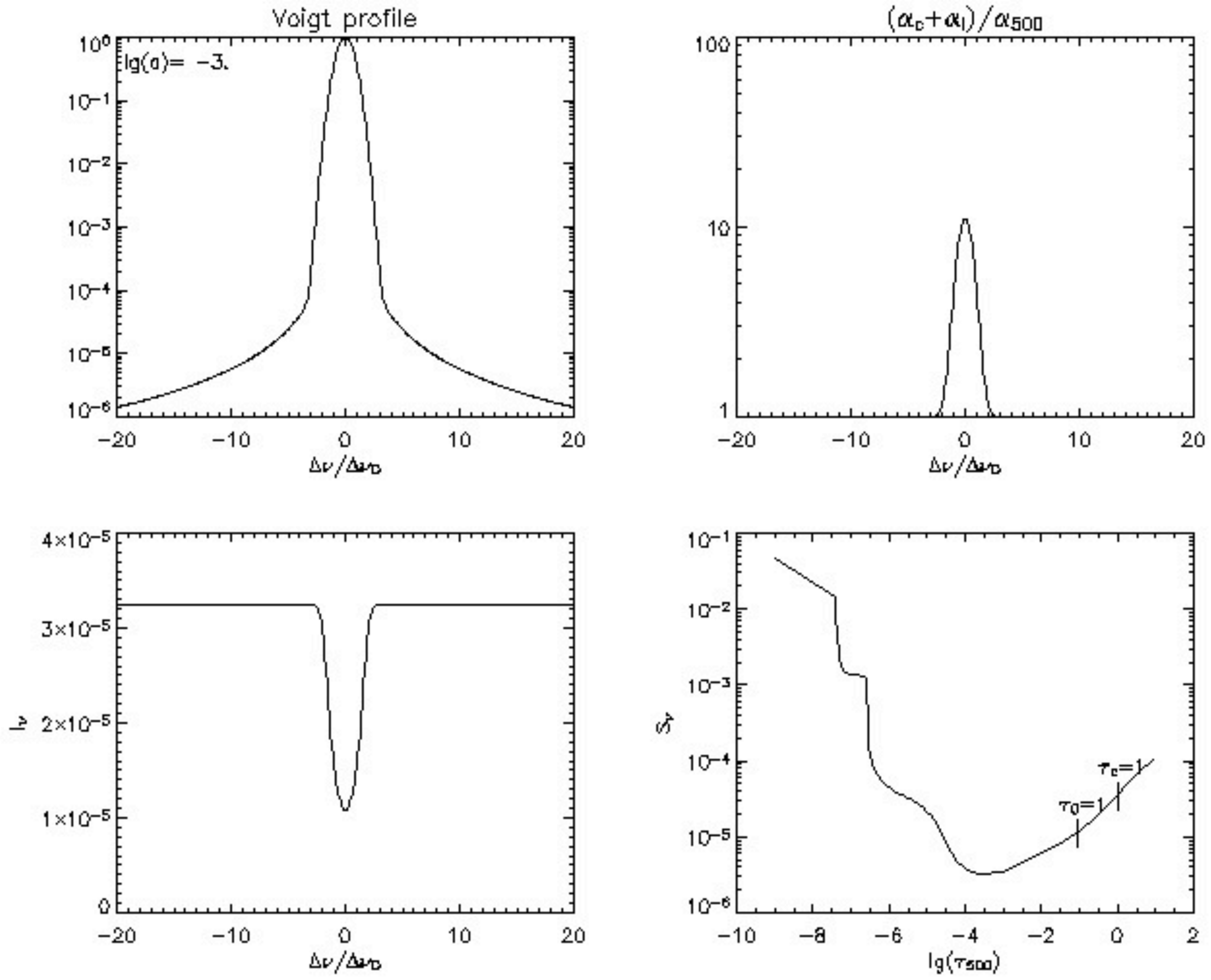
$$I_\nu(\tau_\nu, \mu) = S_\nu(\tau'_\nu = \tau_\nu + \mu)$$



Optically thick line formation 1



Optically thick line formation



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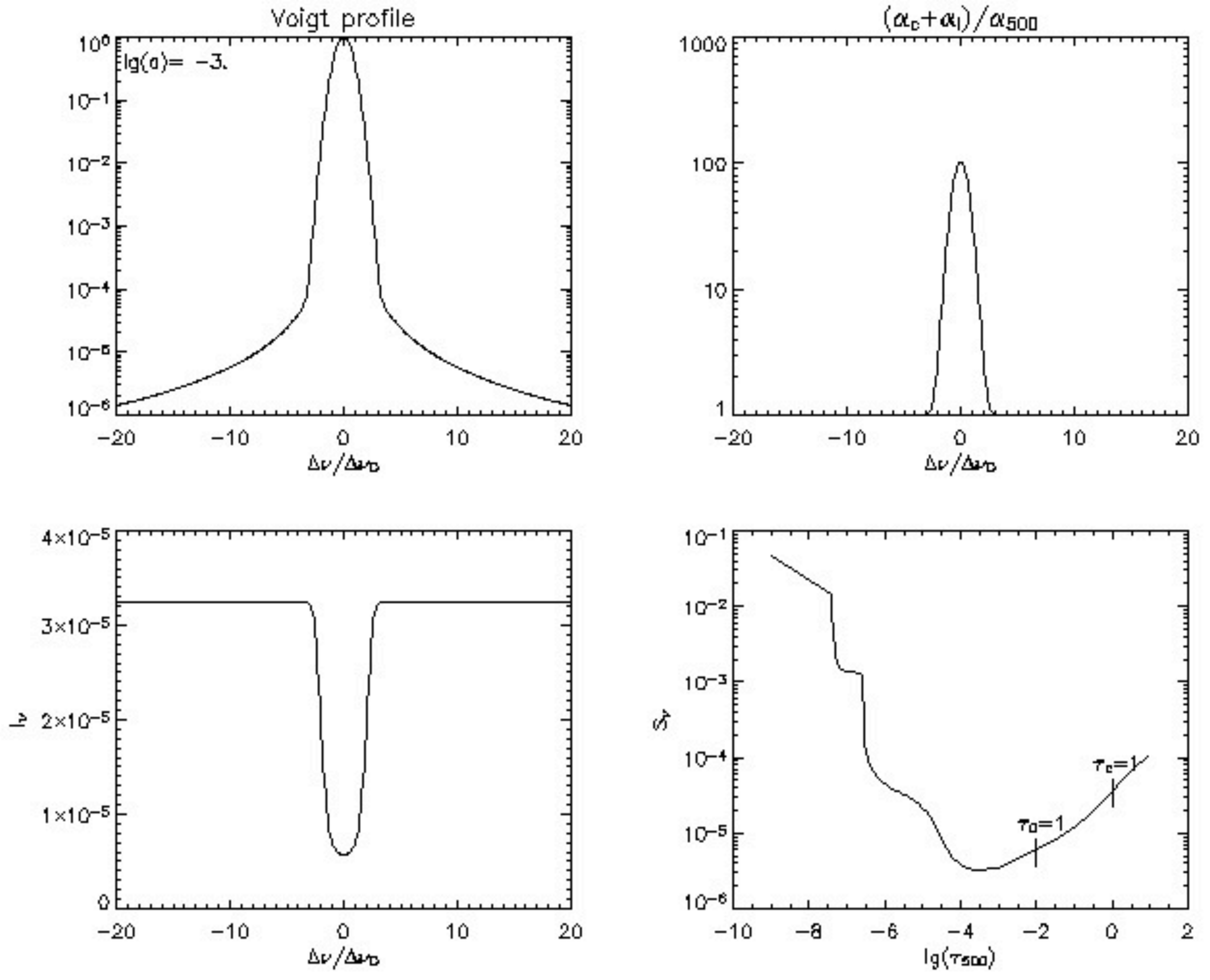

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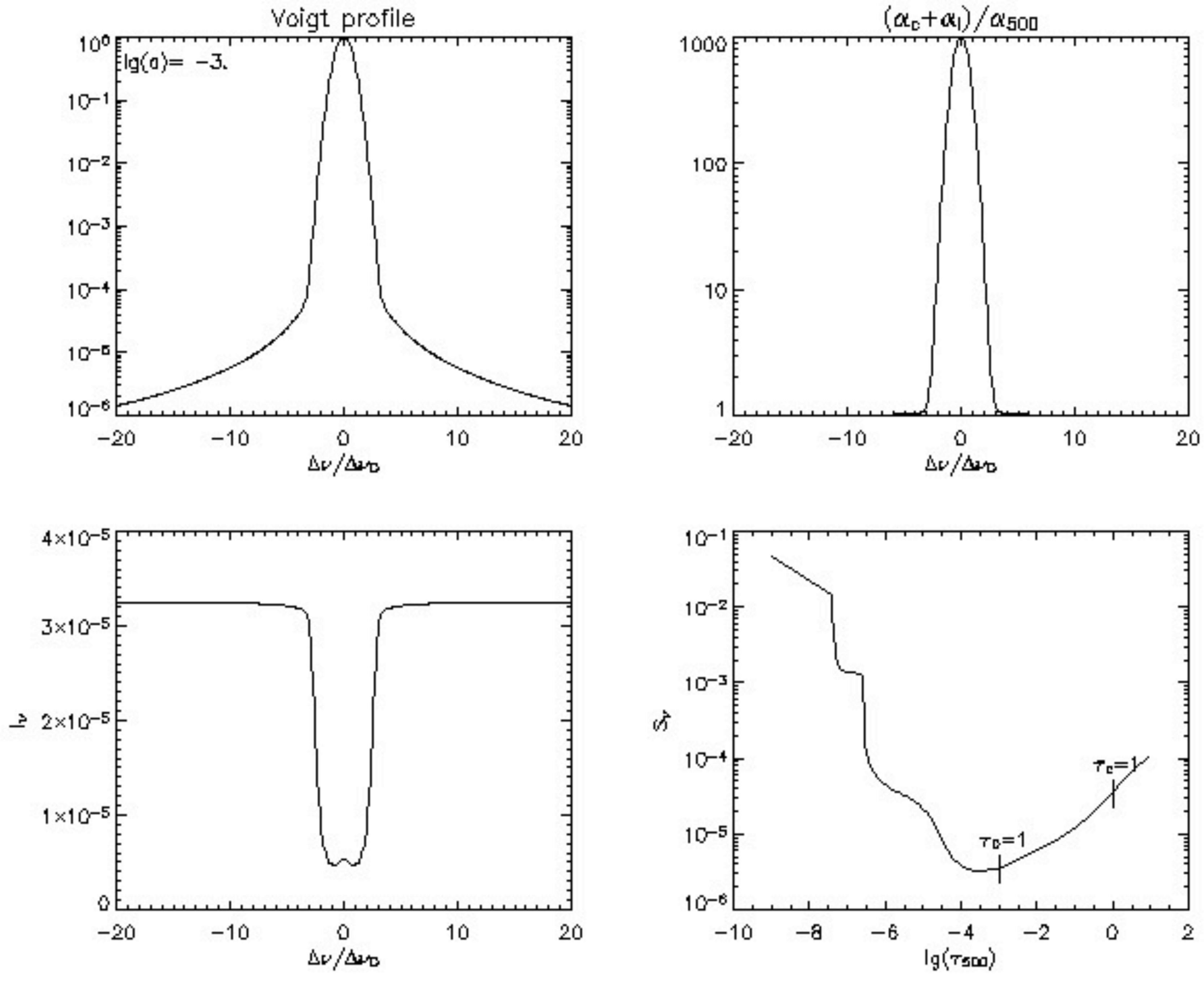

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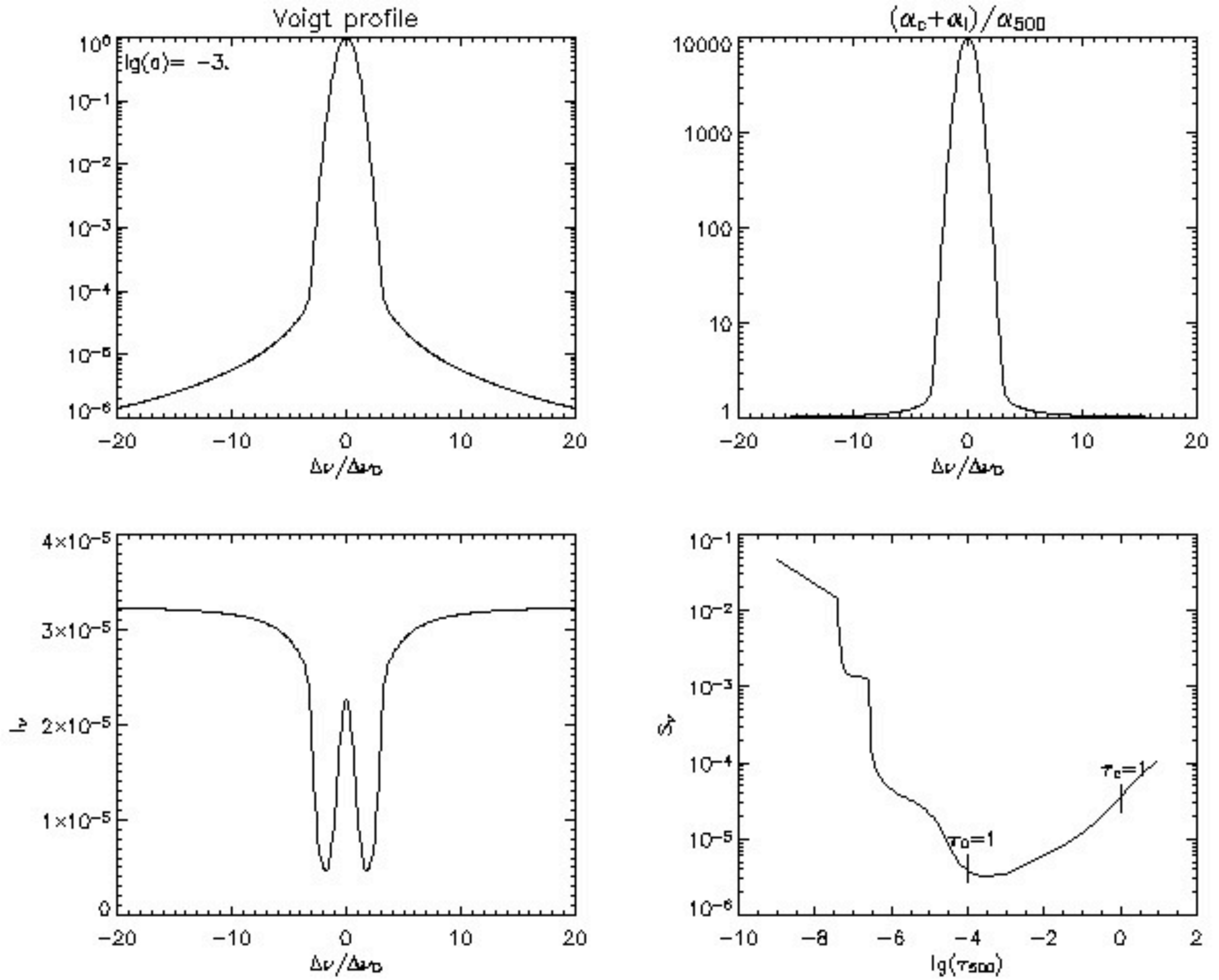
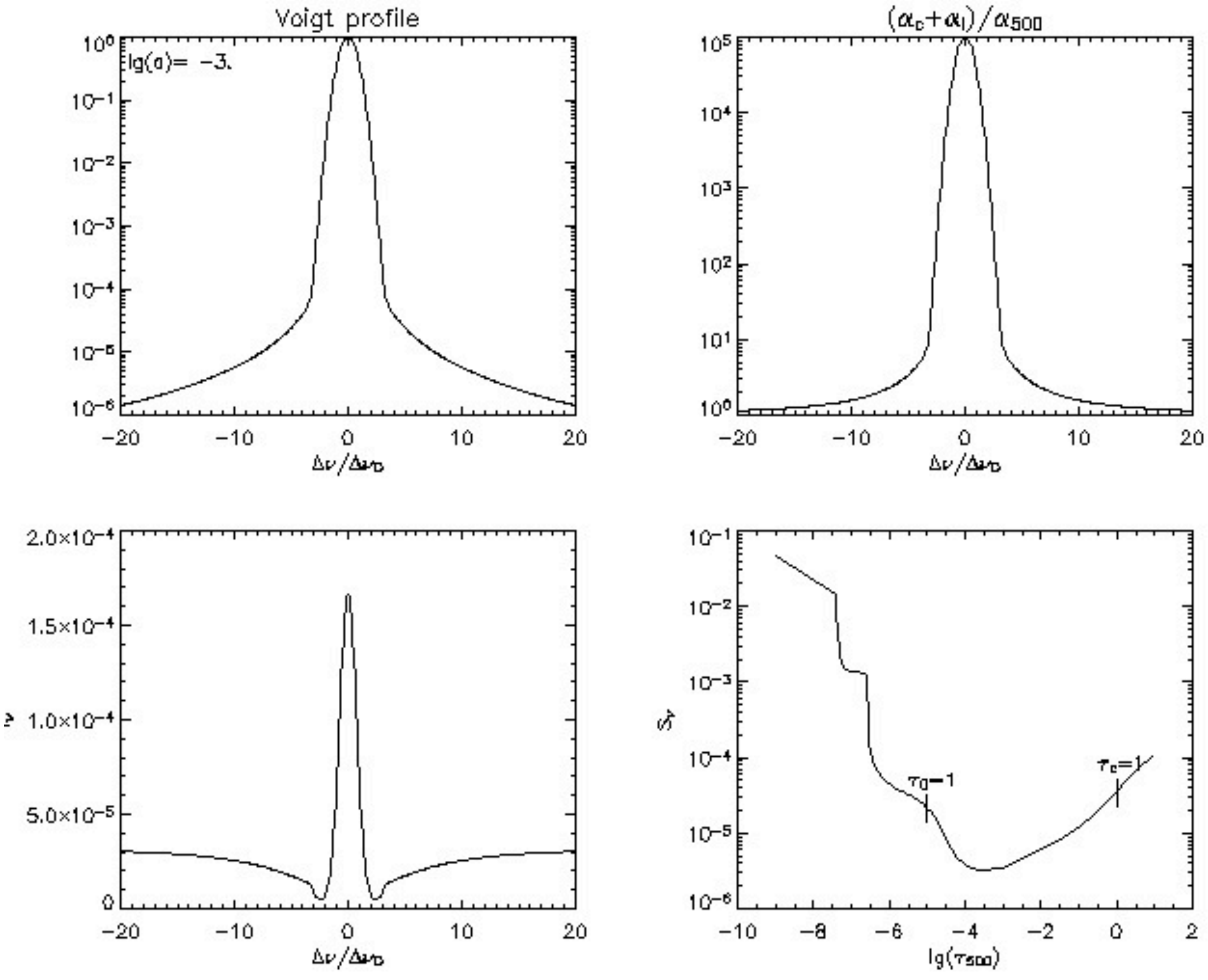
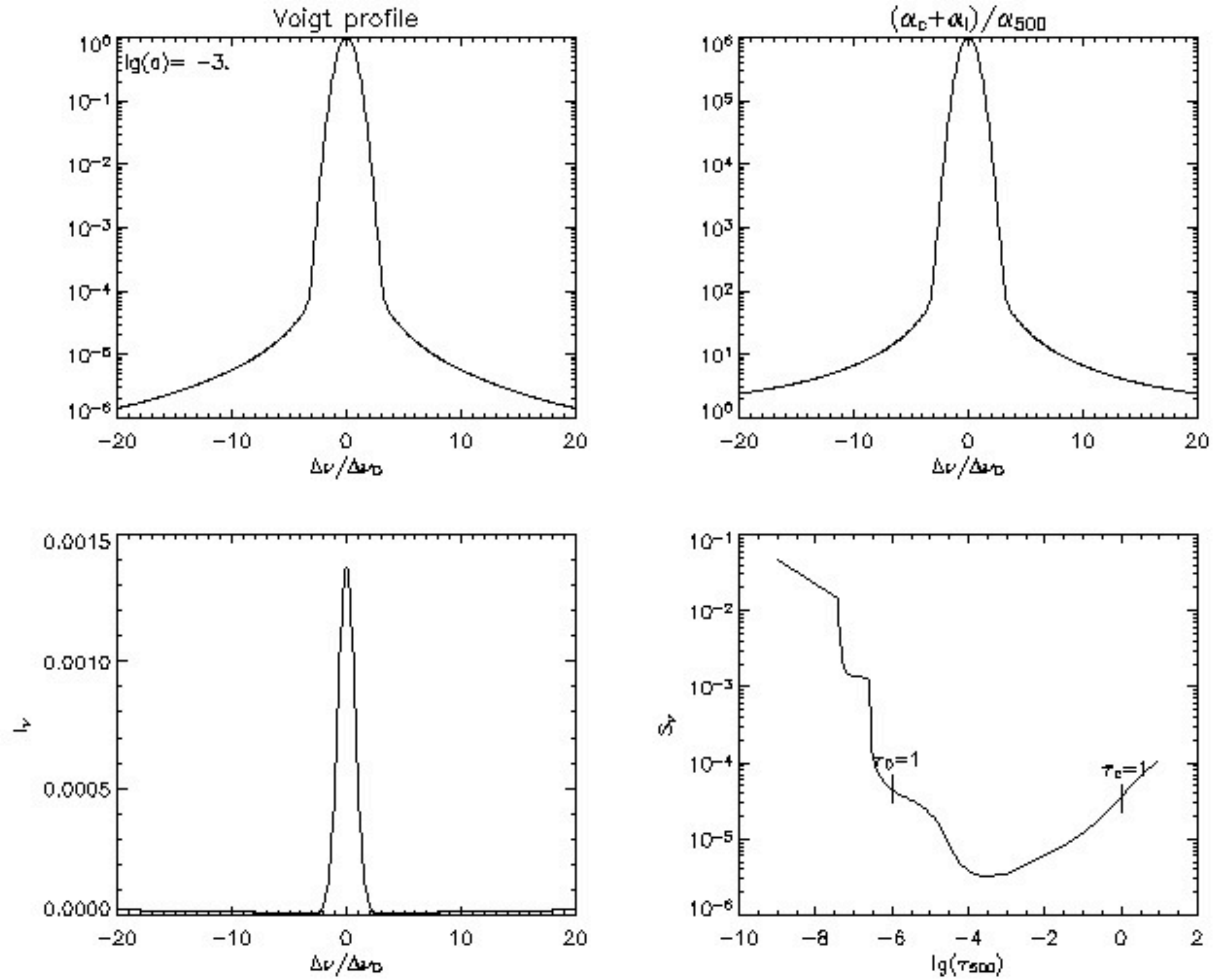


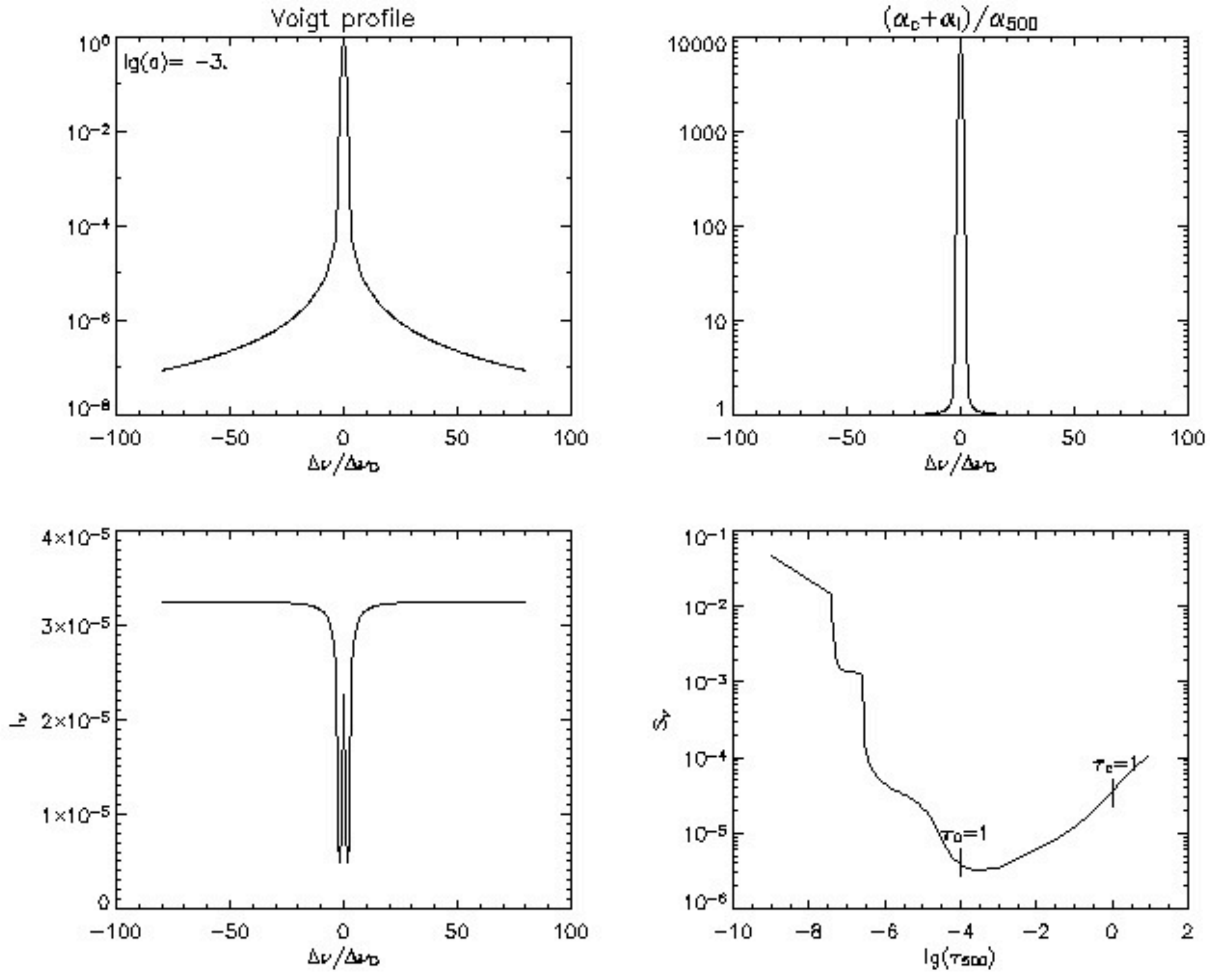
Optically thick line formation



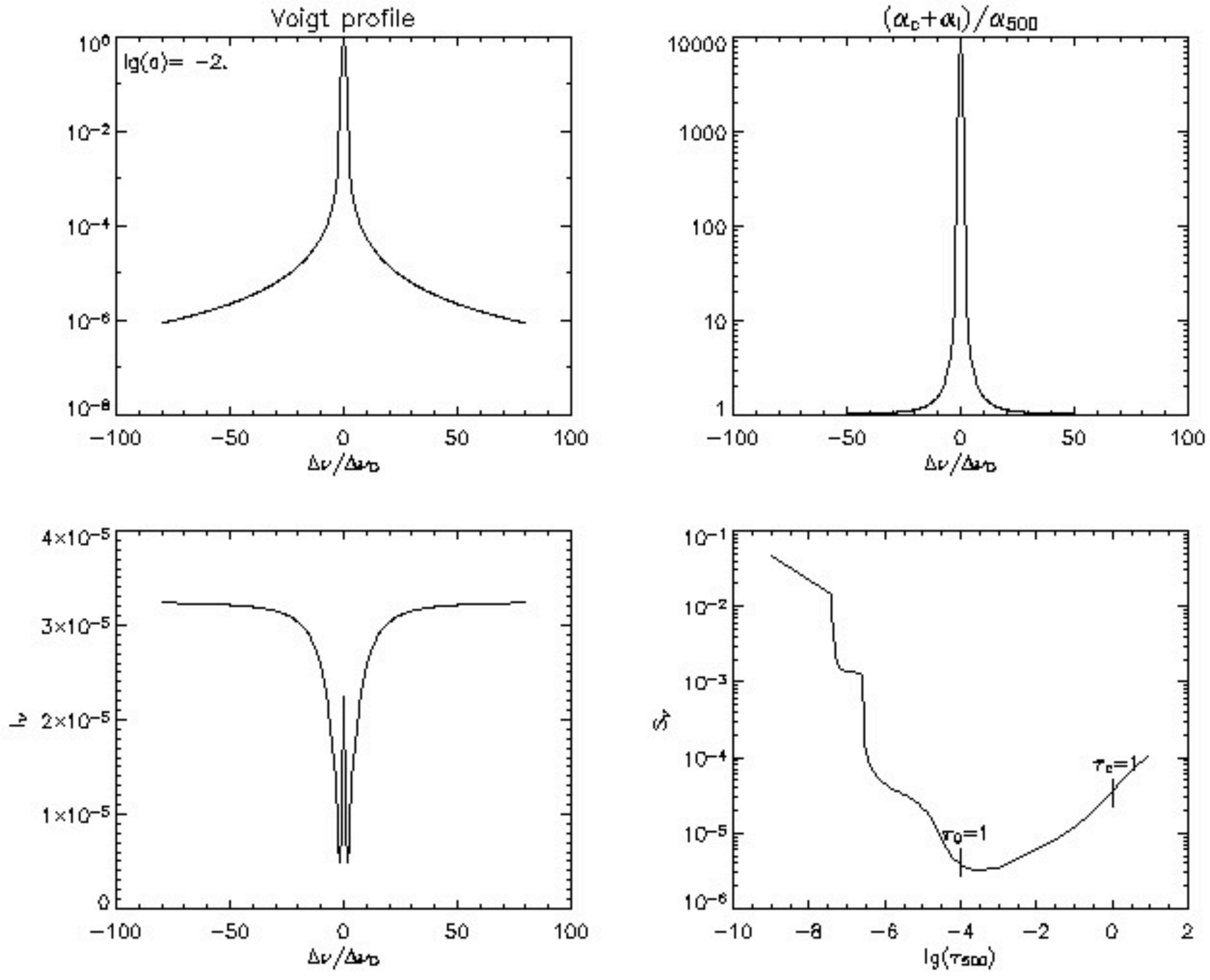
Optically thick line formation



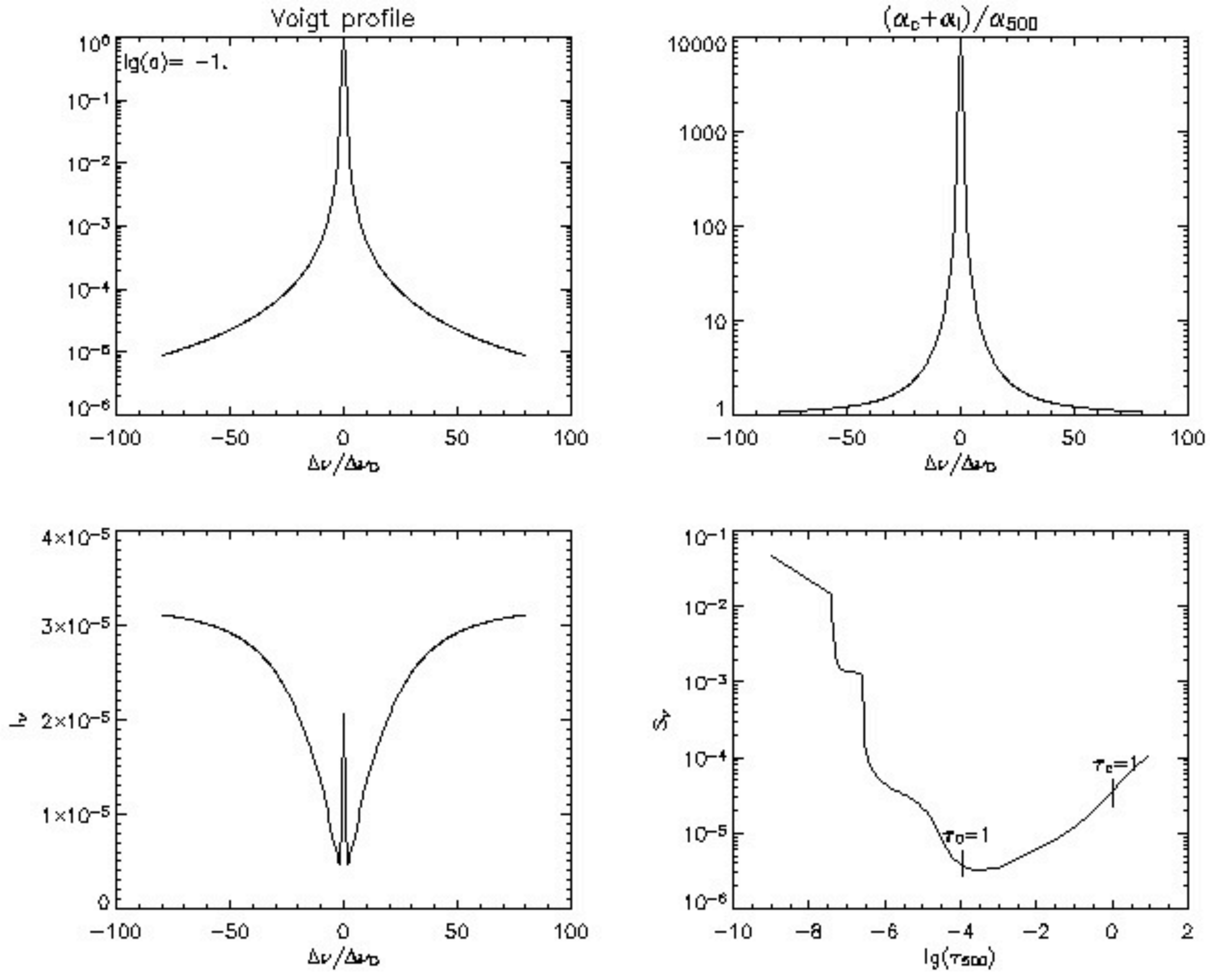
Optically thick line formation 2



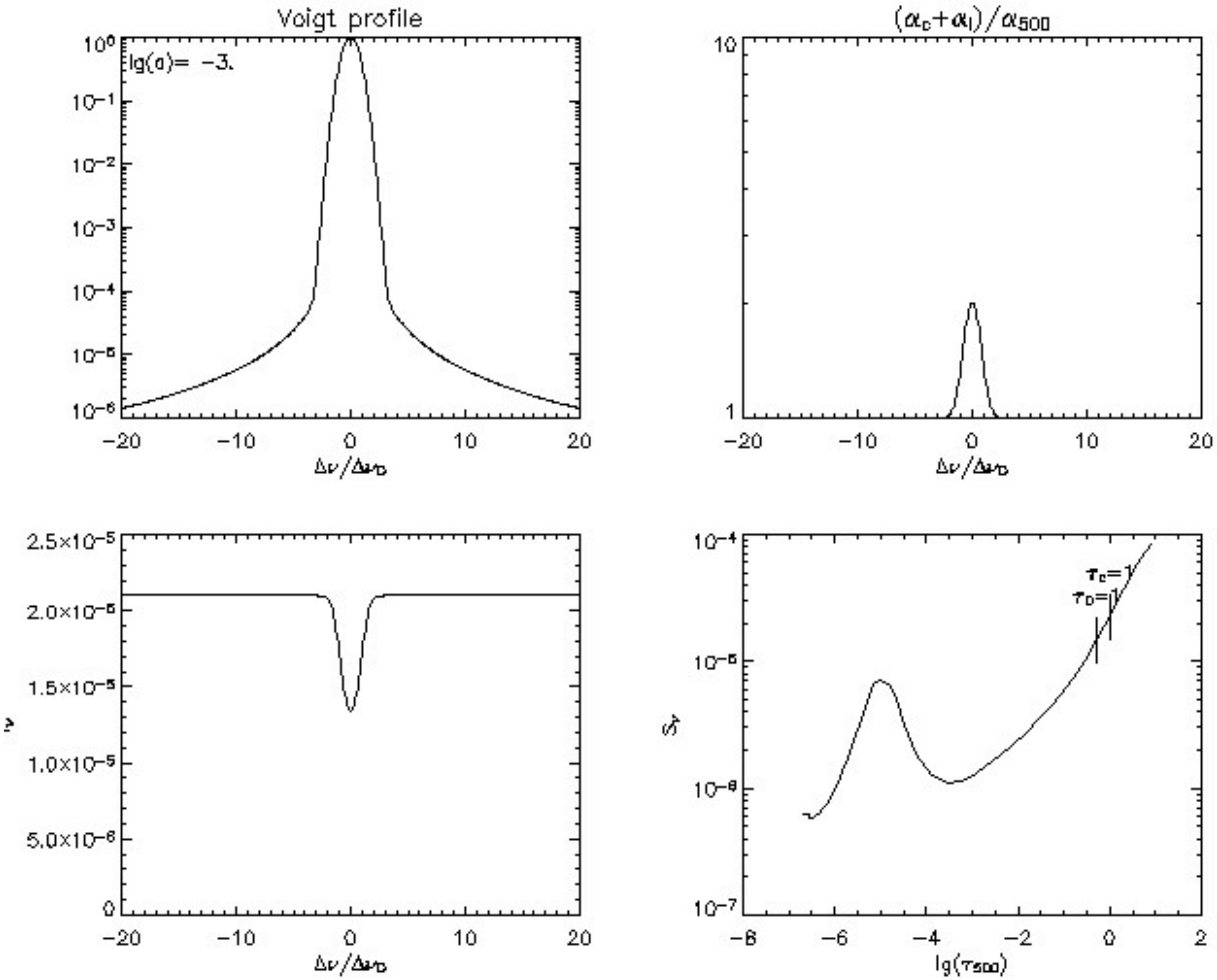
Optically thick line formation



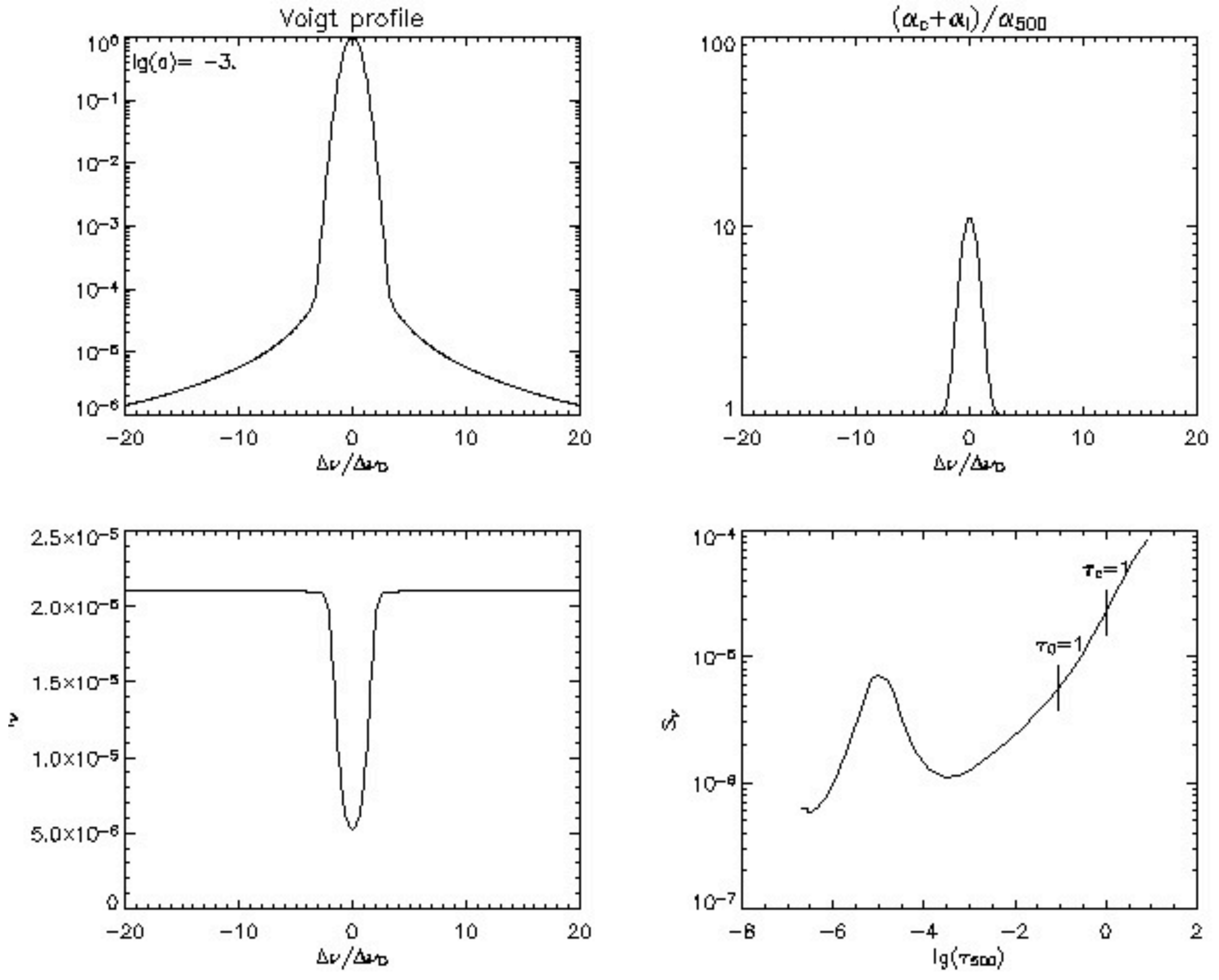
Optically thick line formation



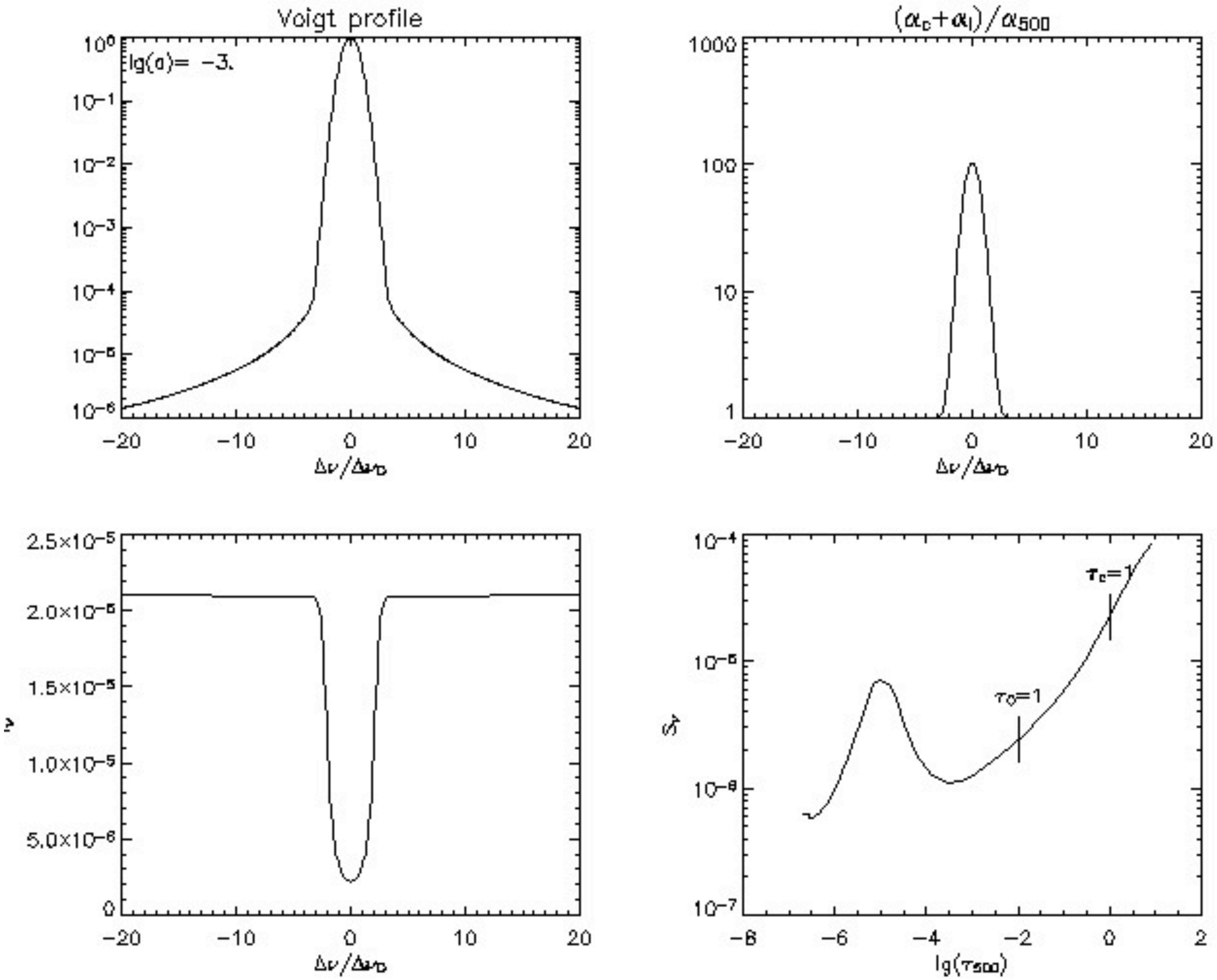
Optically thick line formation 3



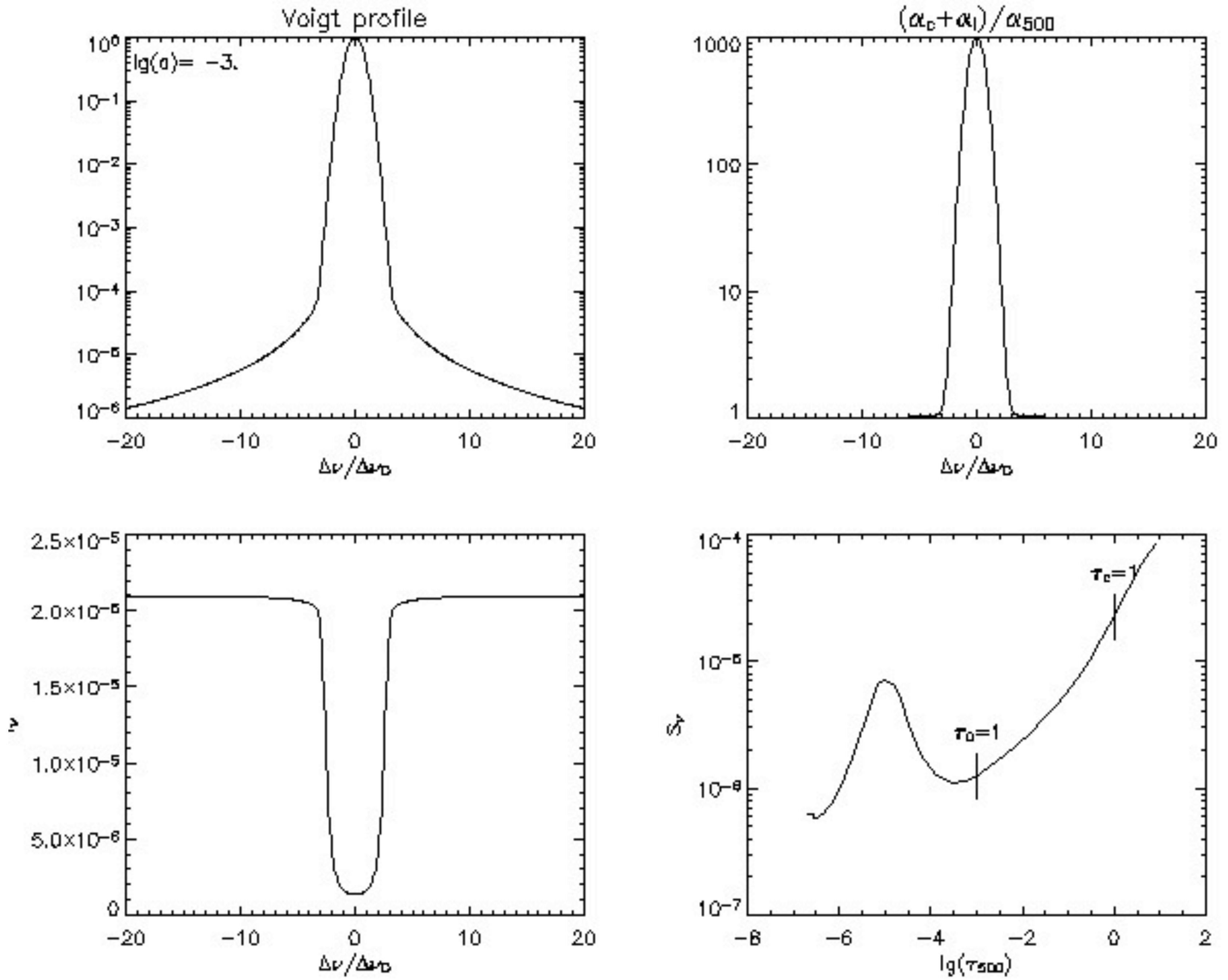
Optically thick line formation



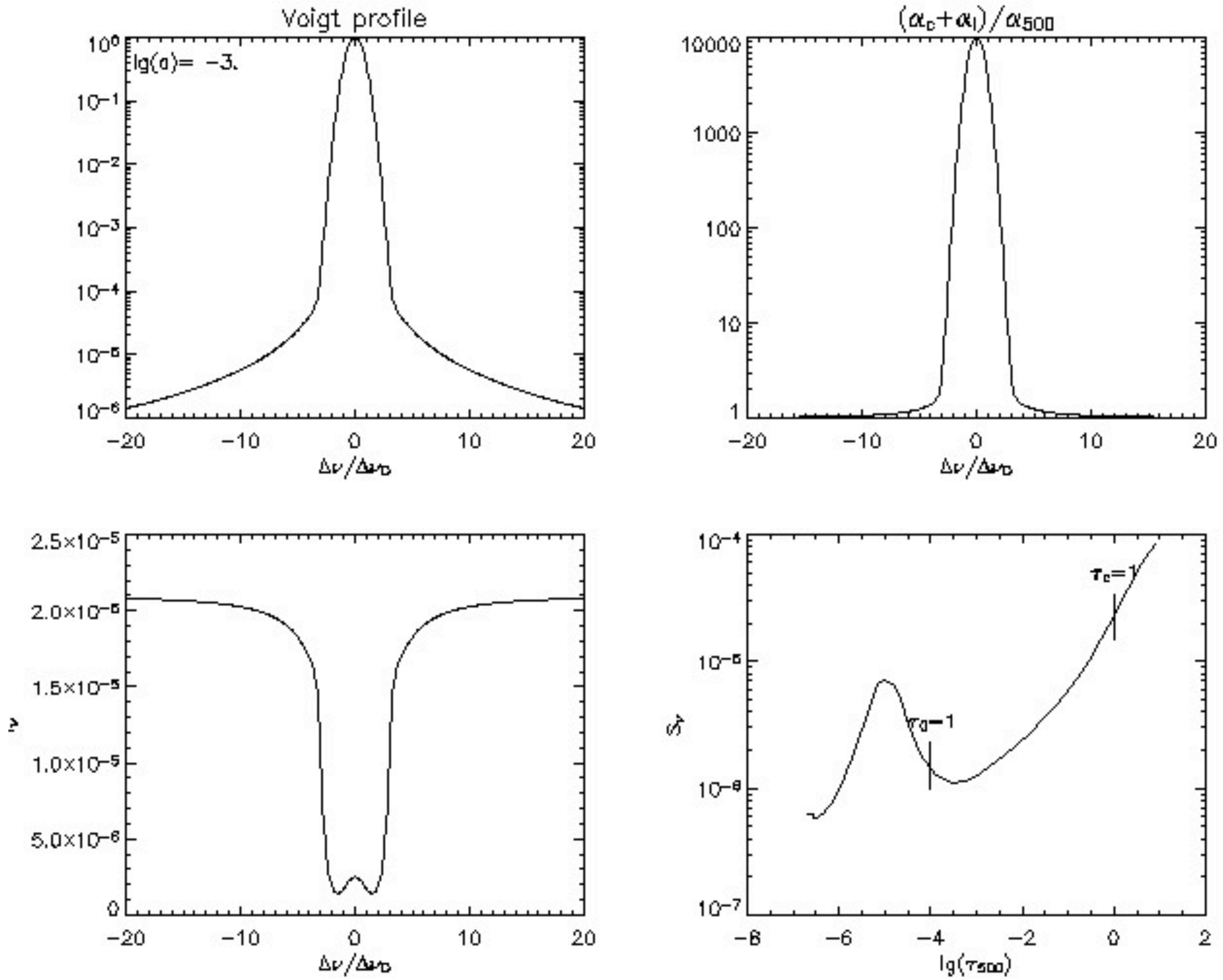
Optically thick line formation

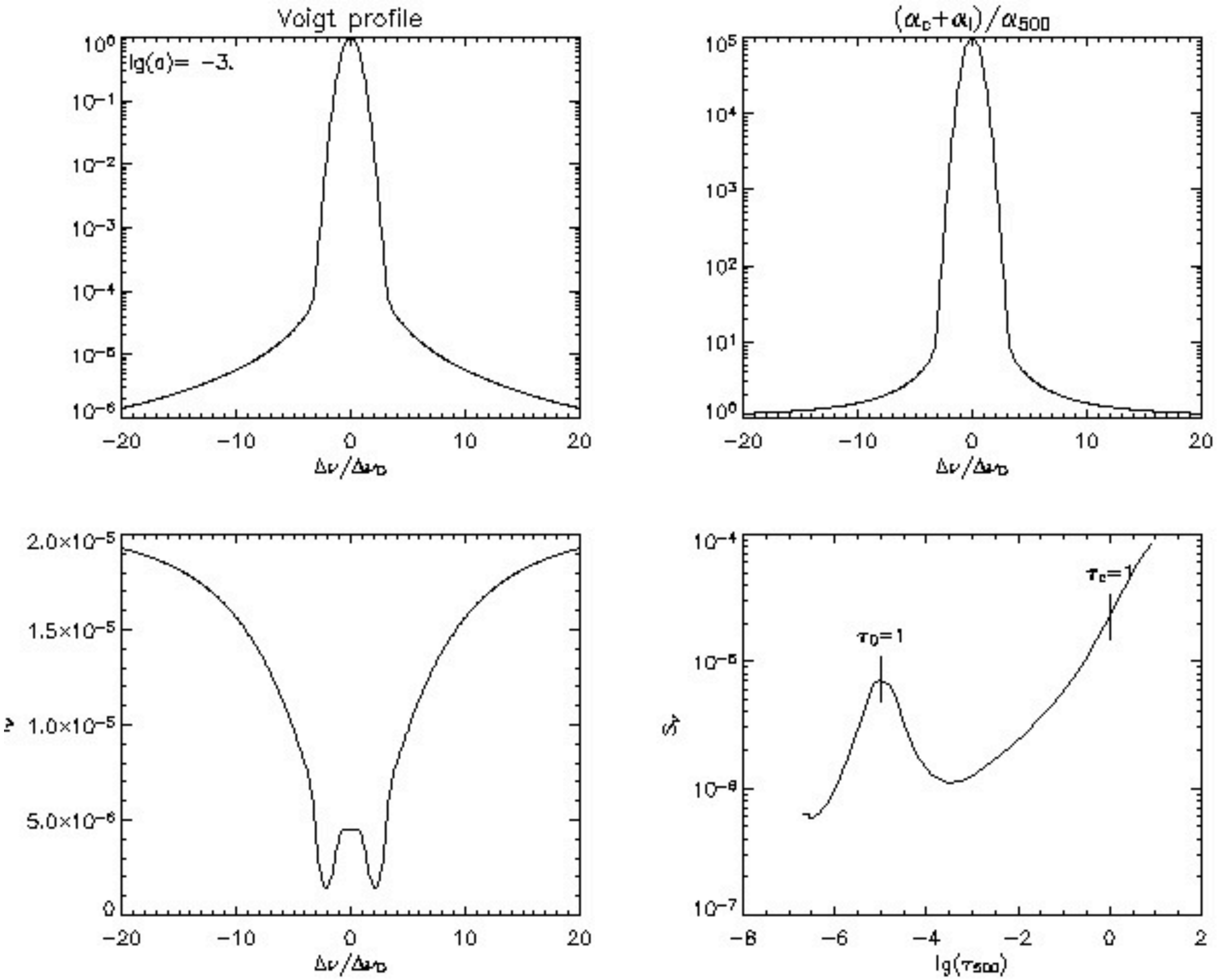


Optically thick line formation

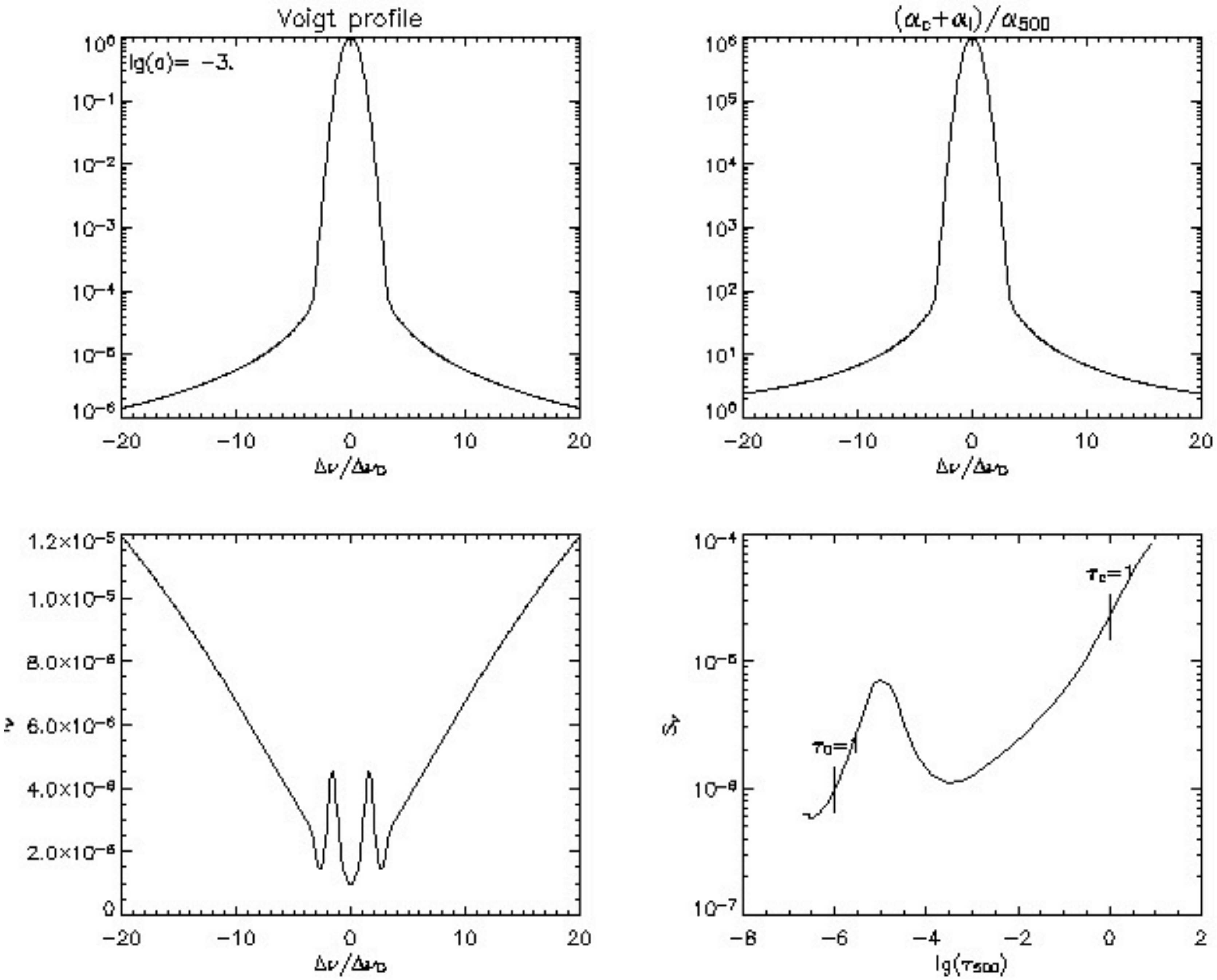


Optically thick line formation





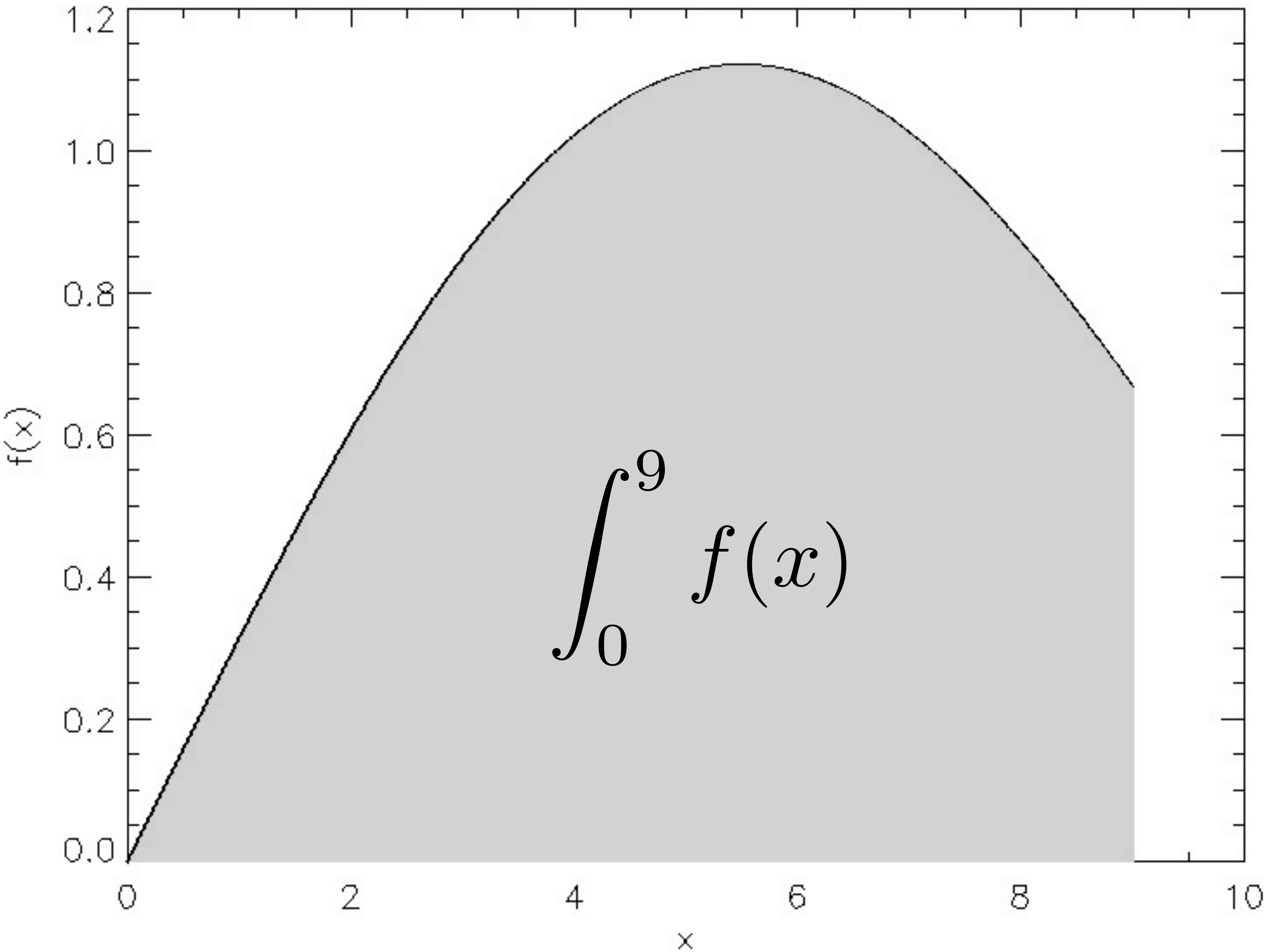
Voigt profile
lg(a)= -3.
Δν/Δν_D
(α_c+α_l)/α_500
Δν/Δν_D
Δν/Δν_D
τ_0=1
τ_c=1
S_ν
lg(τ_500)

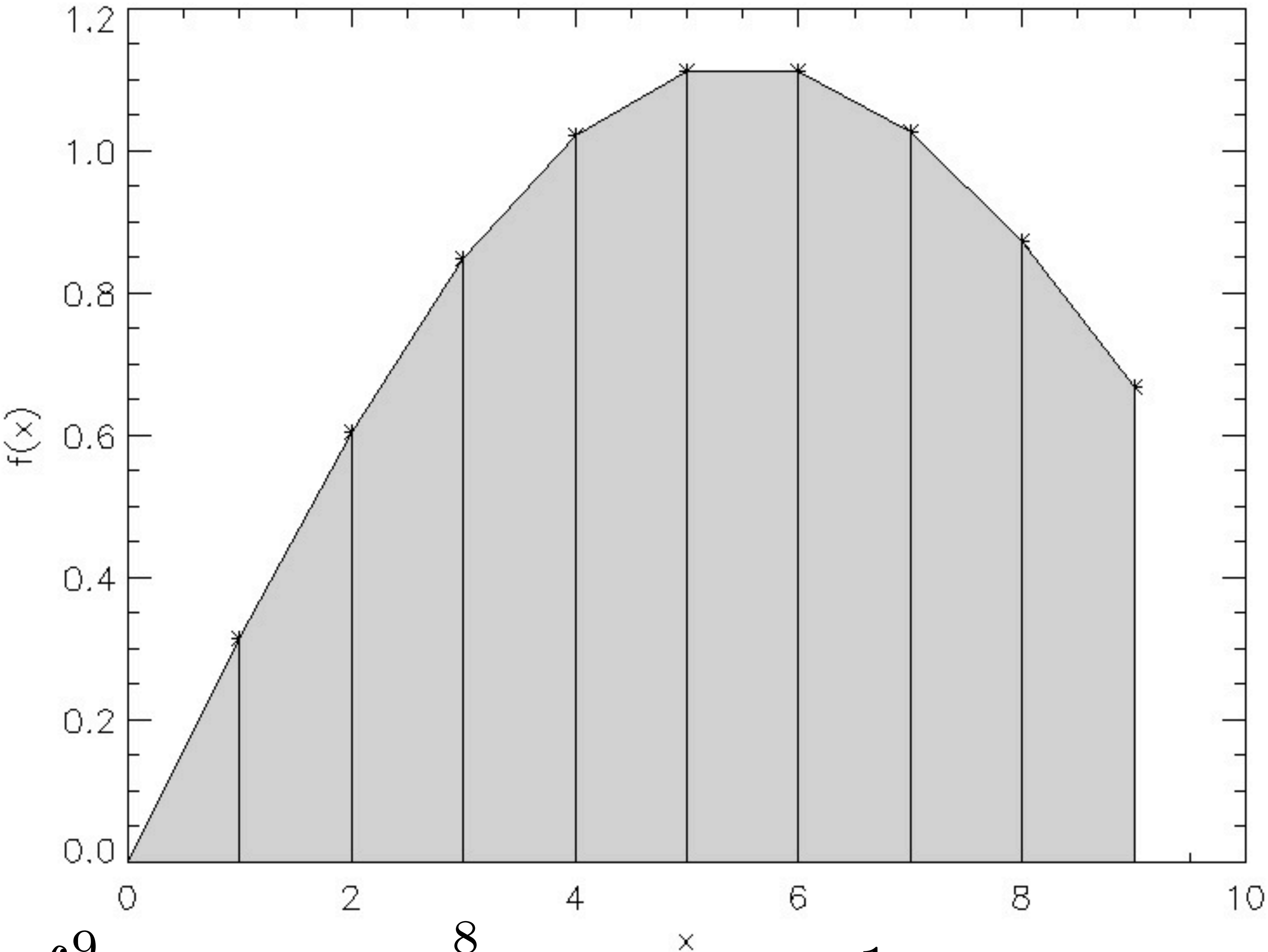


Voigt profile
lg(a)= -3.
Δν/Δν_D
(α_c+α_l)/α_500
Δν/Δν_D
Δν/Δν_D
τ_c=1
τ_0=1
lg(τ_500)

Numerical integration

Numerical integration (quadrature)





$$\int_0^9 f(x)dx \sim \sum_{i=0}^{8}(x_{i+1}-x_i)\frac{1}{2}(f(x_{i+1}+f(x_i))$$

$$\int_0^9 f(x)dx \sim \sum_{i=0}^{8} (x_{i+1} - x_i)\frac{1}{2}(f(x_{i+1} + f(x_i)) =$$

$$\frac{1}{2}(x_1 - x_0)f(x_0) + \sum_{i=1}^{7} \frac{1}{2}(x_{i+1} - x_{i-1})f(x_i) +$$

$$\frac{1}{2}(x_9 - x_8)f(x_9)$$

In general:

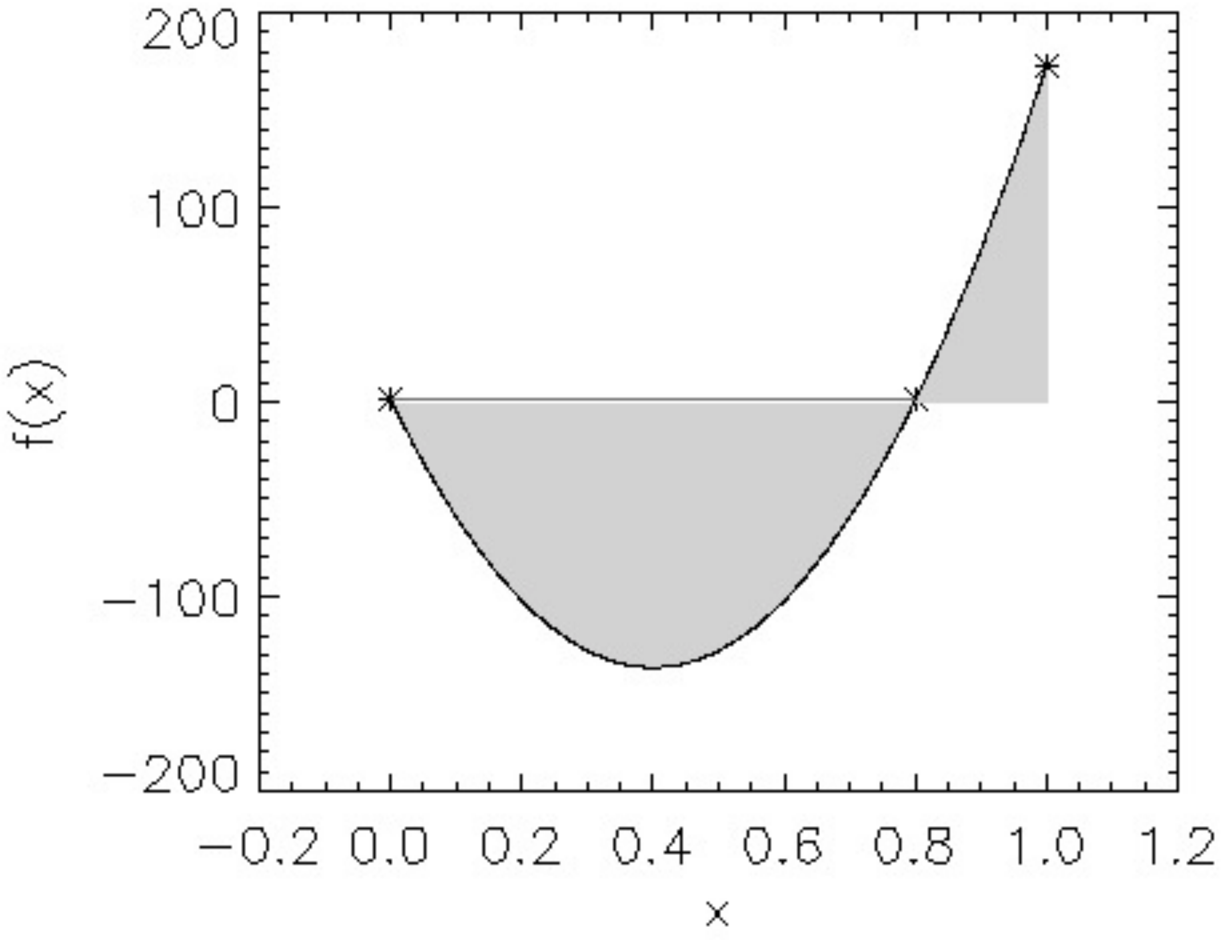
$$\int_a^b f(x)dx \sim \sum_{i=0}^{N-1} w_i f(x_i)$$

1. Grid points given

Trapezoidal: linear approximation between points

Simpson: parabolic between points

Higher accuracy but risk of overshoot



2. Integration method can determine points:

Gaussian quadratures

$$\int_a^b f(x)g(x)dx \sim \sum_{i=0}^{N-1} w_i f(x_i)$$

$g(x) = 1$ Gauss (-Legendre)

$g(x) = e^{-x}; a = 0; b = \infty$ Gauss-Laguerre

Mean intensity: Gaussian quadrature

$$J_\nu(\tau_\nu) = \frac{1}{2}\int_{-1}^{1} I_\nu(\tau_\nu,\mu)d\mu = \int_0^1 \frac{1}{2}(I_\nu^+(\tau_\nu,\mu) + I_\nu^-(\tau_\nu,\mu))d\mu =$$

$$\sum_{i=0}^{N_\mu - 1} w_i \frac{1}{2}(I_\nu^+(\tau_\nu,\mu_i) + I_\nu^-(\tau_\nu,\mu_i))$$

$$N_\mu = 3$$

w_i	μ_i
0.277778	0.112702
0.444444	0.500000
0.277778	0.887298

Intensity: Gauss-Laguerre quadrature

$$I_\nu(0) = \frac{1}{\mu}\int_0^\infty S_\nu(\tau_\nu) e^{-\tau_\nu/\mu} d\tau_\nu$$

$$d\tau_{\nu\mu} \equiv \frac{1}{\mu} d\tau_\nu \quad \tau_{\nu\mu} = \frac{1}{\mu}\tau_\nu$$

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

	$(\tau_{\nu\mu})_i$	w_i	
$N_{\tau_{\nu\mu}} = 1$	1.0	1.0	=Eddington-Barbier
$N_{\tau_{\nu\mu}} = 2$	0.58579	0.85355	
	3.41421	0.14645	

Source function with scattering

Source function with scattering

$$\eta_\nu = \kappa_\nu B_\nu + \sigma_\nu J_\nu$$
$$\chi_\nu = \kappa_\nu + \sigma_\nu$$

$$S_\nu \equiv \frac{\eta_\nu}{\chi_\nu} = \frac{\kappa_\nu}{\kappa_\nu + \sigma_\nu} B_\nu + \frac{\sigma_\nu}{\kappa_\nu + \sigma_\nu} J_\nu$$

$$S_\nu = B_\nu + \frac{\sigma_\nu}{\kappa_\nu + \sigma_\nu}(J_\nu - B_\nu)$$

$$\rho_\nu \equiv \frac{\sigma_\nu}{\kappa_\nu + \sigma_\nu}$$

$$S_\nu = B_\nu + \rho_\nu (J_\nu - B_\nu)$$

Transfer equation, plane parallel atmosphere

$$\mu \frac{dI_\nu}{d\tau_\nu} = I_\nu - S_\nu$$

Boundary conditions:

$$\lim_{\tau_\nu \to \infty} (I_\nu e^{-\tau_\nu/\mu}) = 0 \qquad I_\nu^-(0) = 0$$

$$I_\nu^+(\tau_\nu) = \frac{1}{\mu} \int_{\tau_\nu}^{\infty} S_\nu(\tau'_\nu) e^{-(\tau'_\nu - \tau_\nu)/\mu} d\tau'_\nu$$

$$I_\nu^-(\tau_\nu) = \frac{1}{\mu} \int_0^{\tau_\nu} S_\nu(\tau'_\nu) e^{-(\tau_\nu - \tau'_\nu)/\mu} d\tau'_\nu$$

$$J_\nu(\tau_\nu) = \frac{1}{2} \int_{-1}^{1} I_\nu(\tau_\nu, \mu) d\mu = \int_0^1 \frac{1}{2} (I_\nu^+(\tau_\nu, \mu) + I_\nu^-(\tau_\nu, \mu)) d\mu \equiv \Lambda_\nu[S_\nu]$$

$$J_\nu(\tau_\nu) = \Lambda_\nu[S_\nu] = \Lambda_\nu[B_\nu] + \Lambda_\nu[\rho_\nu(J_\nu - B_\nu)]$$

Λ-iteration:

$$\begin{cases} J_\nu^{(n+1)}(\tau_\nu) & = \Lambda_\nu[B_\nu] + \Lambda_\nu[\rho_\nu(J_\nu^{(n)} - B_\nu)] \\ J^{(0)}(\tau_\nu) & = B_\nu \end{cases}$$

If $\rho_\nu \sim 1$ this scheme won't work

Cases when scattering dominates:

Hot stars, opacity dominated by electron scattering

Cool stars, low [Fe/H]: Rayleigh scattering dominates

Spectral lines: $1 - \rho_\nu \sim 10^{-8}$

Alternative form

$$S_\nu = (1 - \epsilon_\nu) J_\nu + \epsilon_\nu B_\nu$$

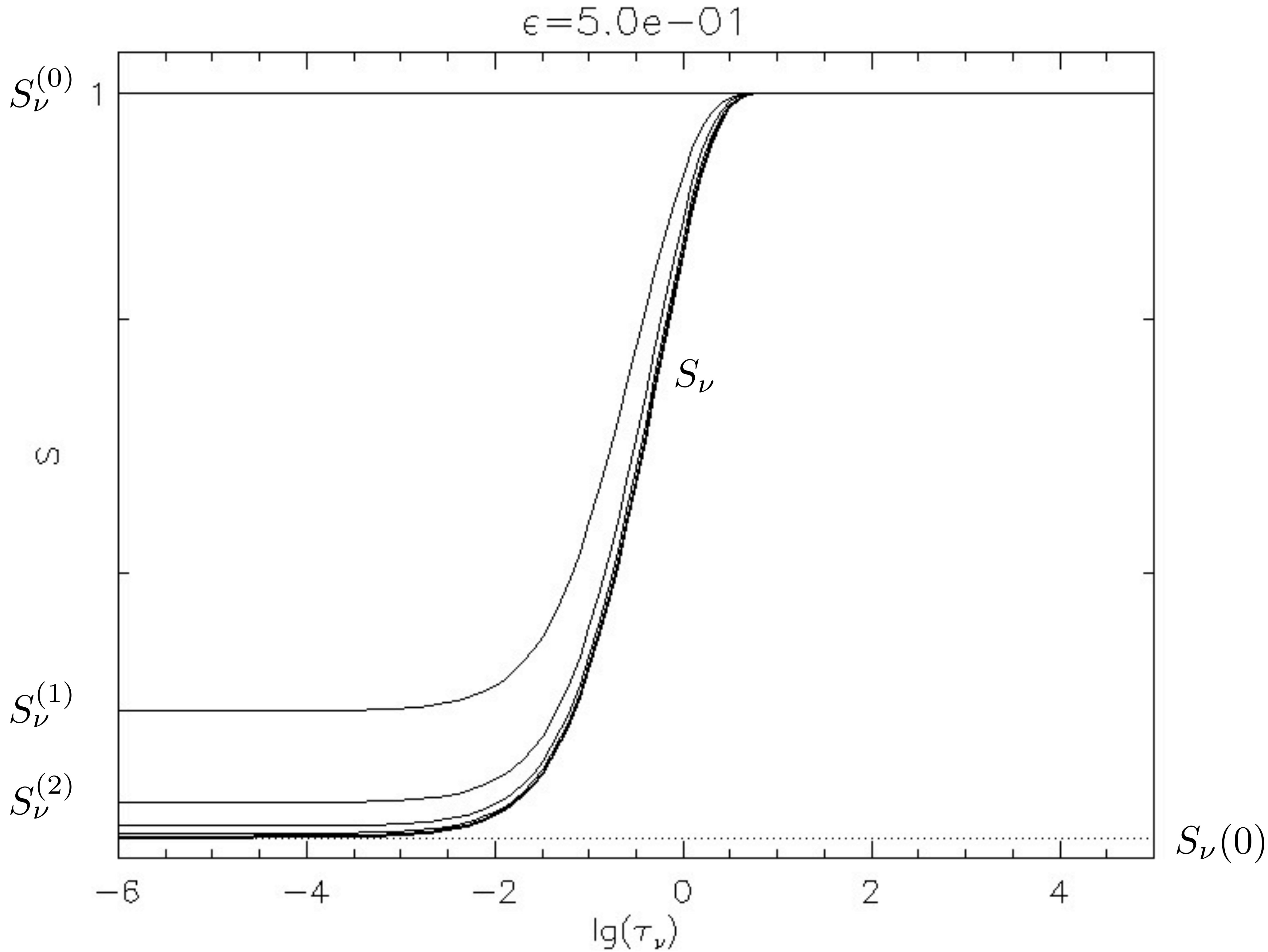
$$S_\nu = (1 - \epsilon_\nu) \Lambda_\nu [S_\nu] + \epsilon_\nu B_\nu$$

Λ-iteration:

$$\begin{cases} S_\nu^{(n+1)} & = (1 - \epsilon_\nu) \Lambda_\nu [S_\nu^{(n)}] + \epsilon_\nu B_\nu \\ S_\nu^{(0)} & = B_\nu \end{cases}$$

Lambda-iteration in practice, 100 iterations

$$S_\nu = \epsilon_\nu B_\nu + (1 - \epsilon_\nu) J_\nu \quad ; \quad B_\nu = 1$$



Lambda-iteration in practice, 100 iterations

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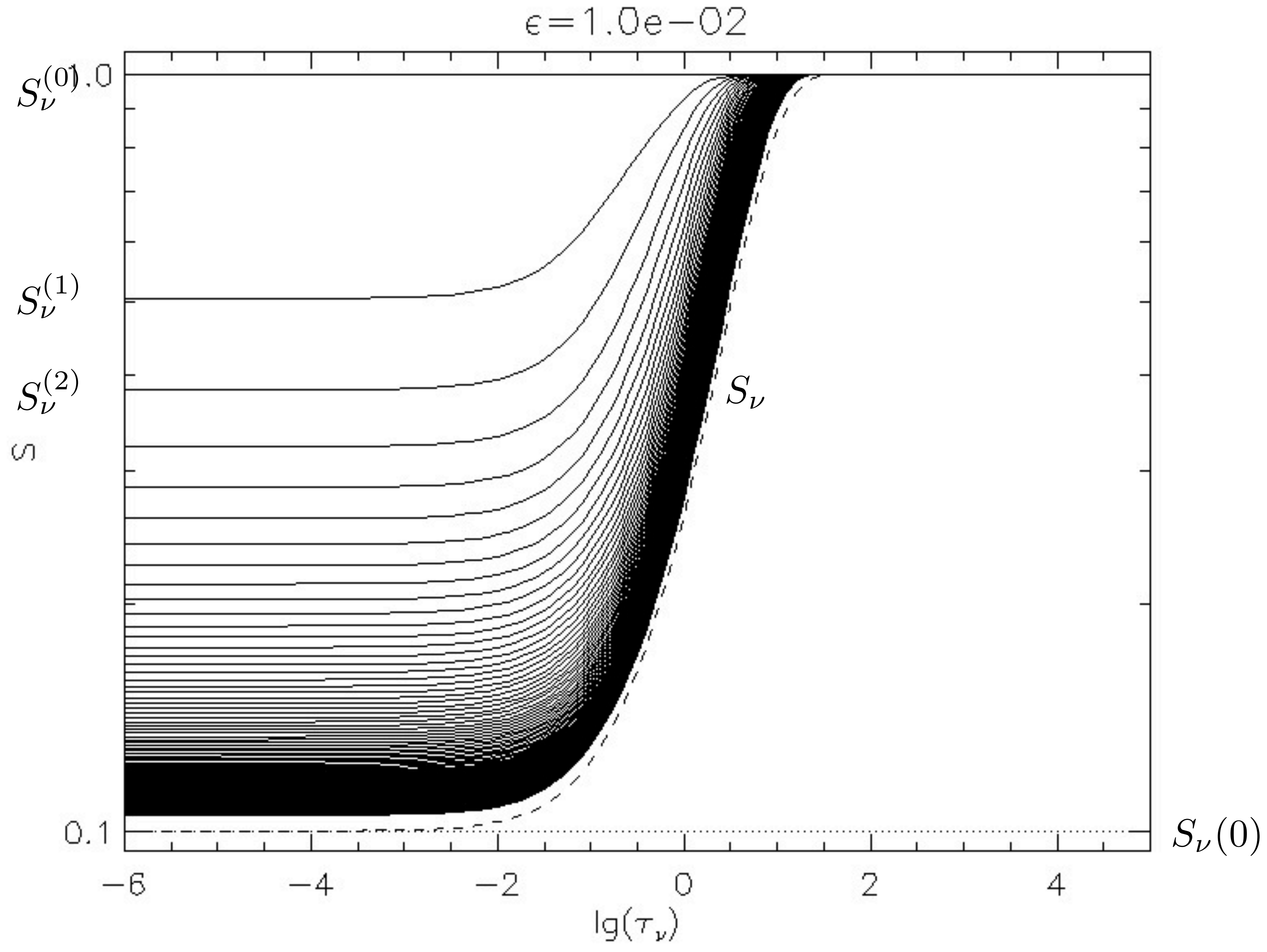

Lambda-iteration in practice, 100 iterations

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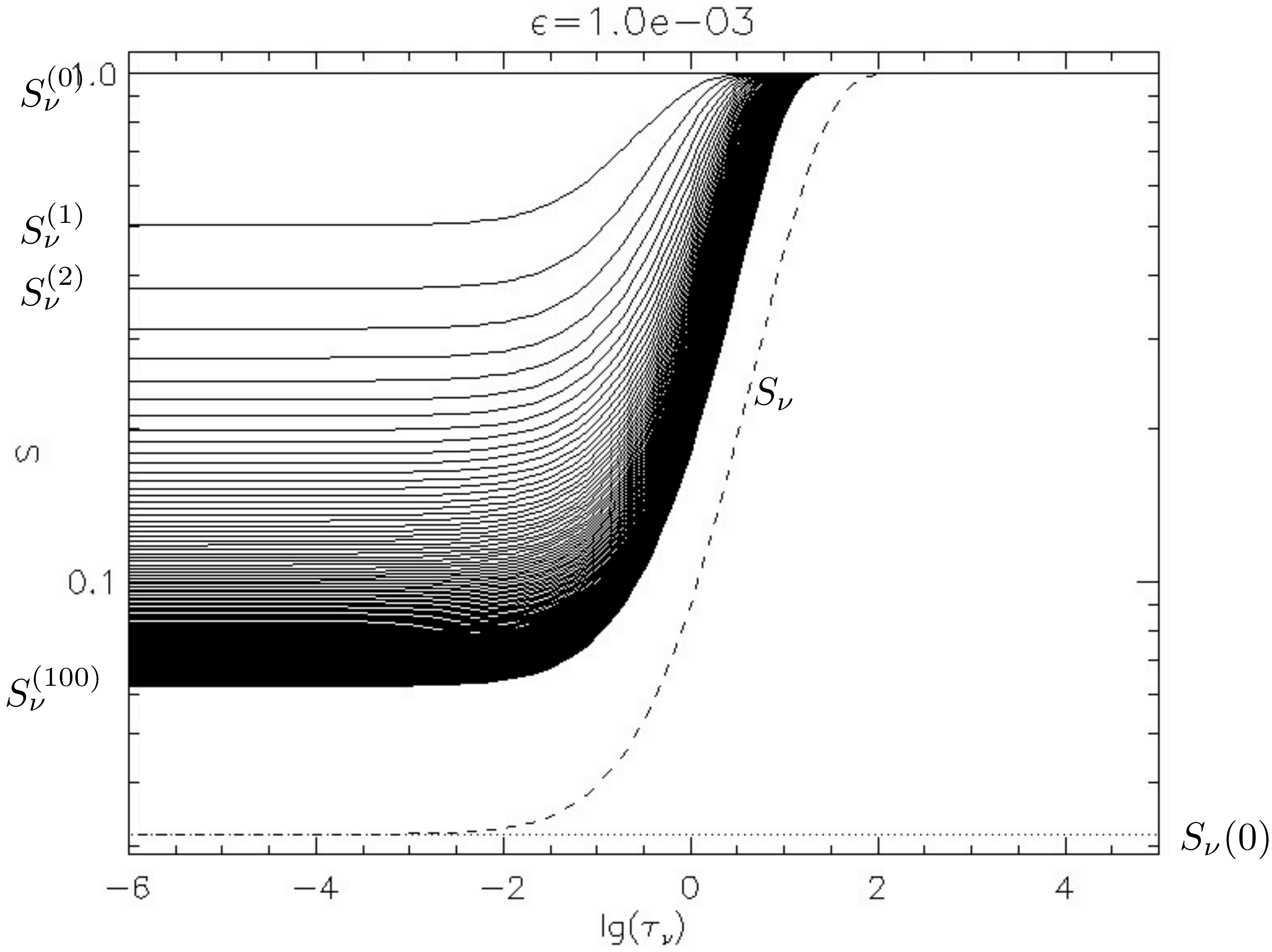

Lambda-iteration in practice, 100 iterations

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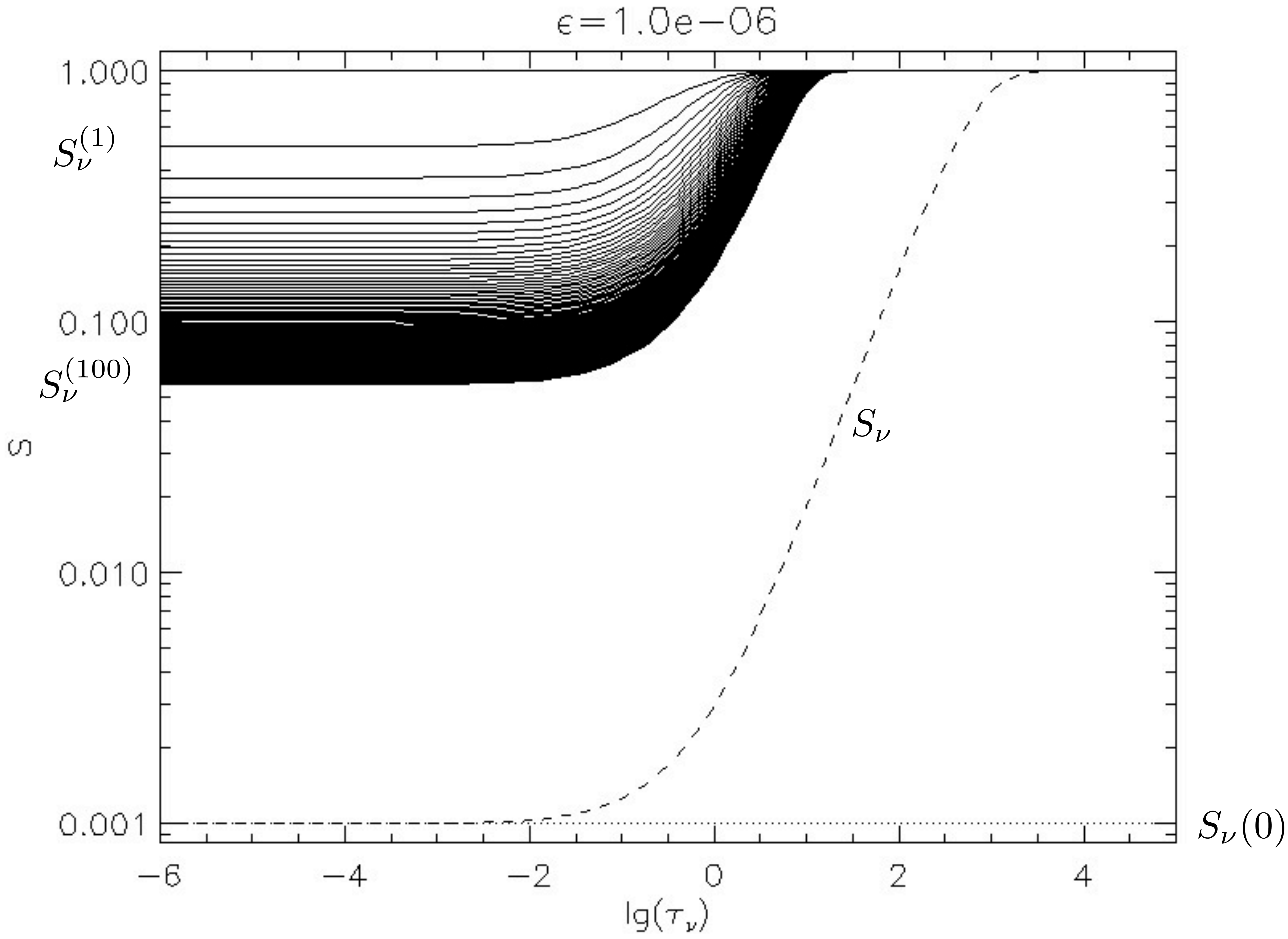


Lambda-iteration in practice

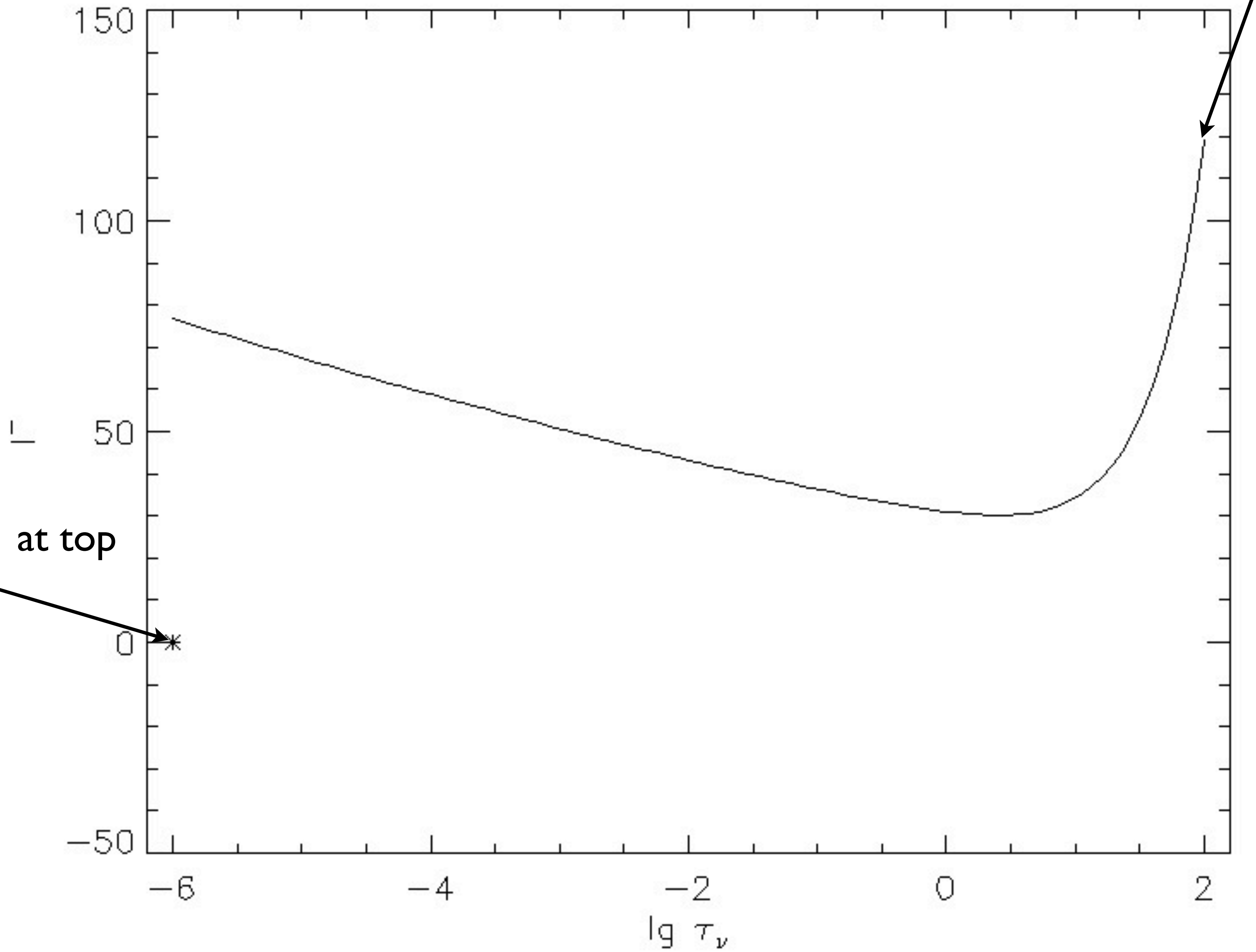
- OK if scattering is small
- Disaster for small epsilon
- Stabilizes instead of converging when epsilon is small (0.5% correction at iteration 100 for $\varepsilon=10^{-6}$ when solution is a factor of 55 from correct solution)

Shooting

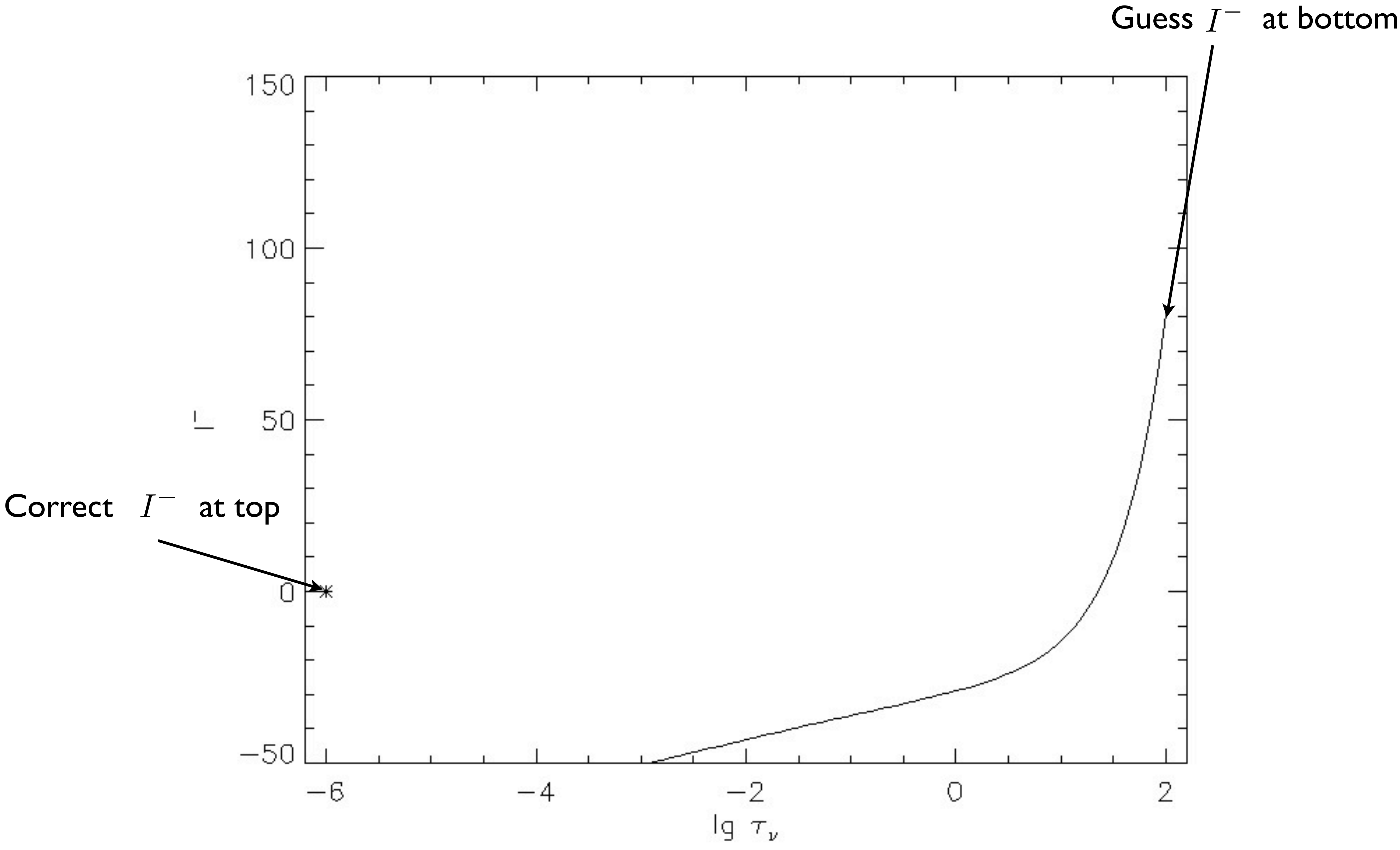
Principles

Guess I^- at bottom

Correct I^- at top

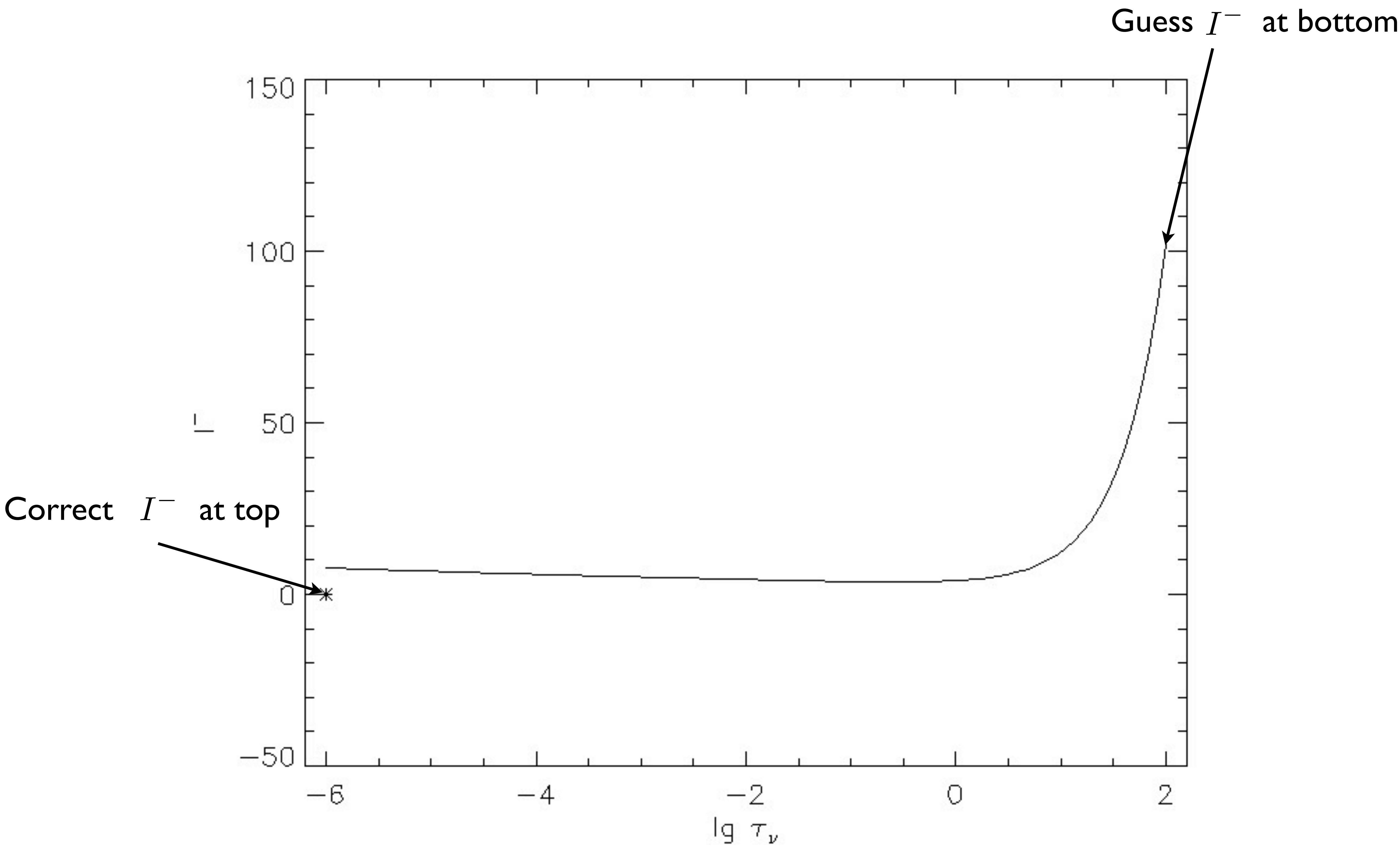


Shooting



Guess I^- at bottom
Correct I^- at top
150
100
50
0
−50
I^-
−6
−4
−2
0
2
lg τ_ν

Shooting



Guess I^- at bottom
Correct I^- at top
150
100
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−50
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−4
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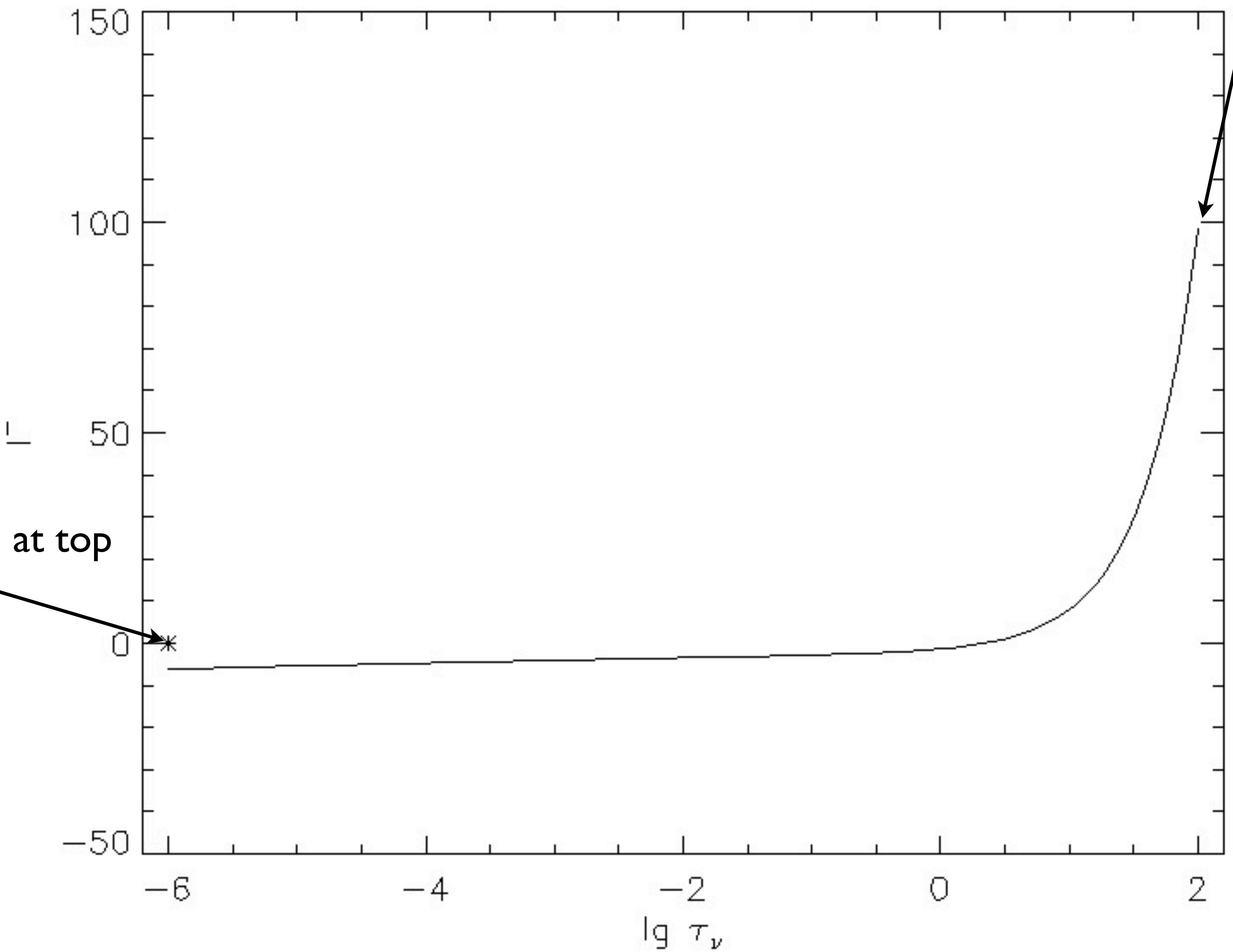
0
2
lg τ_ν

Shooting

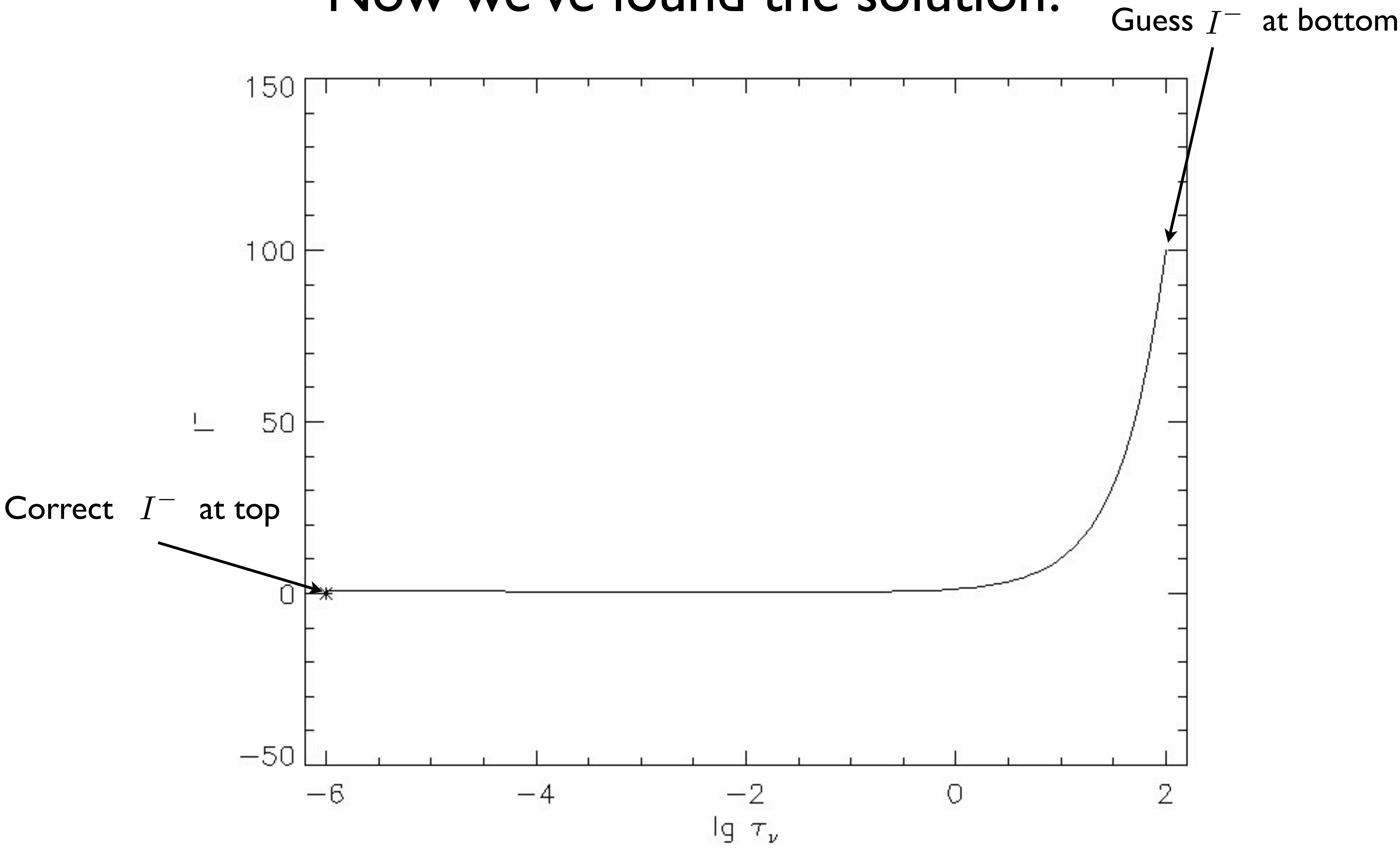
Guess I^- at bottom



Correct I^- at top

Shooting

Now we've found the solution!

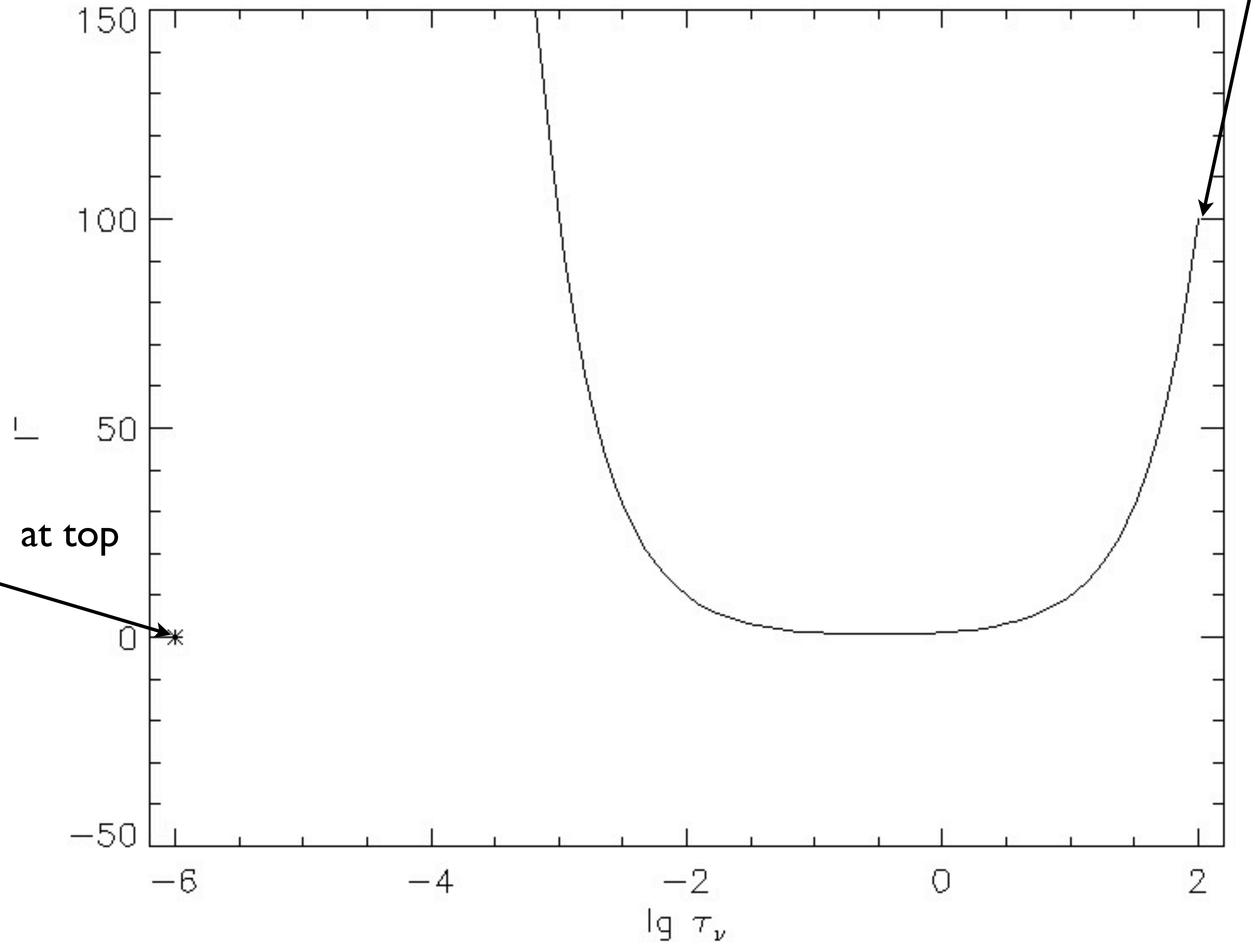


Shooting

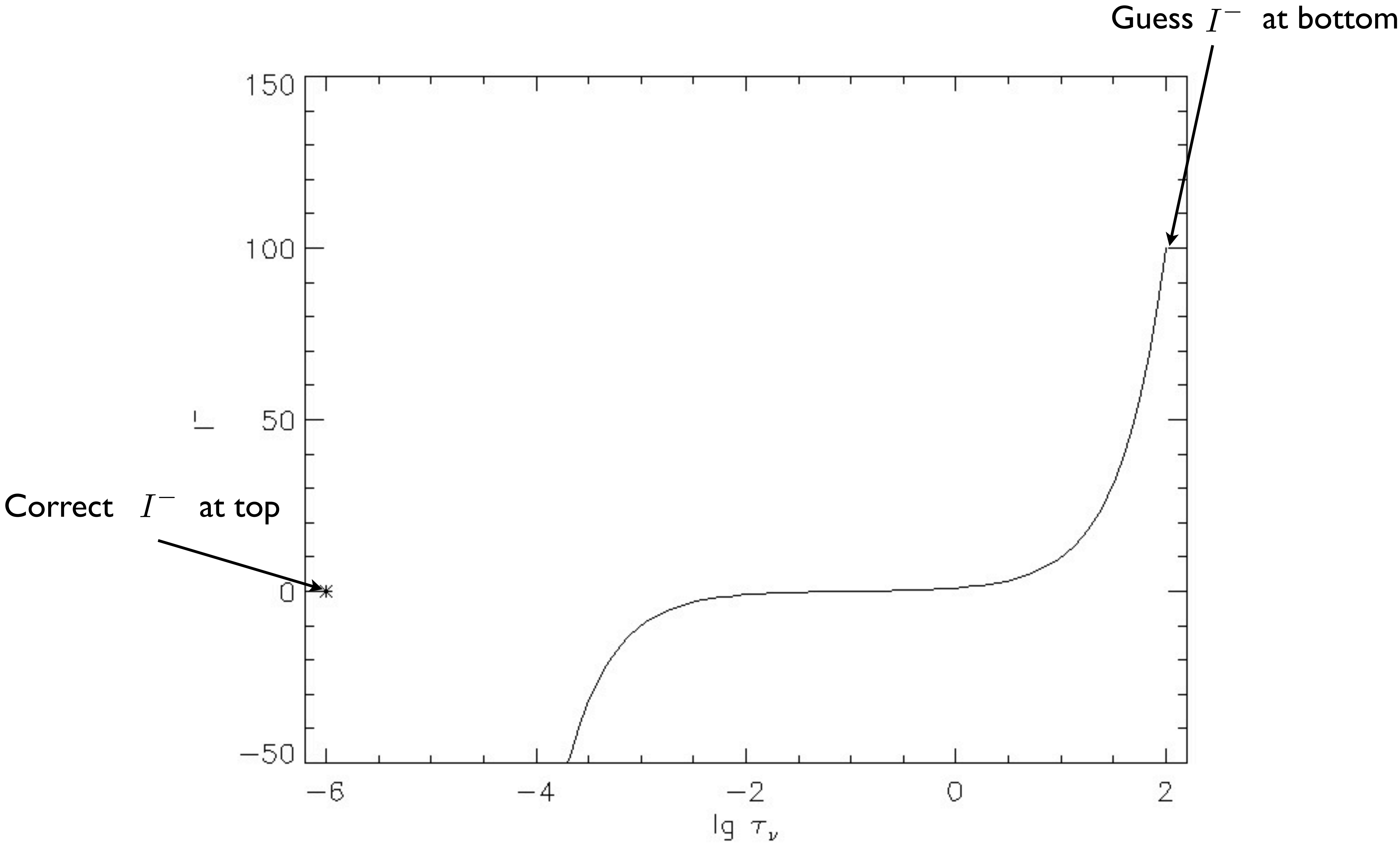
Realistic case

Guess I^- at bottom

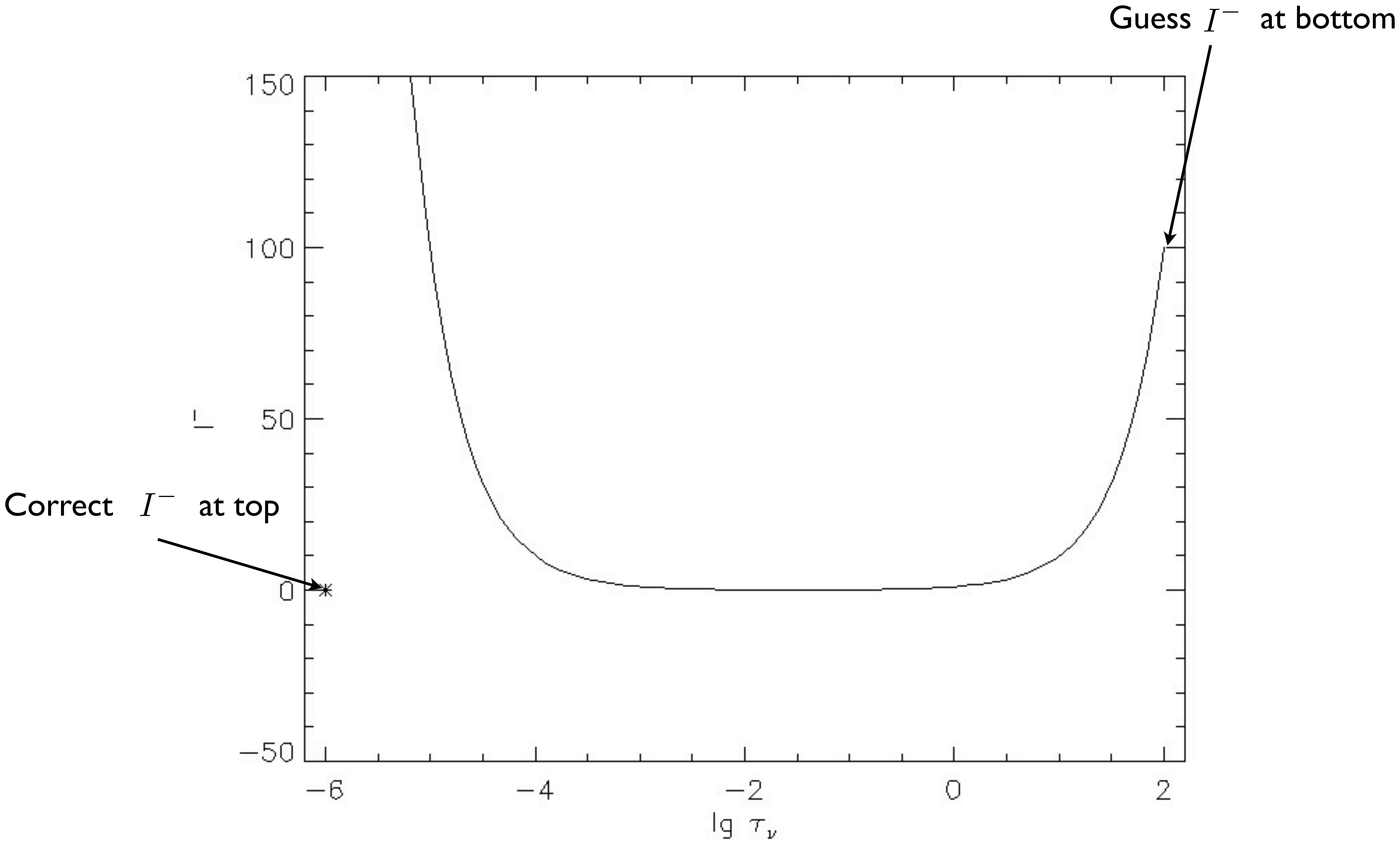
Correct I^- at top



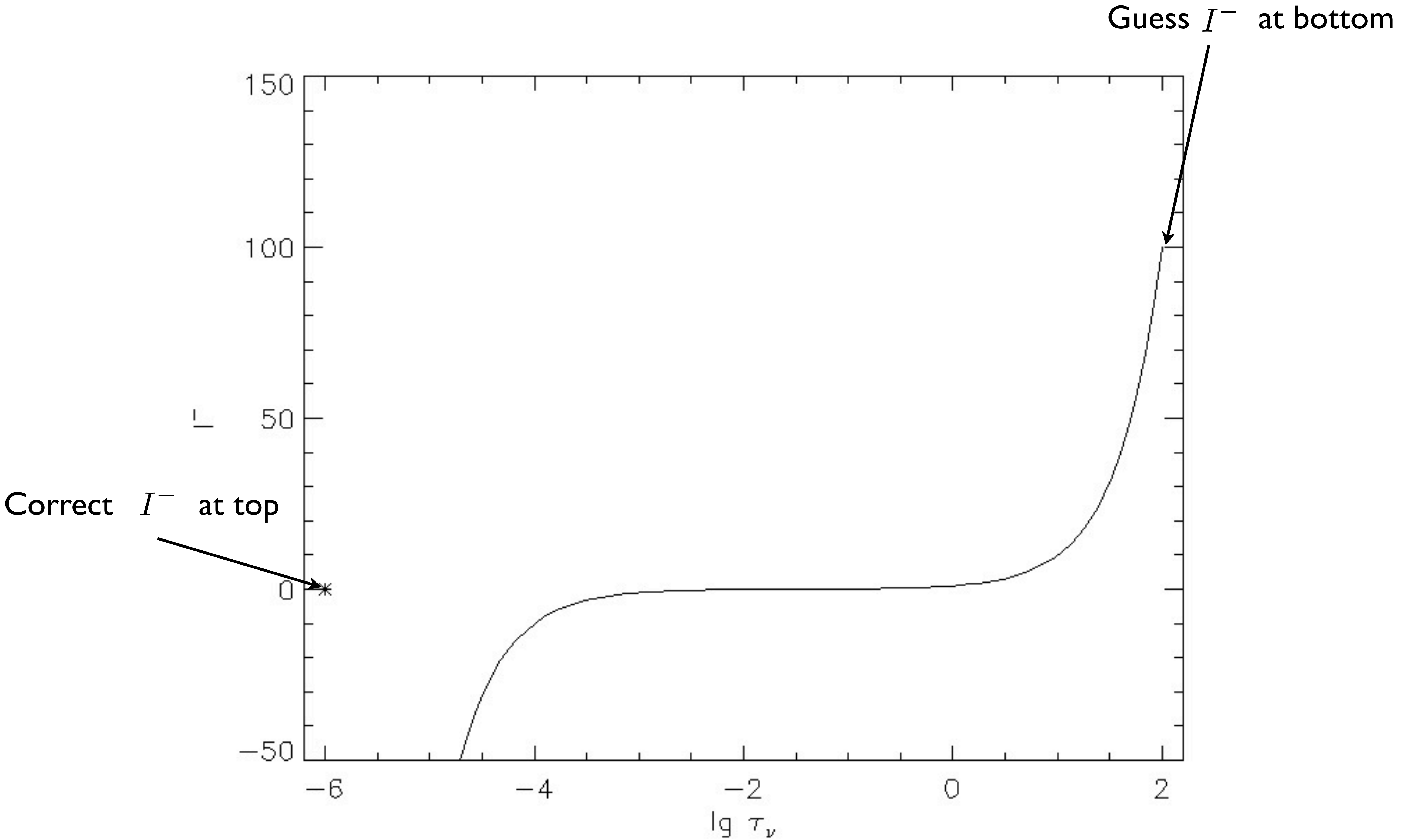
Shooting


Guess I^- at bottom
Correct I^- at top
150
100
50
0
−50
−6
−4
−2
0
2
lg τ_ν

Shooting


Guess I^- at bottom
Correct I^- at top
150
100
50
0
−50
−6
−4
−2
0
2
lg τ_ν

Shooting

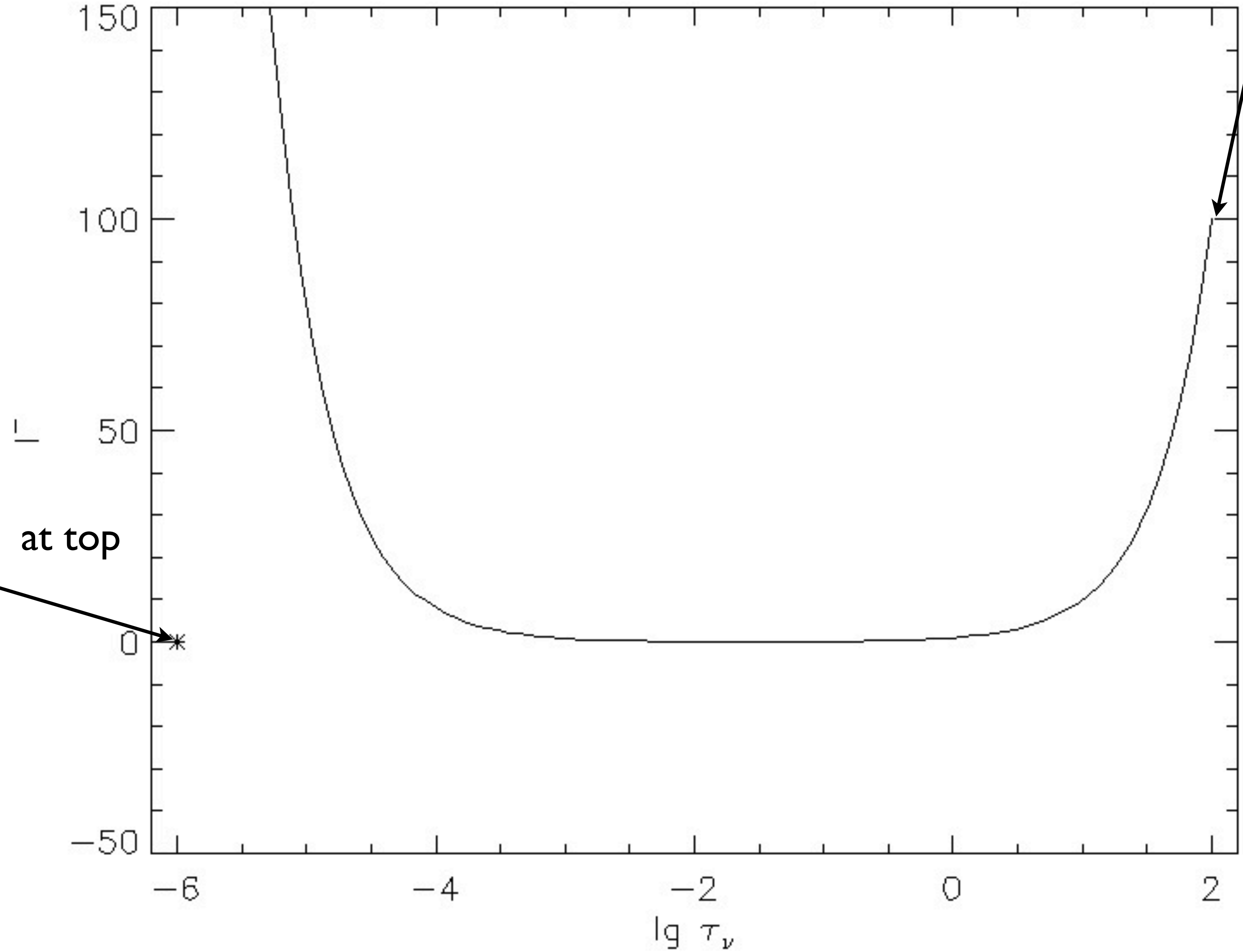


Guess I^- at bottom
Correct I^- at top
150
100
50
0
−50
−6
−4
−2
0
2
lg τ_ν

Shooting

Guess I^- at bottom

Correct I^- at top

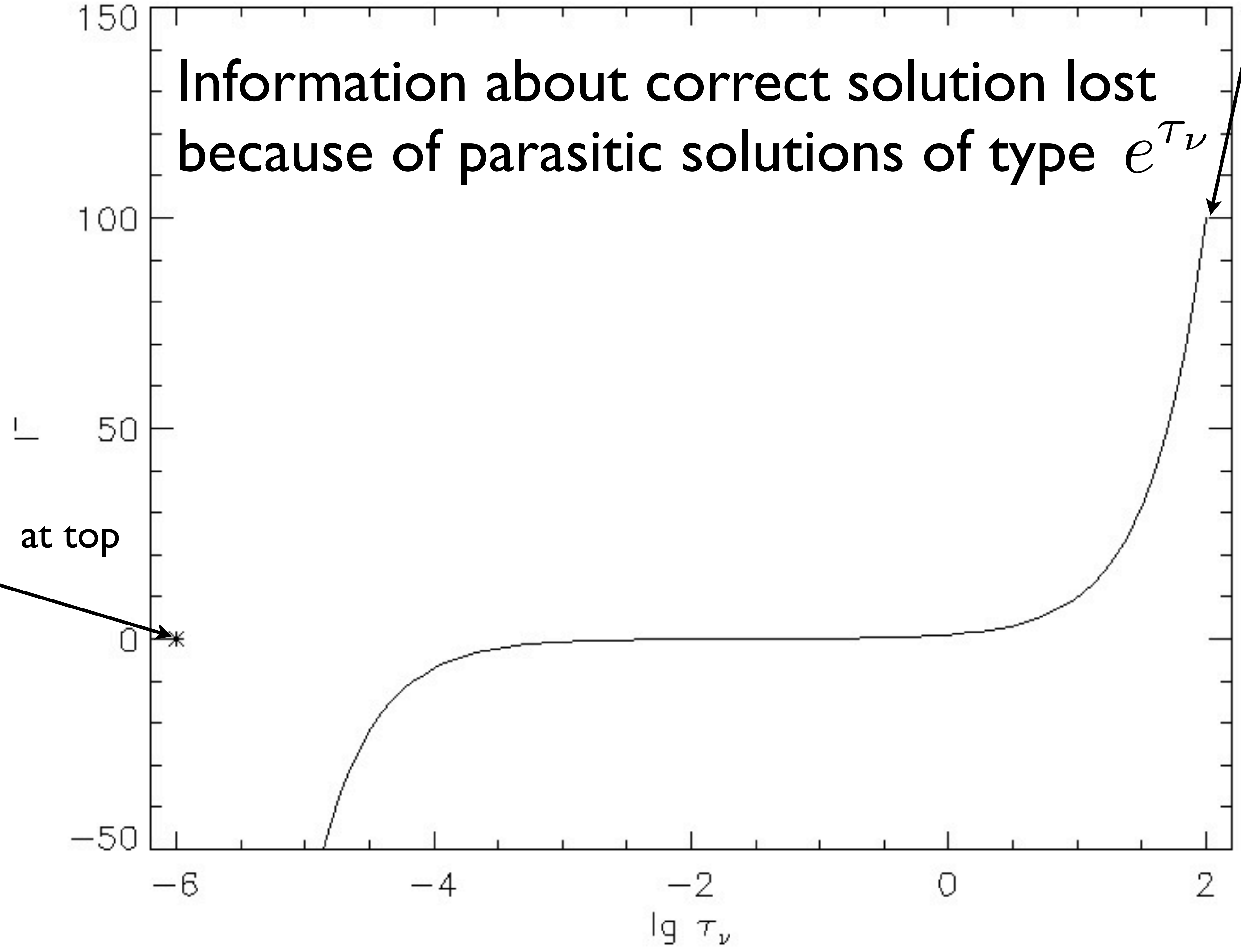


Shooting

Guess I^- at bottom

Information about correct solution lost because of parasitic solutions of type e^{τ_ν}

Correct I^- at top



Why is there a problem?

- Boundary condition partially given at one boundary, partially at the other
- Need to solve for whole atmosphere and take into account bouth boundaries at the same time

Feautrier’s method

Feautrier's method

We drop index ν and location τ_ν :

$$\mu \frac{dI_\mu}{d\tau} = I_\mu - S$$

We write separately for outgoing and incoming rays:

$$\mu \frac{dI_\mu^+}{d\tau} = I_\mu^+ - S^+$$

$$-\mu \frac{dI_\mu^-}{d\tau} = I_\mu^- - S^-$$

Multiplying by $\frac{1}{2}$, assuming $S^+ = S^-$
and adding and subtracting we get

$$\mu \frac{d\frac{1}{2}(I_\mu^+ - I_\mu^-)}{d\tau} = \frac{1}{2}(I_\mu^+ + I_\mu^-) - S^+$$

$$\mu \frac{d\frac{1}{2}(I_\mu^+ + I_\mu^-)}{d\tau} = \frac{1}{2}(I_\mu^+ - I_\mu^-)$$

Using the second equation in the first and introducing

$$P \equiv \frac{1}{2}(I_\mu^+ + I_\mu^-) \qquad R \equiv \frac{1}{2}(I_\mu^+ - I_\mu^-)$$

we get

$$\boxed{\mu^2 \frac{d^2 P}{d\tau^2} = P - S}$$

We discretize: $\tau_\nu \longrightarrow \tau_i \qquad \mu \longrightarrow \mu_j$

Define differences:

$$[\Delta\tau]_{i+1/2} \approx \tau_{i+1} - \tau_i \equiv \Delta\tau_i \tag{5.20}$$

$$[\Delta\tau]_{i-1/2} \approx \tau_i - \tau_{i-1} \equiv \Delta\tau_{i-1} \tag{5.21}$$

Replace derivatives with differences

$$\left[\frac{\mathrm{d}P(\tau,\mu_j)}{\mathrm{d}\tau}\right]_{i+1/2} \equiv \lim_{\Delta\tau\to 0} \frac{[\Delta P(\tau,\mu_j)]_{i+1/2}}{[\Delta\tau]_{i+1/2}}$$

$$\approx \frac{P(\tau_{i+1},\mu_j) - P(\tau_i,\mu_j)}{\tau_{i+1}-\tau_i} = \frac{P_{i+1}-P_i}{\Delta\tau_i},$$

2nd derivative replaced by difference between 1st derivatives:

$$
\begin{aligned}
\left[\frac{\mathrm{d}^2 P(\tau,\mu_j)}{\mathrm{d}\tau^2}\right]_i &\approx \frac{\left[\Delta P(\tau,\mu_j)/\Delta\tau\right]_{i+1/2} - \left[\Delta P(\tau,\mu_j)/\Delta\tau\right]_{i-1/2}}{[\Delta\tau]_i} \\
&\approx \frac{\left[\Delta P(\tau,\mu_j)/\Delta\tau\right]_{i+1/2} - \left[\Delta P(\tau,\mu_j)/\Delta\tau\right]_{i-1/2}}{\frac{1}{2}\left([\Delta\tau]_{i+1/2} + [\Delta\tau]_{i-1/2}\right)} \\
&\approx \frac{2}{\Delta\tau_{i-1} + \Delta\tau_i}\left[\frac{P_{i+1}}{\Delta\tau_i} - \frac{P_i}{\Delta\tau_i} - \frac{P_i}{\Delta\tau_{i-1}} + \frac{P_{i-1}}{\Delta\tau_{i-1}}\right] \\
&= \frac{2P_{i-1}}{\Delta\tau_{i-1}\left(\Delta\tau_{i-1} + \Delta\tau_i\right)} - \frac{2P_i}{\Delta\tau_i\,\Delta\tau_{i-1}} + \frac{2P_{i+1}}{\Delta\tau_i\left(\Delta\tau_{i-1} + \Delta\tau_i\right)}.
\end{aligned}
$$

With these (5.17) can be written as:

$$\mu^2 \left[\frac{\mathrm{d}^2 P}{\mathrm{d}\tau^2}\right]_i - P_i = A_i P_{i-1} - B_i P_i + C_i P_{i+1} = -S_i \tag{5.22}$$

with

$$A_i = \frac{2\mu^2}{\Delta\tau_{i-1}\left(\Delta\tau_{i-1} + \Delta\tau_i\right)} \tag{5.23}$$

$$B_i = 1 + \frac{2\mu^2}{\Delta\tau_i\,\Delta\tau_{i-1}} \tag{5.24}$$

$$C_i = \frac{2\mu^2}{\Delta\tau_i\left(\Delta\tau_{i-1} + \Delta\tau_i\right)}. \tag{5.25}$$

Numerically unstable for small $\Delta\tau_i$ (use Stein's trick)

2 level atom with coherent scattering:

$$\mu^2 \frac{\mathrm{d}^2 P(\tau,\mu)}{\mathrm{d}\tau^2} = P(\tau,\mu) - \varepsilon(\tau)B(\tau) - \left(1-\varepsilon(\tau)\right)J(\tau) \tag{5.27}$$

$$= P(\tau,\mu) - \varepsilon(\tau)B(\tau) - \left(1-\varepsilon(\tau)\right)\sum_{j=1}^{m} a_j P_j(\tau,\mu_j), \tag{5.28}$$

Source function thus introduces all angles for the equation of a given angle

$$\mathbf{TP} = -\varepsilon\mathbf{B}$$

Structure of matrix:

$$
\mathbf{T} = \begin{pmatrix}
x & x & x & x & & & & & & & & & & & & & & \\
x & x & x & & x & & & & & & & & & & & & & \\
x & x & x & & & x & & & & & & & & & & & & \\
x & & & x & x & x & x & & & & & & & & & & & \\
& x & & x & x & x & & x & & & & & & & & & & \\
& & x & x & x & x & & & x & & & & & & & & & \\
& & & x & & & x & x & x & x & & & & & & & & \\
& & & & x & & x & x & x & & x & & & & & & & \\
& & & & & x & x & x & x & & & x & & & & & & \\
& & & & & & \ddots & & & \ddots & & & \ddots & & & & & \\
& & & & & & & & & & & & & & & & & \\
& & & & & & & & & & & & x & x & x & x & & \\
& & & & & & & & & & & & x & x & x & & x & \\
& & & & & & & & & & & & x & x & x & & & x \\
& & & & & & & & & & & & x & & & x & x & x \\
& & & & & & & & & & & & & x & & x & x & x \\
& & & & & & & & & & & & & & x & x & x & x
\end{pmatrix}
$$

Solve for all depths at the same time

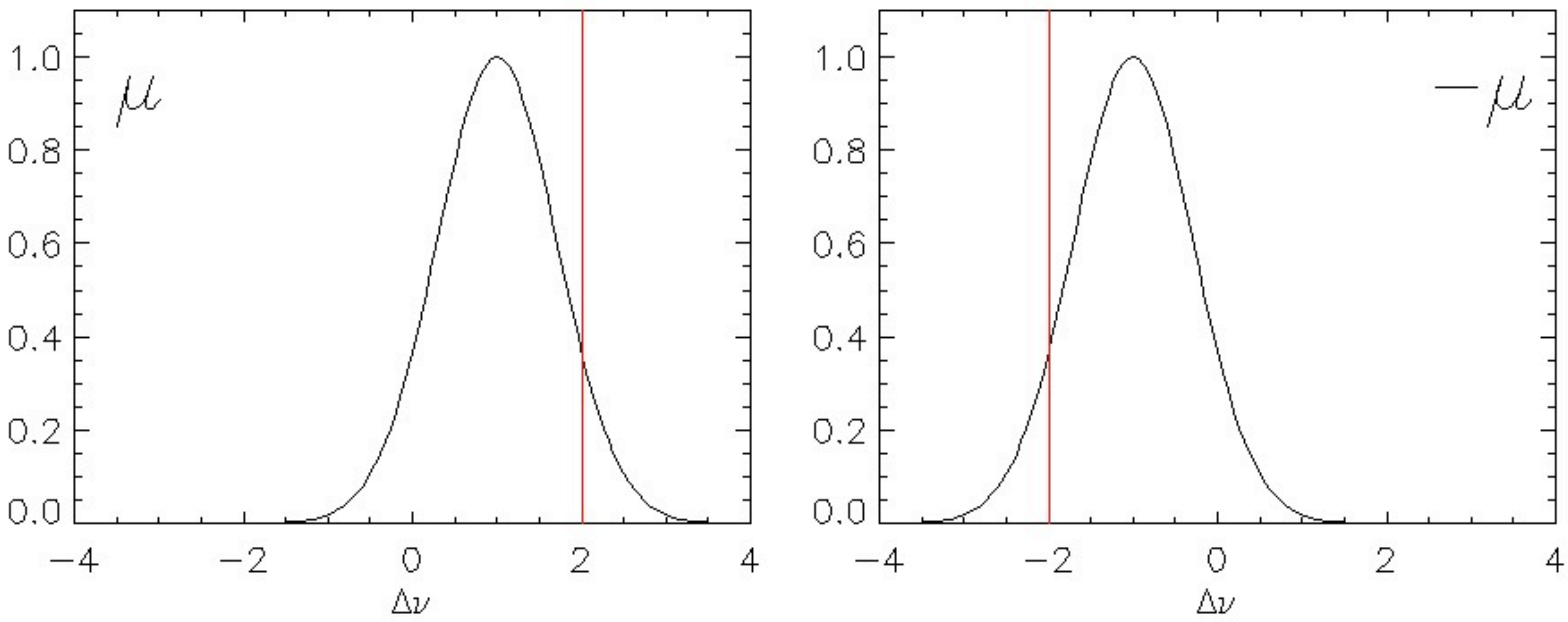
Boundaries at both ends taken into account simultaneously

Note that Feautrier's method assumes $S^+ = S^-$

With velocities in the atmosphere this condition is not fulfilled!!

If the absorption profile of a line is symmetric, we can redefine P (and R):

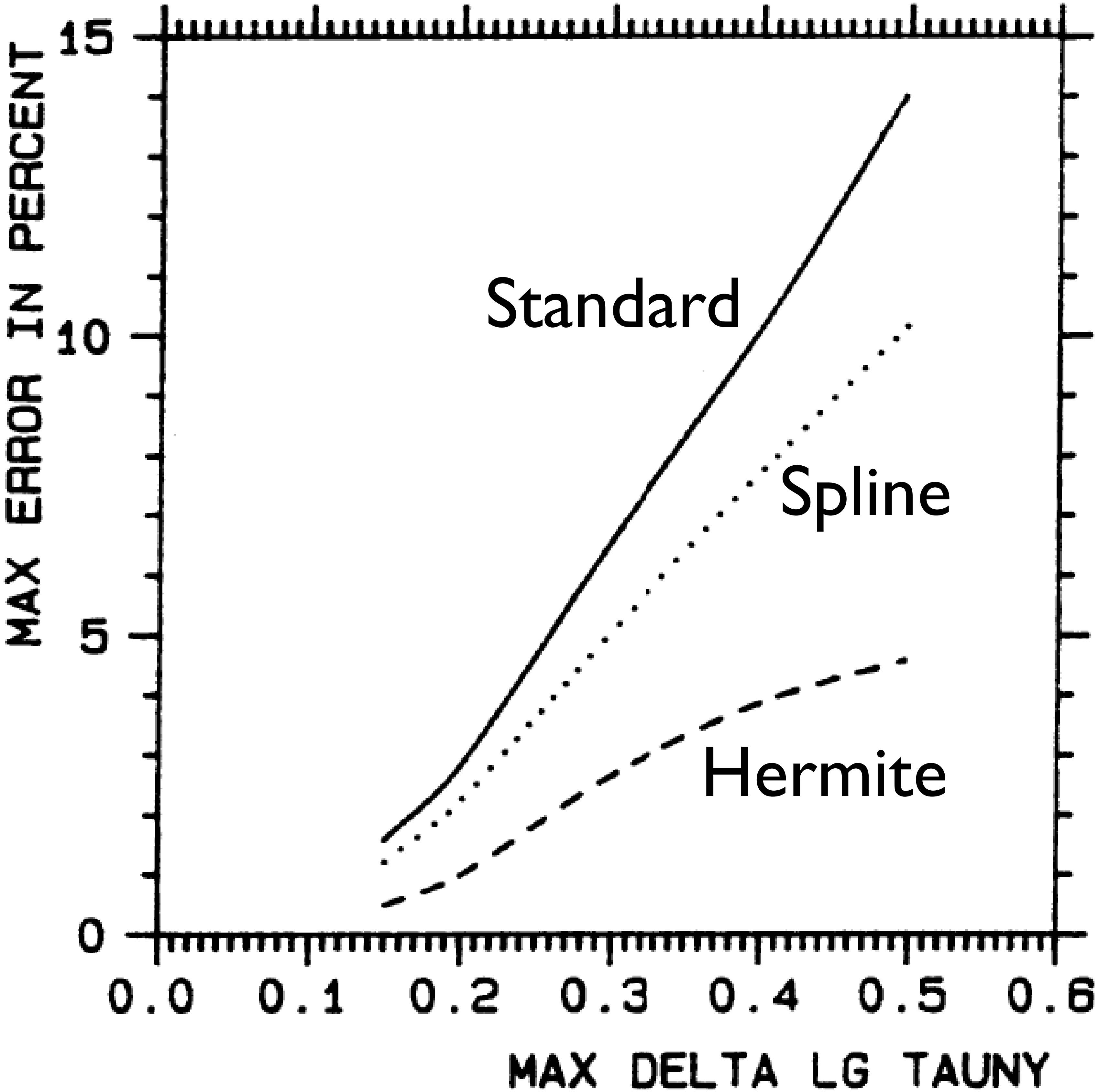
$$P_\mu(\tau, \Delta\nu) \equiv \frac{1}{2}(I_\mu^+(\tau, \Delta\nu) + I_\mu^-(\tau, -\Delta\nu))$$

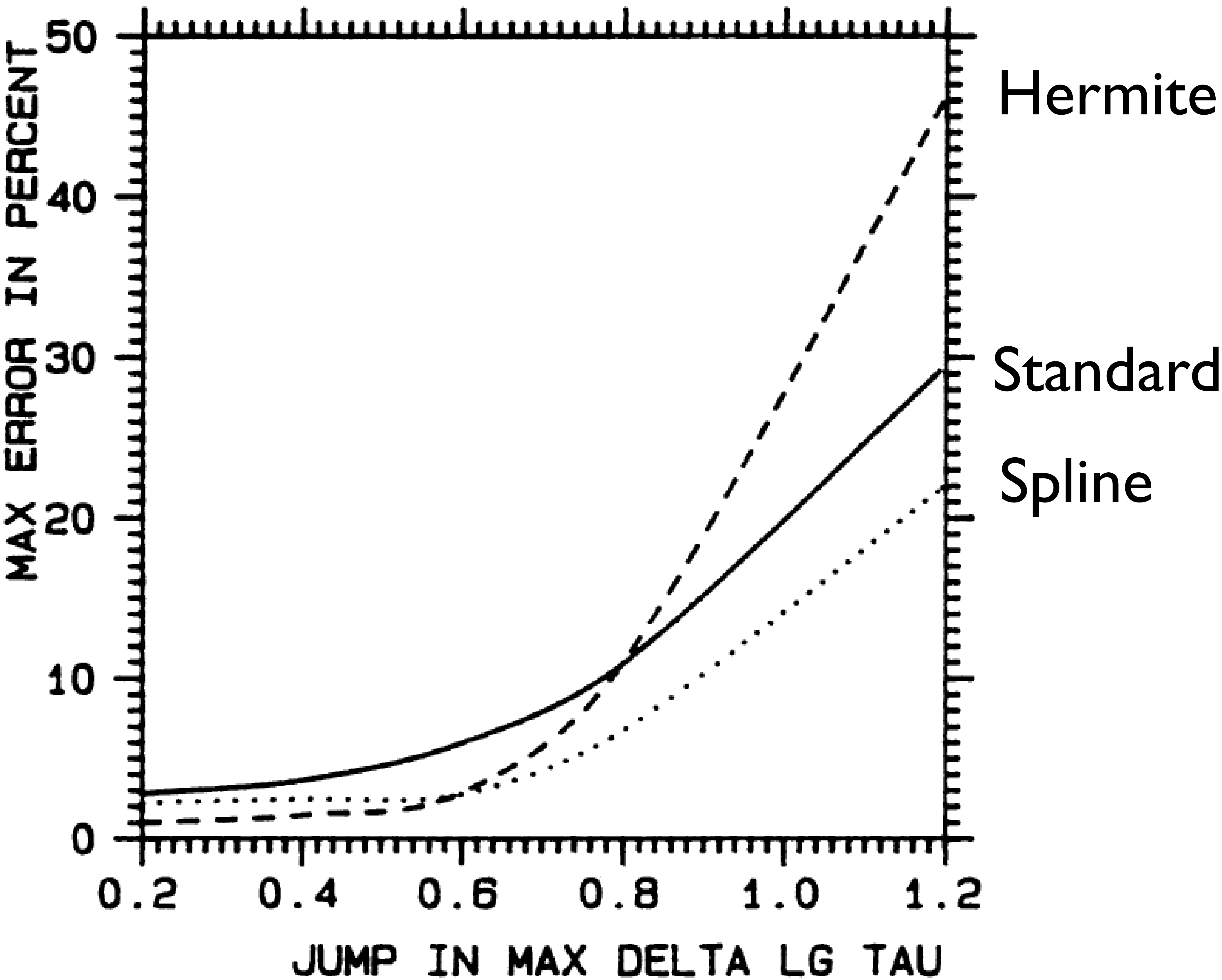


Feautrier's method is fast and accurate (2nd order) and is the method of choice for the formal solution, even when there is no scattering.

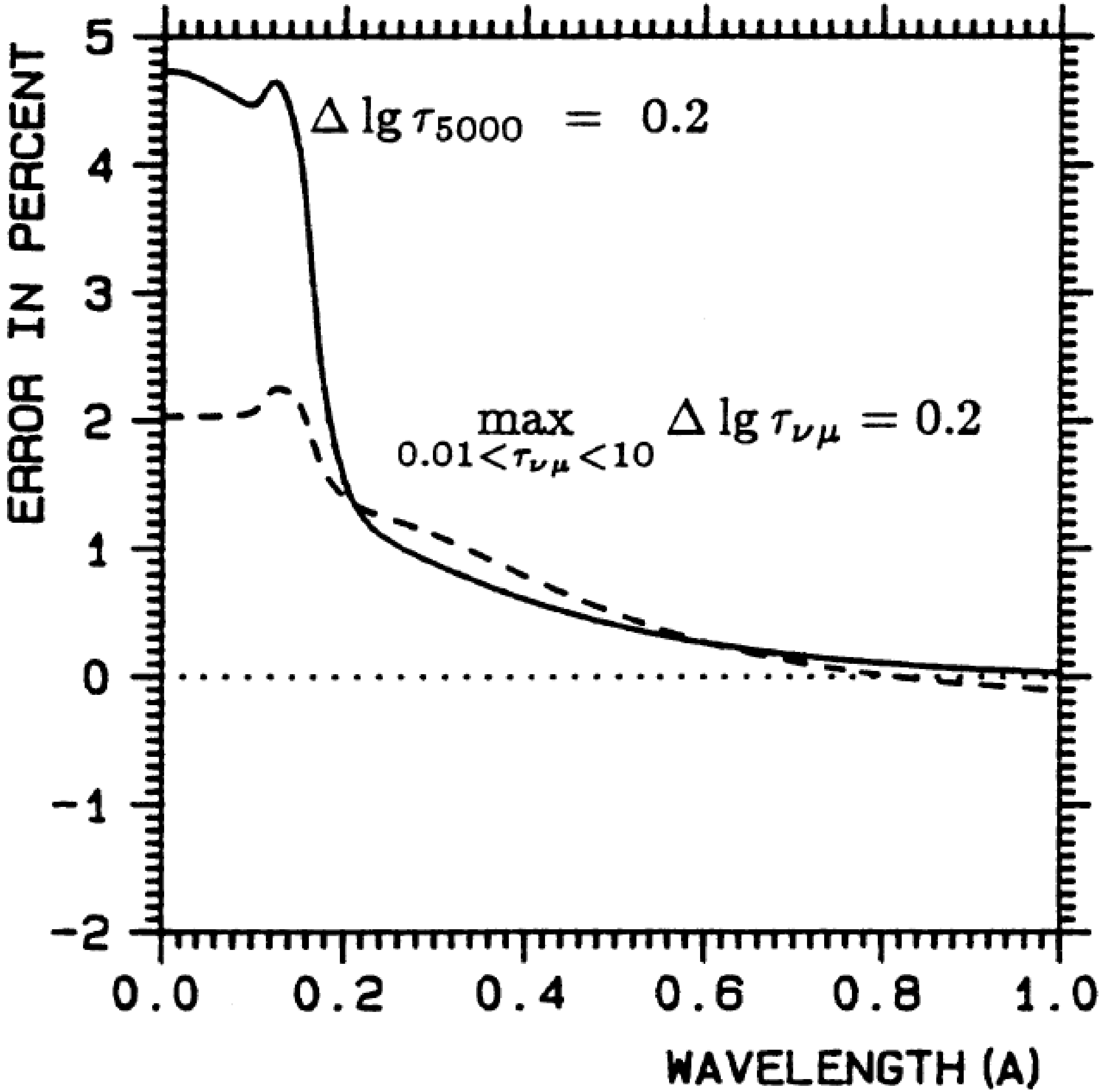
There are versions that are 3rd and 4th order accurate (spline and Hermite forms)

Cannot be used if we have both velocity fields and blends!


MAX ERROR IN PERCENT
15
10
5
0
Standard
Spline
Hermite
0.0
0.1
0.2
0.3
0.4
0.5
0.6
MAX DELTA LG TAUNY



MAX ERROR IN PERCENT
0
10
20
30
40
50
0.2
0.4
0.6
0.8
1.0
1.2
JUMP IN MAX DELTA LG TAU
Hermite
Standard
Spline



5
4
3
2
1
0
−1
−2
ERROR IN PERCENT
$\Delta \lg \tau_{5000} = 0.2$
$\max_{0.01<\tau_{\nu\mu}<10} \Delta \lg \tau_{\nu\mu} = 0.2$
0.0
0.2
0.4
0.6
0.8
1.0
WAVELENGTH (A)

Velocity fields and blends

Integral methods

- Treat outgoing and incoming rays separately
- Fit source function with a function (e.g. cubic spline)
- Integrate fitting function analytically

MULTI

MULTI

http://folk.uio.no/matsc/mul23

Also: ~carlsson/mul23.tar on sagami

- 1D
- Statistical equilibrium
- given atmosphere {T, Ne, Vz, Vmic}(x)
- one element at a time
- continuum opacity in LTE
- Complete Redistribution
- Hydrostatic equilibrium can be solved for

MULTI documentation

in http://folk.uio.no/matsc/mul23

multi_manual.pdf	quick start manual
report33.pdf	version 1.0 documentation
mul23.pdf	version 2.3 documentation
idldoc.pdf	IDL routines documentation
multi_exercises.pdf	exercises

MULTI

Input files

ATMOS	atmospheric structure
DSCALE	depth discretization
ABUND	abundances
ABSDAT	background opacities
ATOM	atomic data
INPUT	switches, run-parameters

Output

IDL files
JOBLOG
OUT

ATMOS

```
  VAL3C
  MASS SCALE
*
* LG G
  4.44
*
* NDEP
  52
*
*LG CMASS         TEMPERATURE       NE            V                 VTURB
  -5.279262E+00   4.470000E+05   1.205000E+09   0.              1.128000E+01
  -5.270430E+00   1.410000E+05   3.839000E+09   0.              9.870000E+00
  -5.269783E+00   8.910000E+04   5.961000E+09   0.              9.820000E+00
  -5.268492E+00   5.000000E+04   9.993000E+09   0.              9.760000E+00
...
*
*  HYDROGEN POPULATIONS
*  NH(1)        NH(2)        NH(3)        NH(4)        NH(5)        NP
   2.3841E+03   7.9839E-04   2.0919E-04   2.3110E-04   2.9470E-04   1.0030E+09
   5.3401E+04   1.8790E-02   7.4560E-03   8.1751E-03   1.0430E-02   3.1990E+09
   2.4030E+05   7.5740E-02   2.9400E-02   3.1550E-02   4.0101E-02   5.0310E+09
...
```

DSCALE

```
* DEPTH SCALE FROM DSCAL2
 DSCAL2 ON equidistant
 MASS SCALE
* NDEP    lg(Tau_500[1])
  80      -6.672232
      -5.225000
      -5.213486
...
```

ABUND

```
H    1.000E+00
HE   1.000E-01
SI   3.548E-05         from Grevesse 1989
MG   3.802E-05         from Grevesse 1989
AL   2.951E-06         from Grevesse 1989
FE   4.677E-05         from Grevesse 1989
C    3.631E-04         from Grevesse 1989
NA   1.514E-06
S    1.622E-05
K    1.122E-07
CA   2.138E-06
NI   1.202E-07
CR   2.951E-07
N    8.511E-05
O    5.888E-04
NE   3.236E-04
SC   1.259e-09         from Grevesse 1989
TI   9.772e-08         from Grevesse 1989
V    1.000e-08         from Grevesse 1989
MN   2.455e-07         from Grevesse 1989
CO   8.318e-08         from Grevesse 1989
```

ABUND

```
H   12.00     abundances from
HE  10.93     Asplund, Grevesse, Sauval, Scott 2009, ARAA 47, 481
SI   7.51
MG   7.60
AL   6.45
FE   7.50
C    8.43
NA   6.24
S    7.12
K    5.03
CA   6.34
NI   6.22
CR   5.64
N    7.83
O    8.69
NE   7.93
SC   3.15
TI   4.95
V    3.93
MN   5.43
CO   4.99
```

ABSDAT

```
         21
H  HE C   N   O   NE NA MG AL SI S   K   CA SC TI V   CR MN FE CO NI
      1.008      4.003      12.01      14.01      16.00      20.18
      23.00      24.32      26.97      28.06      32.06      39.10
      40.08      45.0       47.9       50.9       52.01      54.9
      55.85      58.9       58.69
     2    3    4    4    4    4    4    4    4    4    4    4
     4    4    4    4    4    4    4    4    4
     2    1
H I
13.595   2 11.0     2
H I
...
/CA II 3P6 4S 2SE      CA III GROUND TERM   P.JUDGE / COMPILATION
 2           0.000    2.0
   ILOGL=1   KVADL=0   MINEX=0   MAXEX=0  NLATB= 11
      510.       600.       750.       850.       950.      1000.
     1020.      1026.      1030.      1035.      1045.
   ILOGT=0   KVADT=0   MINET=0   MAXET=0  NTETB=  1   ITETA=0
 1.557E-19 1.836E-19 2.101E-19 2.183E-19 2.142E-19 2.122E-19
 2.101E-19 2.081E-19 2.060E-19 2.060E-19 2.040E-19
...
```

ATOM

```
CA II
* ABUND   AWGT
  6.36   40.08
*NK NLINE NCONT NRFIX
  6   5    5     0
*   E          G         LABEL                  ION
   0.00000   2.00000   'CA II 3P6 4S 2SE     '   2
 13650.248   4.00000   'CA II 3P6 3D 2DE 3/2'   2
 13710.900   6.00000   'CA II 3P6 3D 2DE 5/2'   2
 25191.535   2.00000   'CA II 3P6 4P 2PO 1/2'   2
 25414.465   4.00000   'CA II 3P6 4P 2PO 3/2'   2
 95785.470   1.00000   'CA III GROUND TERM  '   3
* J  I      F        NQ  QMAX  Q0 IW    GA       GVW      GS
  4  1  3.1600E-01 101  300.  3. 0  1.42E08  234.223  3.0E-06
  5  1  6.3700E-01 101  300.  3. 0  1.46E08  234.223  3.0E-06
  4  2  4.7300E-02 101  150.  1. 0  1.42E08    2.04   3.0E-06
  5  2  9.6000E-03 101  150.  1. 0  1.46E08    2.01   3.0E-06
  5  3  5.7400E-02 101  150.  1. 0  1.46E08    2.01   3.0E-06
* UP  LO   F        NQ   QMAX    Q0
   6  1  2.036E-19  5   -1.     0.0
  1044.2   2.0360E-19
   911.7   2.1400E-19
   850.0   2.1720E-19
   750.0   2.1030E-19
   600.0   1.8200E-19
*
...
 GENCOL
 TEMP
  7     2000.     3000.     6000.     12000.     24000.     48000.     96000.
OHMEGA
  2  1  5.60e+00  5.60e+00  5.60e+00  5.60e+00  5.60e+00  5.60e+00  5.60e+00
OHMEGA
...
```

INPUT

```
DIFF=2.0,ELIM1=0.1,ELIM2=0.001,QNORM=12.85,THIN=0.1,
IATOM2=0,ICONV=1,IHSE=0,ILAMBD=2,IOPAC=1,ISTART=1,ISUM=0,
ITMAX=40,ITRAN=0,NMU=5,
IWABND=0,IWATMS=0,IWATOM=0,IWCHAN=0,IWDAMP=0,IWEMAX=1,IWEQW=0,
IWEVEC=0,IWHEAD=0,IWHSE=0,IWLGMX=1,IWLINE=0,IWLTE=0,IWN=0,IWNIIT=0,
IWOPAC=0,IWRAD=0,IWRATE=0,IWSTRT=0,IWTAUQ=0,IWTEST=0,IWWMAT=0,
IWJFIX=0,IWARN=0,IOPACL=0,ISCAT=0,INCRAD=0,INGACC=0,ICRSW=0,
IOSMET=0,EOSMET=0.5,
IDL1=1,IDLNY=1,IDLCNT=1,IDLOPC=1
```

ALI

Split the lambda operator into an approximate part and a correction

$$\boldsymbol{\Lambda}_\nu = \boldsymbol{\Lambda}^* + (\boldsymbol{\Lambda}_\nu - \boldsymbol{\Lambda}^*) \tag{5.39}$$

$$J_\nu = \boldsymbol{\Lambda}^*_\nu[S] + (\boldsymbol{\Lambda}_\nu - \boldsymbol{\Lambda}^*_\nu)[S] \tag{5.40}$$

Classical lambda-iteration: $S^{(n+1)} = (1-\varepsilon)\,\boldsymbol{\Lambda}[S^{(n)}] + \varepsilon B,$ then becomes (5.33)

NB!

$$S^{(n+1)} = (1-\varepsilon)\,\boldsymbol{\Lambda}^*[S^{(n+1)}] + (1-\varepsilon)(\boldsymbol{\Lambda}_\nu - \boldsymbol{\Lambda}^*)[S^{(n)}] + \varepsilon B \tag{5.41}$$

$$\begin{aligned} S^{(n+1)} - (1-\varepsilon)\,\boldsymbol{\Lambda}^*[S^{(n+1)}] &= \boxed{(1-\varepsilon)\,\boldsymbol{\Lambda}_\nu[S^{(n)}] + \varepsilon B} - (1-\varepsilon)\,\boldsymbol{\Lambda}^*[S^{(n)}] \\ &= \boxed{S^{\mathrm{FS}}} - (1-\varepsilon)\,\boldsymbol{\Lambda}^*[S^{(n)}], \end{aligned} \tag{5.42}$$

$$S^{(n+1)} = (1-(1-\varepsilon)\,\boldsymbol{\Lambda}^*)^{-1}\left[S^{\mathrm{FS}} - (1-\varepsilon)\,\boldsymbol{\Lambda}^*[S^{(n)}]\right]. \tag{5.43}$$

Classical lambda-iteration: $S^{(n+1)} - S^{(n)} = S^{\mathrm{FS}} - S^{(n)},$ (5.44)

Accelerated lambda-iteration:

$$S^{(n+1)} - S^{(n)} = (1-(1-\varepsilon)\,\boldsymbol{\Lambda}^*)^{-1}\,[S^{\mathrm{FS}} - S^{(n)}]. \tag{5.45}$$

Different choices of approximate lambda operator

Core saturation

Scharmer modified core saturation

Scharmer operator: one point quadrature formula

$$I_\nu(\tau_{\nu\mu},\mu) \equiv I^{\pm}_{\nu\mu} = \mathbf{\Lambda}^*_{\nu\mu}[S_\nu(\tau_{\nu\mu})] \approx W^{\pm}_{\nu\mu}(\tau_{\nu\mu})\, S_\nu\left(f^{\pm}_{\nu\mu}(\tau_{\nu\mu})\right), \tag{5.52}$$

Use a linear test source function to deduce the W and f

$\mu > 0$

$$\begin{aligned} W^{+}_{\nu\mu} &= 1 \\ f^{+}_{\nu\mu} &= \tau_{\nu\mu} + 1 \end{aligned} \tag{5.60}$$

=EB

$\mu < 0$

$$\begin{aligned} W^{-}_{\nu\mu} &= 1 - \mathrm{e}^{-\tau_{\nu\mu}} \\ f^{-}_{\nu\mu} &= \frac{\tau_{\nu\mu}}{1 - \mathrm{e}^{-\tau_{\nu\mu}}} - 1 \end{aligned} \tag{5.62}$$

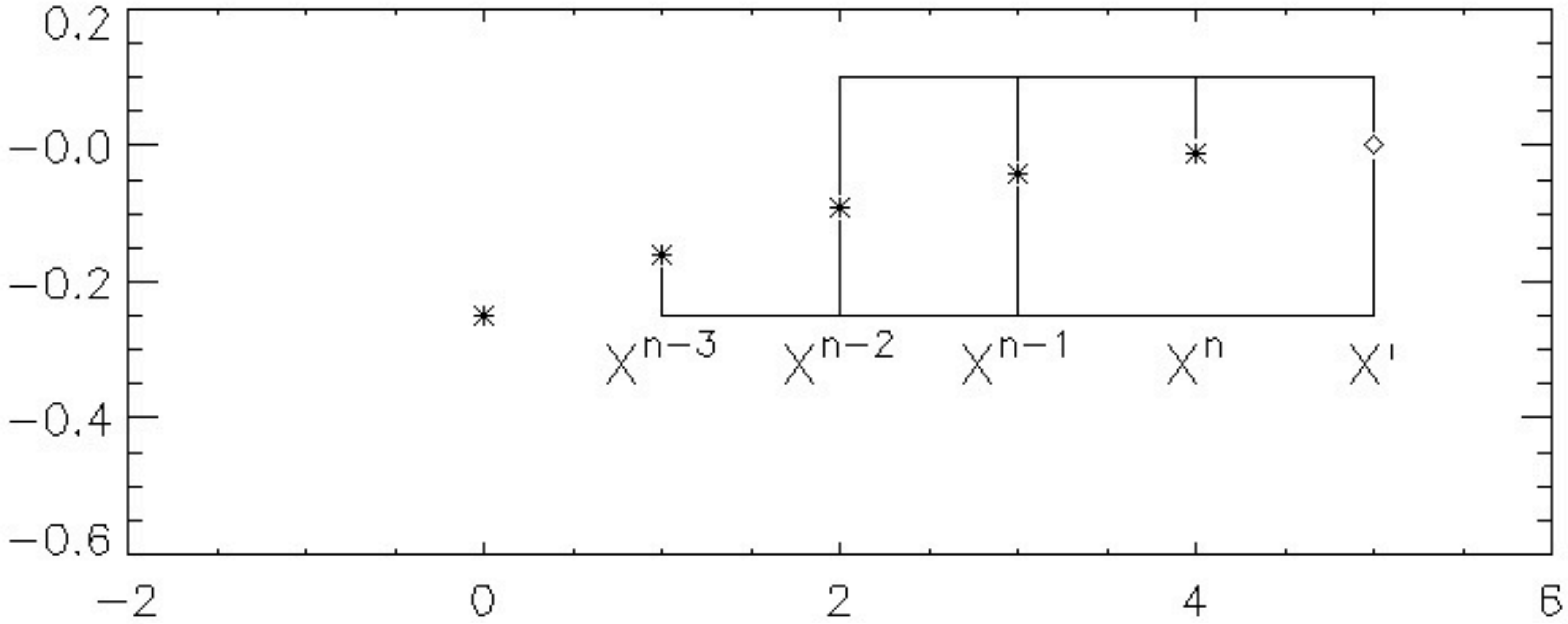
Olson-Auer-Buchler (OAB) operator

The diagonal of the full lambda operator

- Easy to construct (Rybicki-Hummer 1991)
- Easy to “invert” (diagonal matrix)
- Easy to adopt to 3D geometry
- Slow convergence - needs acceleration steps

Convergence acceleration

Ng-acceleration



We use M previous iterations to extrapolate $\mathbf{x}$

$$\mathbf{x} = \left(1 - \sum_{m=1}^{M} \alpha_m\right)\mathbf{x}^{(n)} + \sum_{m=1}^{M} \alpha_m \mathbf{x}^{(n-m)}$$

$= \alpha_0$ because $\sum_{m=0}^{M} \alpha_m = 1$

Same coefficients applied to one iteration back

$$\mathbf{x}' = \left(1 - \sum_{m=1}^{M} \alpha_m\right)\mathbf{x}^{(n-1)} + \sum_{m=1}^{M} \alpha_m \mathbf{x}^{(n-m-1)}$$

α_m determined by minimizing distance between vectors $\mathbf{x}$ and $\mathbf{x}'$ with weights w

minimize $\quad r^2 = \sum w_d (x_d - x'_d)^2$

$$\frac{\partial}{\partial \alpha_i}\left[r^2\right] = 0, \forall i \qquad \text{gives}$$

$$0 = \sum_{d=1}^{N} w_d (x_d - x'_d)\left(\frac{\partial x_d}{\partial \alpha_i} - \frac{\partial x'_d}{\partial \alpha_i}\right), \forall i$$

$$0 = \sum_{d=1}^{N} w_d \left[(1 - \sum_{j=1}^{M} \alpha_j) x_d^{(n)} + \sum_{j=1}^{M} \alpha_j x_d^{(n-j)} - (1 - \sum_{j=1}^{M} \alpha_j) x_d^{(n-1)} - \sum_{j=1}^{M} \alpha_j x_d^{(n-j-1)}\right] \times$$

$$\times \left[-x_d^{(n)} + x_d^{(n-i)} + x_d^{(n-1)} - x_d^{(n-i-1)}\right]$$

introducing

$$\Delta x_d^{(n)} \equiv x_d^{(n)} - x_d^{(n-1)}$$

we get

$$\sum_{d=1}^{N} w_d \sum_{j=1}^{M} \alpha_j(-x_d^{(n)} + x_d^{(n-j)} + x_d^{(n-1)} - x_d^{(n-j-1)})[\Delta x_d^{(n-i)} - \Delta x_d^{(n)}] =$$

$$-\sum_{d=1}^{N} w_d[x_d^{(n)} - x_d^{(n-1)}][\Delta x_d^{(n-i)} - \Delta x_d^{(n)}]$$

we thus get a matrix equation

$$\boldsymbol{A\alpha} = \boldsymbol{b}$$

$$A_{ij} = \sum_{d=1}^{N} w_d(\Delta x_d^{(n)} - \Delta x_d^{(n-j)})(\Delta x_d^{(n)} - \Delta x_d^{(n-i)})$$

$$b_i = \sum_{d=1}^{N} w_d \Delta x_d^{(n)}(\Delta x_d^{(n)} - \Delta x_d^{(n-i)})$$

Linearization

$$x^2 = 2$$

$$(x^{(n)})^2 = 2 + E^{(n)}$$

$$(x^{(n)} + \delta x^{(n)})^2 = 2$$

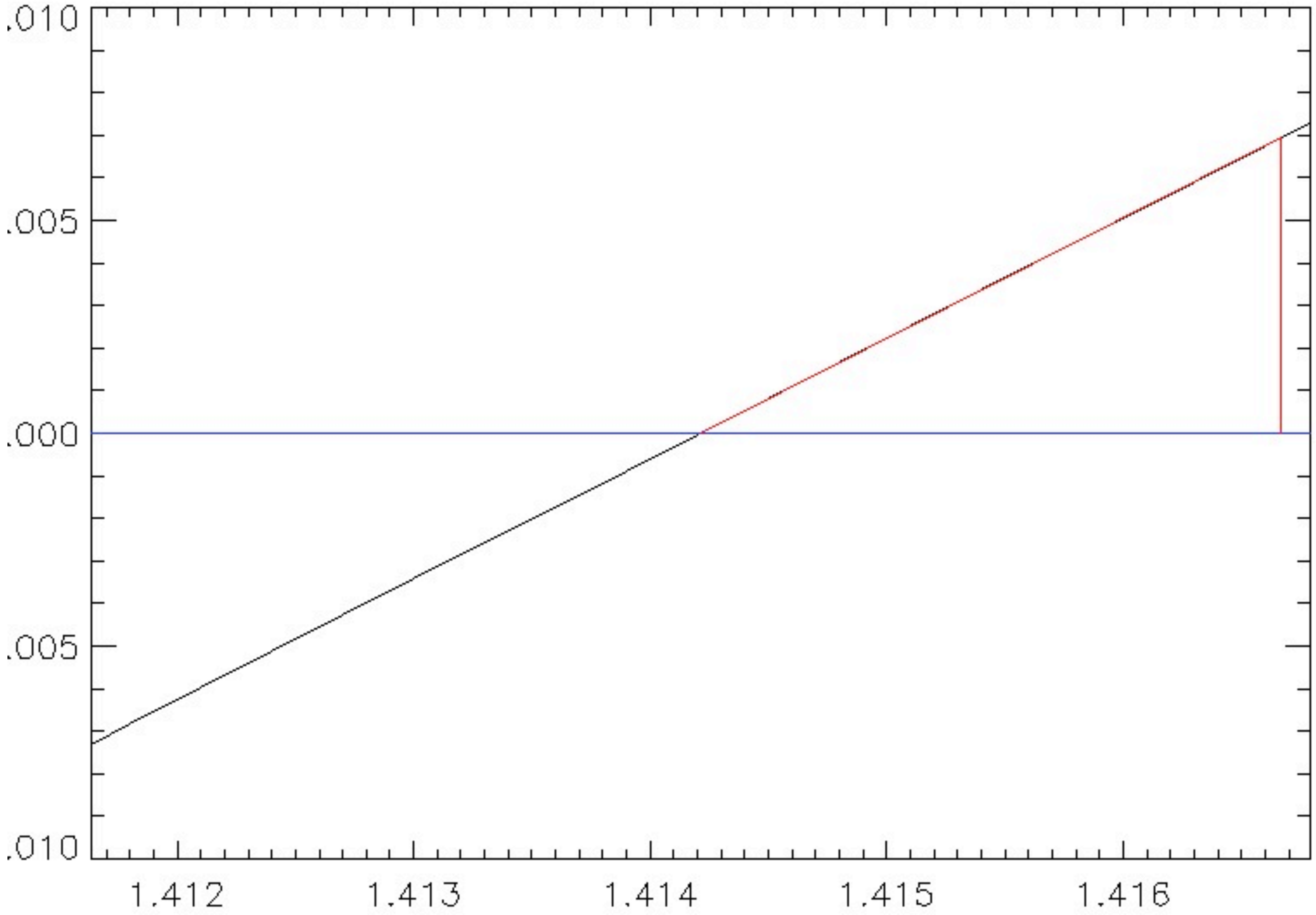
$$(x^{(n)})^2 + 2x^{(n)}\delta x^{(n)} + \cancel{(\delta x^{(n)})^2} = 2$$

$$\boxed{2x^{(n)}\delta x^{(n)} = -E^{(n)}}$$

$$\delta x^{(n)} = \frac{-E^{(n)}}{2x^{(n)}} = \frac{2 - (x^{(n)})^2}{2x^{(n)}}$$

n	$x^{(n)}$	$lg\|x - \sqrt{2}\|$
0	1	-0.4
1	1.5	-1.1
2	1.416	-2.6
3	1.414216	-5.7
4	1.414213562	-11.8

Newton-Raphson



Convergence radius

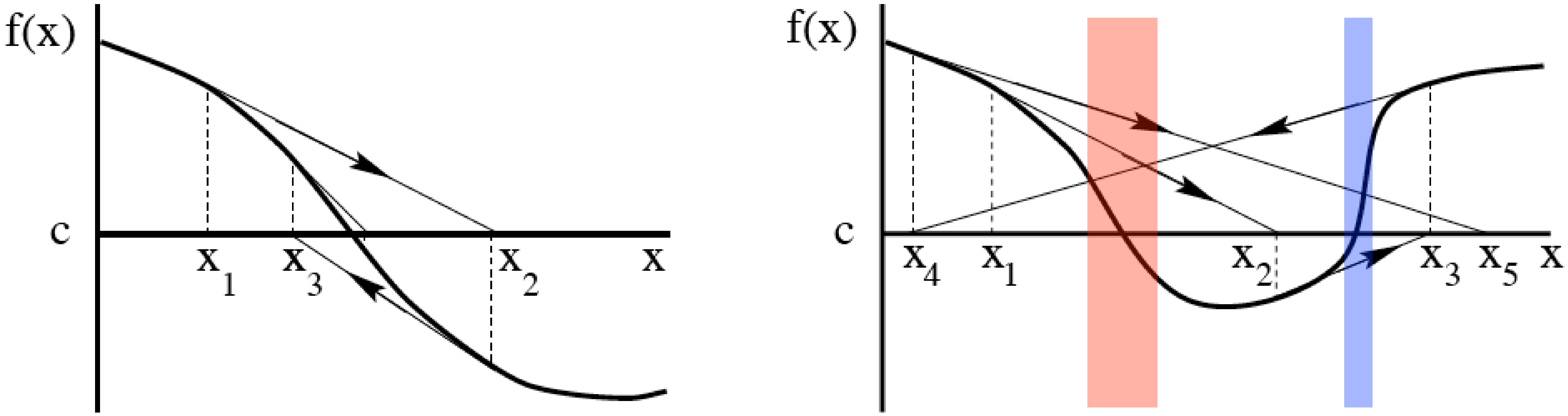
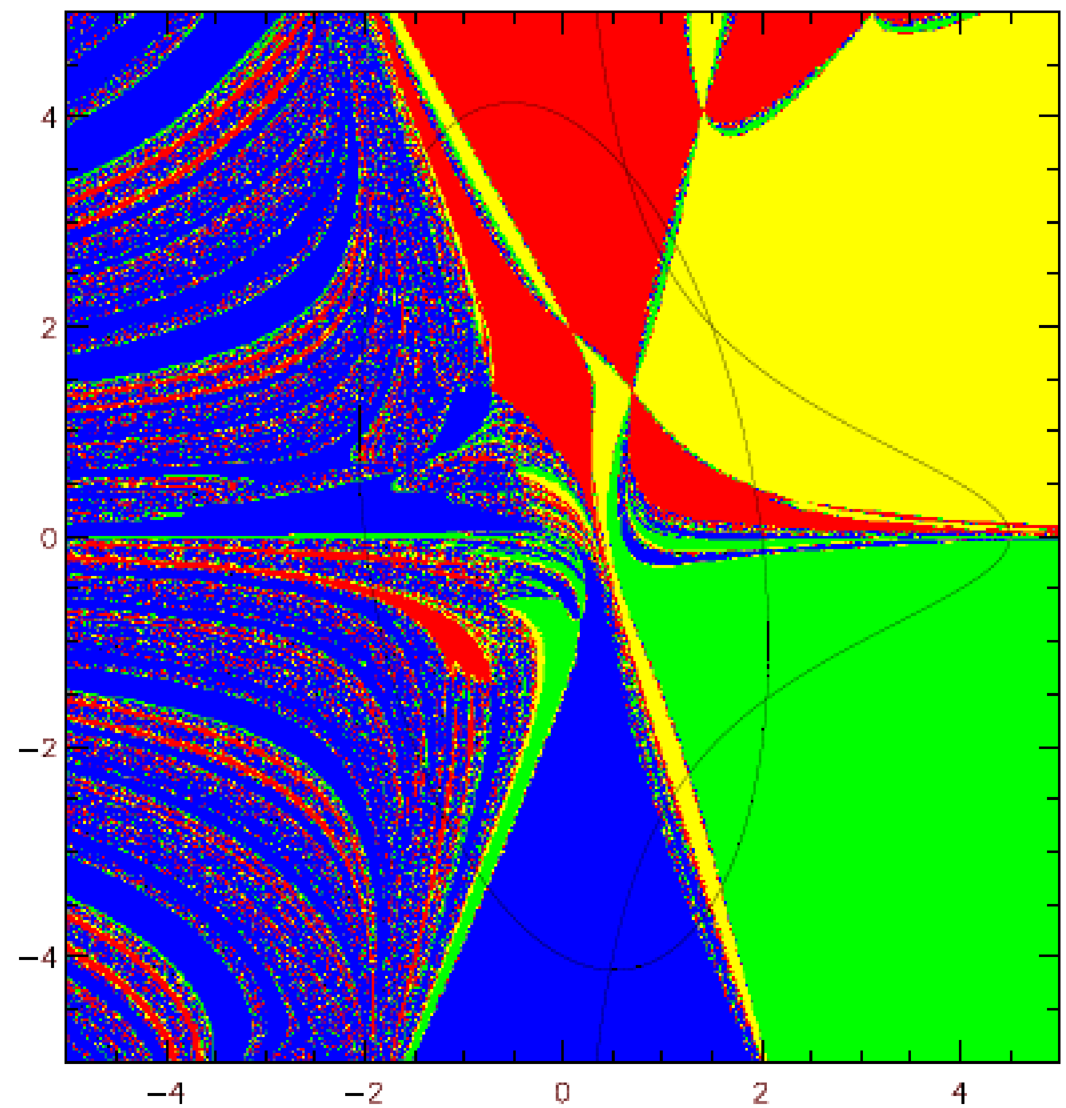


Figure 5.3: Newton-Raphson iteration to find the x for which $f(x) = c$. Find the tangent to $f(x)$ at the first estimate $x = x_1$, find its intersection $x = x_2$ with the constant c, find the tangent to $f(x)$ there, locate its intersection at $x = x_3$, and so on. It works well at left but won't find either solution at right. The convergence region around the solution is small.

Systems of equations

$$\begin{cases} 4x^2 + xy + y^2 - 16 = & 0 \\ 2x + xy^2 - 9 = & 0 \end{cases}$$

$$\begin{pmatrix} 8x^{(n)} + y^{(n)} & x^{(n)} + 2y^{(n)} \\ 2 + (y^{(n)})^2 & 2x^{(n)}y^{(n)} \end{pmatrix} \begin{pmatrix} \delta x^{(n)} \\ \delta y^{(n)} \end{pmatrix} = \begin{pmatrix} -4(x^{(n)})^2 - x^{(n)}y^{(n)} - (y^{(n)})^2 + 16 \\ -2x^{(n)} - x^{(n)}(y^{(n)})^2 + 9 \end{pmatrix}$$



non-LTE

Transfer equation

The intensity depends on the opacity and the source function. The opacity depends on population densities.

Local Thermodynamic Equilibrium (LTE):

- Source function: Planck function
- Population densities: f(T,Ne) (Saha, Boltzmann)

non-LTE:

Source function and population densities depend on the non-local radiation field

non-LTE

$$\frac{dI}{d\tau} = S - I \qquad f(\nu, \mu)$$

$$S_l = \frac{n_j A_{ji} \Psi}{n_i B_{ij} \Phi - n_j B_{ji} \Psi_{se}} \qquad f(\nu, \mu)$$

$$\frac{Dn_i}{Dt} = \sum_{j \neq i}^{N} n_j P_{ji} - n_i \sum_{j \neq i}^{N} P_{ij}$$

P_{ij} is the probability for a transition from level i to level j

non-LTE (CRD)

$$P_{ij} = R_{ij} + C_{ij}$$

$$\begin{aligned} R_{ji} &= A_{ji} + B_{ji}\bar{J}_{ij} \\ R_{ij} &= B_{ij}\bar{J}_{ij} \end{aligned}$$

with A_{ji}, B_{ij} and B_{ji} the Einstein coefficients for spontaneous emission, absorption and stimulated emission, respectively. All these are given by atomic physics. $\bar{J}_{ij}$ is the absorption profile ($\phi_{\nu\mu}$) weighted integrated mean intensity:

$$\bar{J}_{ij} = \frac{1}{2}\int_{-1}^{1}\int_{0}^{\infty}\phi_{\nu\mu}I_{\nu\mu}d\nu d\mu$$

non-LTE

$$\frac{Dn_i}{Dt} = \sum_{j \neq i}^{N} n_j P_{ji} - n_i \sum_{j \neq i}^{N} P_{ij}$$

P_{ij} contains the intensities and thus an integral of the source function over the whole atmosphere. The source function depends on the population densities. We thus have a non-local, non-linear problem to solve.

Statistical equilibrium, particle conservation and radiative transfer equations are to be solved together through linearization

(Equation numbers from Uppsala Report 33)

$$n_i \sum_{j \neq i}^{n_l} P_{ij} - \sum_{j \neq i}^{n_l} n_j P_{ji} = 0 \qquad (2.1)$$

$$\sum_{j=1}^{n_l} n_j = n_{tot} \qquad (2.2)$$

$$\mu \frac{dI_{\nu\mu}}{dz} = -\kappa_{\nu\mu} I_{\nu\mu} + j_{\nu\mu} \qquad (2.3)$$

Rates are the sum of radiative and collisional rates

$$P_{ij} = R_{ij} + C_{ij} \tag{2.4}$$

Radiative (bb) and (bf) rates can be written in general form

$$R_{ij} = \begin{cases} \frac{1}{2} \int\limits_{-1}^{1} \int\limits_{0}^{\infty} \frac{4\pi}{h\nu} \alpha_{ji} G_{ji} (I_{\nu\mu} + \frac{2h\nu^3}{c^2}) d\nu d\mu & \text{if } i > j \\ \frac{1}{2} \int\limits_{-1}^{1} \int\limits_{0}^{\infty} \frac{4\pi}{h\nu} \alpha_{ij} I_{\nu\mu} d\nu d\mu & \text{if } i < j \end{cases} \tag{2.5}$$

$$\alpha_{ij} = \begin{cases} B_{ij} \frac{h\nu_{ij}}{4\pi} \phi_{\nu\mu} & \text{(b-b);} \\ \alpha_c(\nu) & \text{(b-f).} \end{cases} \tag{2.6}$$

$$G_{ij} = \begin{cases} g_i / g_j & \text{(b-b);} \\ \frac{n_i^\star}{n_j^\star} e^{\frac{-h\nu}{kT}} & \text{(b-f).} \end{cases} \tag{2.7}$$

For bb transitions this simplifies to the familiar form:

$$R_{ij} = \begin{cases} A_{ij} + B_{ij}\bar{J}_{ij}, & \text{if } i > j; \\ B_{ij}\bar{J}_{ij}, & \text{if } i < j. \end{cases} \tag{2.8}$$

$$\bar{J}_{ij} = \frac{1}{2}\int\limits_{-1}^{1}\int\limits_{0}^{\infty} \phi_{\nu\mu} I_{\nu\mu} d\nu d\mu \tag{2.9}$$

$$\frac{1}{2}\int_{-1}^{1}\int_{0}^{\infty} \phi_{\nu\mu} d\nu d\mu = 1$$

Opacity and emissivity in general form:

Background (continuum) contribution

$$\kappa_{\nu\mu} = \kappa_{\nu c} + \alpha_{ij}(\nu, \mu)(n_i - G_{ij} n_j) \tag{2.10}$$

$$j_{\nu\mu} = j_{\nu c} + \frac{2h\nu^3}{c^2} G_{ij} \alpha_{ij}(\nu, \mu) n_j \tag{2.11}$$

$$S_{\nu\mu} = j_{\nu\mu} / \kappa_{\nu\mu} \tag{2.12}$$

(Equation numbers from Scharmer & Carlsson 1981)

$$n_i^{(n)} \sum_{j \neq i}^{n_l} P_{ij}^{(n)} - \sum_{j \neq i}^{n_l} n_j^{(n)} P_{ji}^{(n)} = E_i^{(n)} \qquad (3.1)$$

$$n_i^{(n+1)} = n_i^{(n)} + \delta n_i^{(n)} \qquad (3.2)$$

$$P_{ij}^{(n+1)} = P_{ij}^{(n)} + \delta P_{ij}^{(n)} \qquad (3.3)$$

$$n_i^{(n+1)} \sum_{j \neq i}^{n_l} P_{ij}^{(n+1)} - \sum_{j \neq i}^{n_l} n_j^{(n+1)} P_{ji}^{(n+1)} = 0 \qquad (3.4)$$

We insert 3.2 and 3.3 in 3.4, subtract 3.1 and neglect non-linear terms

$$\delta n_i^{(n)} \sum_{j \neq i}^{n_l} P_{ij}^{(n)} + n_i^{(n)} \sum_{j \neq i}^{n_l} \delta P_{ij}^{(n)} - \sum_{j \neq i}^{n_l} \delta n_j^{(n)} P_{ji}^{(n)} \quad (3.5)$$

$$- \sum_{j \neq i}^{n_l} n_j^{(n)} \delta P_{ji}^{(n)} = -E_i^{(n)}$$

$$\delta P_{ij}^{(n)} = B_{ij} \delta \bar{J}_{ij}^{(n)} = B_{ij} \frac{1}{2} \int_{-1}^{1} \int_0^{\infty} \phi_{\nu\mu} \delta I_{\nu\mu}^{(n)} d\nu d\mu \quad (3.6)$$

We need to express $\delta I_{\nu\mu}^{(n)}$ in terms of $\delta n_i^{(n)}$ and $\delta n_j^{(n)}$

We use the transfer equation:

$$\mu \frac{dI_{\nu\mu}^{(n)}}{dz} = -\kappa_{\nu\mu}^{(n)} I_{\nu\mu}^{(n)} + j_{\nu\mu}^{(n)} \tag{3.7}$$

$$\mu \frac{d}{dz} \delta I_{\nu\mu}^{(n)} = -\kappa_{\nu\mu}^{(n)} \delta I_{\nu\mu}^{(n)} - I_{\nu\mu}^{(n)} \delta \kappa_{\nu\mu}^{(n)} + \delta j_{\nu\mu}^{(n)} \tag{3.8}$$

Usual definition of optical depth along a ray

$$d\tau_{\nu\mu}^{(n)} = -\kappa_{\nu\mu}^{(n)} dz/\mu \tag{3.9}$$

We *define* an equivalent source function perturbation:

$$\delta S_{\nu\mu}^{(n)} = \delta j_{\nu\mu}^{(n)} / \kappa_{\nu\mu}^{(n)} - I_{\nu\mu}^{(n)} \delta \kappa_{\nu\mu}^{(n)} / \kappa_{\nu\mu}^{(n)} \tag{3.10}$$

This gives the usual transfer equation, now for the perturbations

$$\frac{d}{d\tau_{\nu\mu}^{(n)}} \delta I_{\nu\mu}^{(n)} = \delta I_{\nu\mu}^{(n)} - \delta S_{\nu\mu}^{(n)} \tag{3.11}$$

$$\kappa_{\nu\mu} = \kappa_{\nu c} + \alpha_{ij}(\nu,\mu)(n_i - G_{ij} n_j) \tag{2.10}$$

$$j_{\nu\mu} = j_{\nu c} + \frac{2h\nu^3}{c^2} G_{ij}\alpha_{ij}(\nu,\mu) n_j \tag{2.11}$$

$$\delta S^{(n)}_{\nu\mu} = \delta j^{(n)}_{\nu\mu} / \kappa^{(n)}_{\nu\mu} - I^{(n)}_{\nu\mu} \delta\kappa^{(n)}_{\nu\mu} / \kappa^{(n)}_{\nu\mu} \tag{3.10}$$

Gives

$$\delta S^{(n)}_{\nu\mu} = c^{(n)}_l \delta n^{(n)}_i + c^{(n)}_u \delta n^{(n)}_j \tag{3.13}$$

$$c^{(n)}_l = -\alpha_{ij}(\nu,\mu) I^{(n)}_{\nu\mu} / \kappa^{(n)}_{\nu\mu} \tag{3.14}$$

$$c^{(n)}_u = G_{ij}\alpha_{ij}(\nu,\mu)(\frac{2h\nu^3}{c^2} + I^{(n)}_{\nu\mu}) / \kappa^{(n)}_{\nu\mu} \tag{3.15}$$

We have thus expressed $\delta S^{(n)}_{\nu\mu}$ in $\delta n^{(n)}_i$ and $\delta n^{(n)}_j$

$$\delta I_{\nu\mu}^{(n)} = \Lambda_{\nu\mu}^{(n)}[\delta S_{\nu\mu}^{(n)}] \qquad (3.12)$$

completes the task of expressing

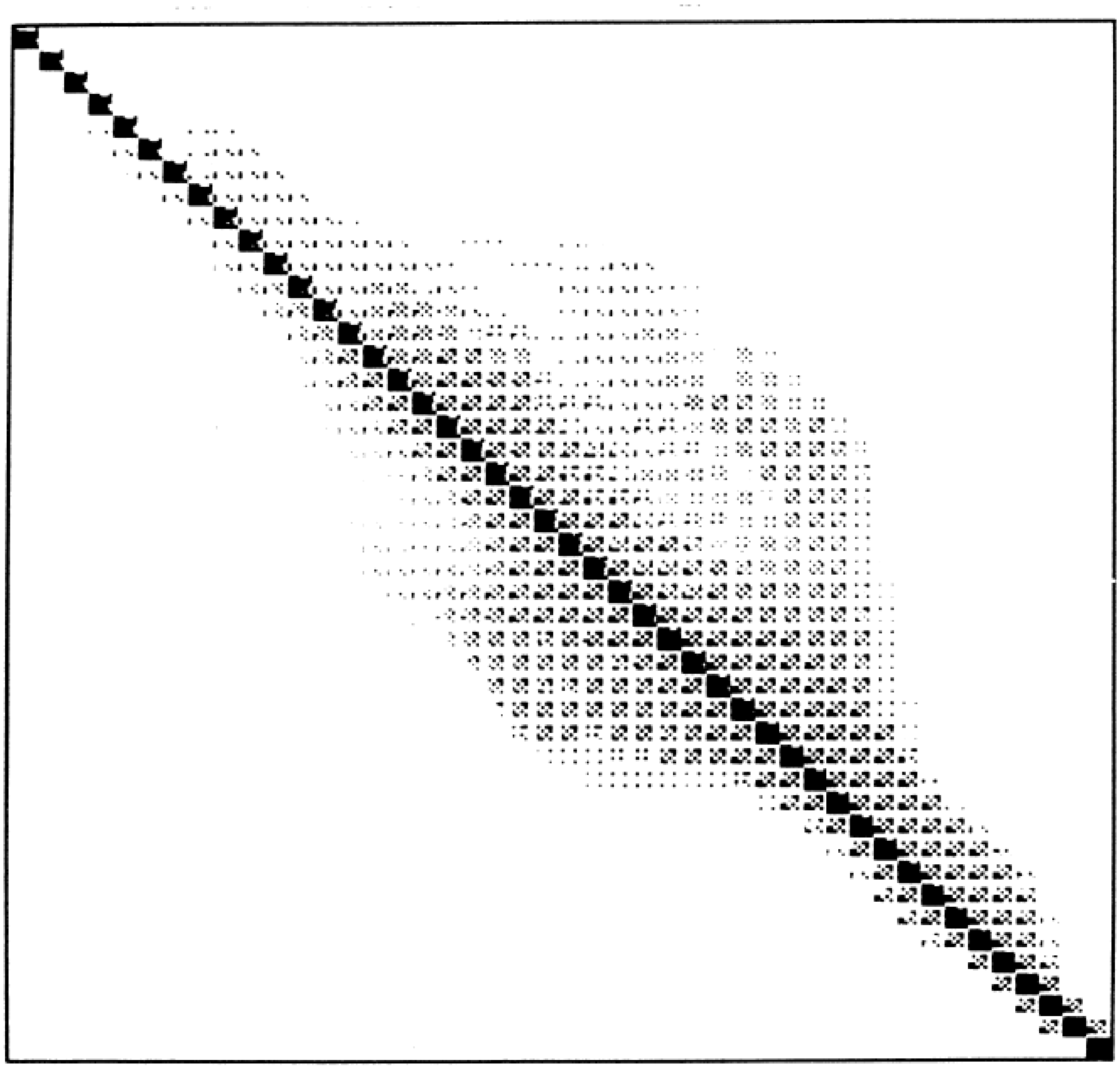
$\delta I_{\nu\mu}^{(n)}$ in terms of $\delta n_i^{(n)}$ and $\delta n_j^{(n)}$

We now have a non-local but linear system of equations for the unknowns $\delta \mathbf{n}$

For $\Lambda_{\nu\mu}^{(n)}$ we may choose

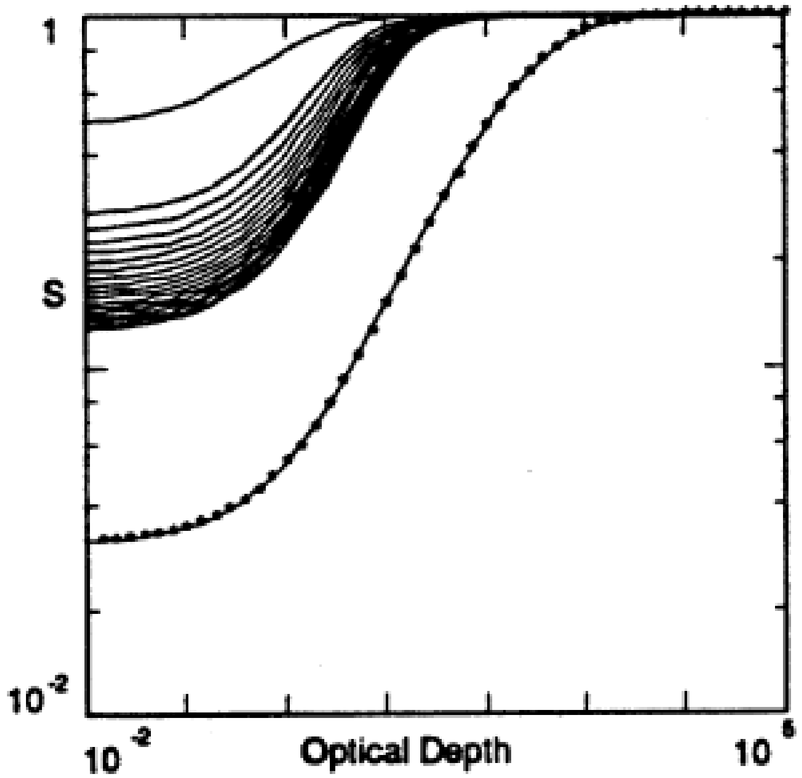
Exact operator: slow to construct, slow to invert
Scharmer's operator: faster and global
Local operator (OAB): fast to construct, invert, but slow convergence.

Coefficient matrix for Scharmer operator

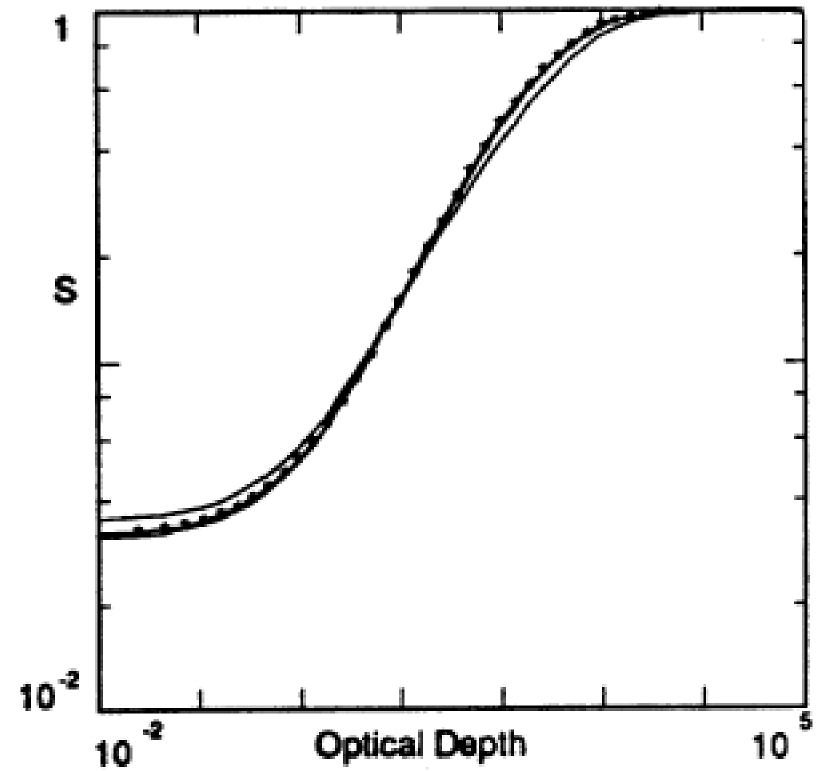


Convergence properties

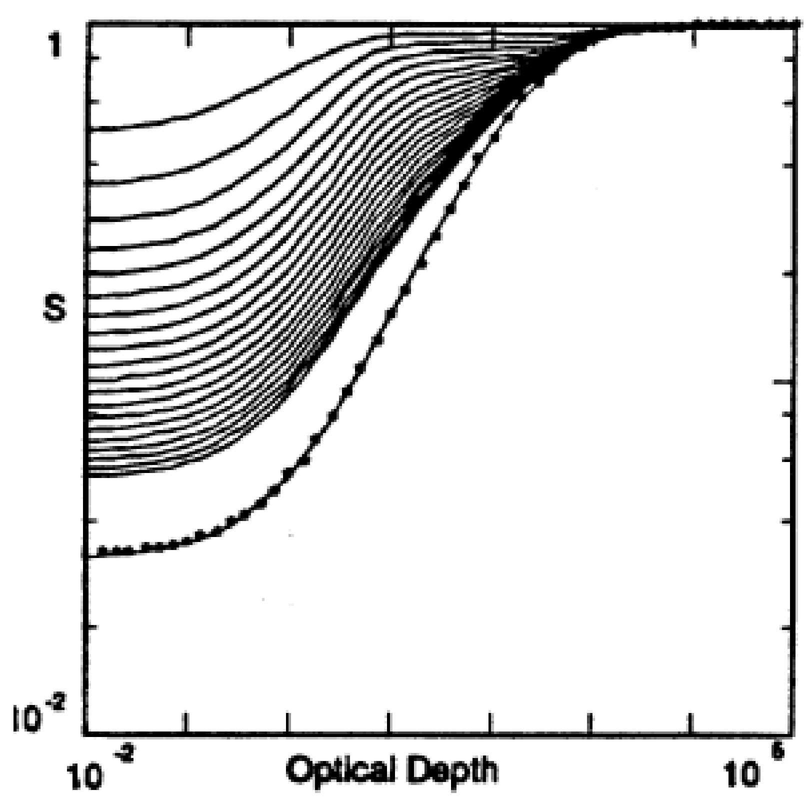
Lambda iteration



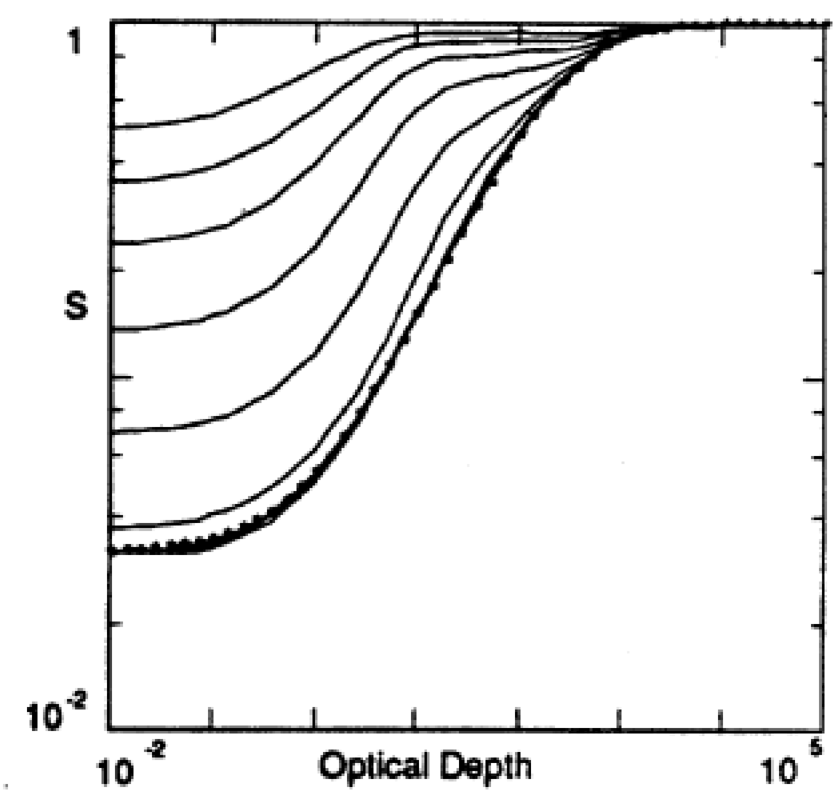
Scharmer operator



Local operator



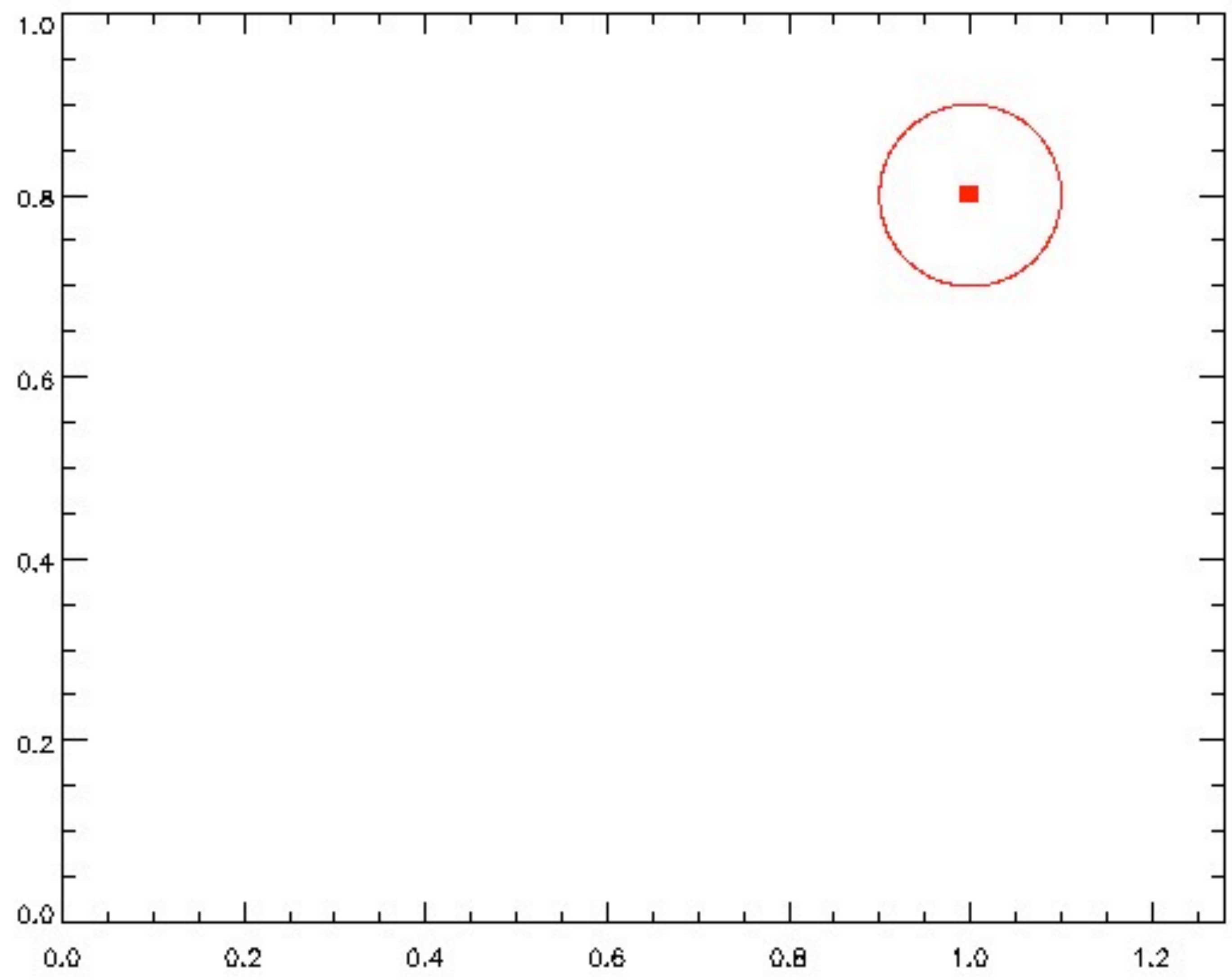
Local + acceleration



CRSW

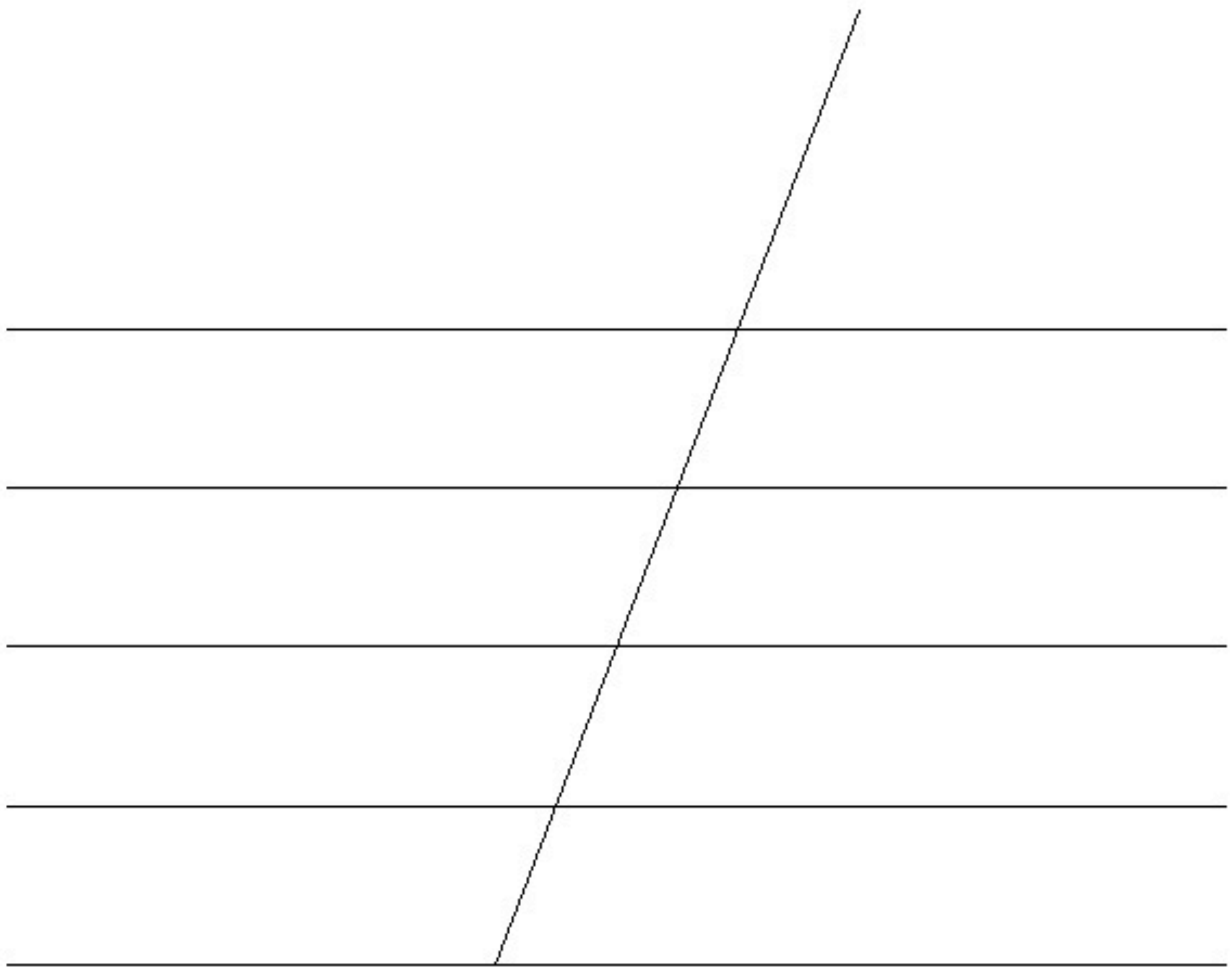
Collisional-Radiative Switching

Multiply collisional rates with a factor that is changed from iteration to iteration

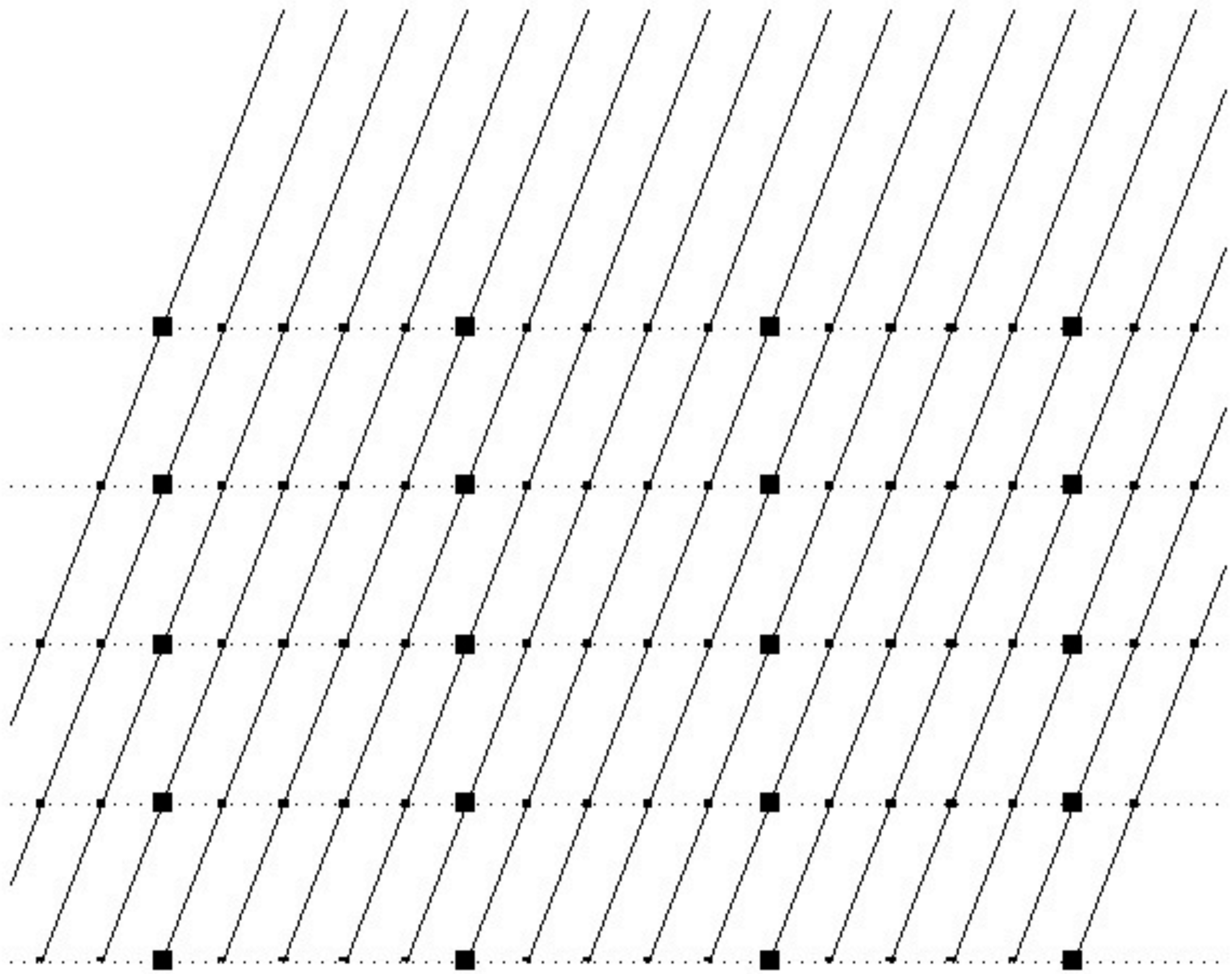


2D-3D

In 1D all rays pass through all grid “points” (planes).

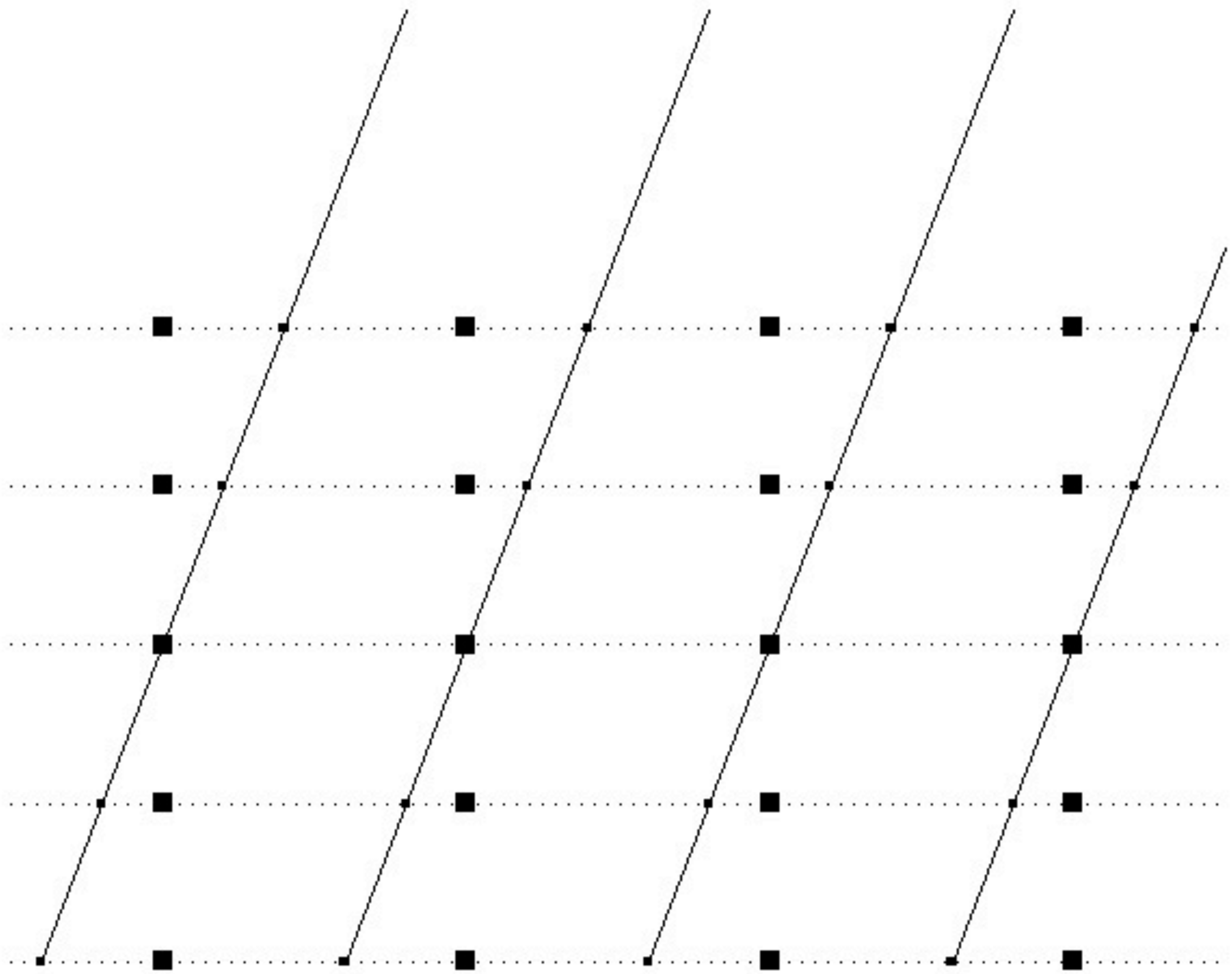


Long characteristics through all grid-points



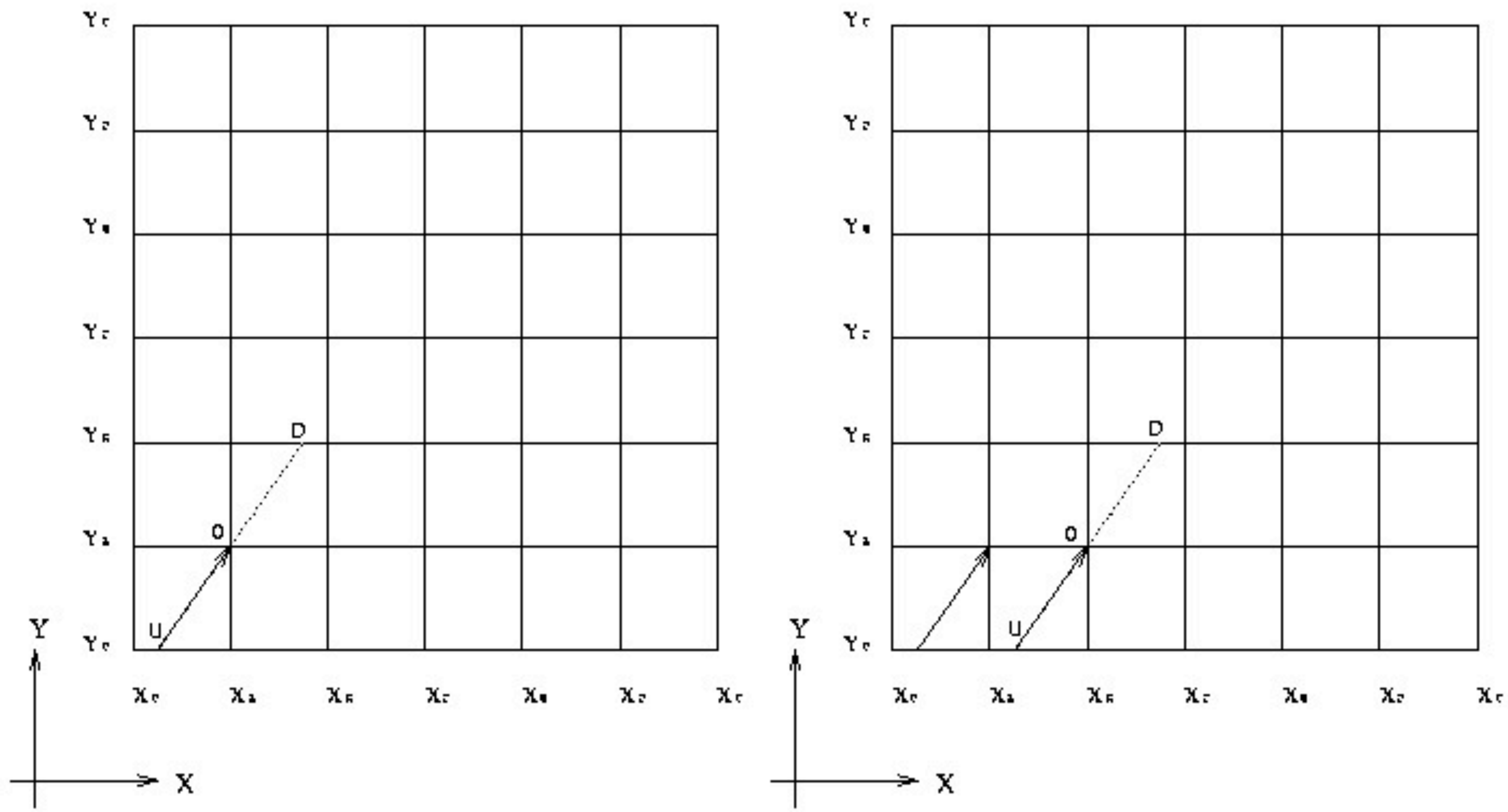
Many rays: slow

Long characteristics through one plane



Fast but may miss localized sources

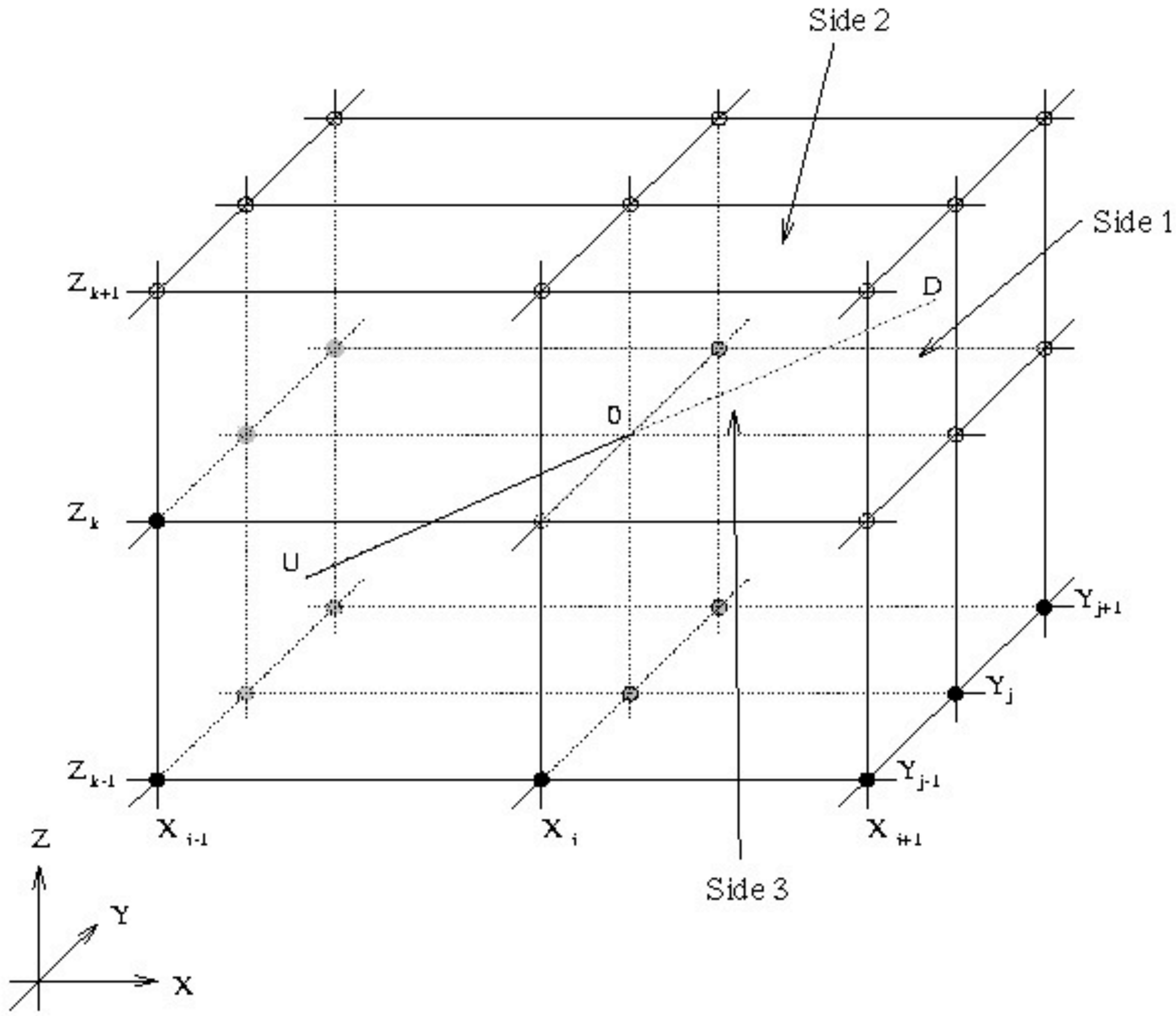
Short characteristics



Approximate S through 3 points (U, O, D), integrate analytically

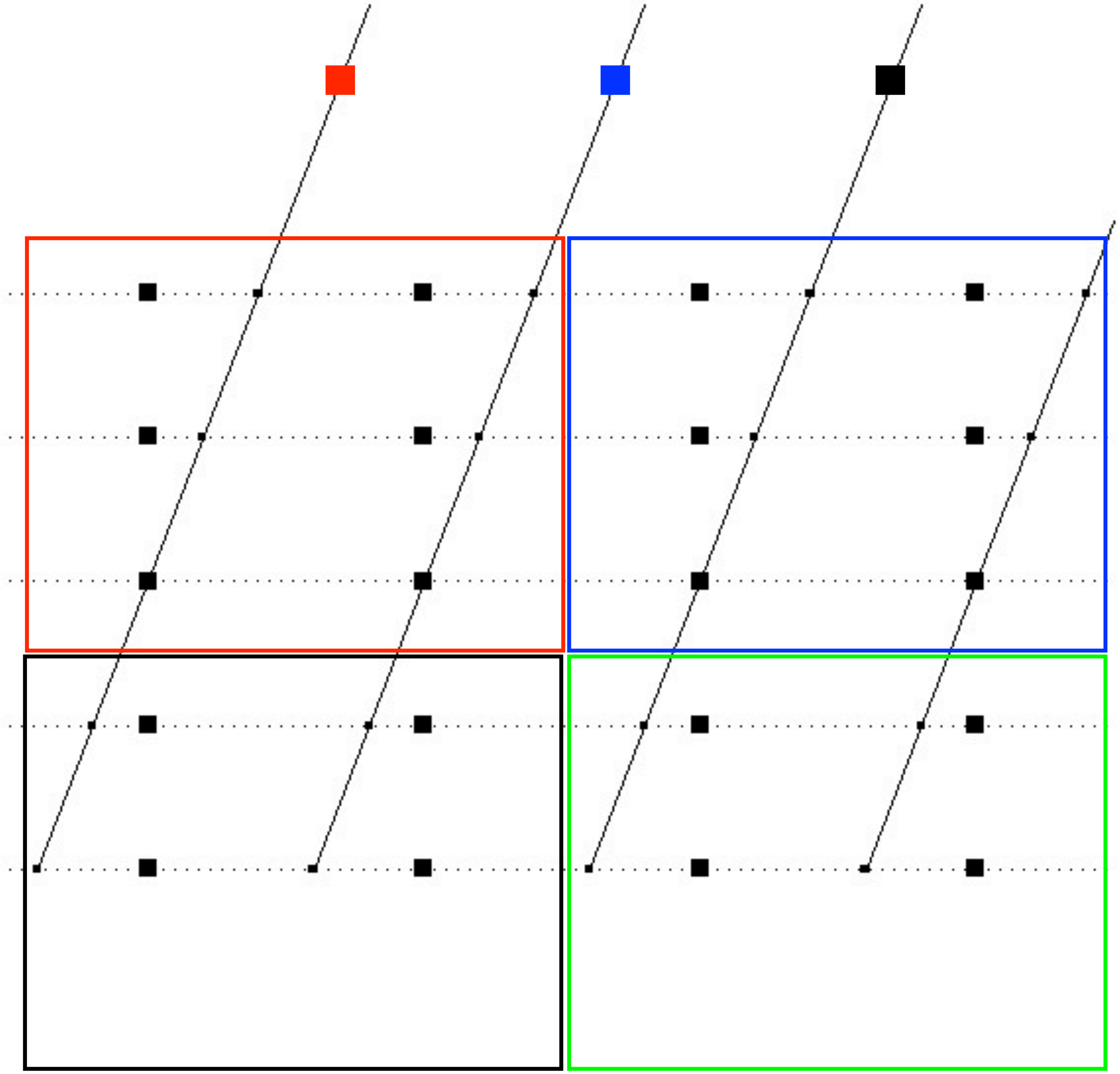
Diffusive

Short characteristics in 3D



Parallelization strategies

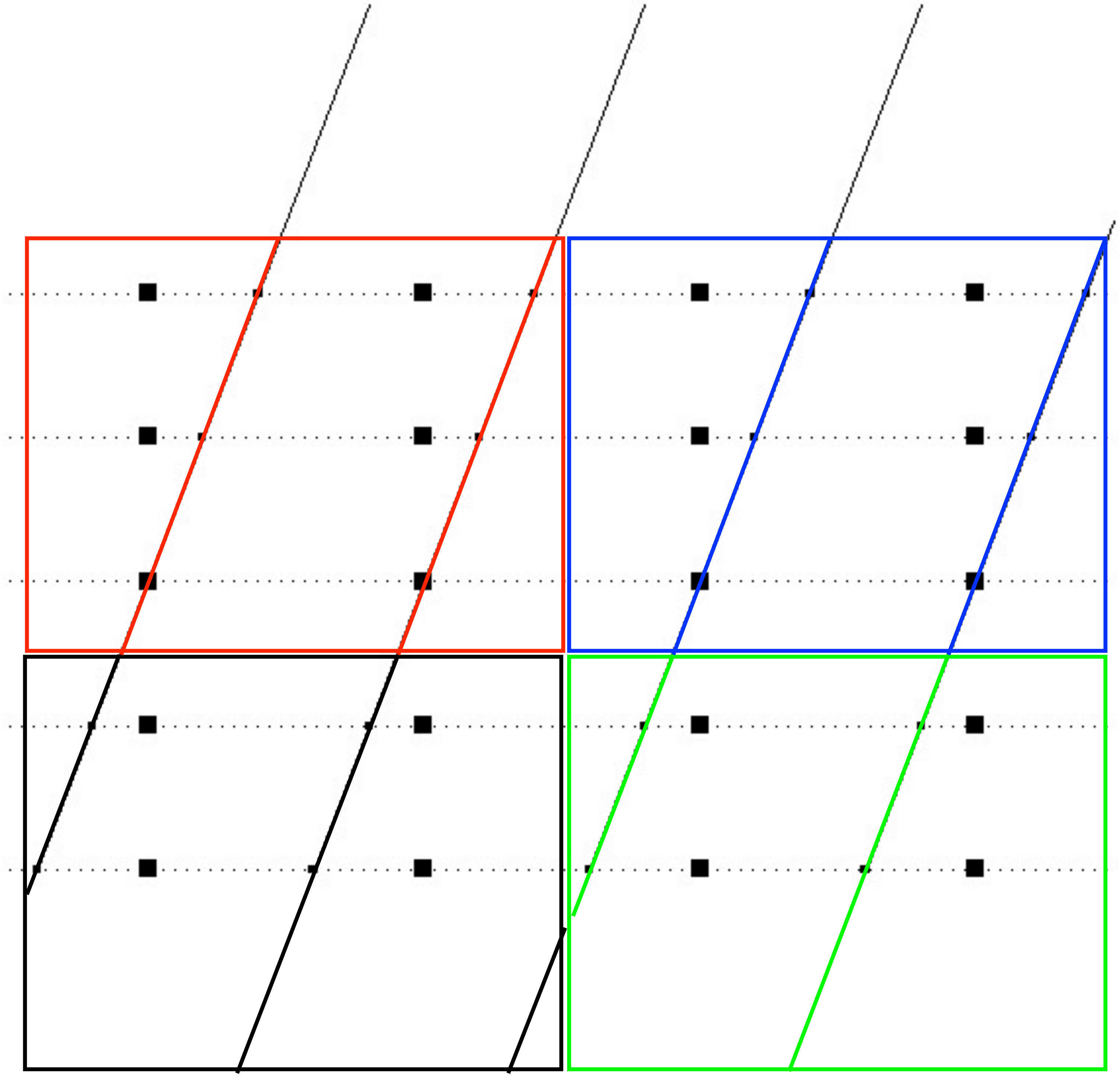
over rays: SMP OK



MPI: massive communication

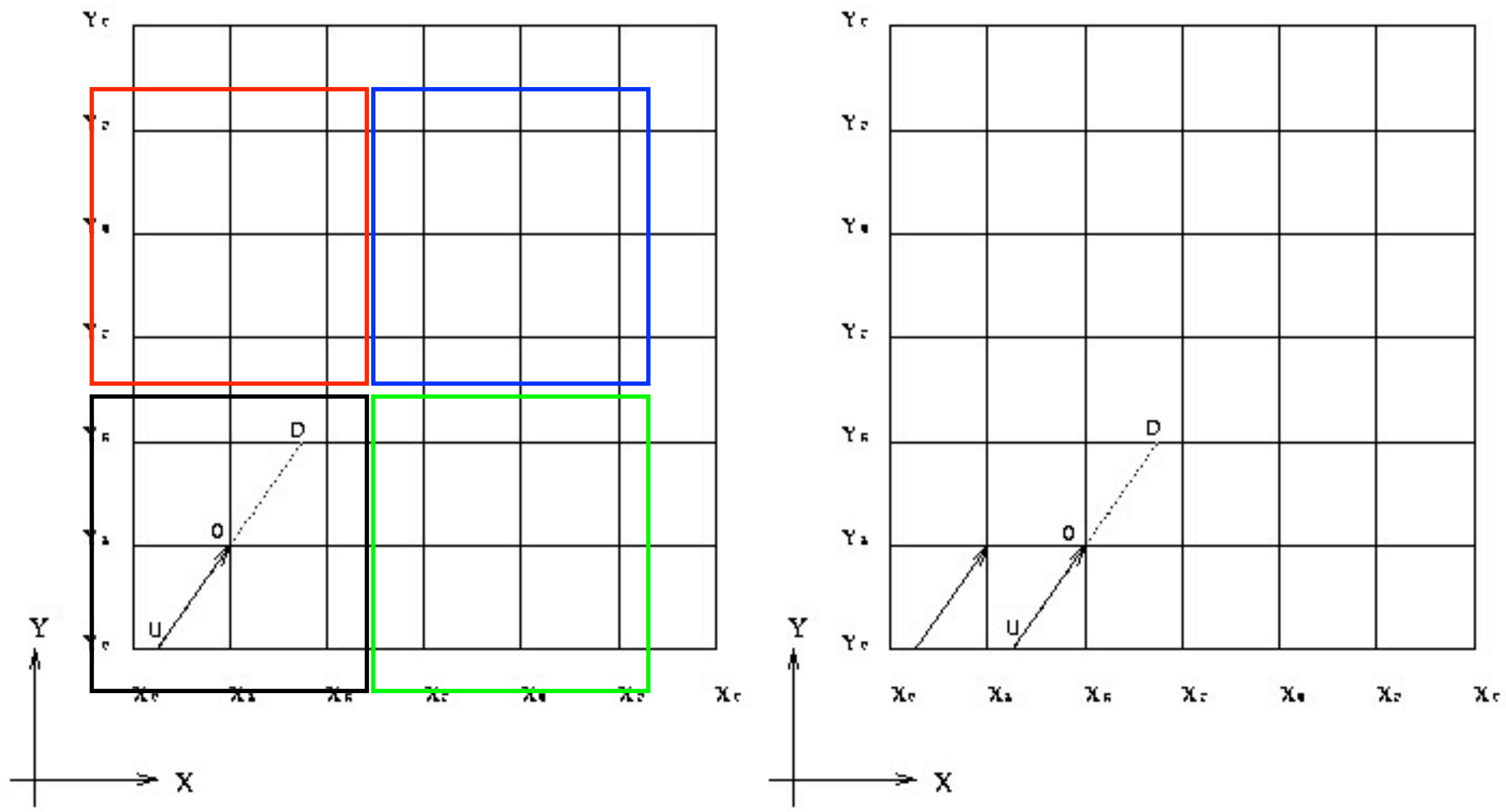
Parallelization strategies

Local rays



MPI: simple communication, complicated admin

Short characteristics



Order: passive processors
multiple sweeps

Energy equation

Radiative equilibrium

$$F_{\rm rad} = \sigma T_{\rm eff}^4$$

$$\nabla F = 0$$

$$\mu \frac{dI_\nu}{dz} = \chi_\nu (S_\nu - I_\nu)$$

integrate over angle

$$\frac{dF_\nu}{dz} = 2\pi \int_{-1}^{1} \chi_\nu (S_\nu - I_\nu) d\mu$$

integrate over frequency

$$\frac{dF}{dz} = 2\pi \int_{-1}^{1} \int_{0}^{\infty} \chi_\nu (S_\nu - I_\nu) d\nu d\mu = 0$$

isotropic χ_ν, S_ν gives

$$\int_{0}^{\infty} \chi_\nu (S_\nu - J_\nu) d\nu = 0$$

NB! flux not specified, only its constancy

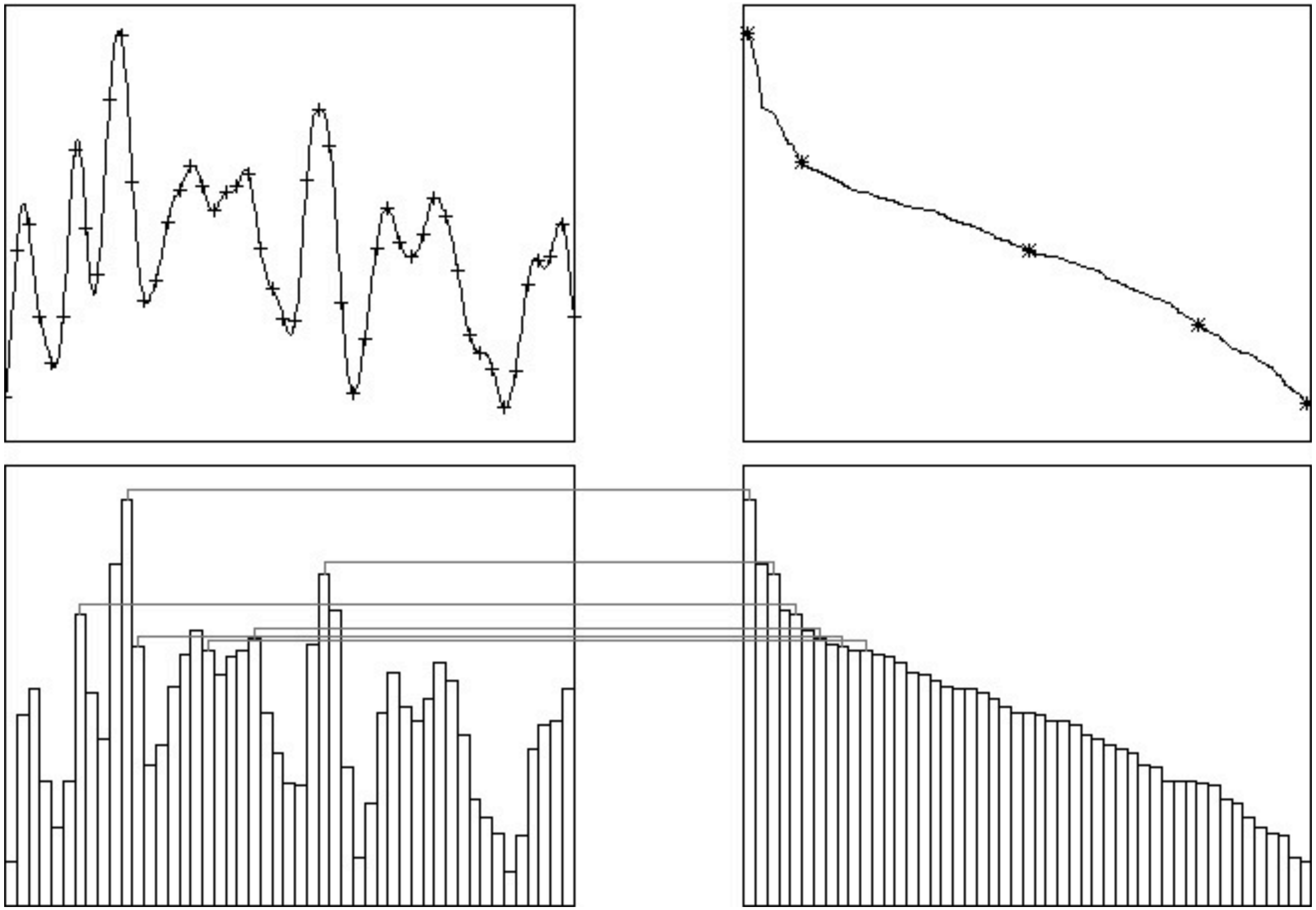
We thus need to solve the transfer equation at many frequencies throughout the spectrum

OS: Opacity sampling. Sample throughout the spectrum, enough points to get a statistically good representation of the integral $\sim$10000 points.

ODF: Opacity distribution function. Reorder frequency points to get smoother function. Fewer points needed $\sim$1000 points. Assumes that high opacity line up.

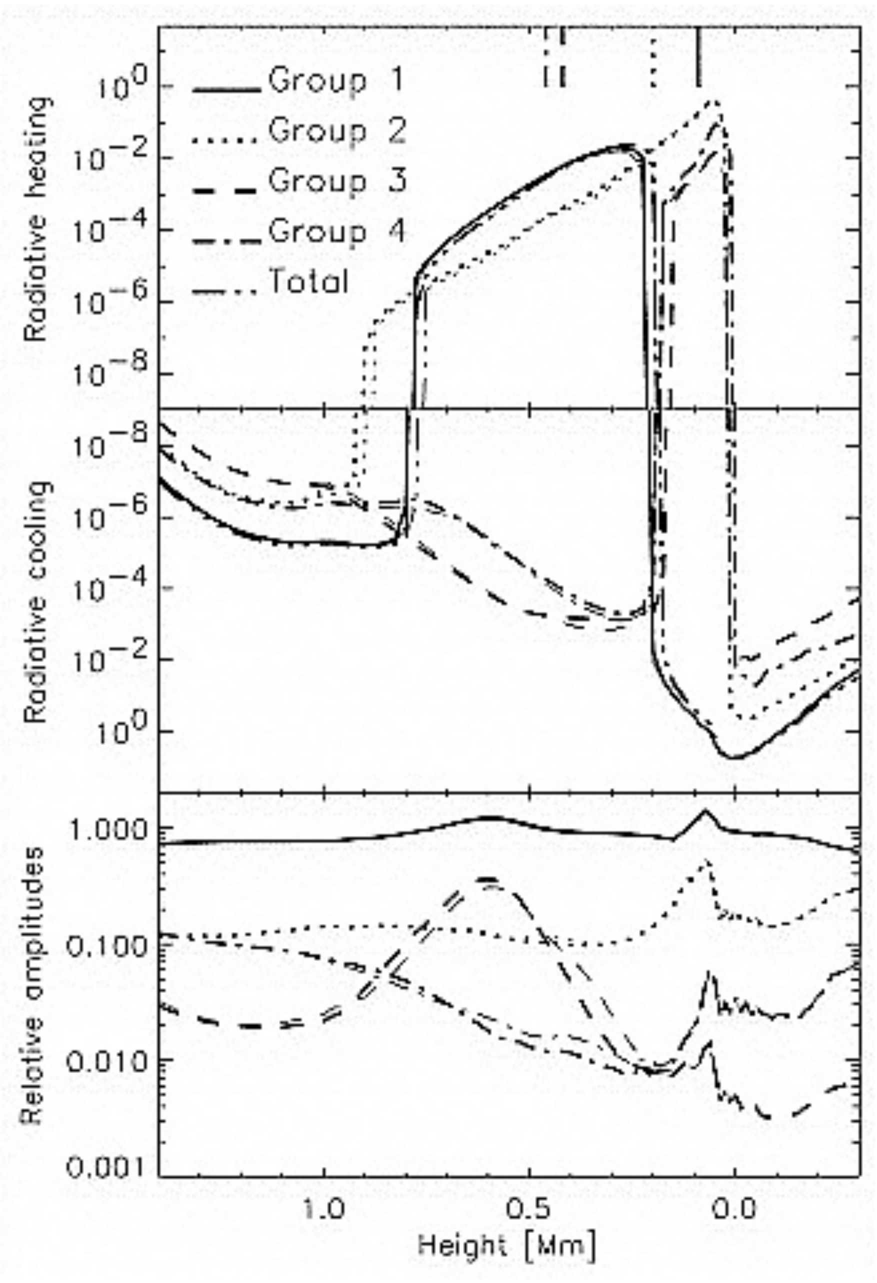
Multi group opacities. As ODF but average also the source function. $\sim$4 points.

ODF



Multi-group opacities

$$\int Y_\lambda d\lambda = \sum_\lambda Y_{\lambda ij} w_{ij} = \sum_i \sum_j Y_{\lambda ij} w_{ij}$$



Linearization

We used to have:

$$\delta j_{\nu\mu} = \frac{\partial j_{\nu\mu}}{\partial n_i}\delta n_i + \frac{\partial j_{\nu\mu}}{\partial n_j}\delta n_j$$

If the atmosphere is not given we get extra variables to solve for:

$$\delta\rho, \delta T, \delta n_e$$

and extra derivatives with respect to these variables

$$\delta j_{\nu\mu} = \frac{\partial j_{\nu\mu}}{\partial \rho}\delta\rho + \frac{\partial j_{\nu\mu}}{\partial T}\delta T + \frac{\partial j_{\nu\mu}}{\partial n_e}\delta n_e + \sum_{i=1}^{N_L} \frac{\partial j_{\nu\mu}}{\partial n_i}\delta n_i$$

$$\frac{\partial j_{\nu c}}{\partial x}, \frac{\partial \kappa_{\nu c}}{\partial x}, \frac{\partial \alpha_{ij}}{\partial x}, \frac{\partial G_{ij}}{\partial x}, \frac{\partial C_{ij}}{\partial x}$$

are no longer zero

Extra equations: Hydrostatic equilibrium
Energy equation, charge conservation

Examples, non-LTE

- non-local, non-linear
- 1D: Accelerated Lambda Iteration (ALI)
  - 500-1000 atomic levels possible
  - codes available (MULTI, RH (Uitenbroek),...)
- 3D: ALI + long or short characteristics
  - 20-30 levels possible
  - not as easy to use as black-box (convergence problems, discretization issues etc) (RH (Uitenbroek), MULTI3D)

Examples

- Contribution & response functions
- non-LTE abundance determinations
- non-LTE modeling of Si I
- non-LTE modeling of O I resonance lines
- intensity from 3D model atmosphere
- non-Statistical equilibrium
- Formation of spectrum in a dynamic chromosphere
- 3D simulations from convection zone to corona

Contribution functions

$$I_{\nu\mu}(0) = \int C_I(x)dx$$

$$C_I(\tau_\nu) = \frac{1}{\mu} S_\nu(\tau_\nu) e^{-\tau_\nu/\mu}$$

$$C_I(z) = \frac{1}{\mu} S_\nu(\tau_\nu) e^{-\tau_\nu/\mu} \chi_\nu$$

Contribution functions give the contributions from different layers of the atmosphere to a given quantity.

Rewrite of contribution function

$$C_I(z) = \frac{1}{\mu} S_\nu(\tau_\nu) e^{-\tau_\nu/\mu} \chi_\nu$$

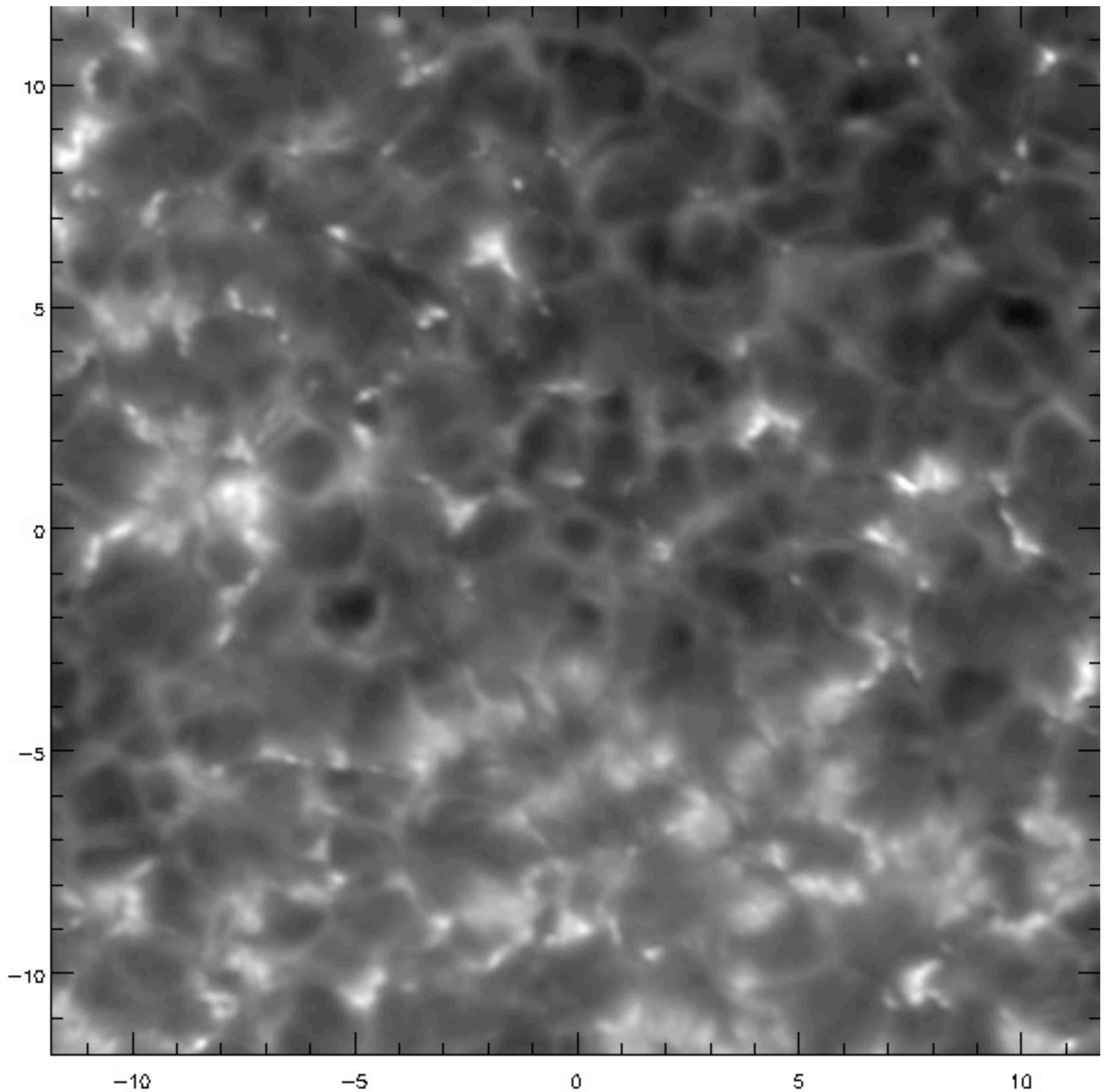
$$C_I(z) = S_\nu(\tau_\nu) \frac{1}{\mu} \tau_\nu e^{-\tau_\nu/\mu} \frac{\chi_\nu}{\tau_\nu}$$

Source term

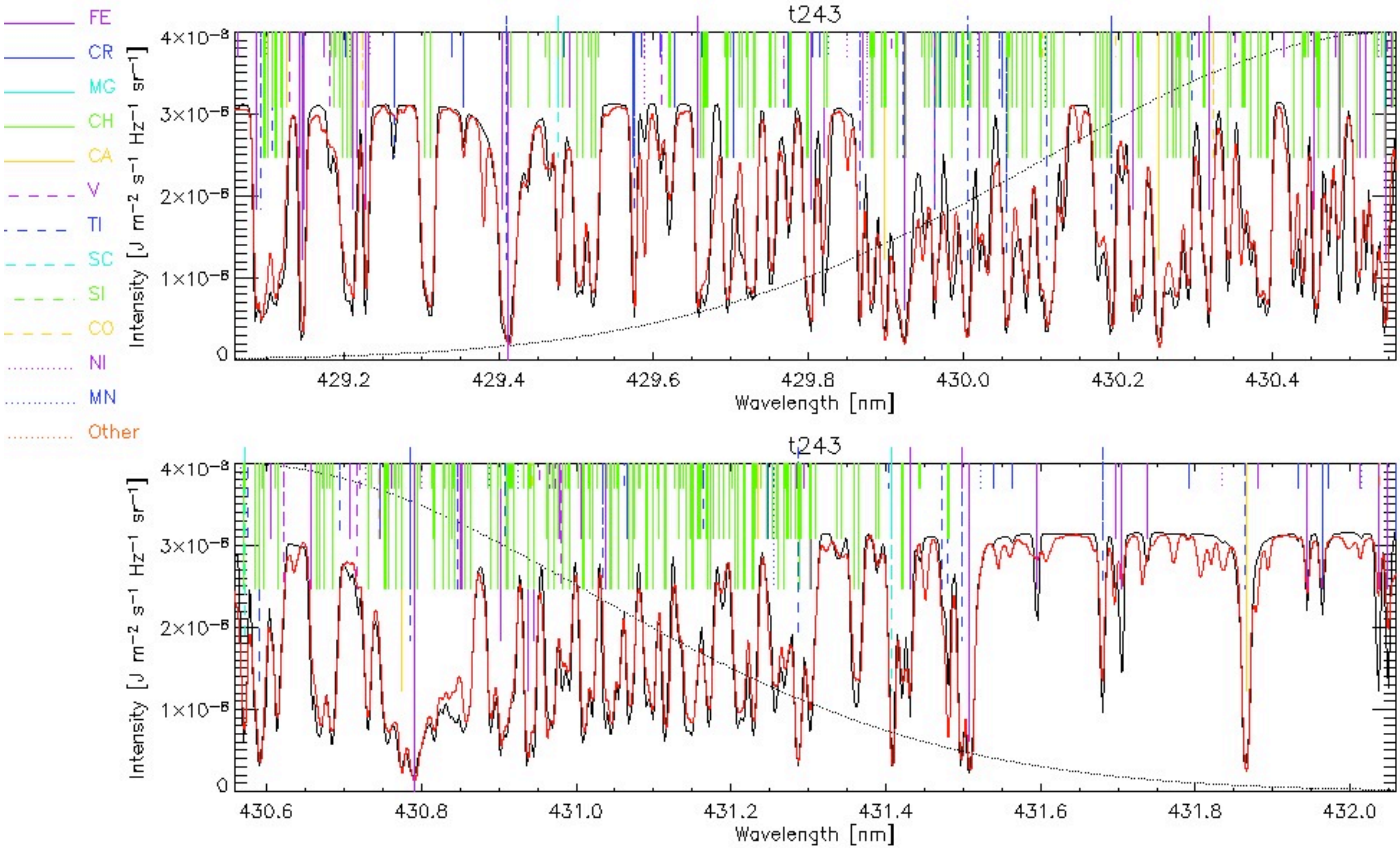
Maximum for $\tau_\nu = \mu$

Dynamic term

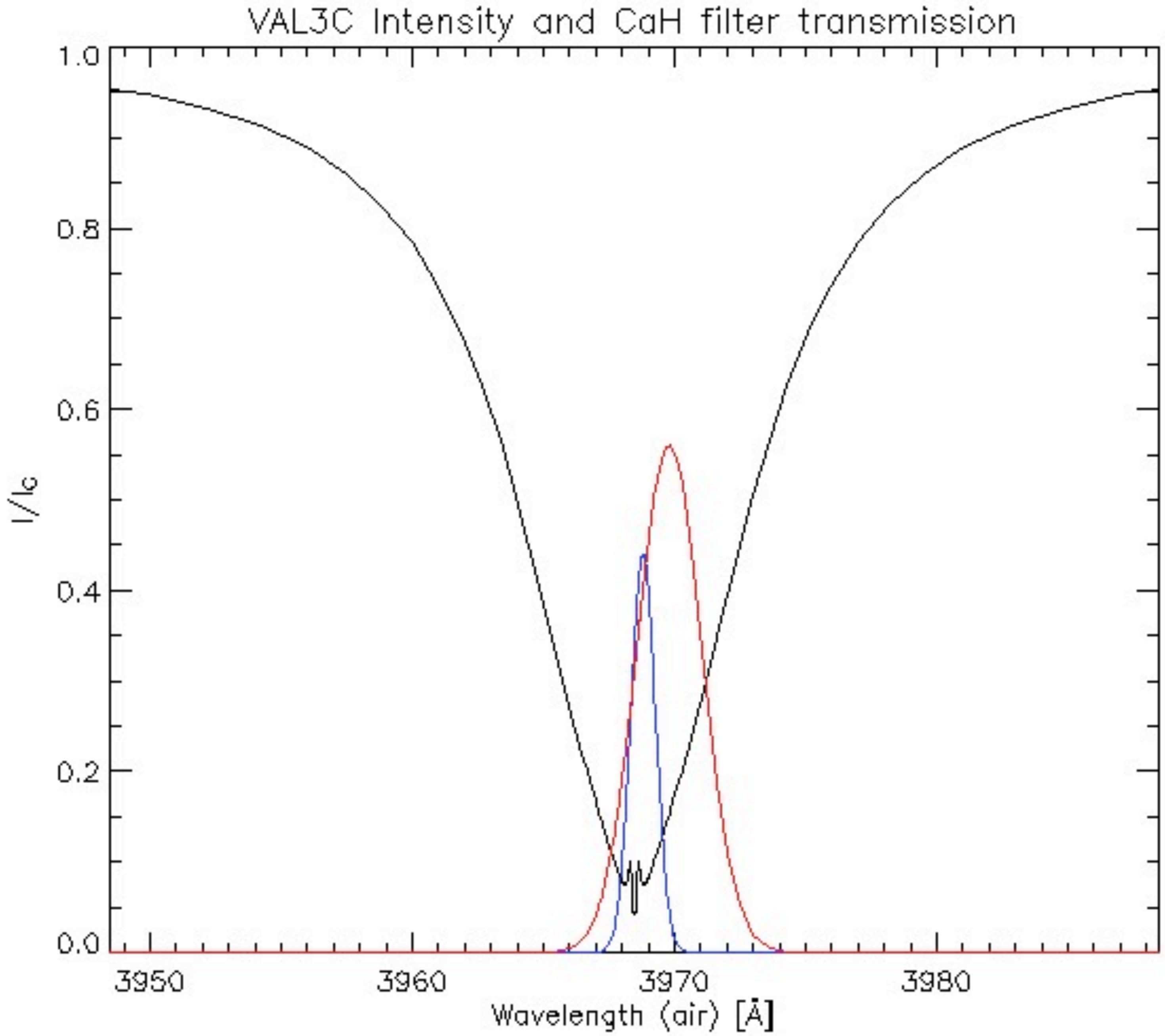
G-band vs Ca H filtergram



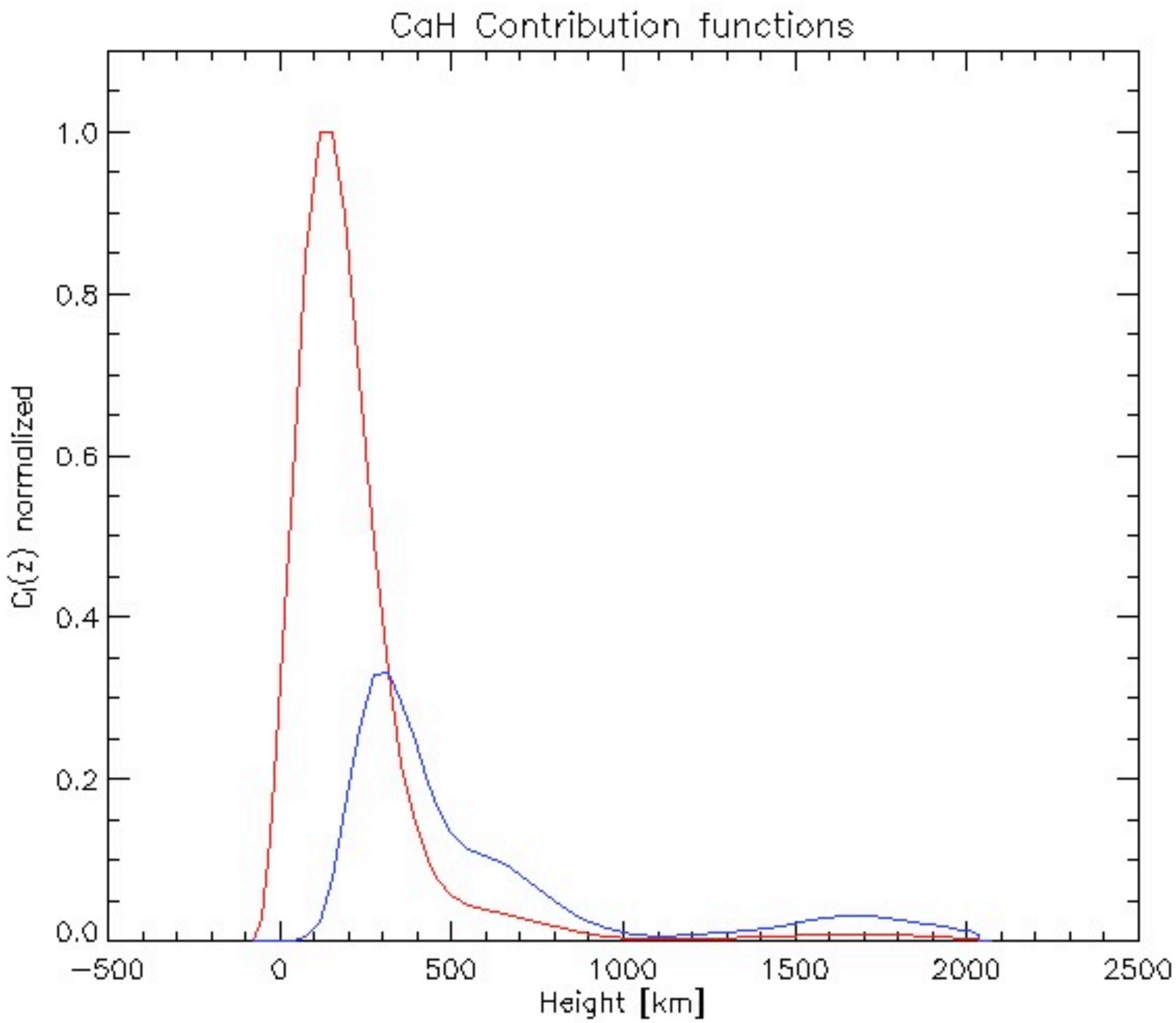
Synthetic spectrum



LaPalma Ca H filters



Contribution to Ca-H filter intensity



Response functions

$$\frac{\Delta I}{I} = \int_{-\infty}^{\infty} R(z) \frac{\Delta T}{T}(z) dz$$

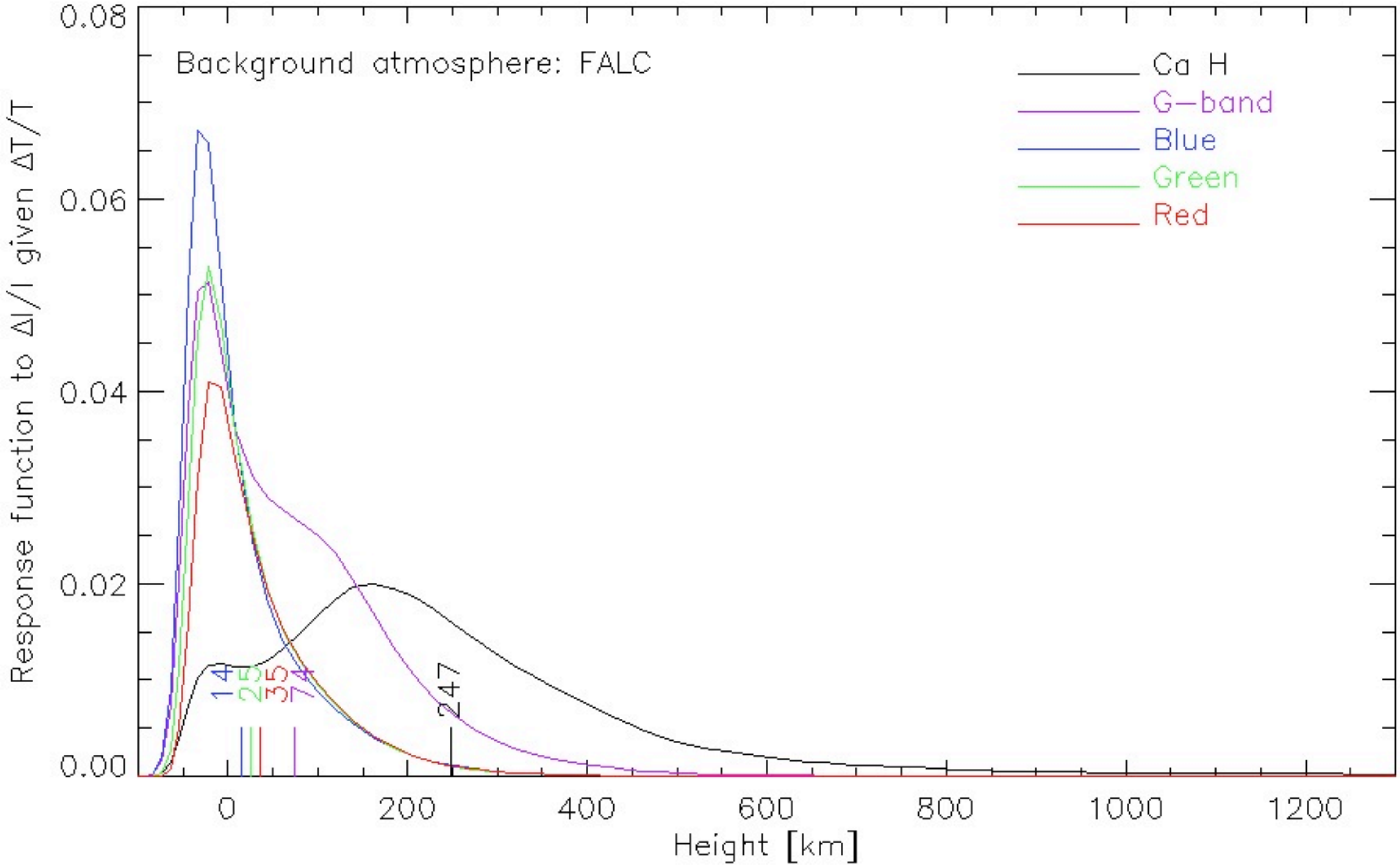
Numerical calculation of a response function

$$\begin{aligned} \frac{\Delta T}{T}(z) &= C, z \leq z' \\ &= 0 \quad z > z' \end{aligned}$$

$$\frac{\Delta I}{I}(z') = C \int_{-\infty}^{z'} R(z) dz$$

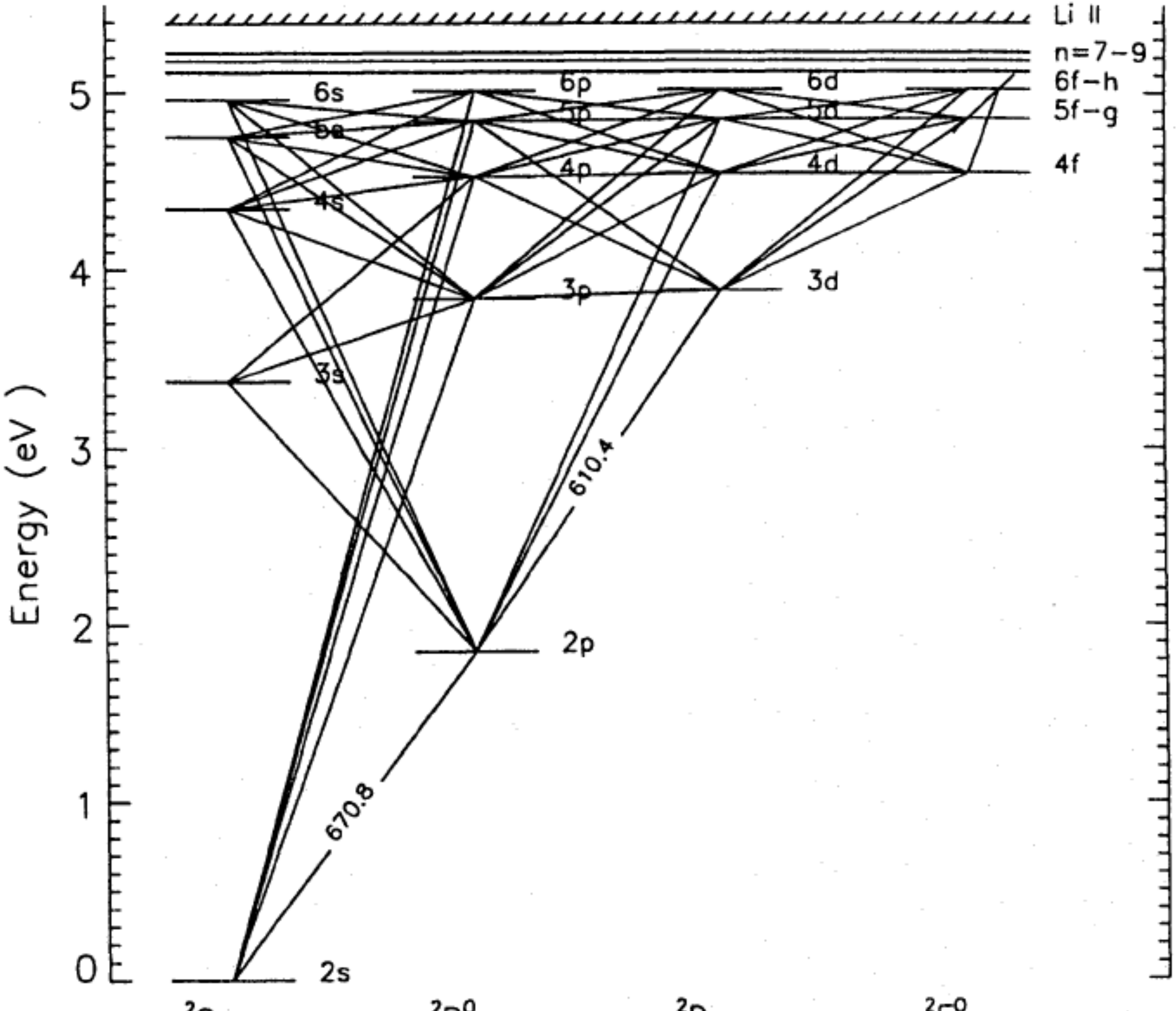
$$R(z') = \frac{1}{C} \frac{d}{dz'} \frac{\Delta I}{I}(z')$$

Response functions of Hinode wide band filters



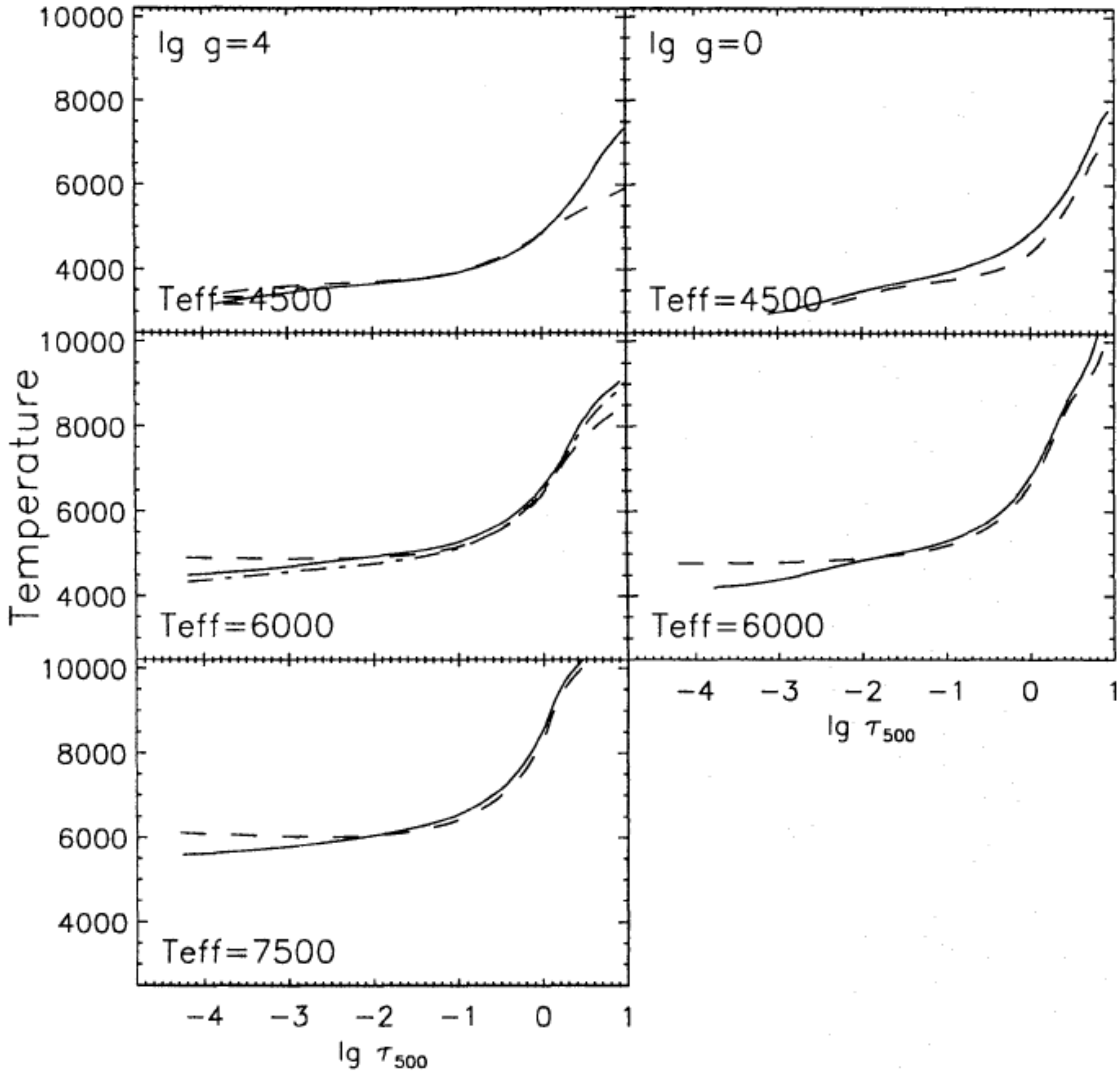
non-LTE abundances of Li

Carlsson, Rutten, Bruls, Shchukina, 1994, A&A 288,860

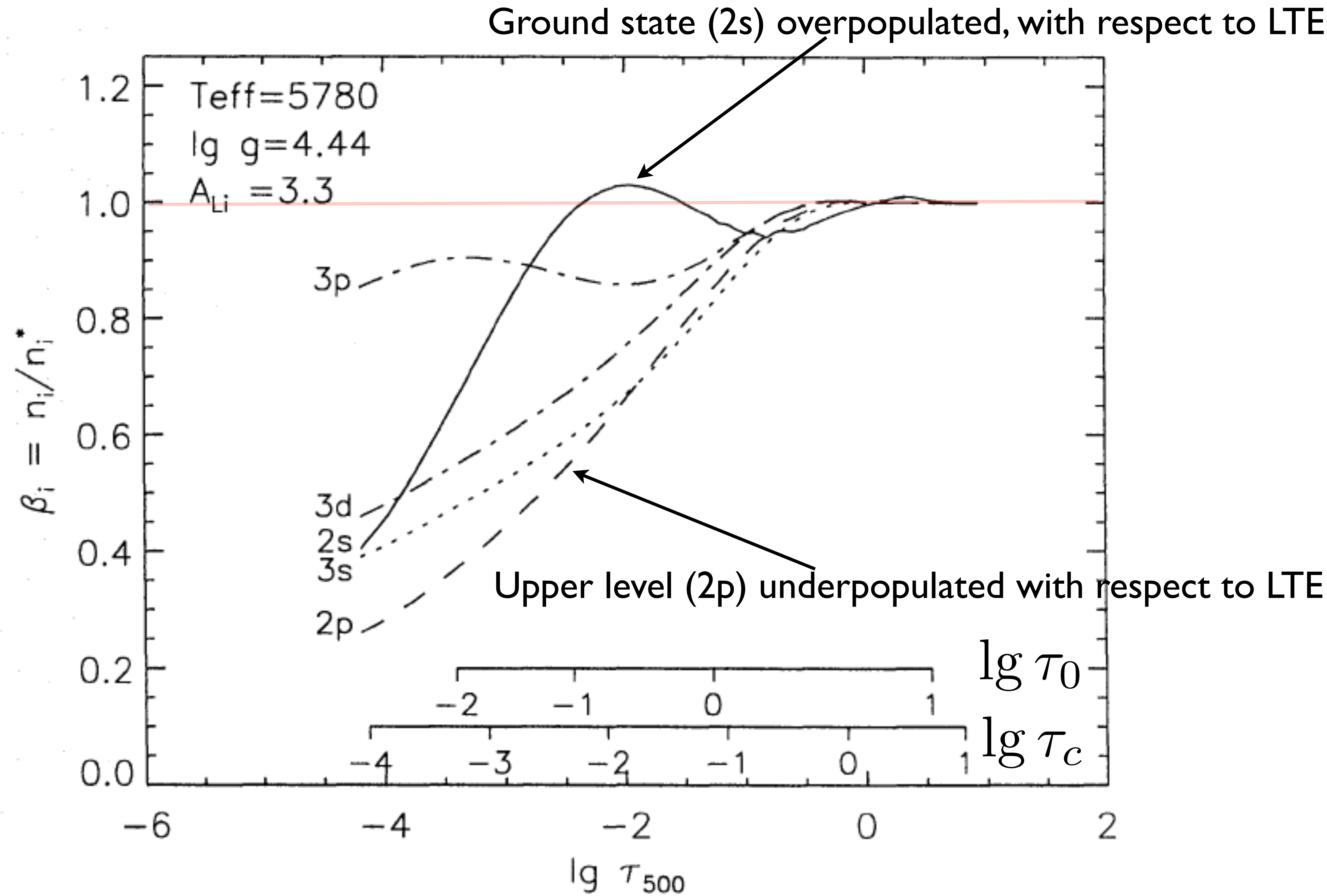


21 levels, 70 lines 20 b-f continua

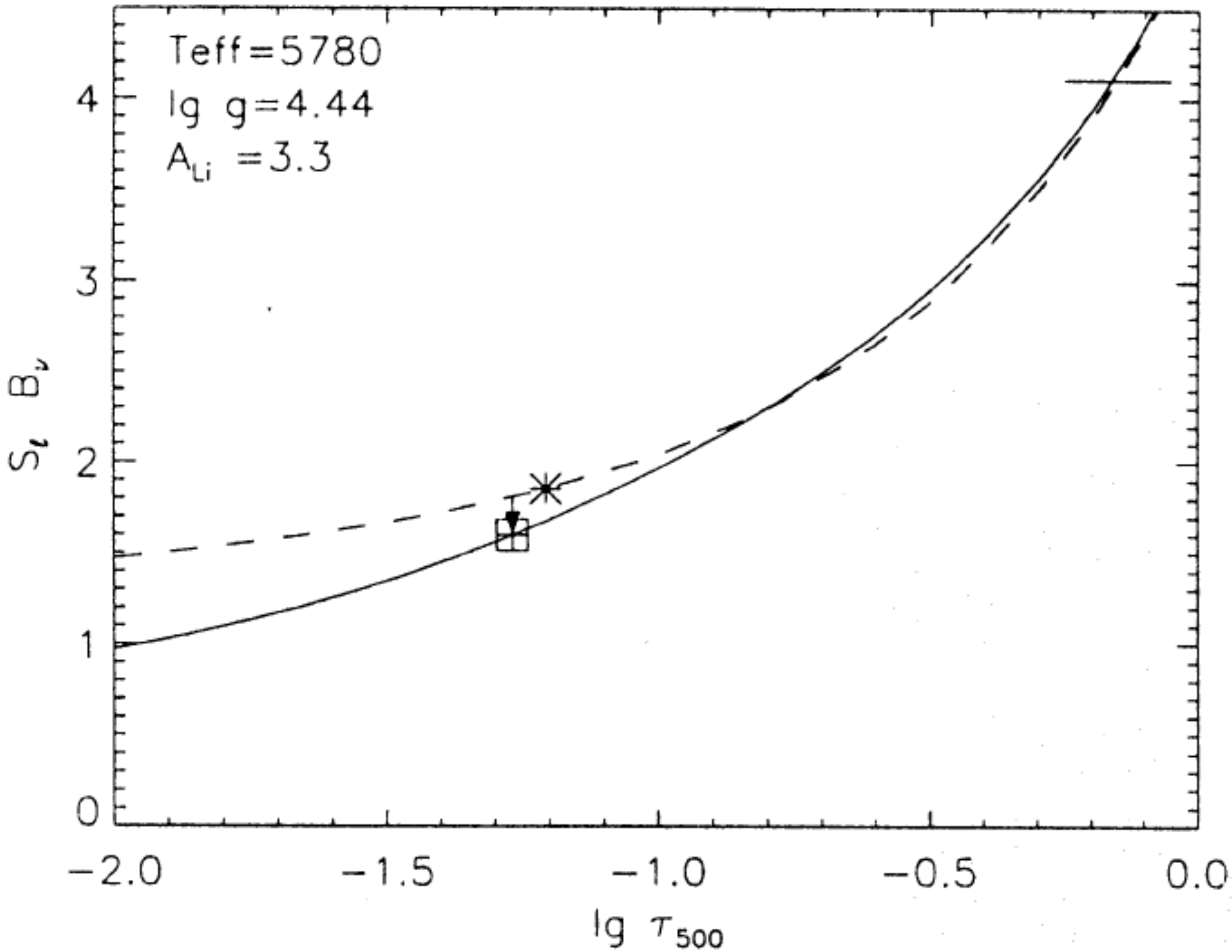
Atmospheric models



departure coefficients

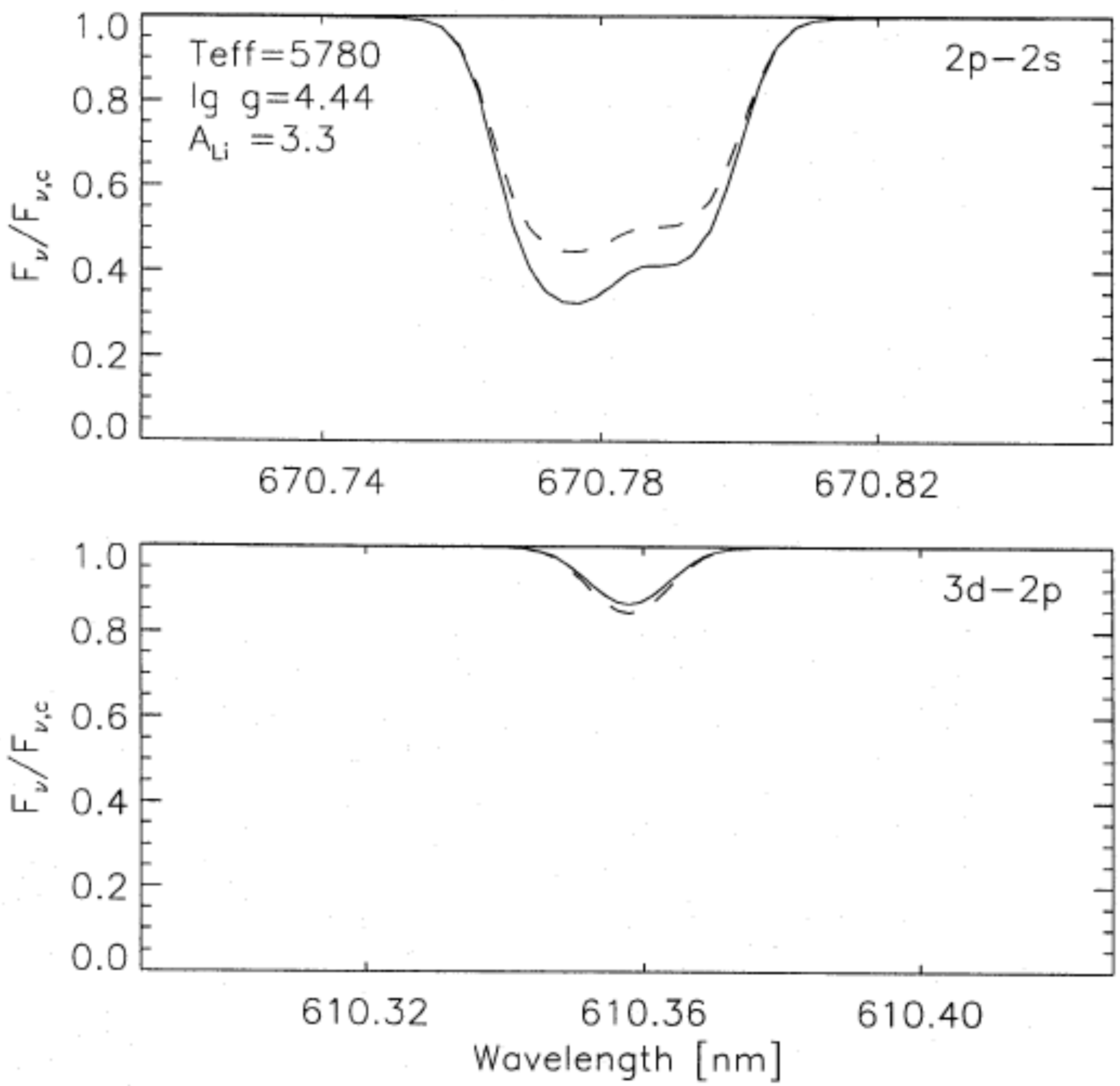


source function



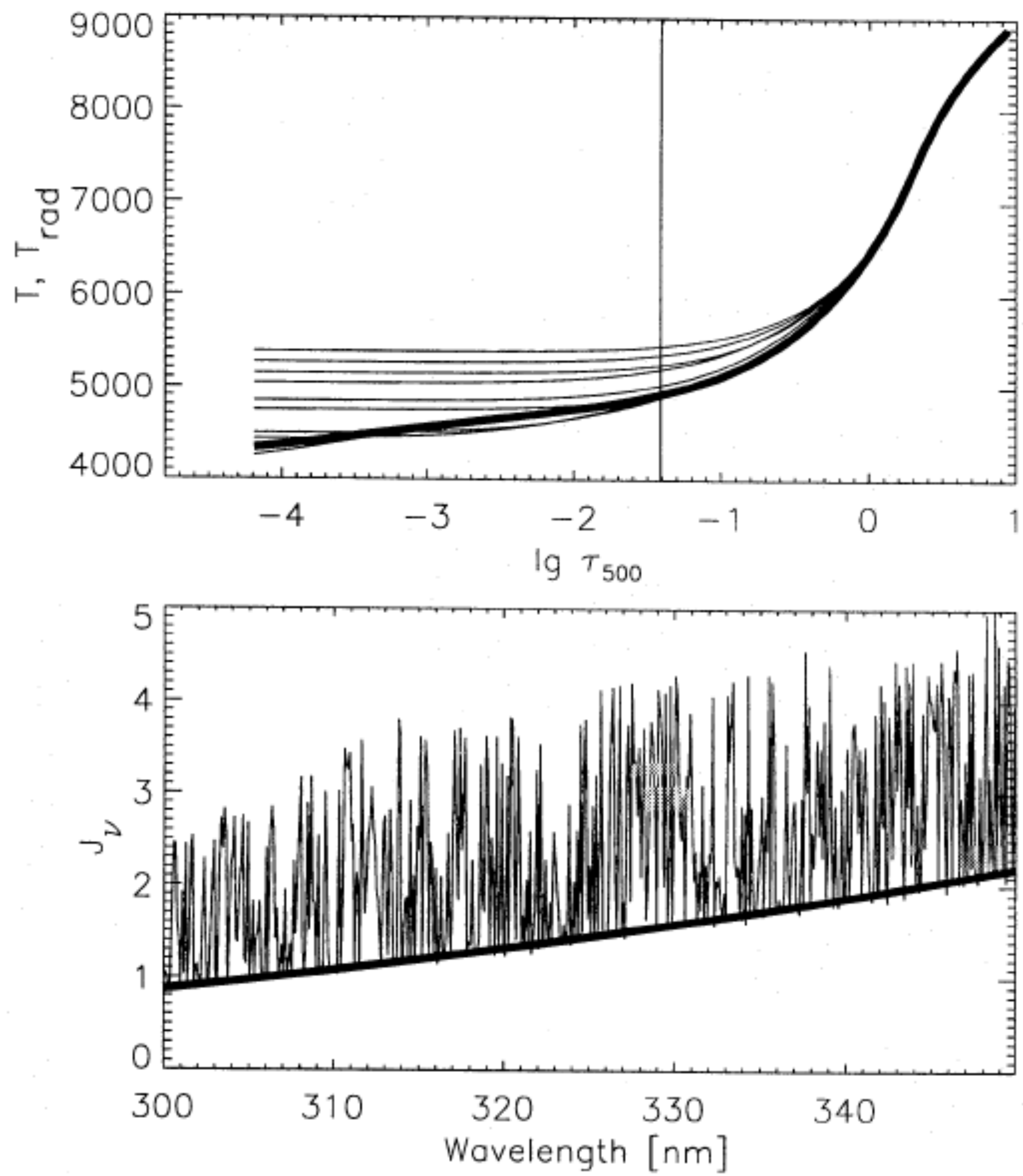
Source function (solid) below Planck function (dashed)
Overpopulated lower level gives tau=1 (square) in non-LTE further out than in LTE (star)

Intensity

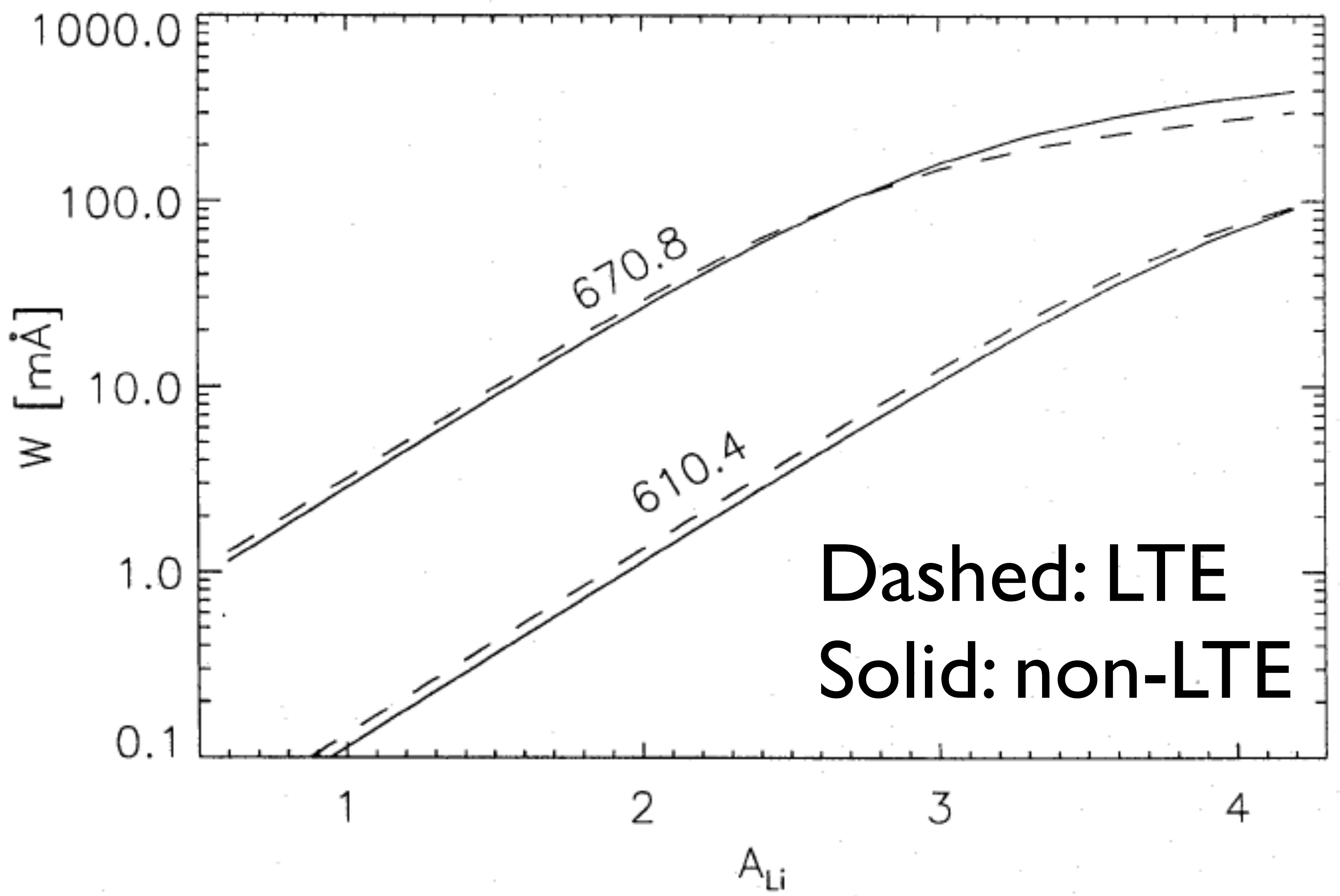


Lower source function and formation further out give stronger line in non-LTE (solid) than in LTE (dashed). Opposite for subordinate line (lower panel)

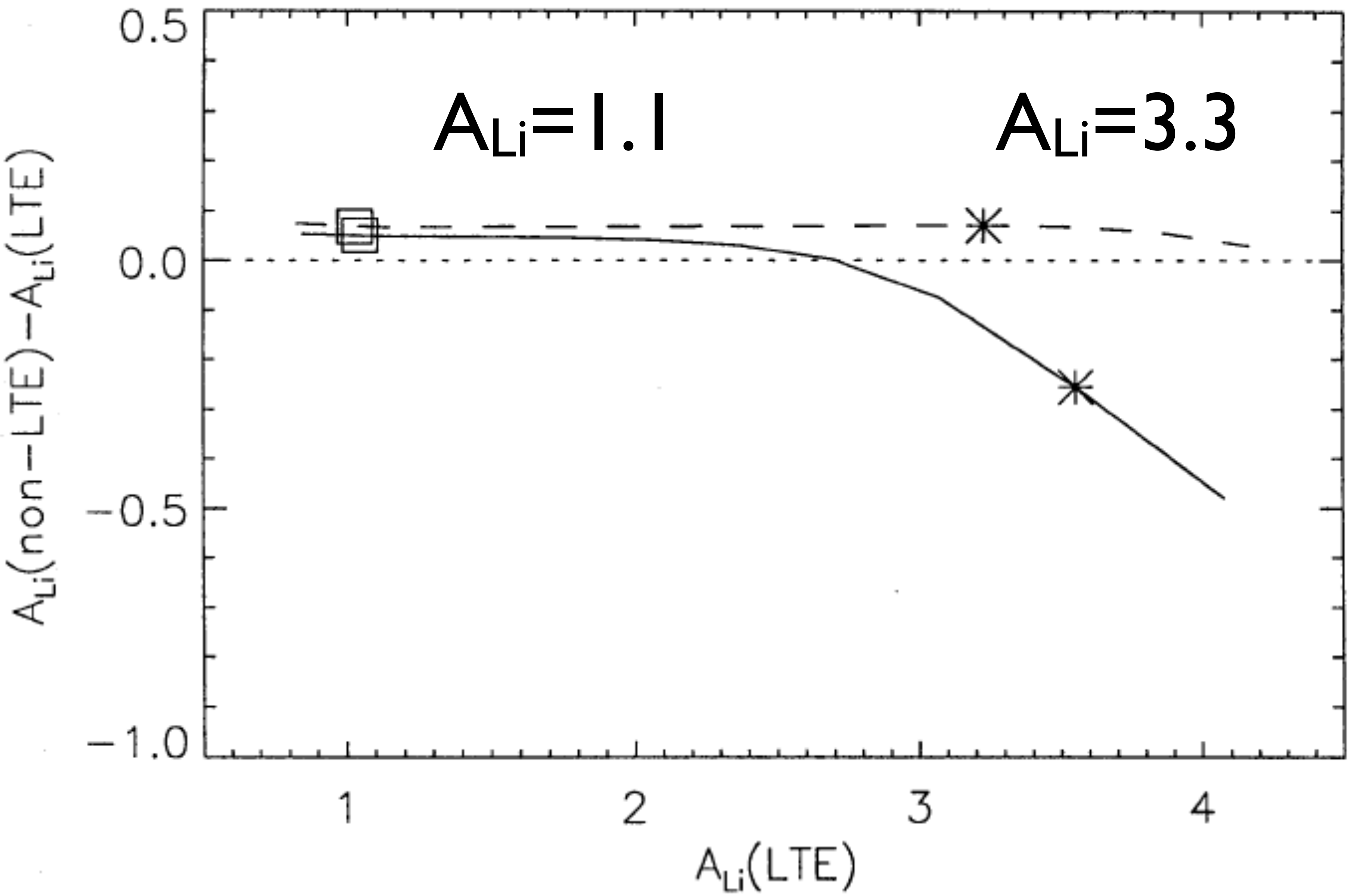
Line blanketing



Curve of growth



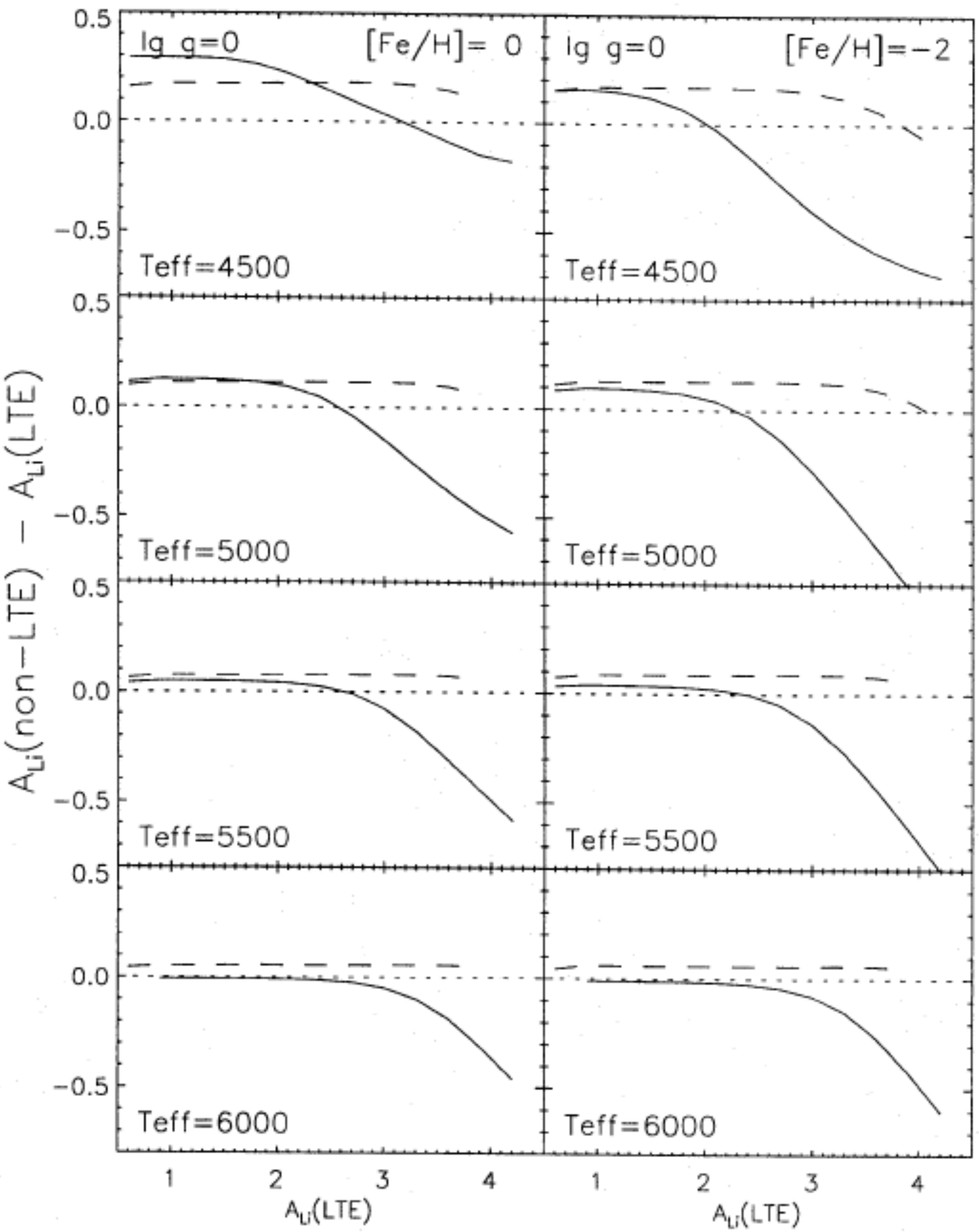
non-LTE abundance correction



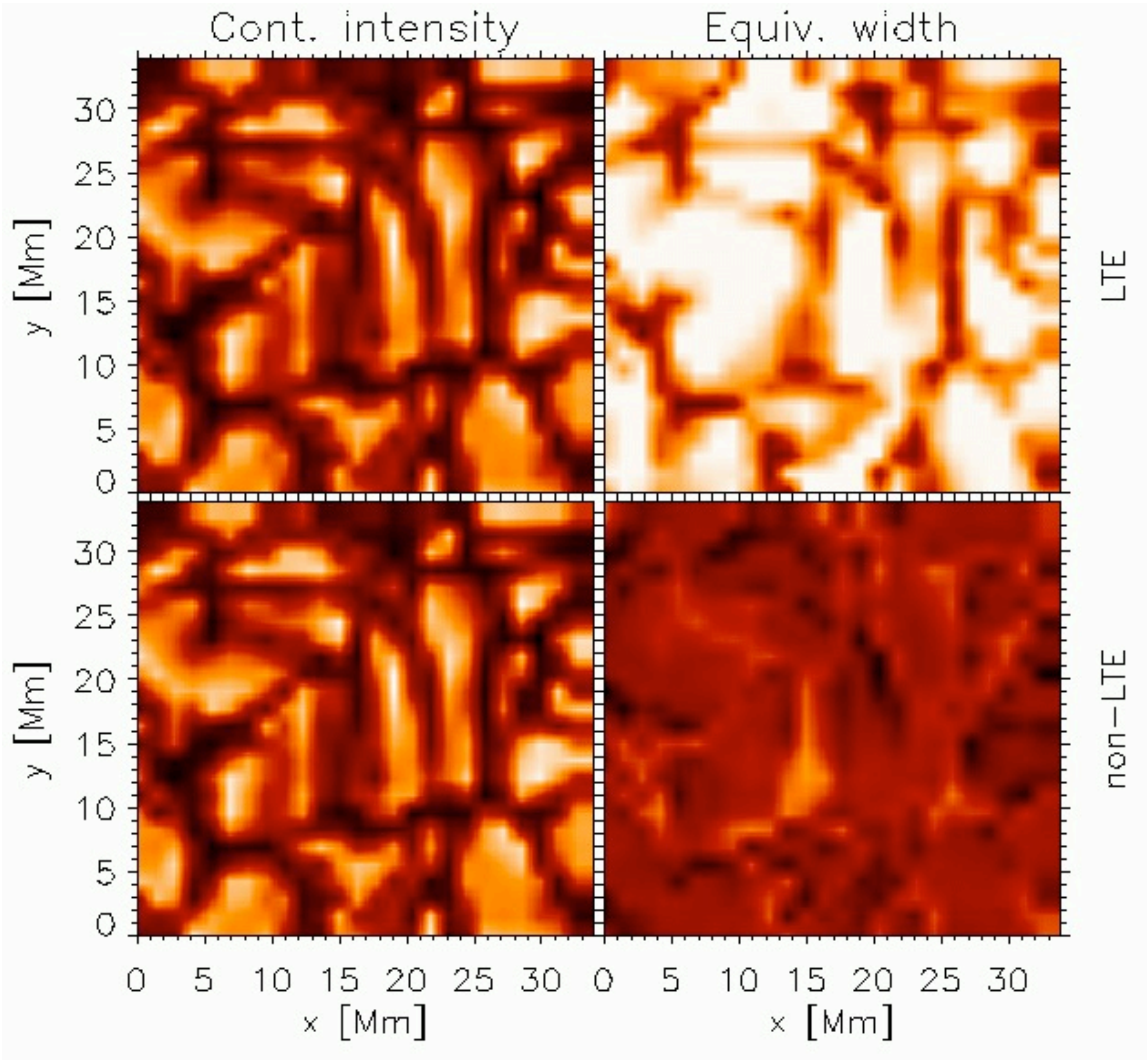
610.4 nm

670.8 nm

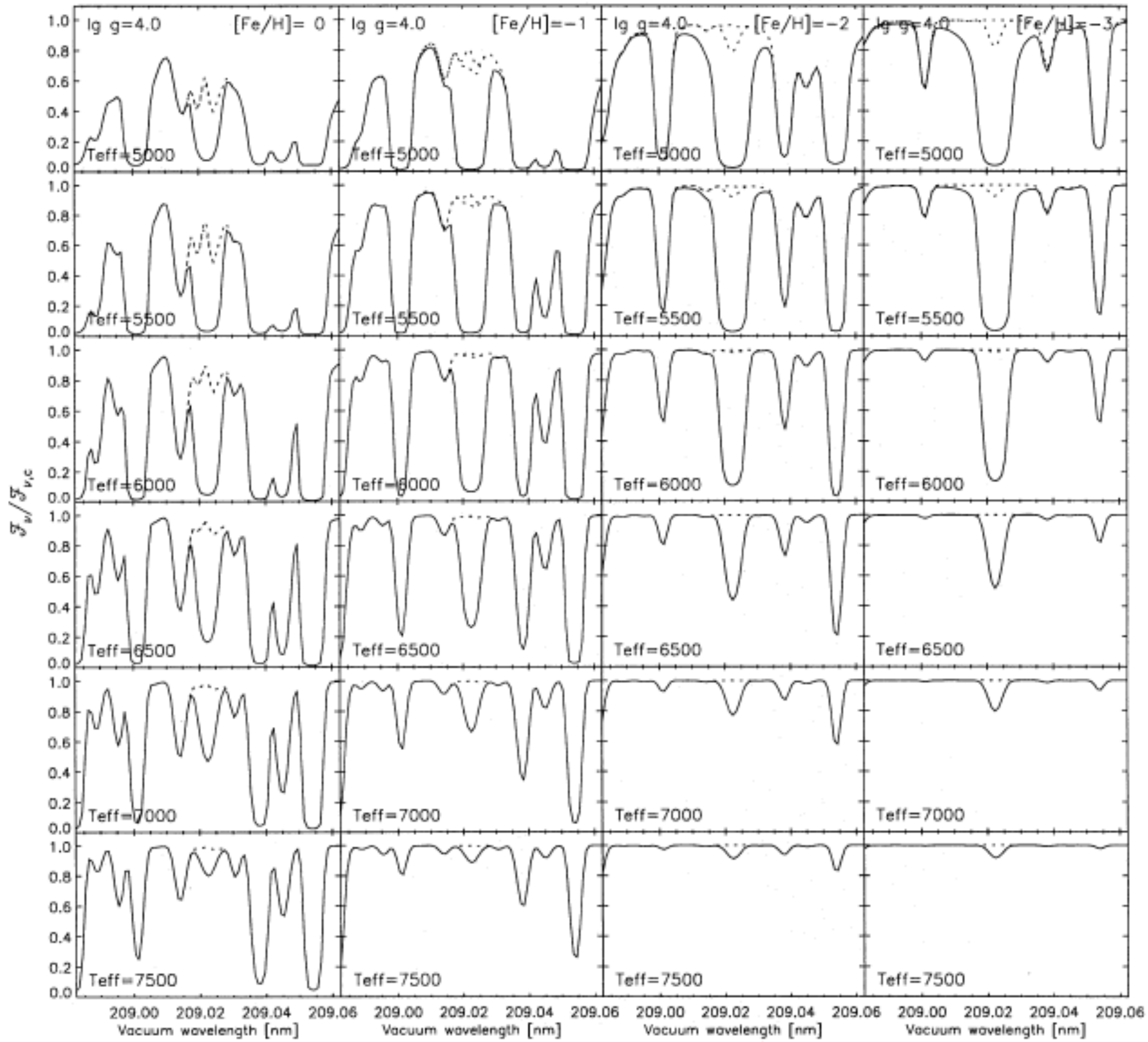
non-LTE abundance corrections for stars



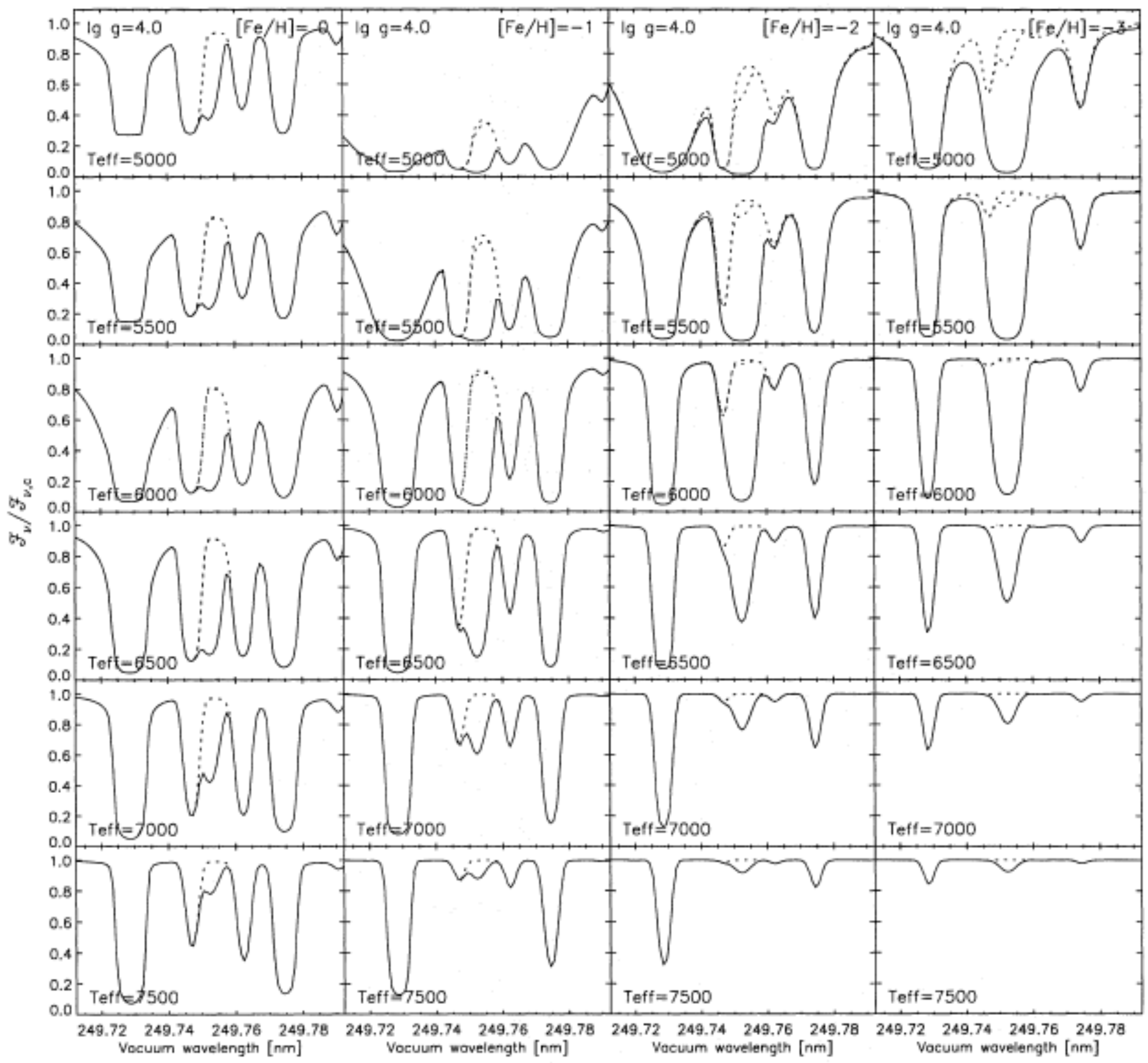
3D non-LTE for Lithium



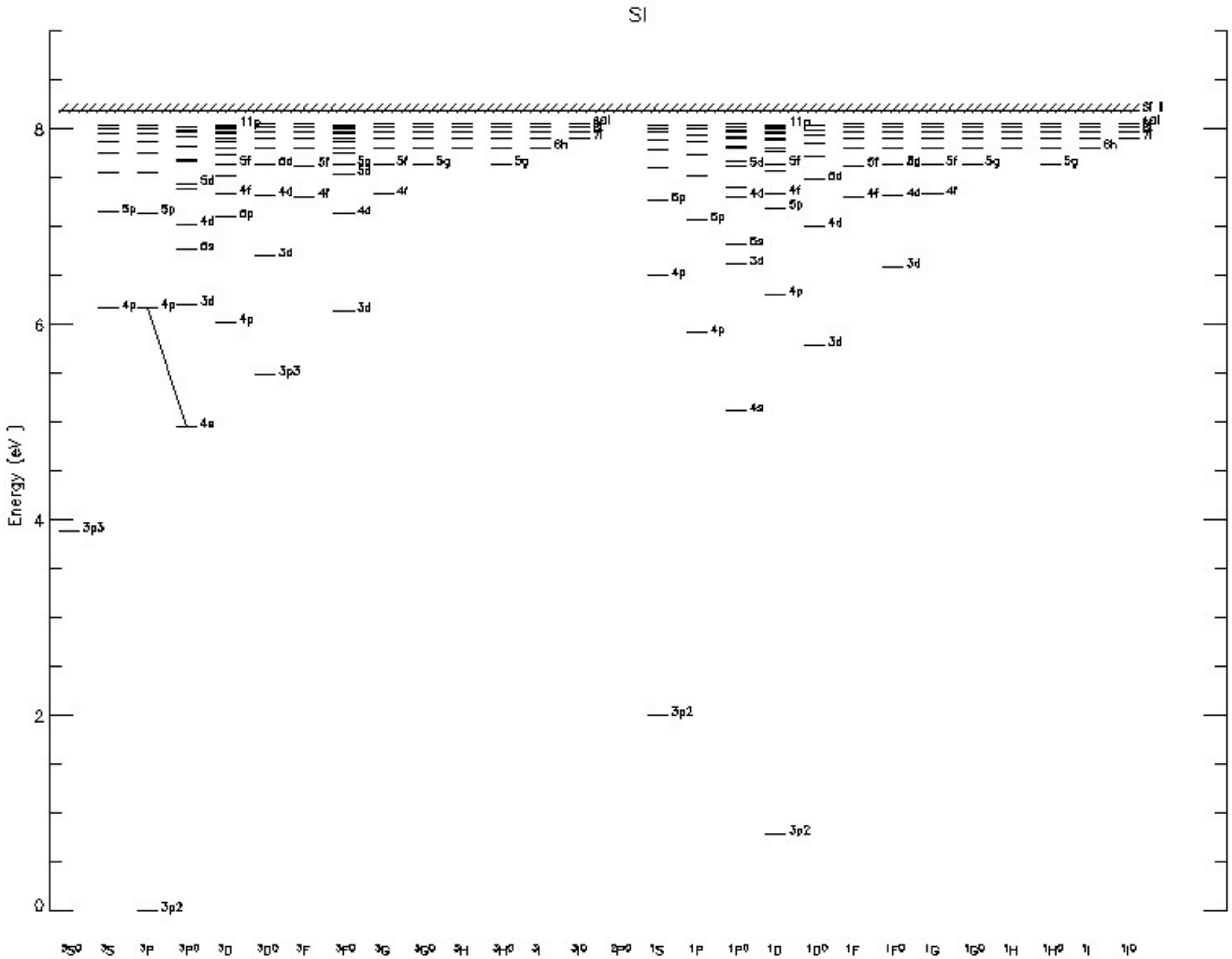
non-LTE B I 209 nm



non-LTE B I 249.75 nm



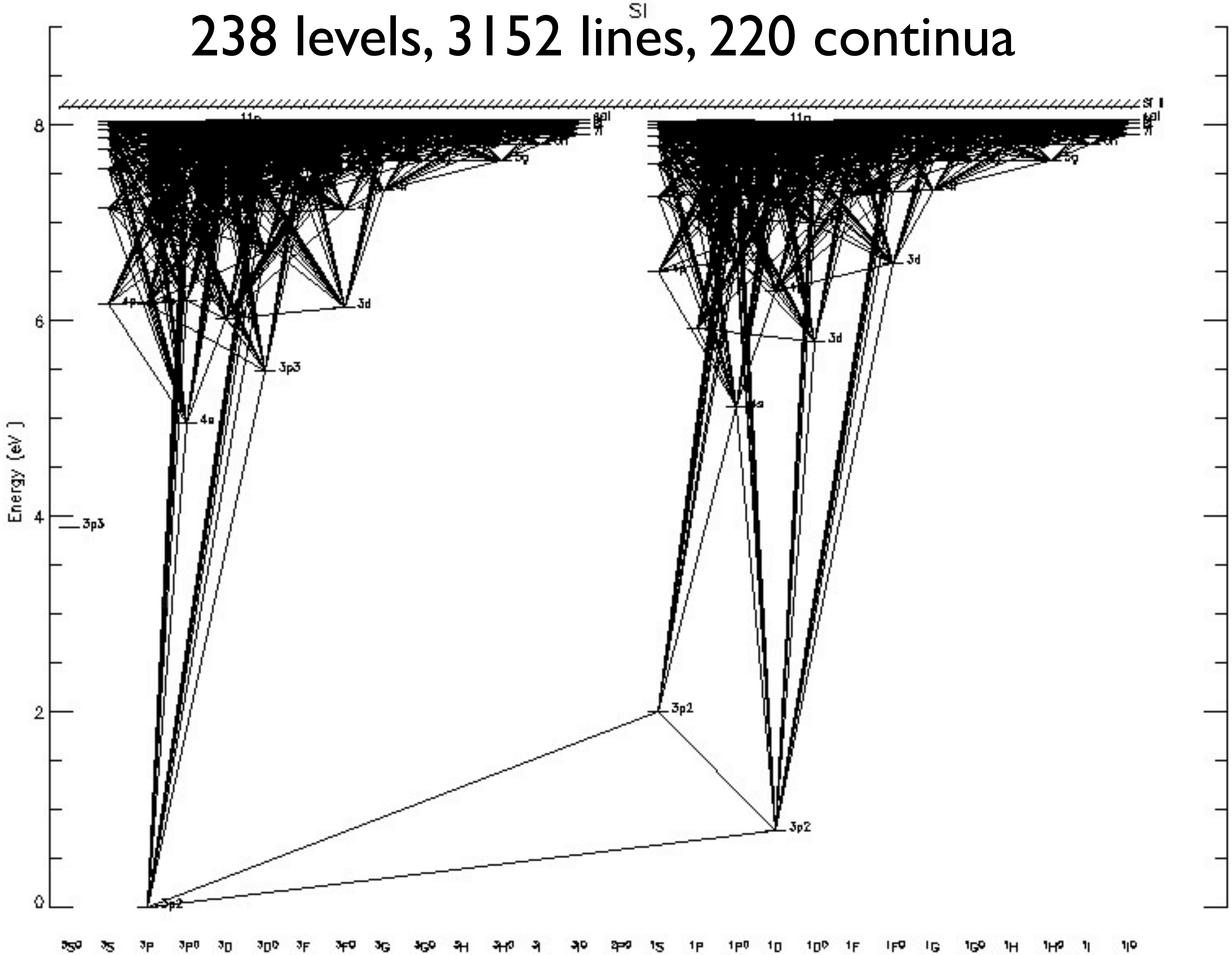
non-LTE modelling of Si I



Bard, Carlsson, 2008, ApJ 682, 1376

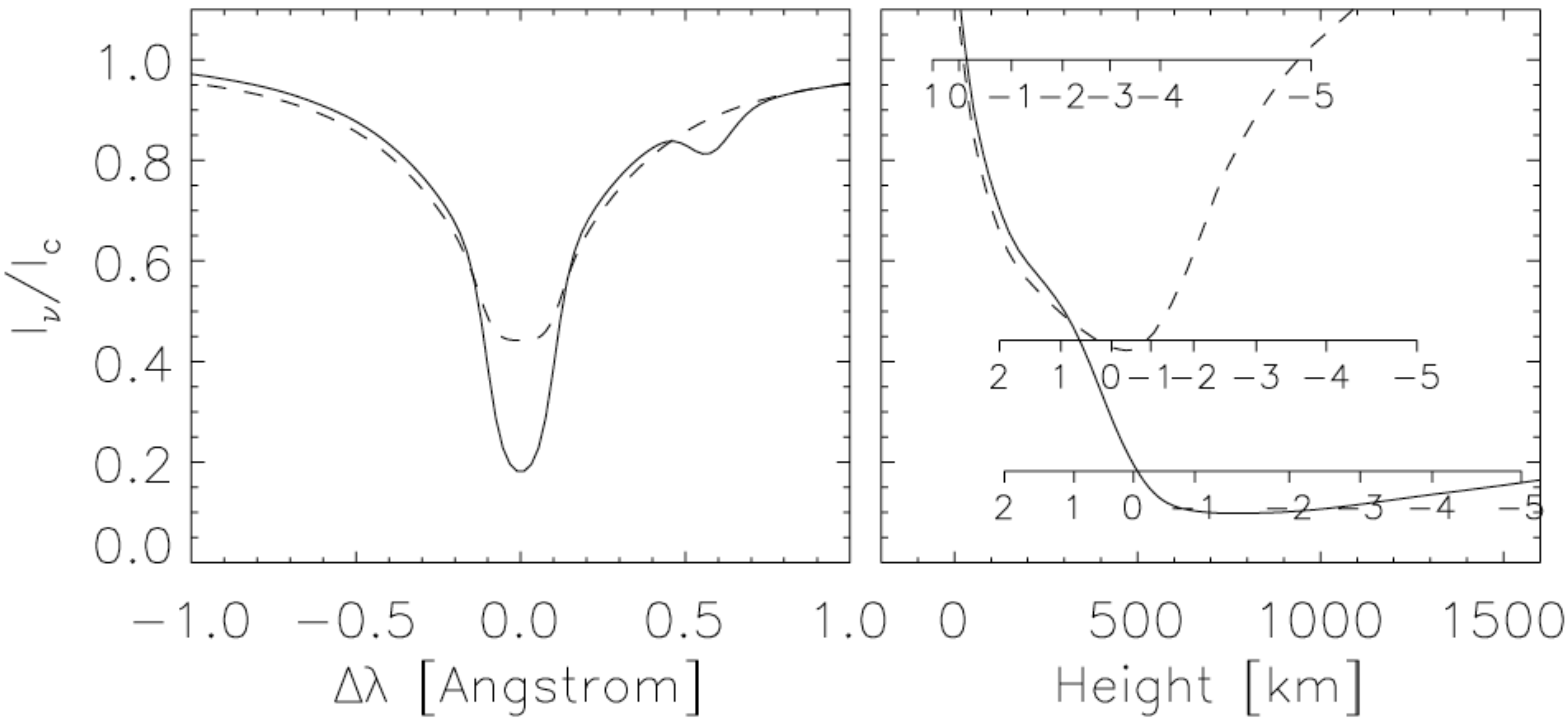
non-LTE modelling of Si I

238 levels, 3152 lines, 220 continua

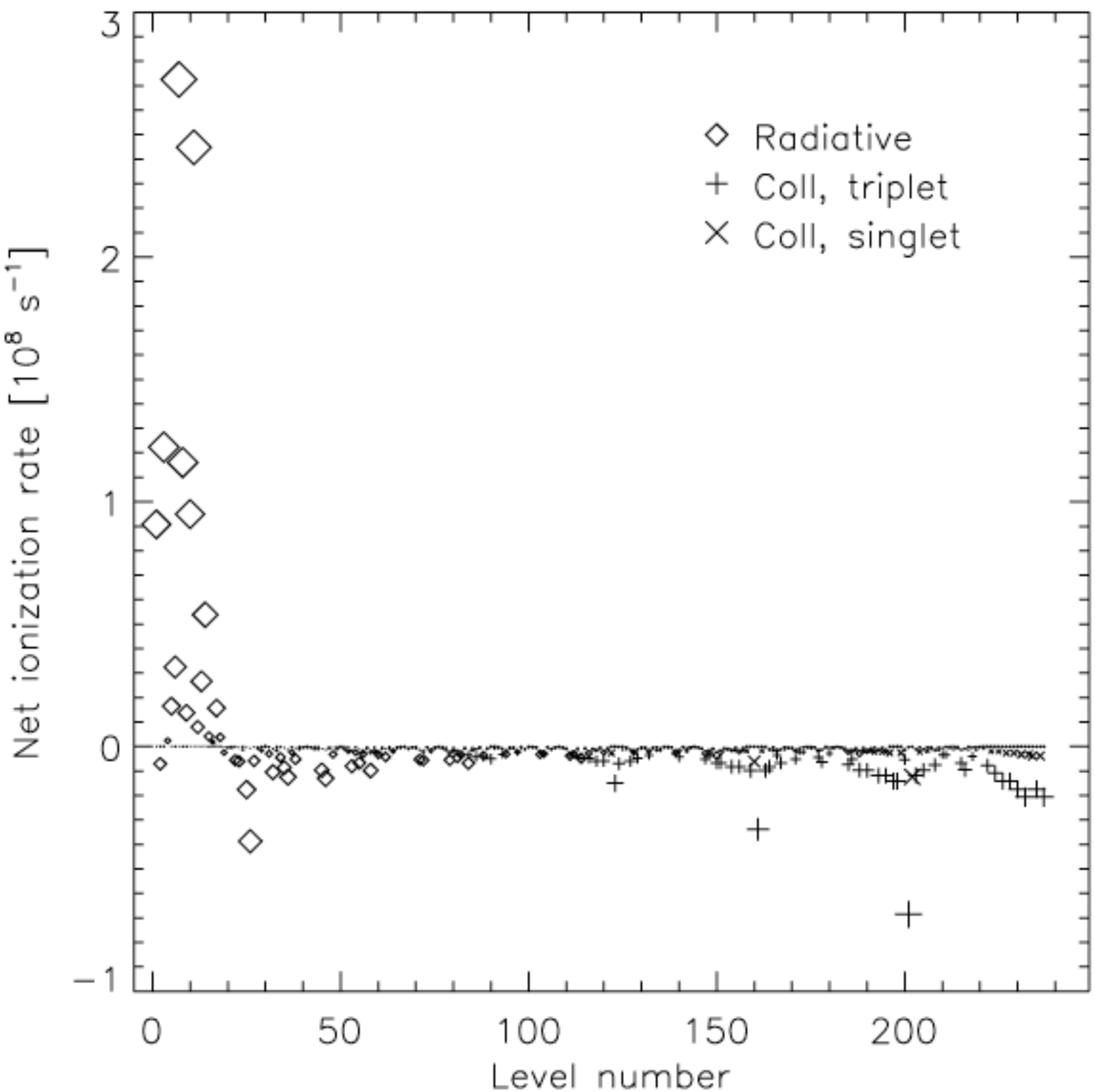


We need a lot of atomic data!

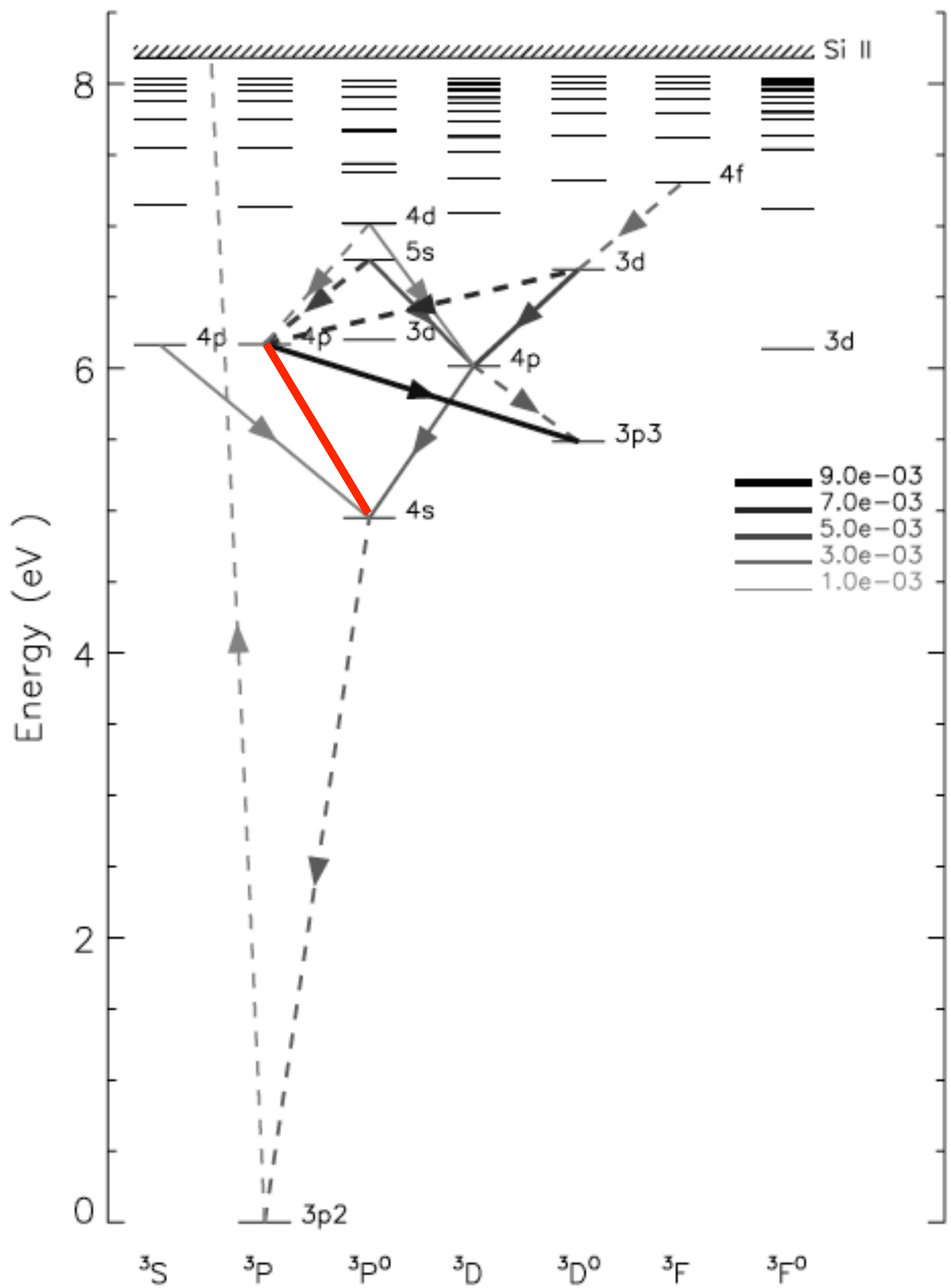
Si 10827 Å line in FALC



Ionization equilibrium

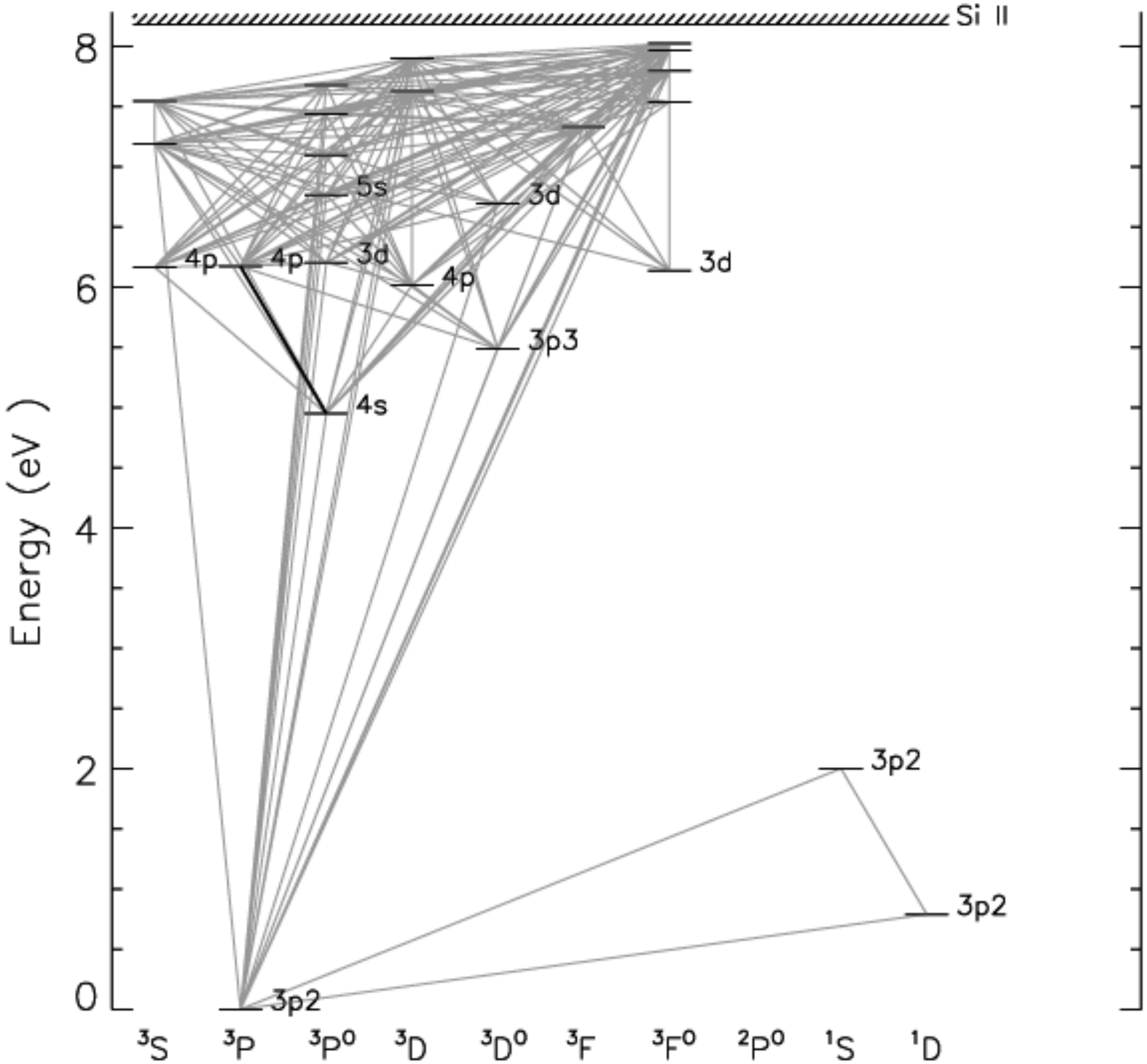


Influence of different rates

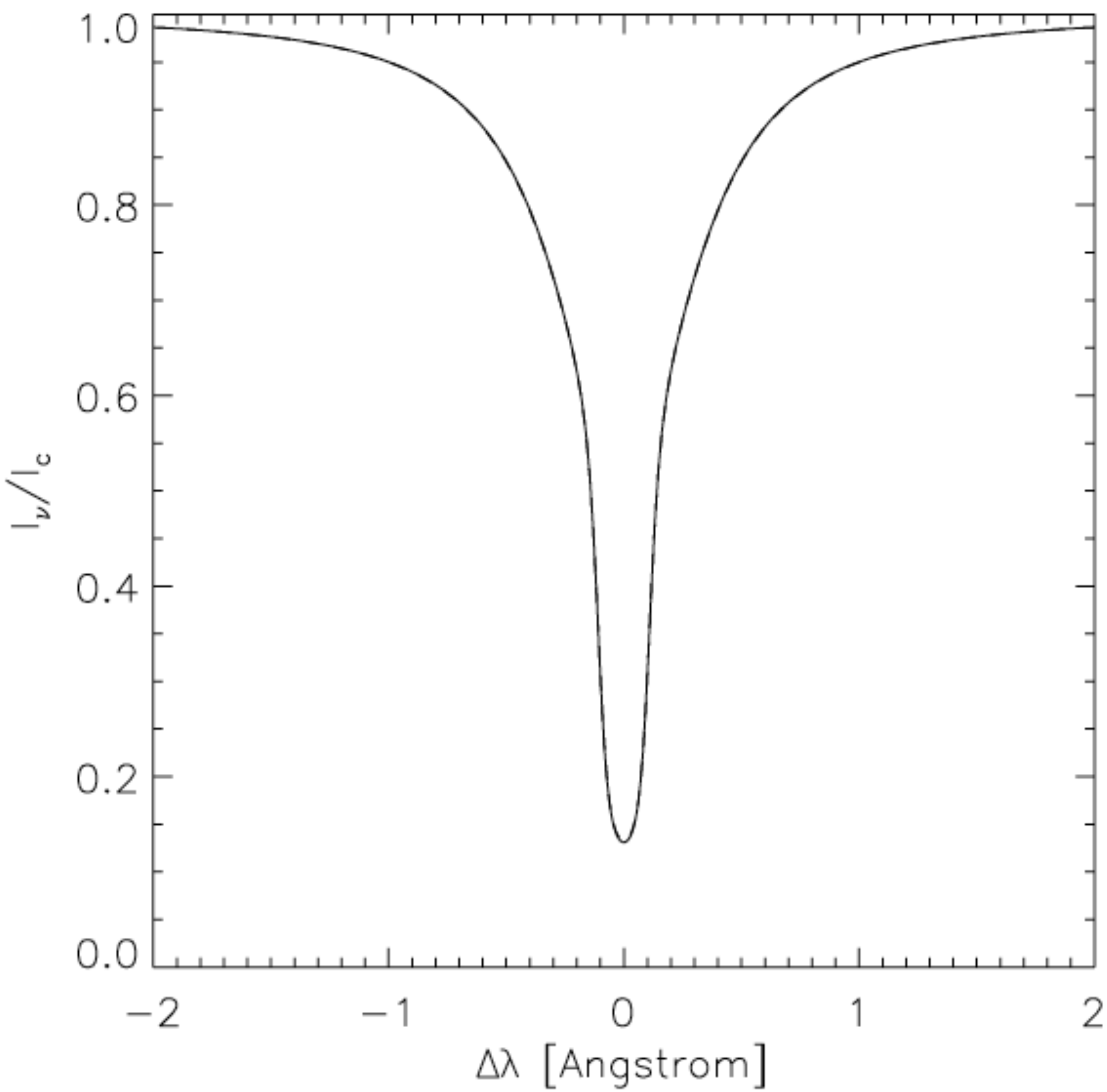


Simplified model atom

23 levels, 149 lines, 22 continua

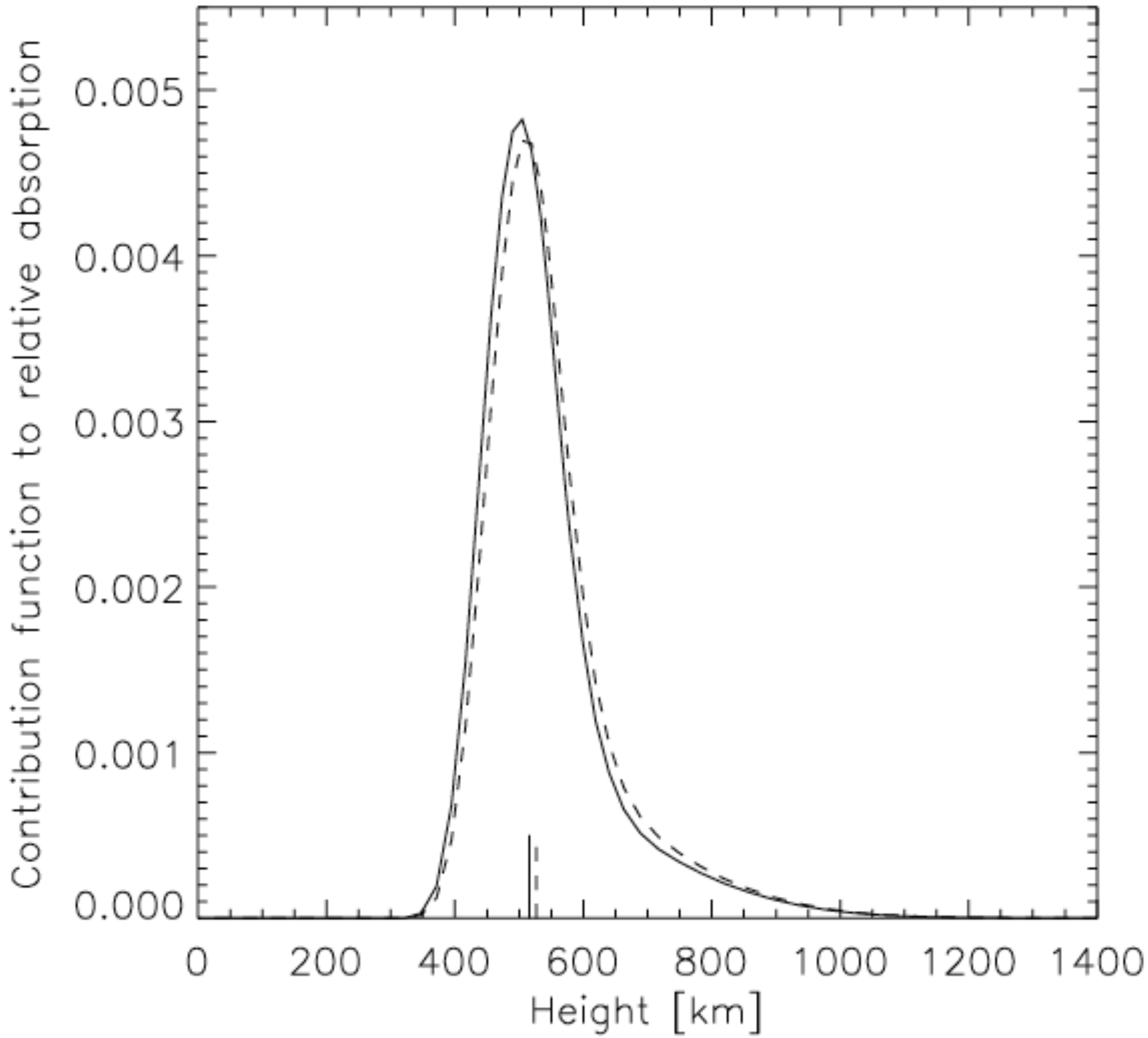


Intensity, FALC



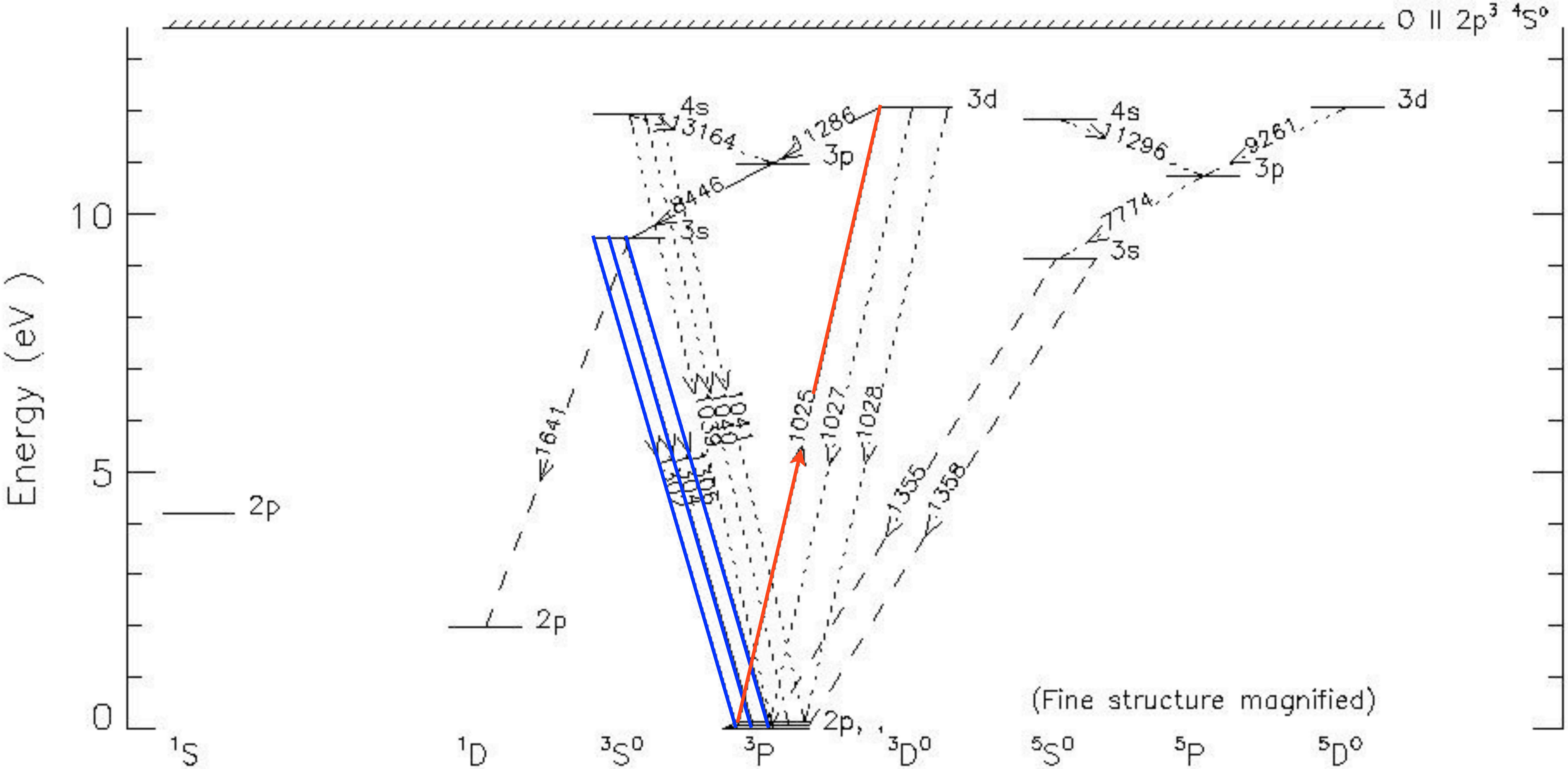
Solid: large model atom
Dashed: simplified model atom

Contribution function to relative absorption



Solid: large model atom
Dashed: simplified model atom

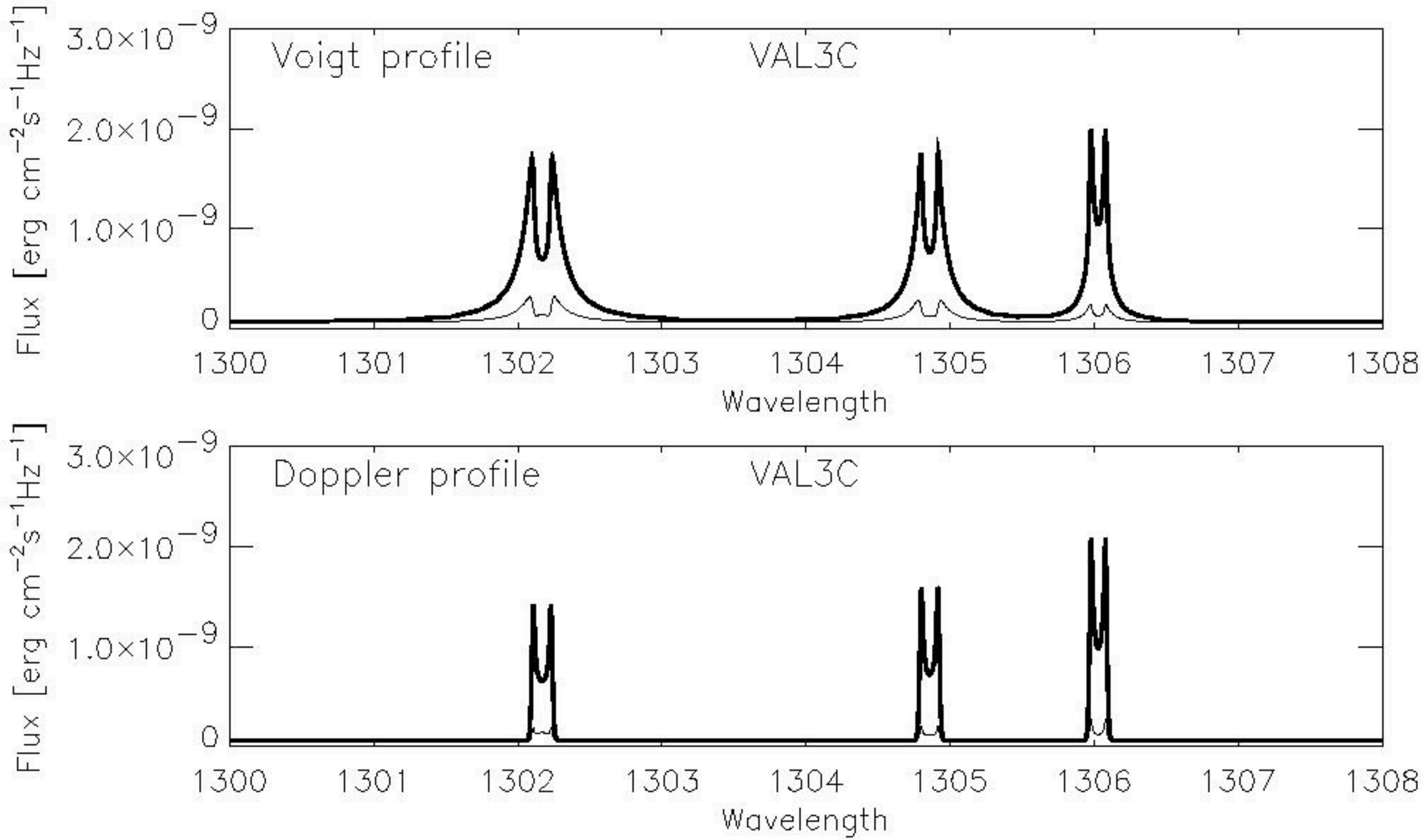
non-LTE modeling of O I resonance lines



Resonance lines pumped by Lyman-beta

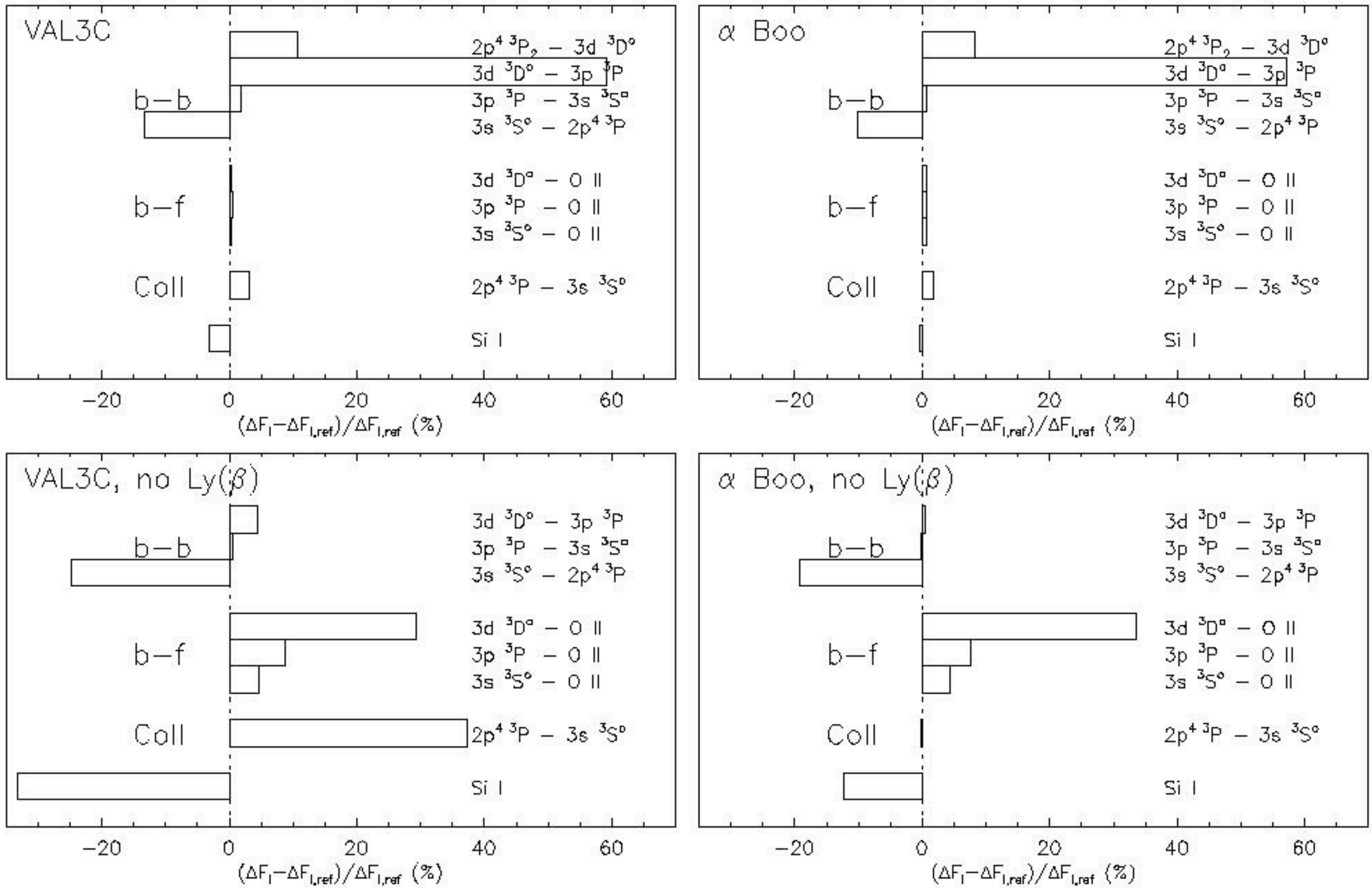
Carlsson, Judge, 1993, ApJ 402, 344

non-LTE modeling of O I resonance lines

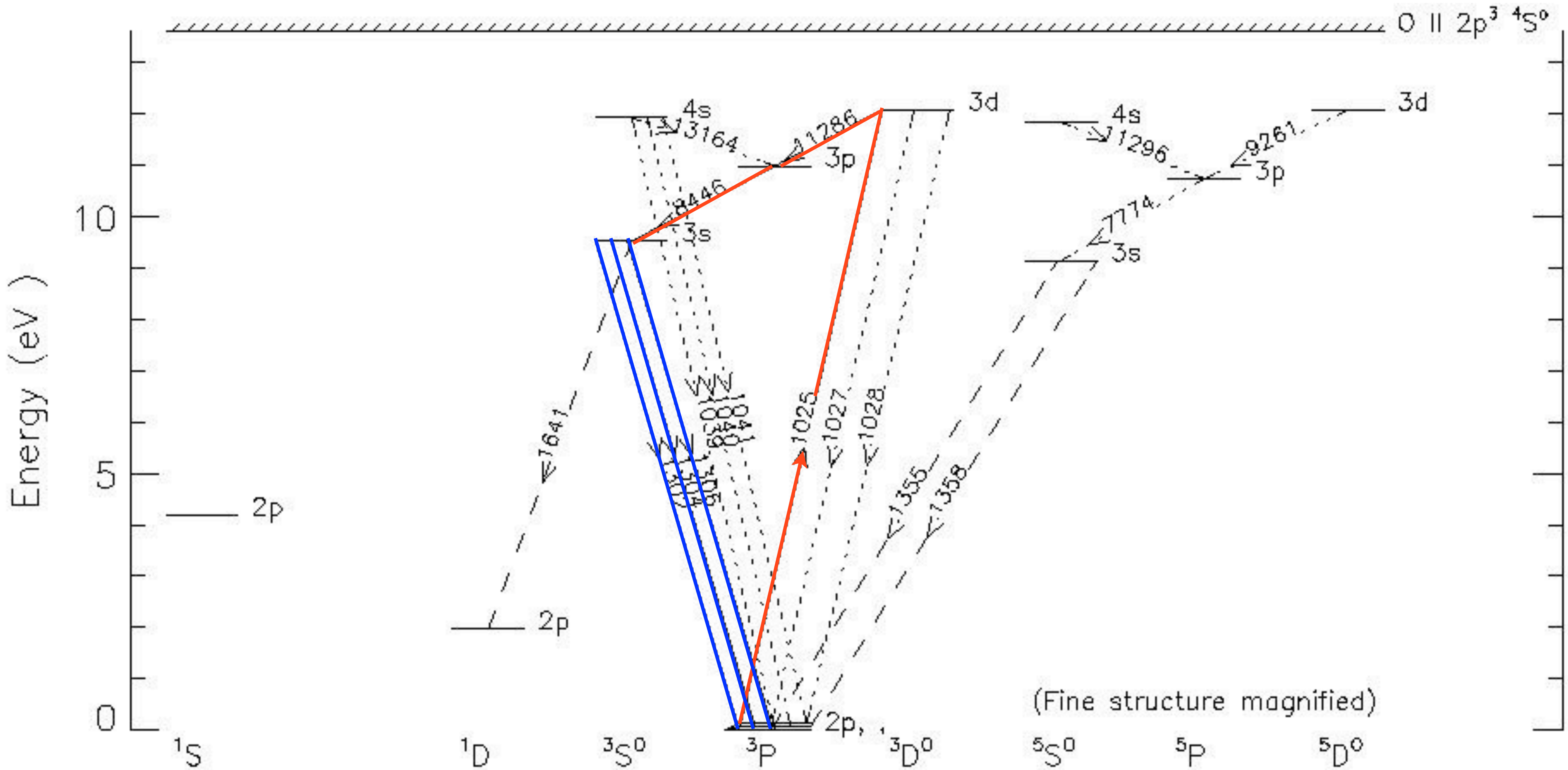


With Lyman-beta pumping (thick) and without (thin)

non-LTE modeling of O I resonance lines



non-LTE modeling of O I resonance lines

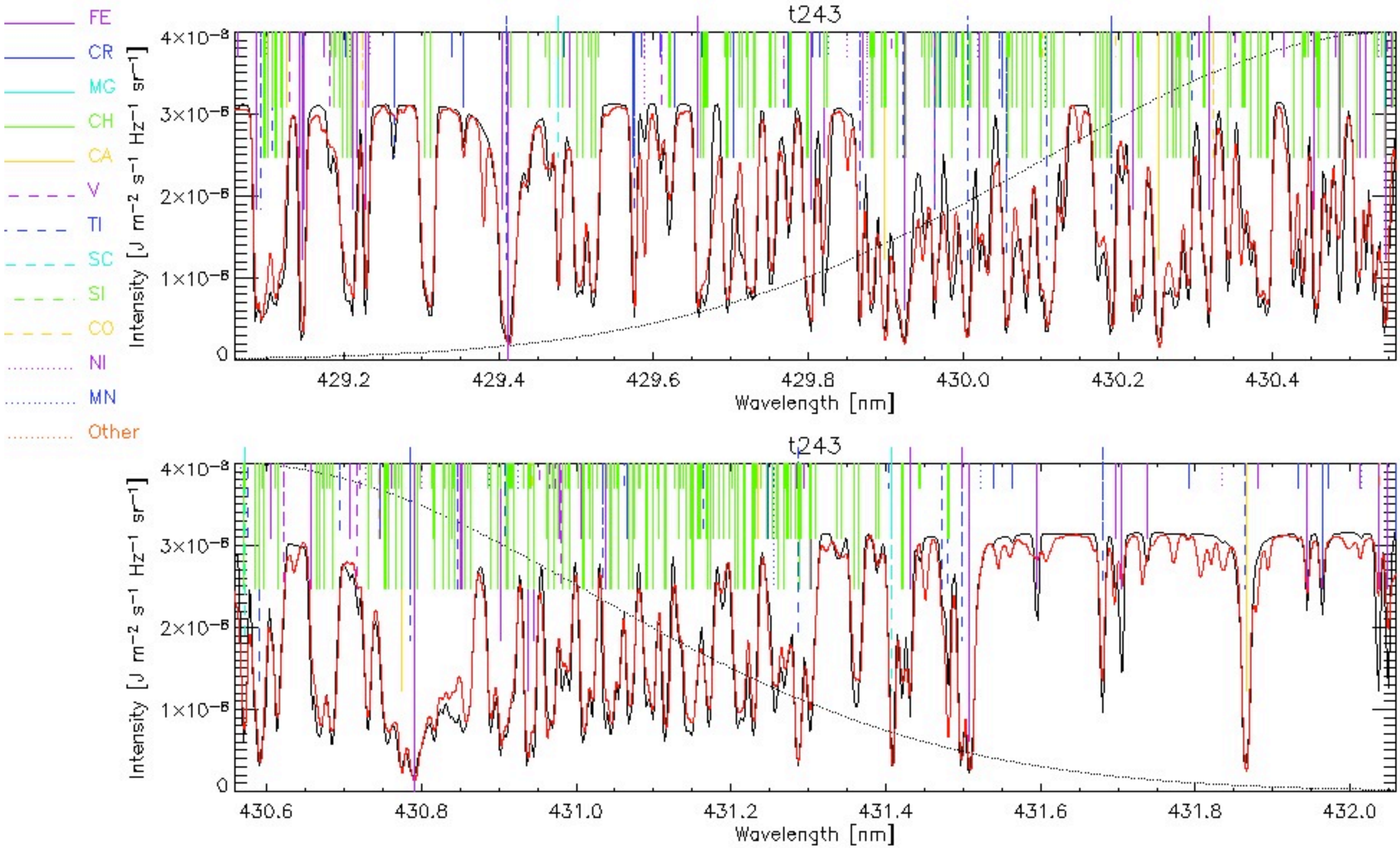


Sensitivity analysis showed importance of pumping chain

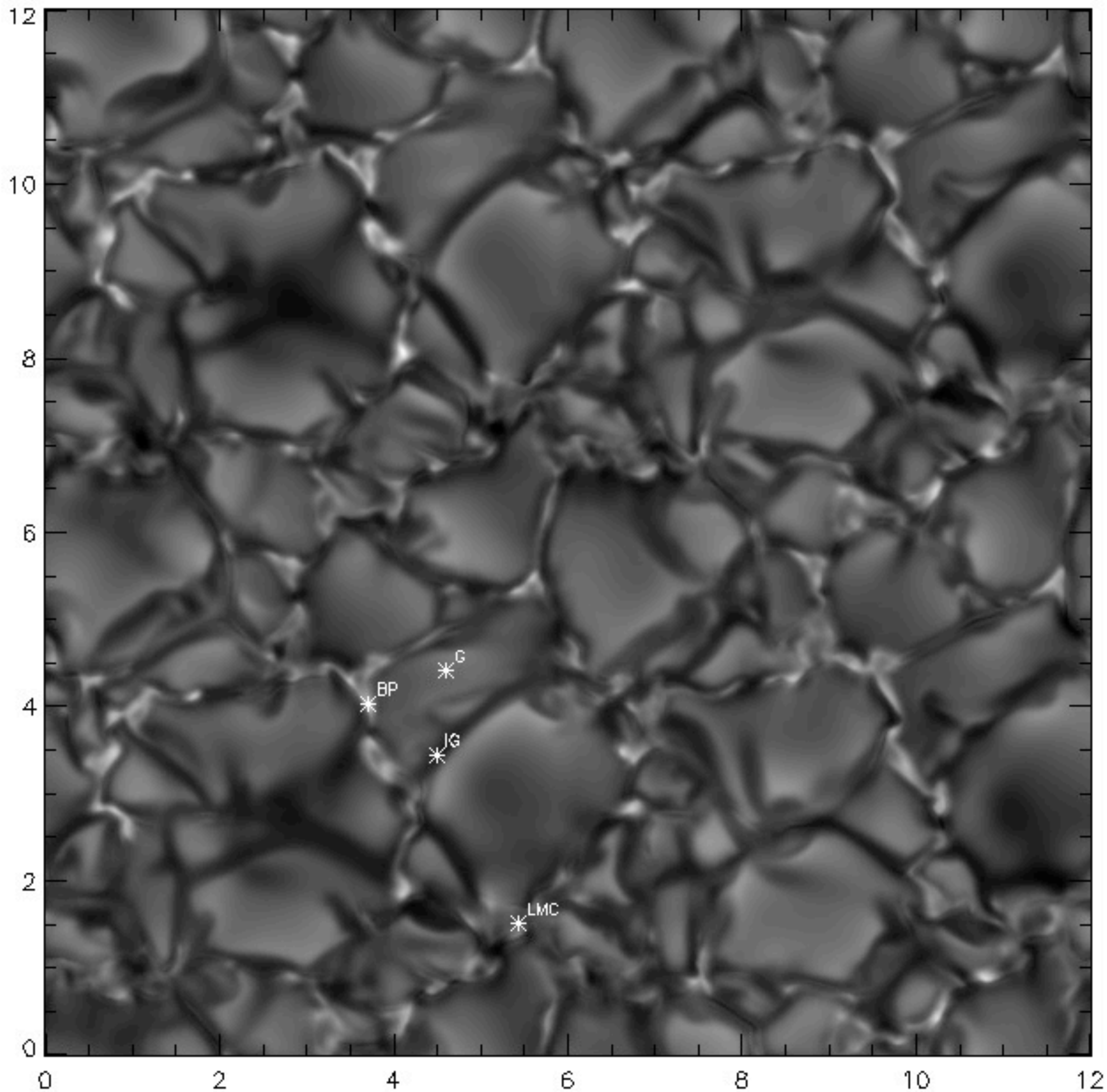
MHD simulation of Solar magneto-convection

- Nordlund/Stein code
- multi-group opacities, 4 bins
- Initial field 250G, vertical, single polarity
- 253x253x163 simulation
- RT each snapshot, 2728 frequency points

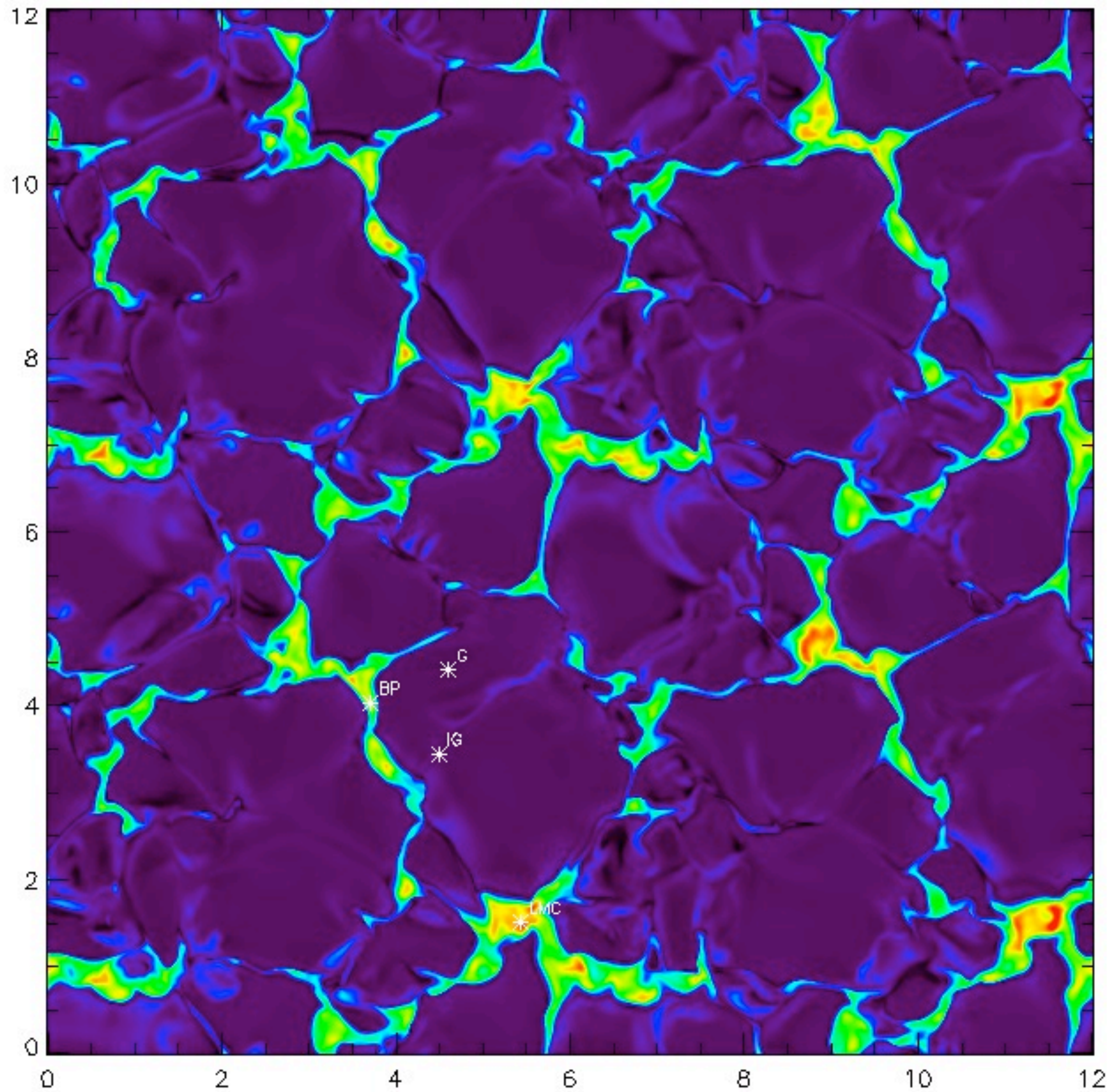
Synthetic spectrum



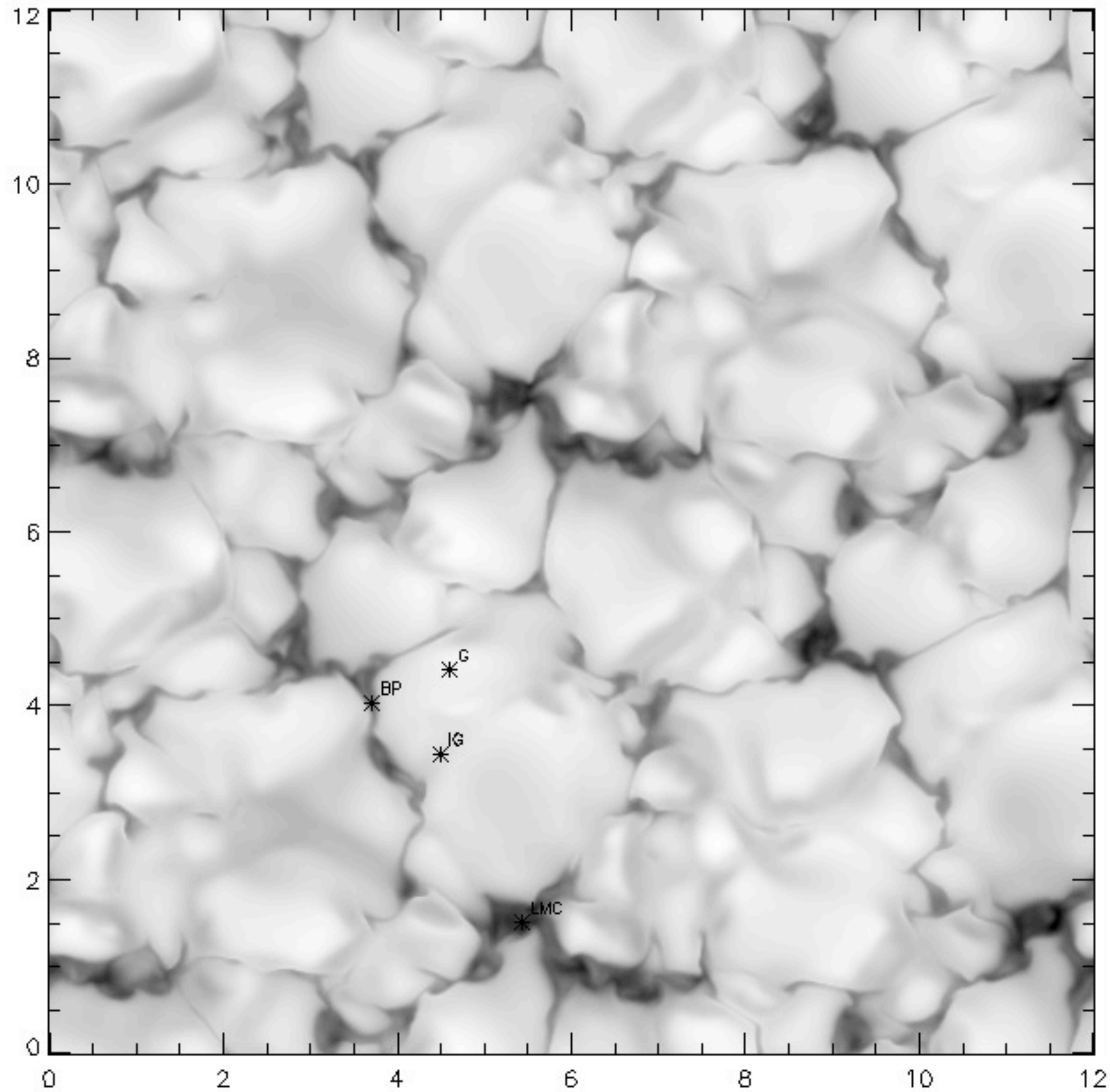
3D MHD simulation



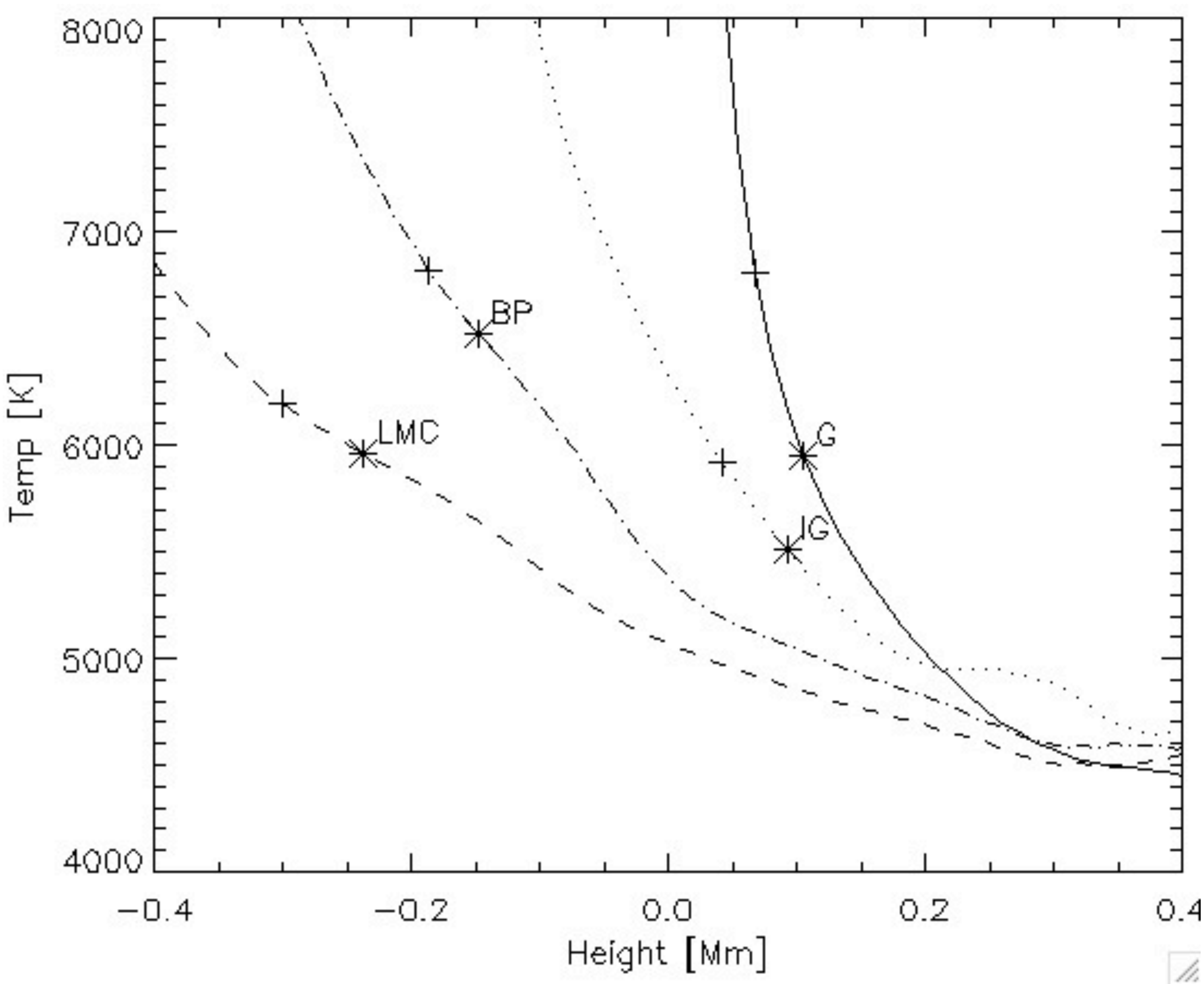
Magnetic field

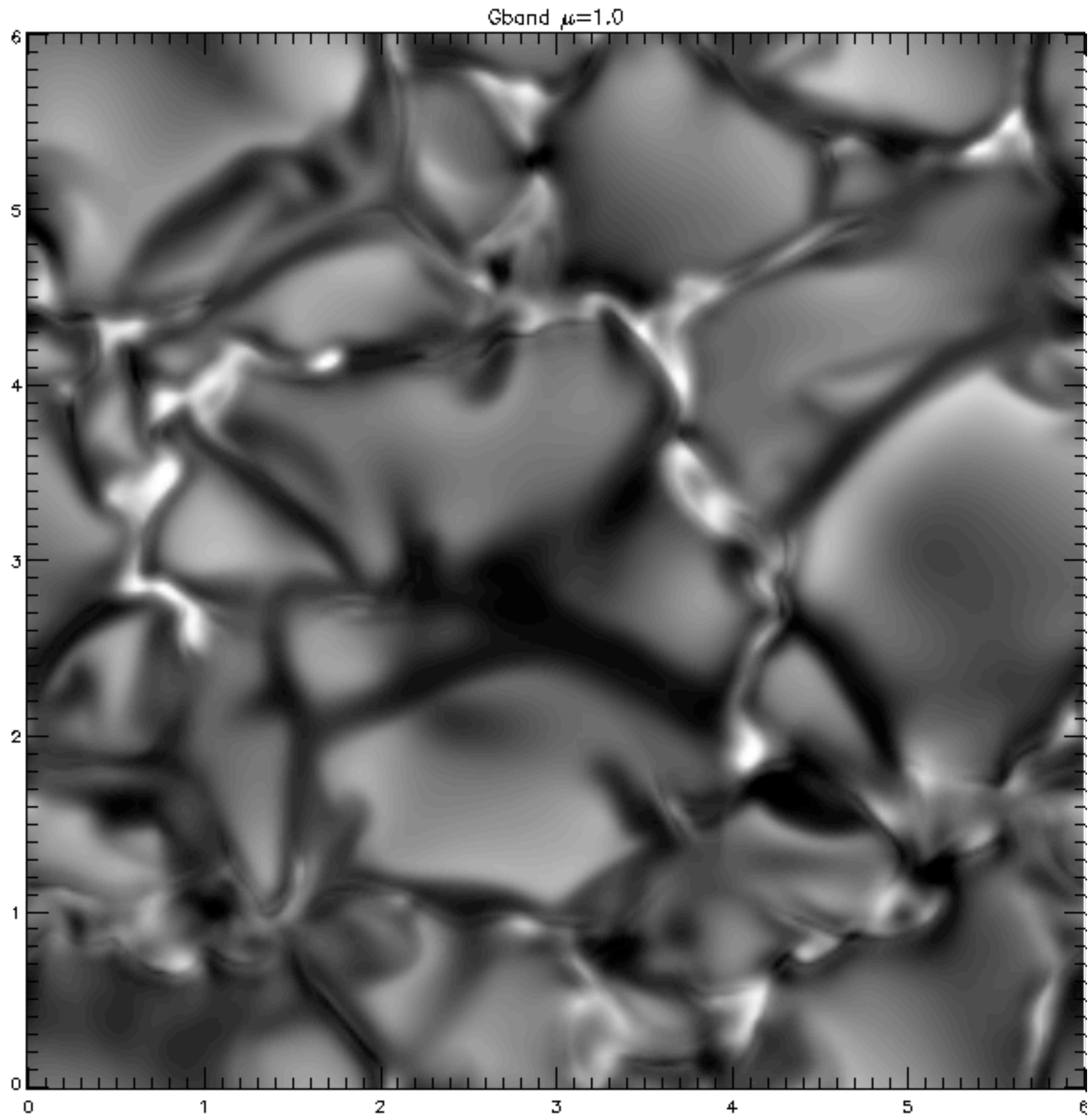


Height where tau=1

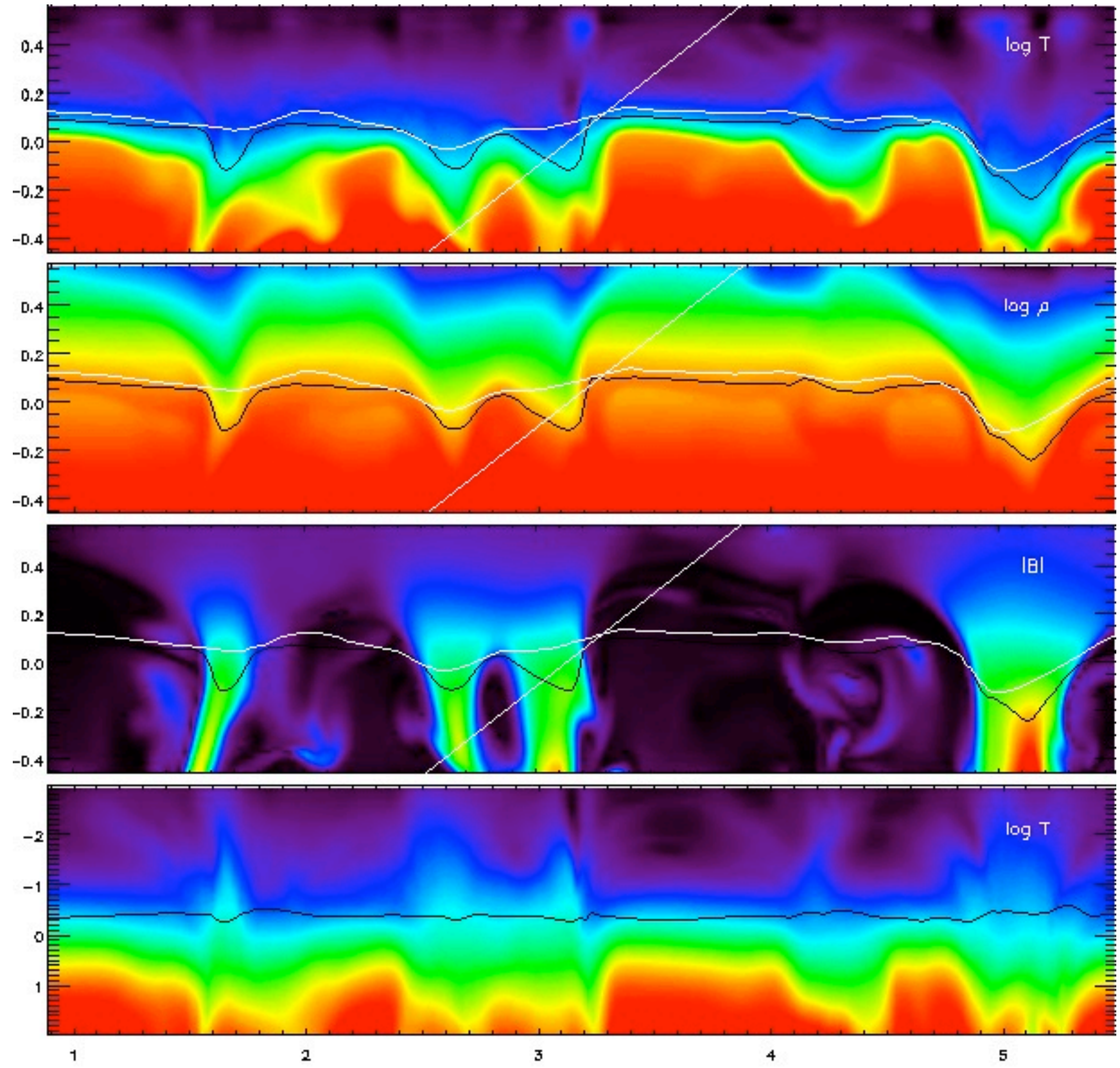


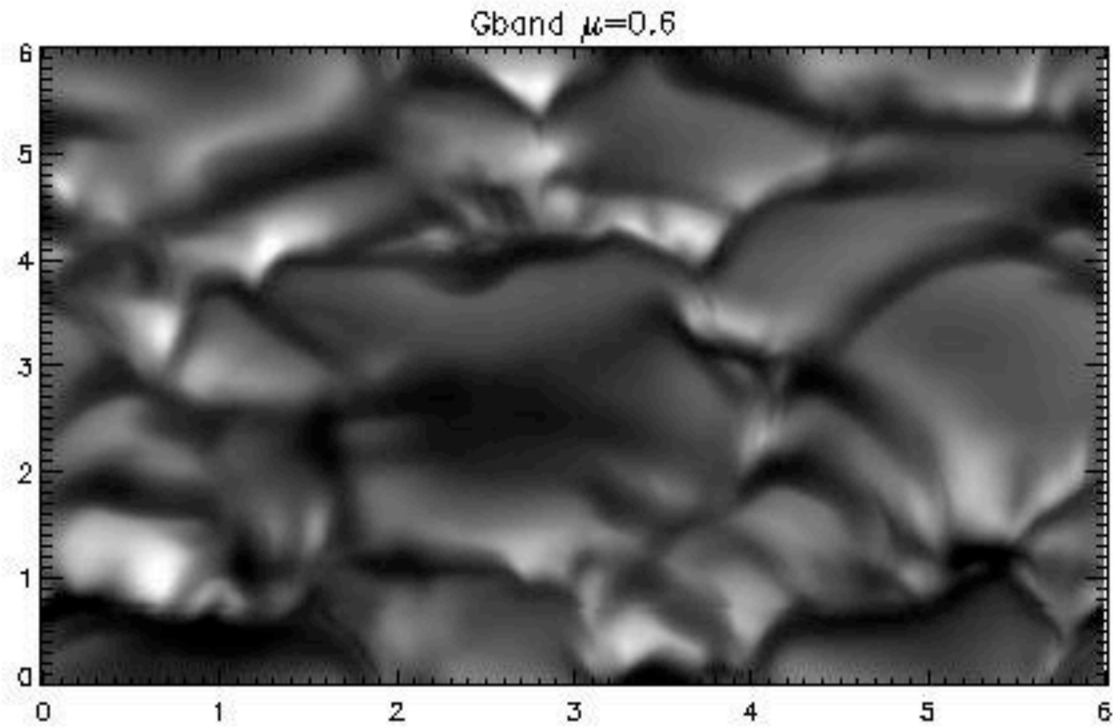
Temperature structure

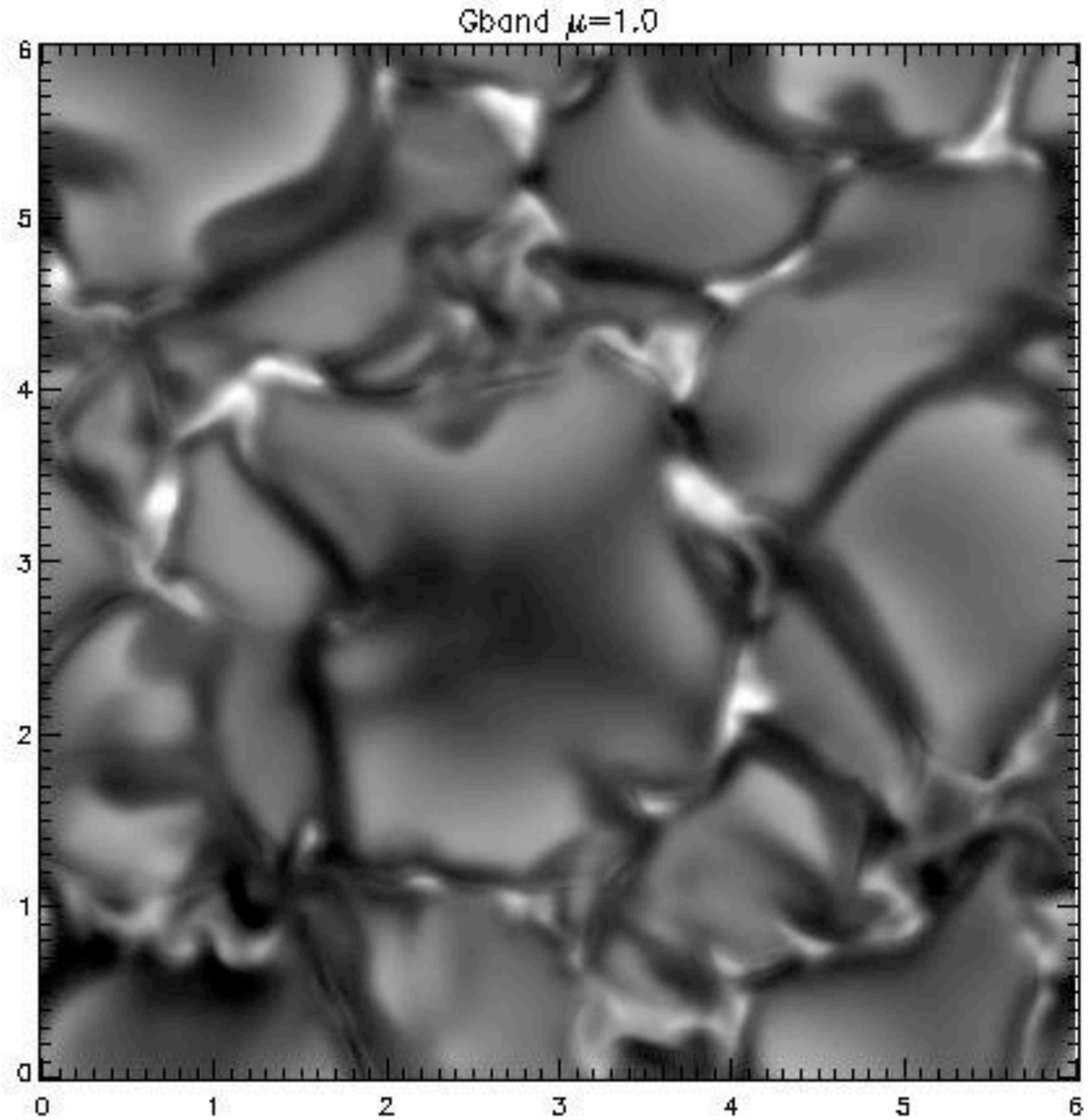



Gband μ=1.0
0
1
2
3
4
5
6
0
1
2
3
4
5
6

Why faculae?

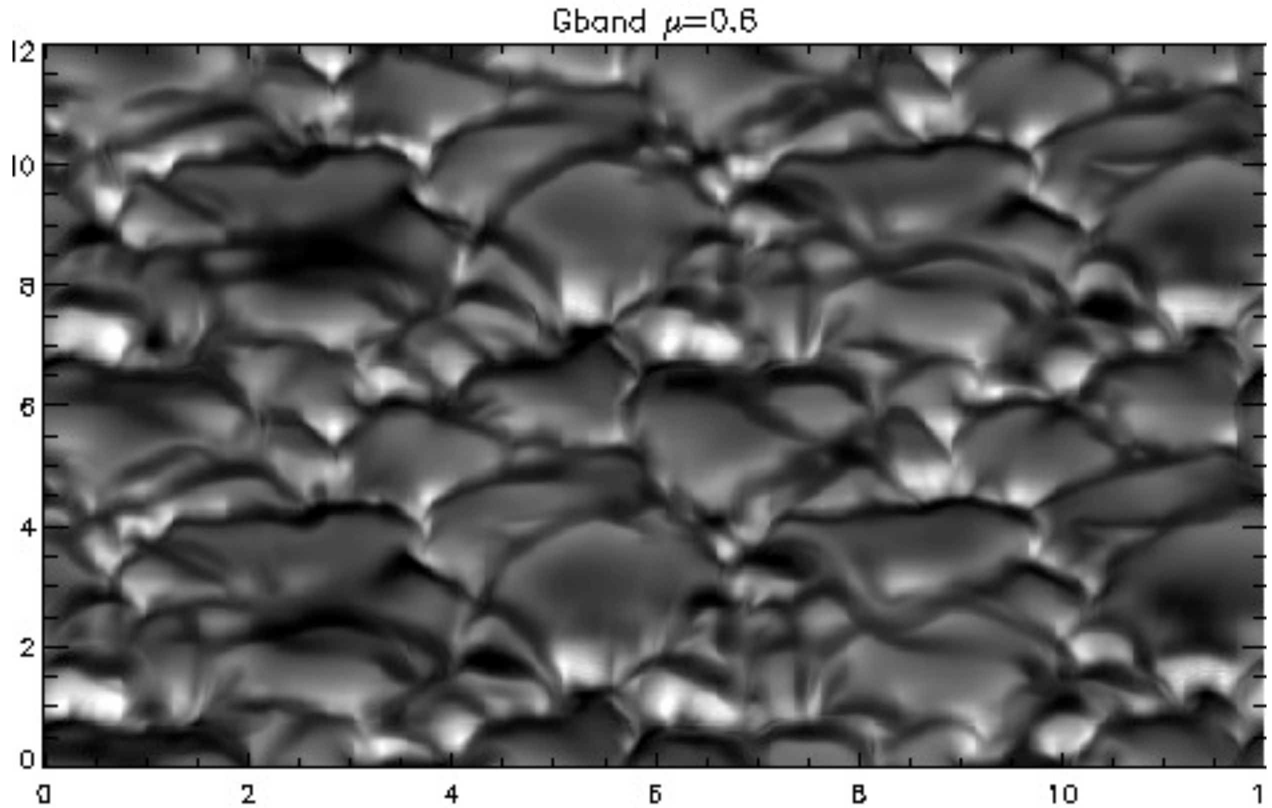



Gband μ=0.6
0
1
2
3
4
5
6

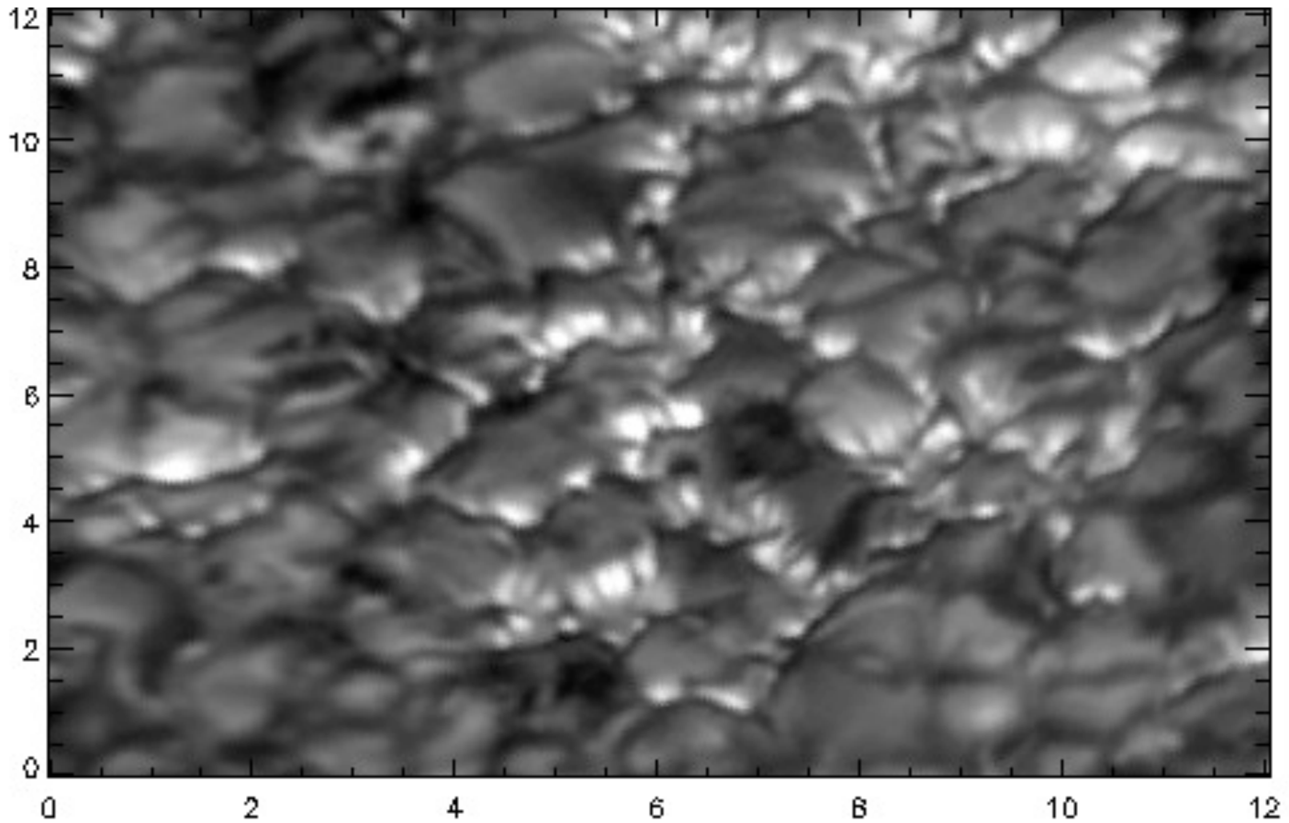

Gband μ=1.0
0
1
2
3
4
5
6

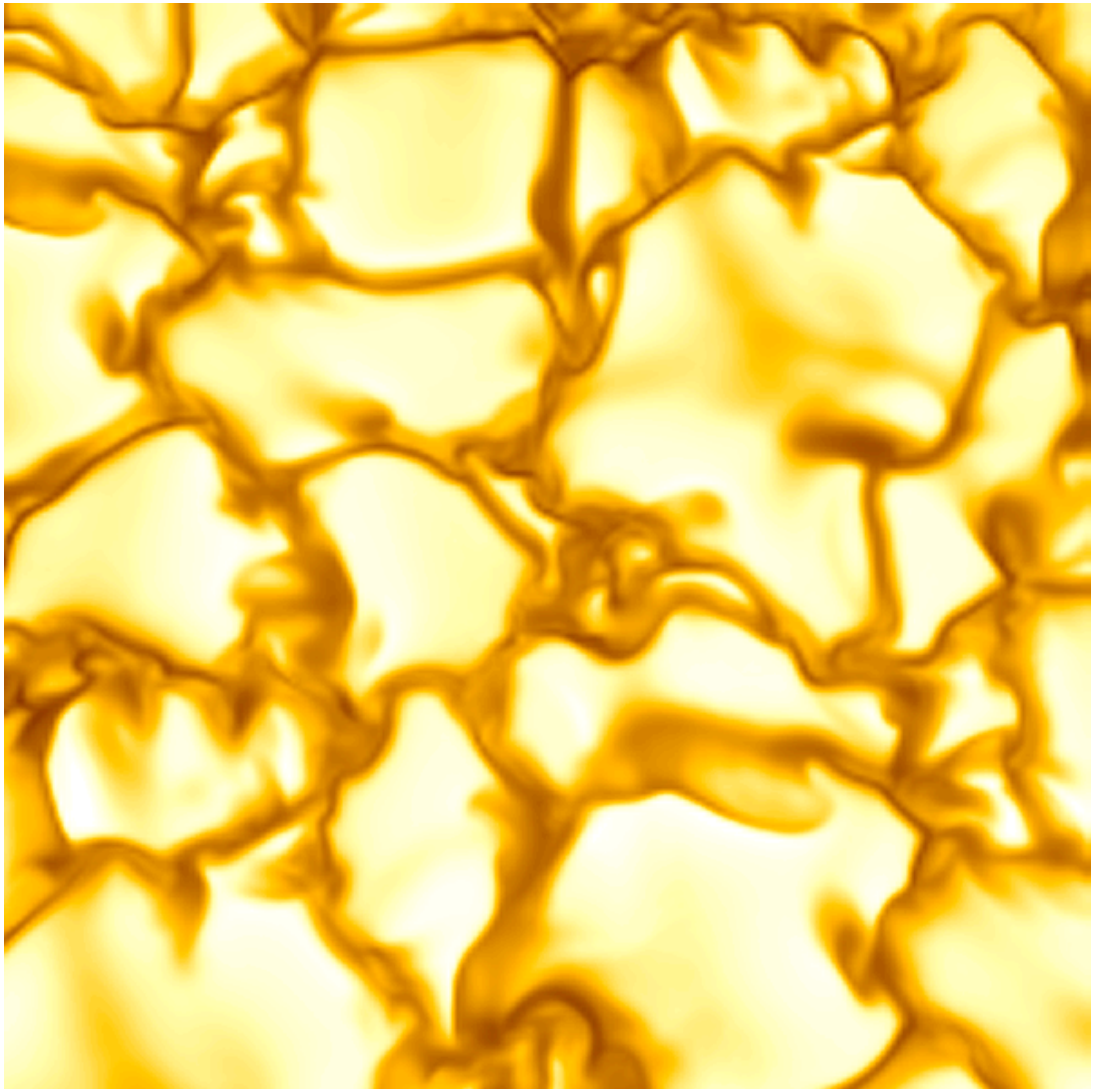
Comparison with observations

Simulation, mu=0.6



Observation, mu=0.63





non-Statistical equilibrium

- 2-level case
- linear rate matrix
- hydrogen ionization

non-Statistical equilibrium

$$\frac{Dn_i}{Dt} = \sum_{j \neq i}^{N} n_j P_{ji} - n_i \sum_{j \neq i}^{N} P_{ij}$$

2-level case:

$$n_1(t) = n_1(\infty) + (n_1(0) - n_1(\infty))e^{-(P_{12}+P_{21})t}$$

Timescale depends on both upward and downward rate

There is only one timescale involved

non-Statistical equilibrium

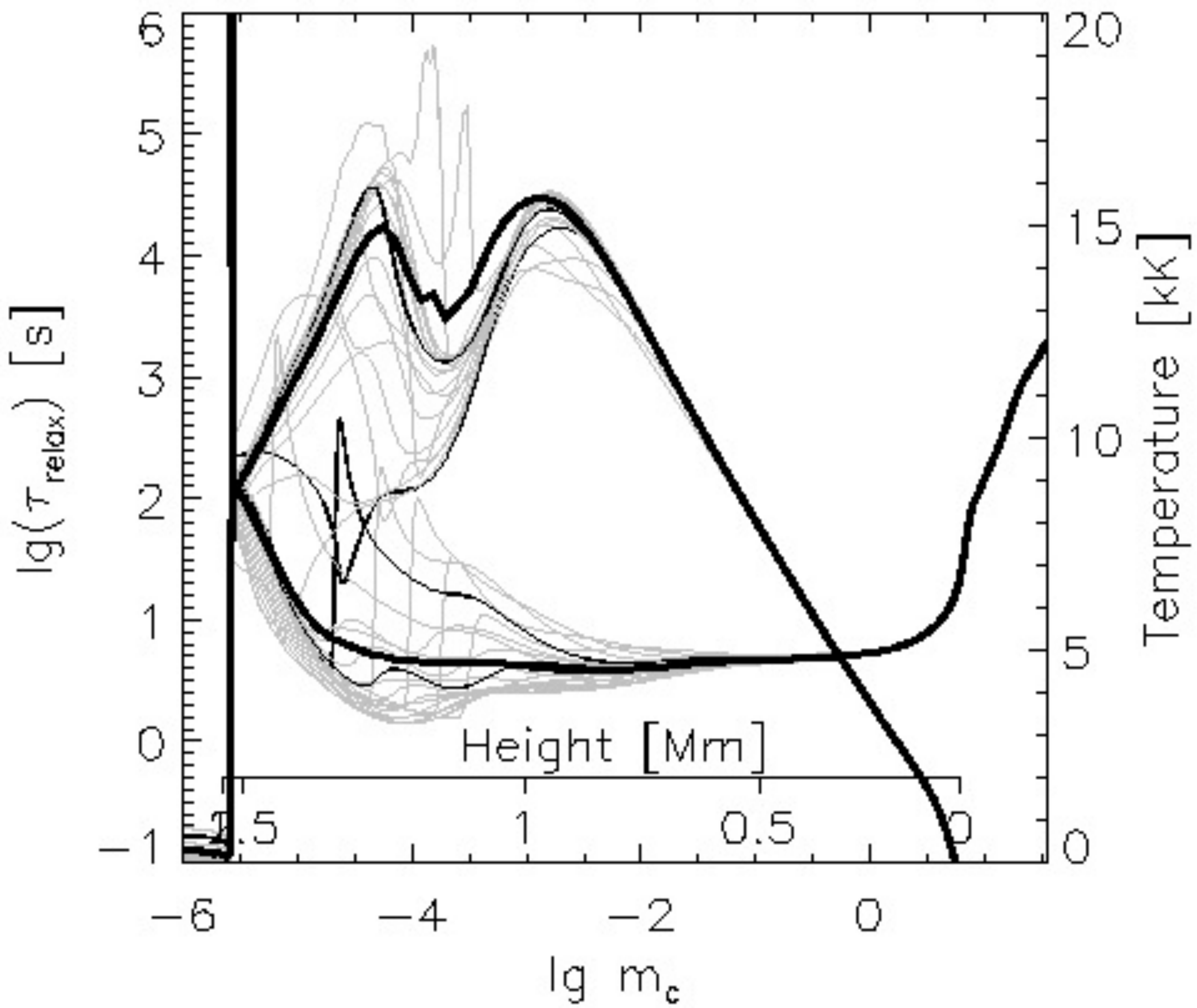
$$\frac{Dn_i}{Dt} = \sum_{j \neq i}^{N} n_j P_{ji} - n_i \sum_{j \neq i}^{N} P_{ij}$$

$$\frac{D\mathbf{n}}{Dt} = \mathbf{W}\mathbf{n}$$

linear rate matrix:

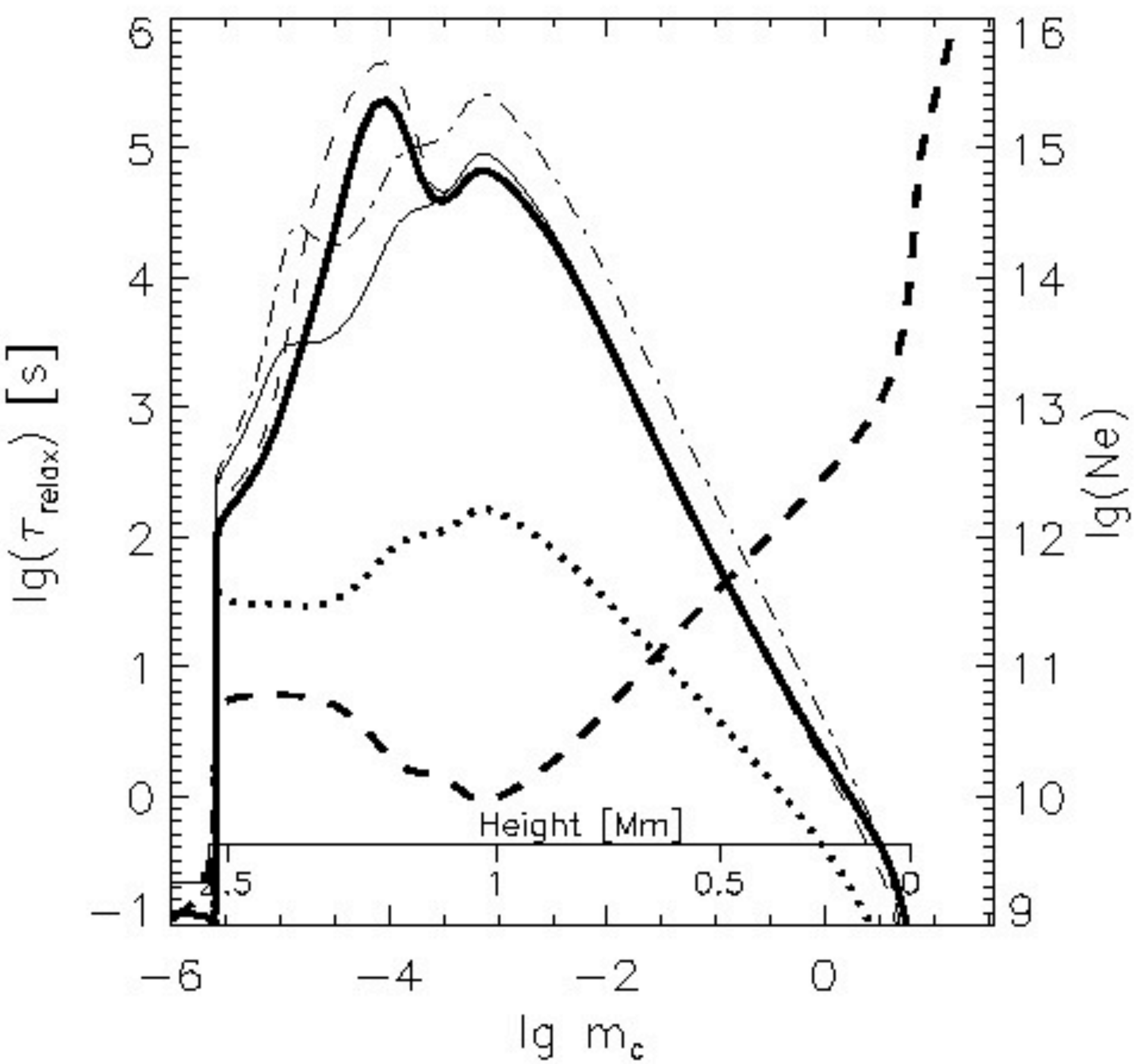
Populations can be written as linear combination of eigenvectors of W with time-evolution given by eigenvalues of W (Judge 2005, JQSRT, 92, 479)

Hydrogen ionization



Time scale for hydrogen ionization/recombination is highly time-varying. Fast rates when temperature is high (ionizing phase), slow rates when temperature is low (recombining phase).

Hydrogen ionization

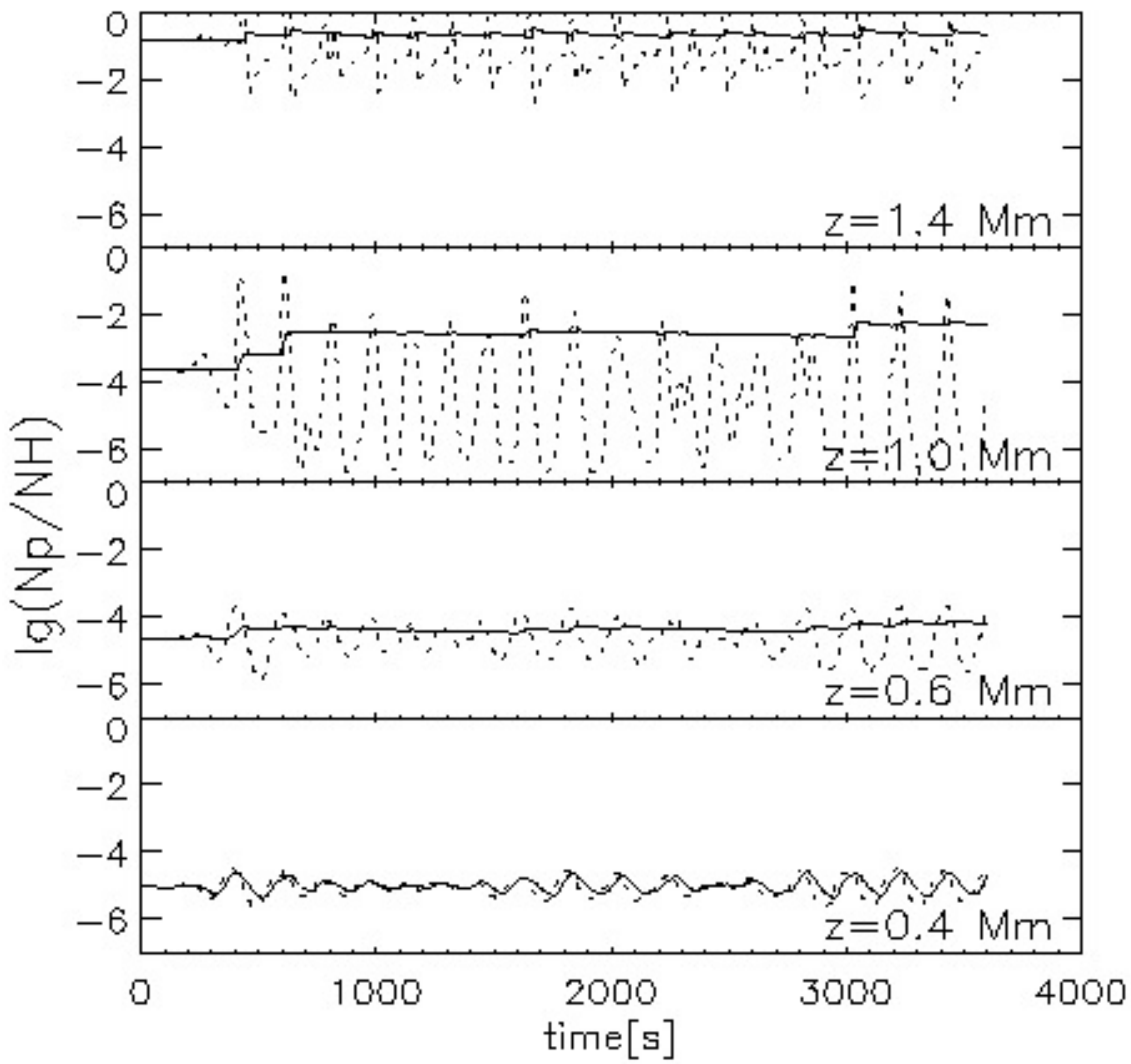


Electron density (thick dashed)
Eigenvalue timescales (thick dotted)
only collisions (dot-dashed)
Lyman lines in detailed balance (thin solid)
Lyman-alpha in escape probability (dashed)
Numerical result (thick solid)

Eigenvalues of rate-matrix give erroneous timescales for non-linear rate-matrix. Exclusion of large, canceling rates (Lyman transitions) give much better results.

(Carlsson & Stein, 2002, ApJ 572,626)

Hydrogen ionization



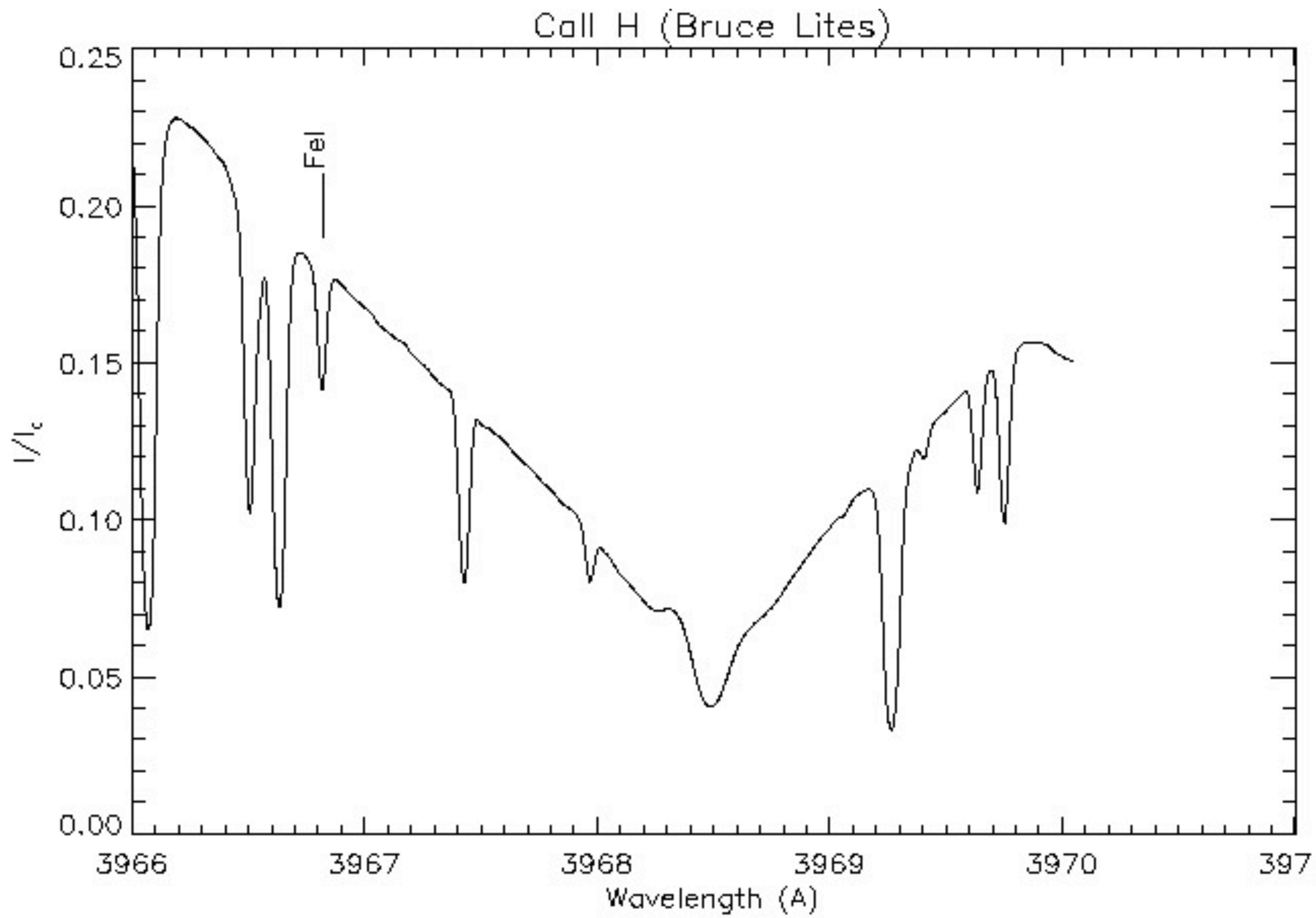
Time dependent ionization (solid)
Equilibrium ionization (dashed)

Slow rates when recombining results in ionization higher than equilibrium values.

Formation of spectrum in a dynamic chromosphere

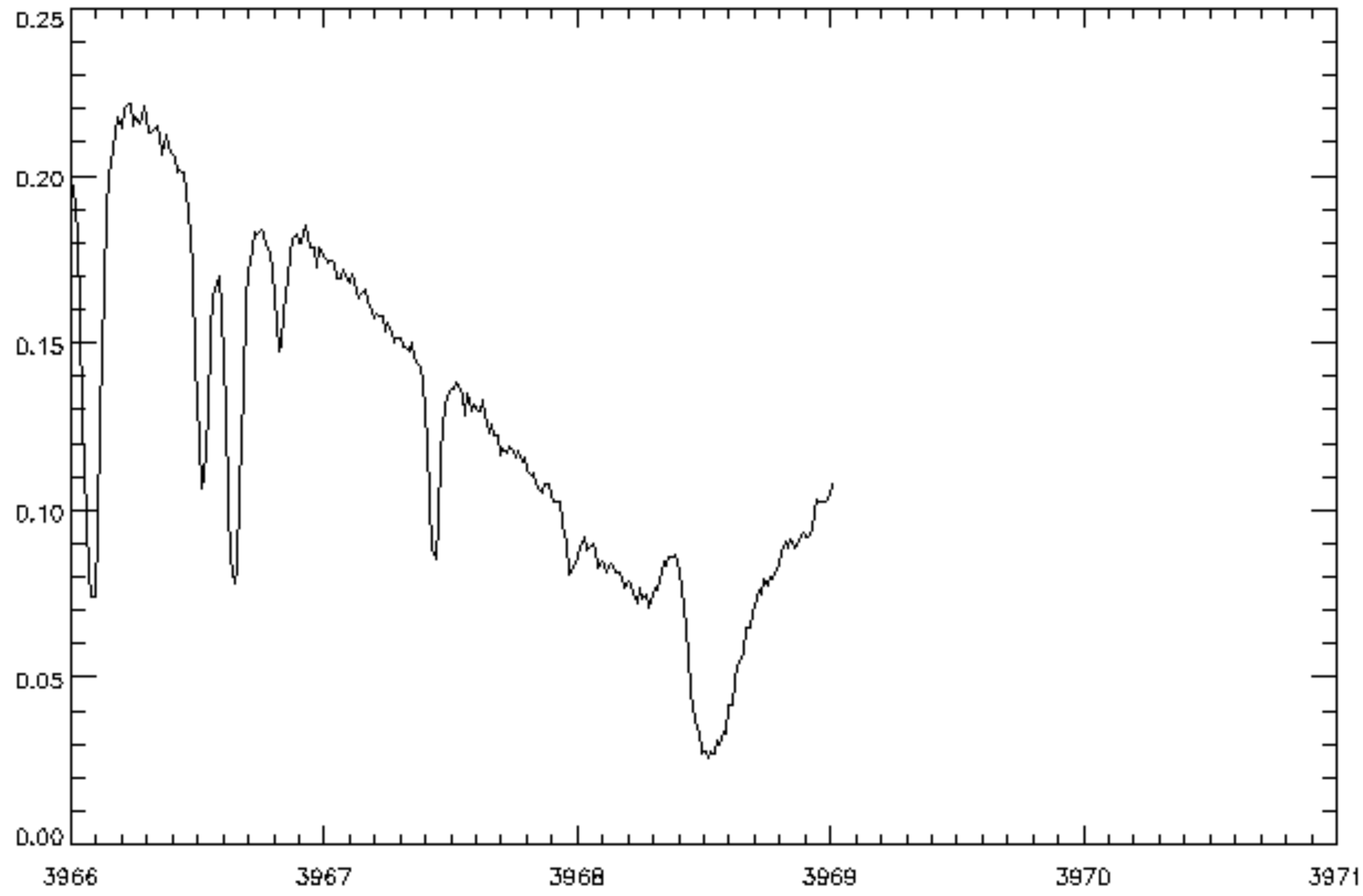
- Observations
- 1D non-LTE simulation
- Continuum formation
- Line formation

Ca II H-line

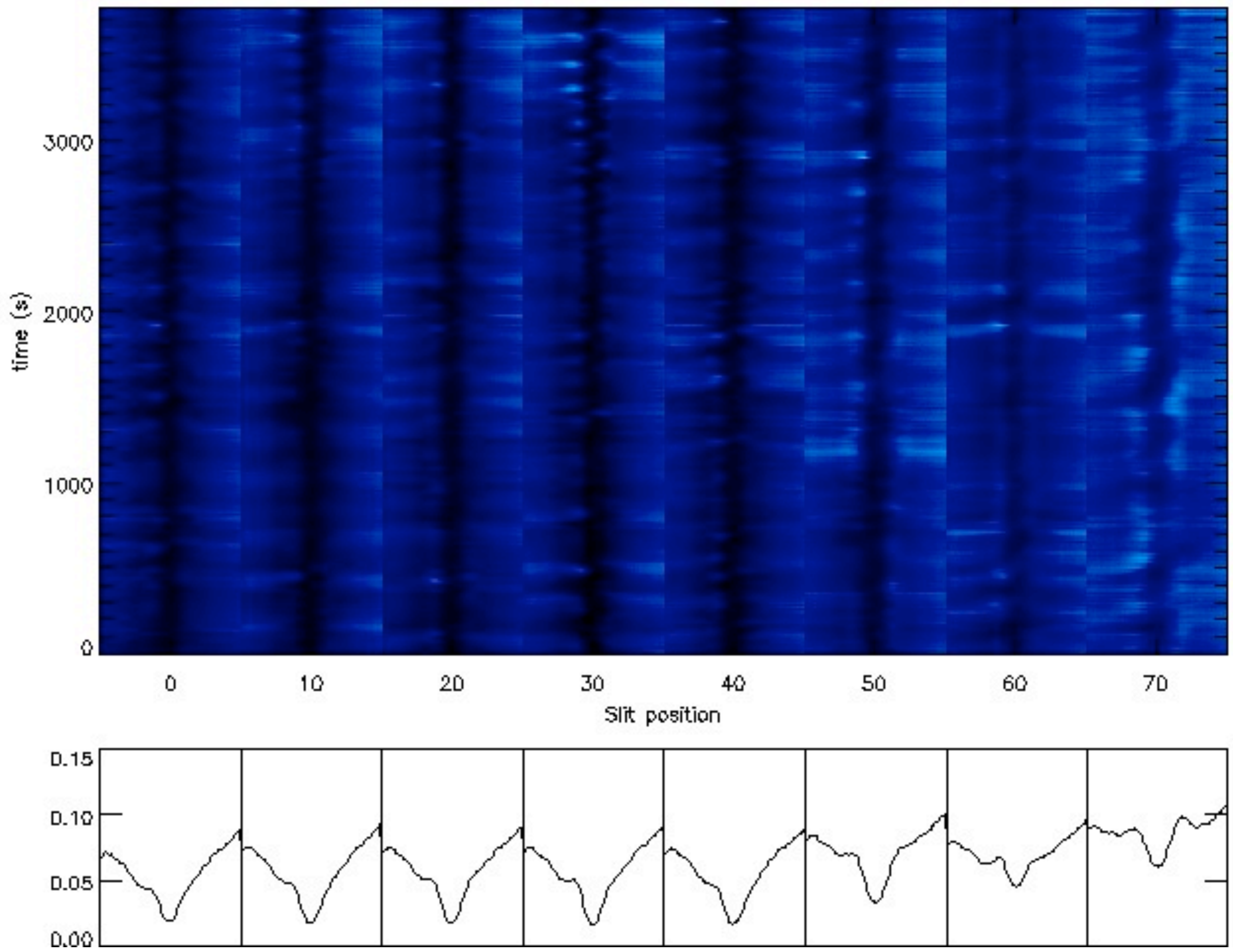


CaII H (Bruce Lites)
FeI
0.25
0.20
0.15
0.10
0.05
0.00
I/I$_c$
3966
3967
3968
3969
3970
3971
Wavelength (A)

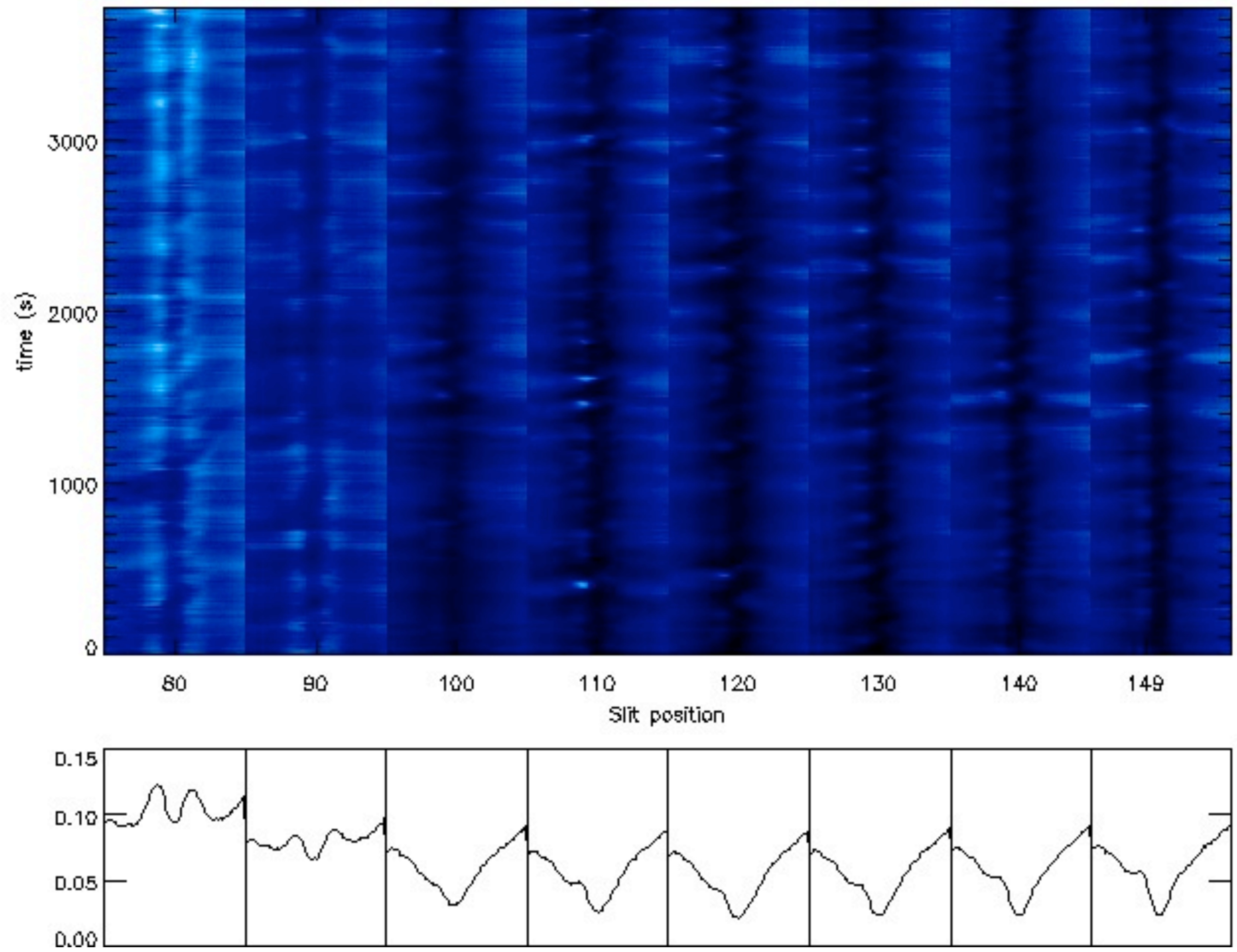
Dynamic behaviour



Spatial variation



Spatial variation



radyn: non-LTE radiation hydrodynamics in 1D

We used to have:

$$\delta j_{\nu\mu} = \frac{\partial j_{\nu\mu}}{\partial n_i}\delta n_i + \frac{\partial j_{\nu\mu}}{\partial n_j}\delta n_j$$

If the atmosphere is not given we get extra variables to solve for:

$$\delta\rho, \delta T, \delta n_e, \delta v_z$$

and extra derivatives with respect to these variables

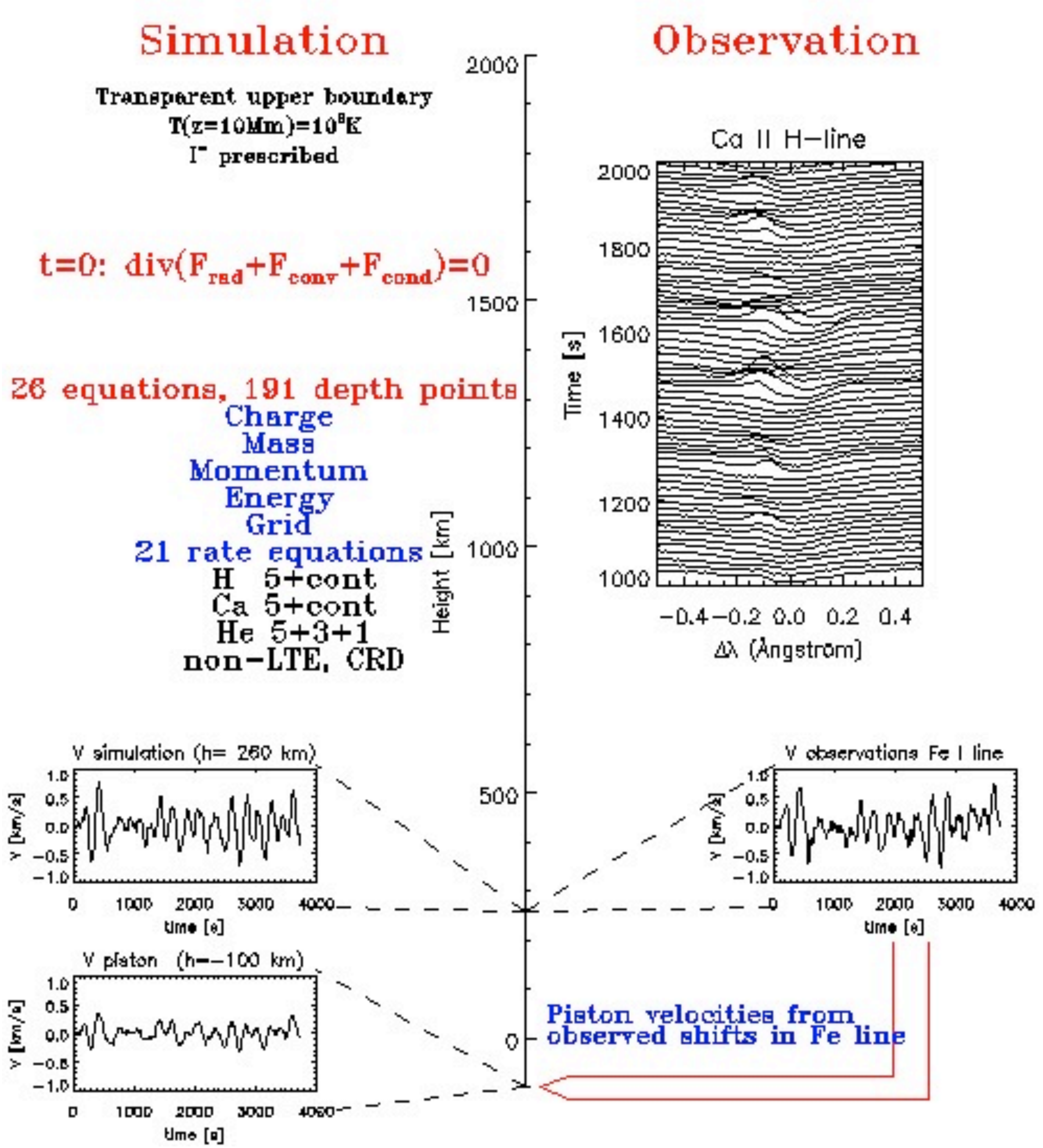
$$\delta j_{\nu\mu} = \frac{\partial j_{\nu\mu}}{\partial \rho}\delta\rho + \frac{\partial j_{\nu\mu}}{\partial T}\delta T + \frac{\partial j_{\nu\mu}}{\partial n_e}\delta n_e + \sum_{i=1}^{N_L} \frac{\partial j_{\nu\mu}}{\partial n_i}\delta n_i + \frac{\partial j_{\nu\mu}}{\partial v_z}$$

$$\frac{\partial j_{\nu c}}{\partial x}, \frac{\partial \kappa_{\nu c}}{\partial x}, \frac{\partial \alpha_{ij}}{\partial x}, \frac{\partial G_{ij}}{\partial x}, \frac{\partial C_{ij}}{\partial x}$$

are no longer zero

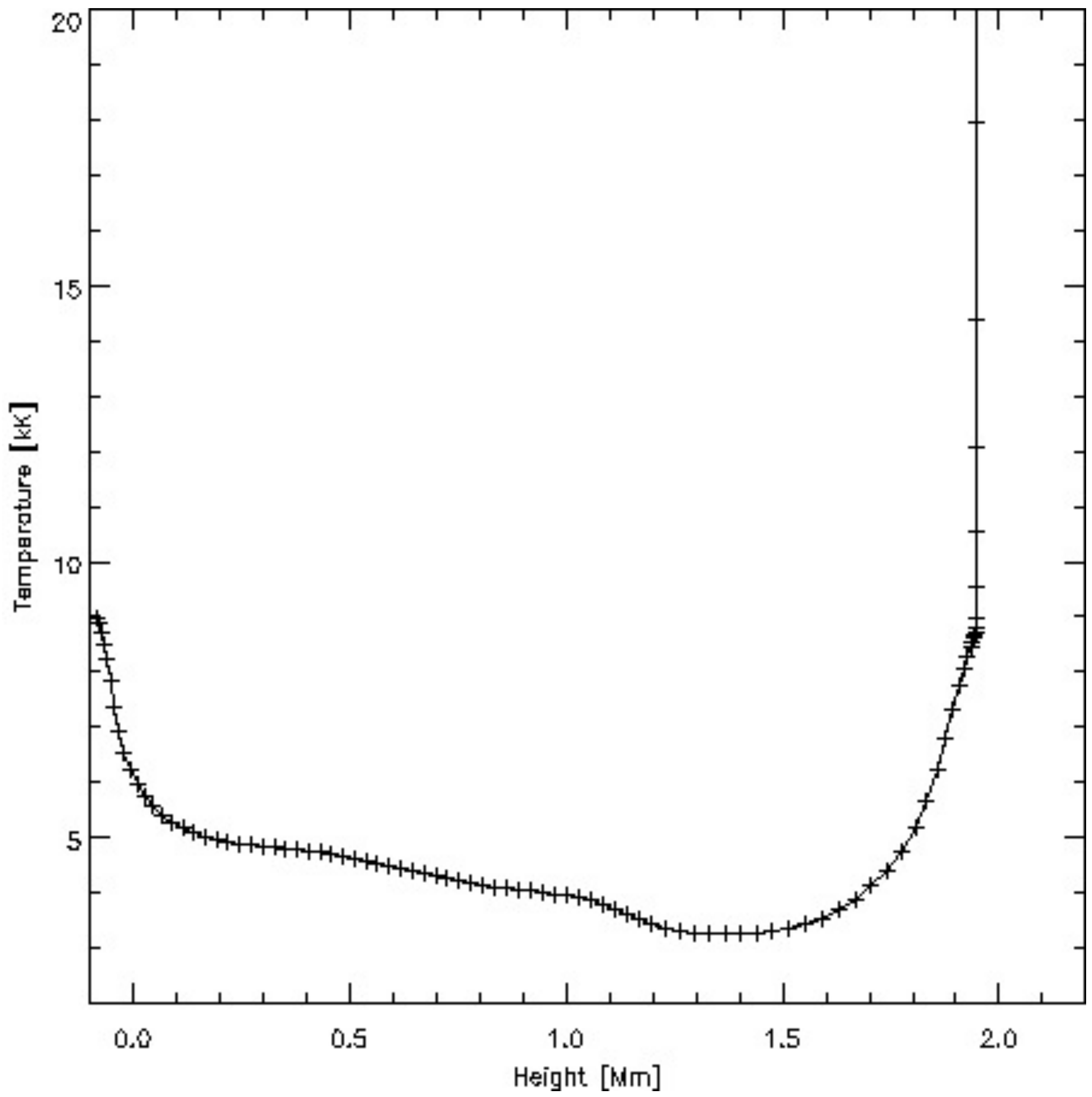
Extra equations: conservation of mass, energy, charge, momentum

1D non-LTE simulation

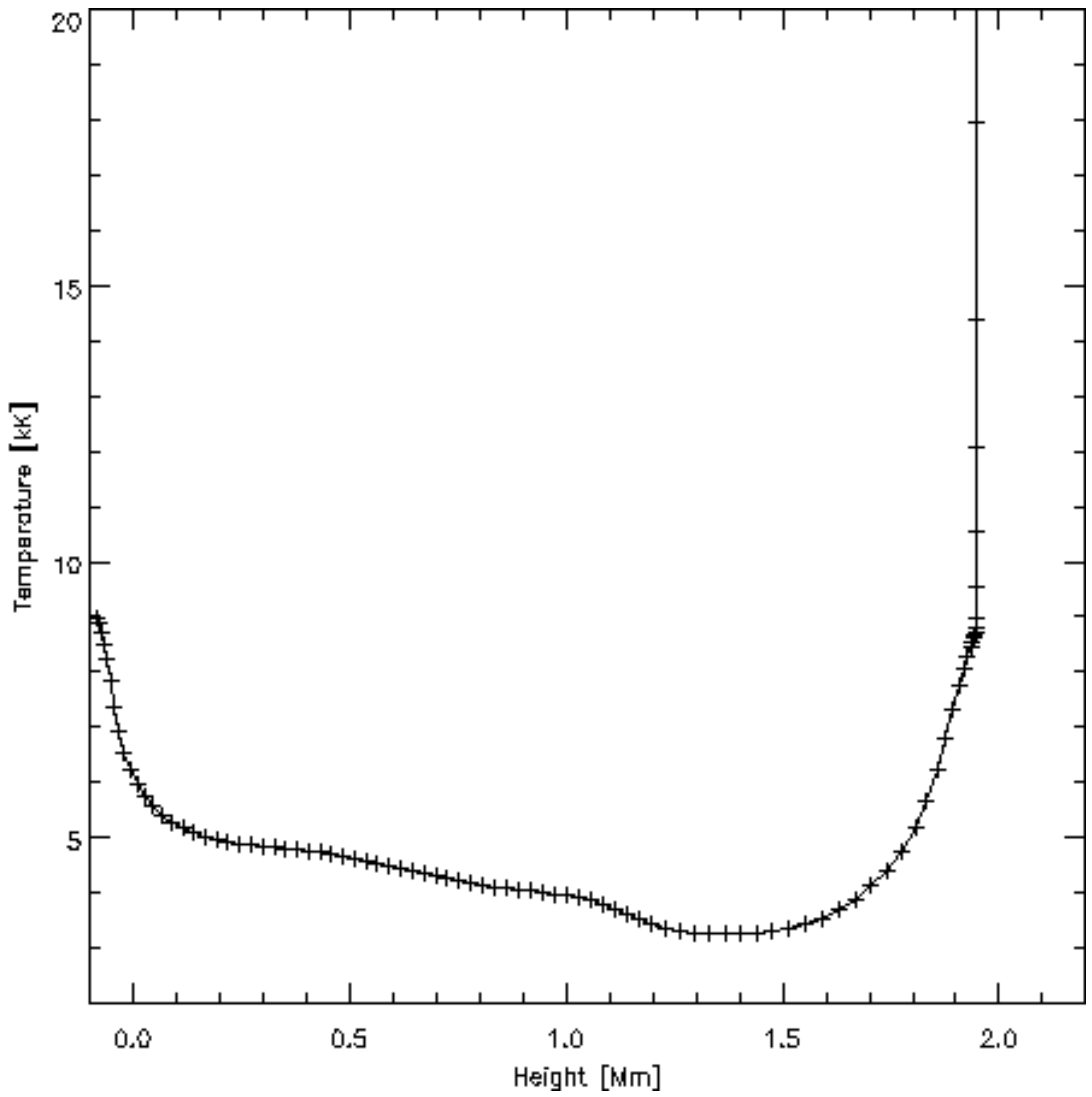


Carlsson & Stein 1992, 1994, 1995, 1997

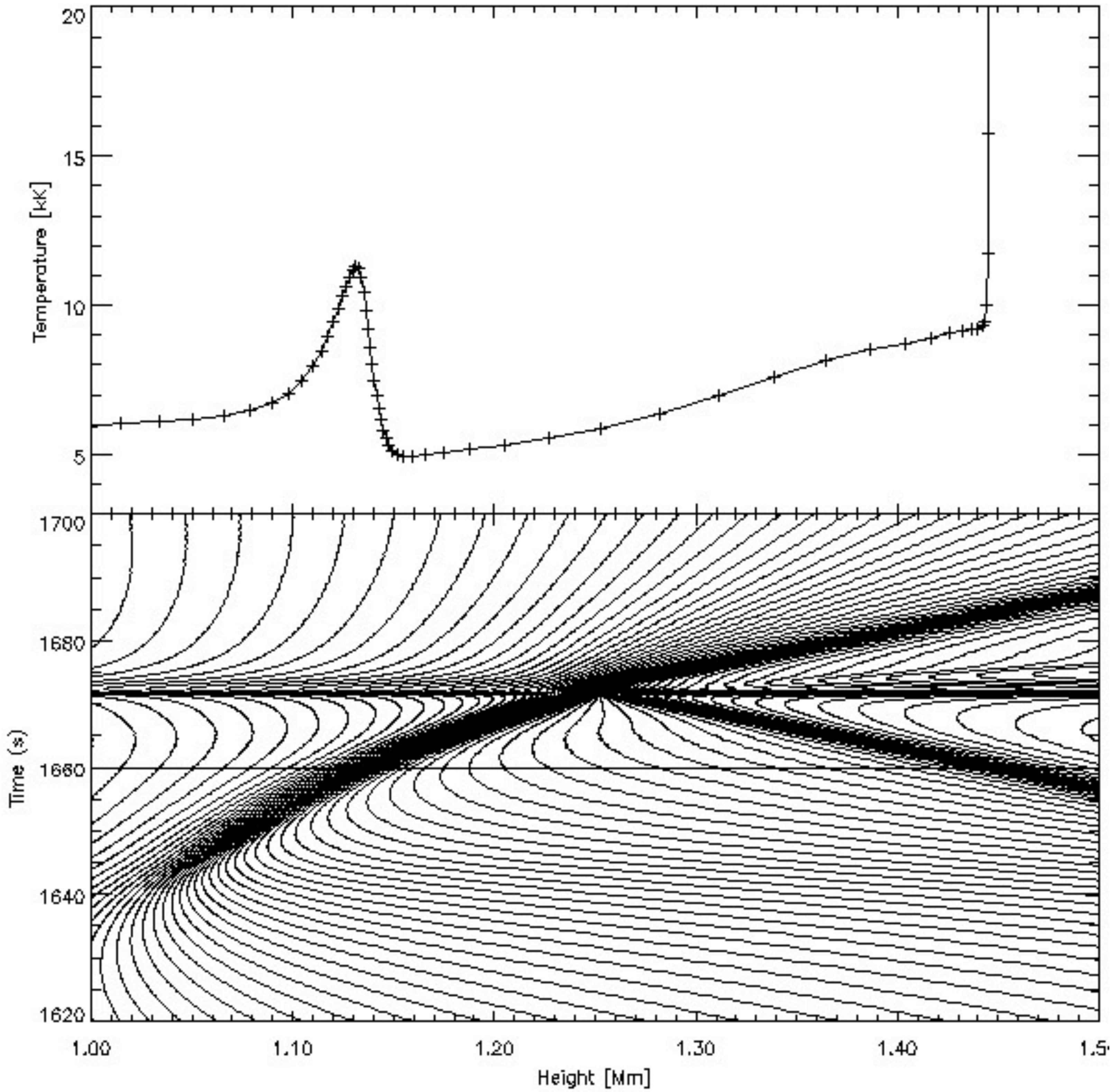
Dynamic behaviour, Temperature



Dynamic behaviour, Temperature

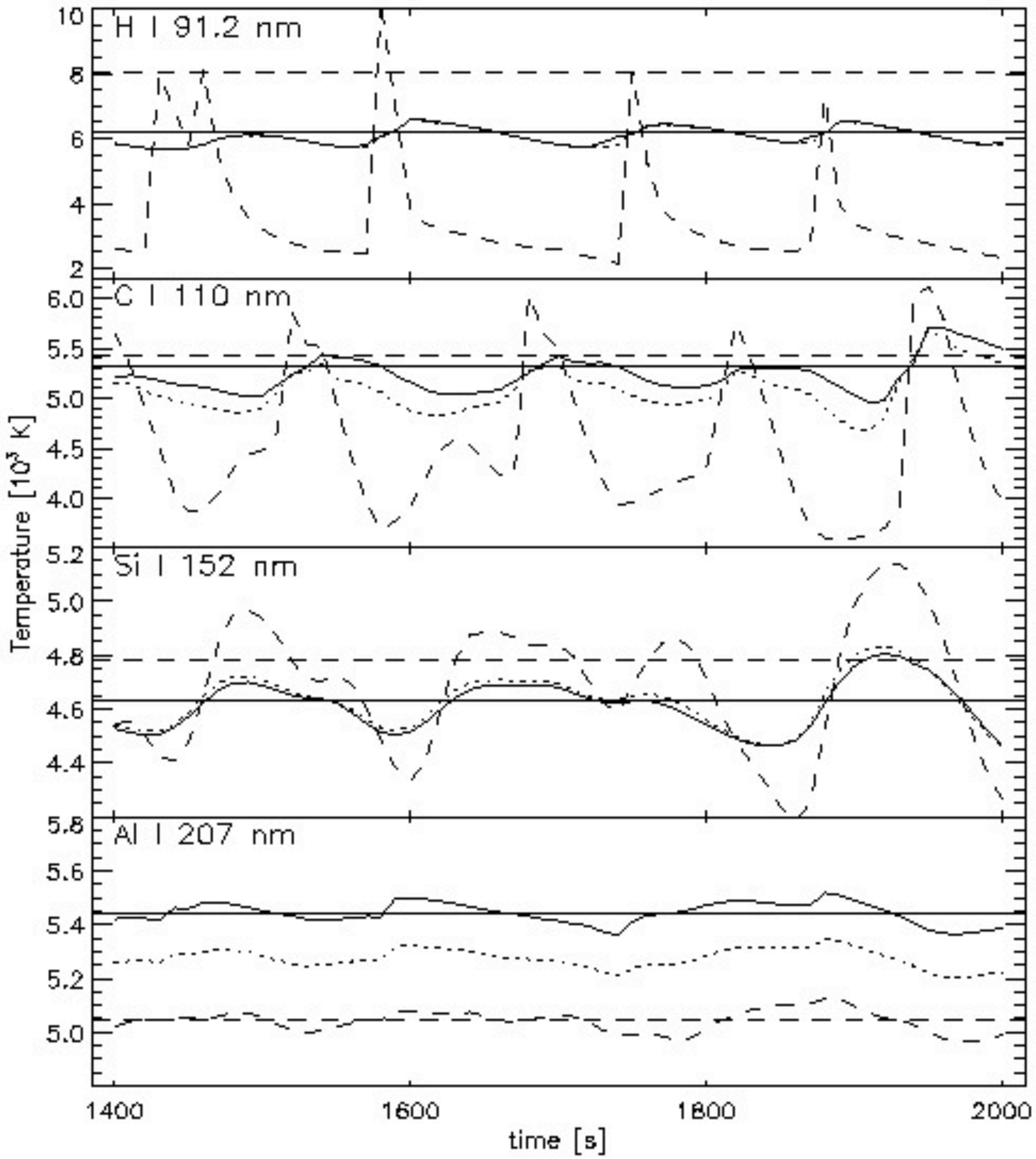


Grid equation



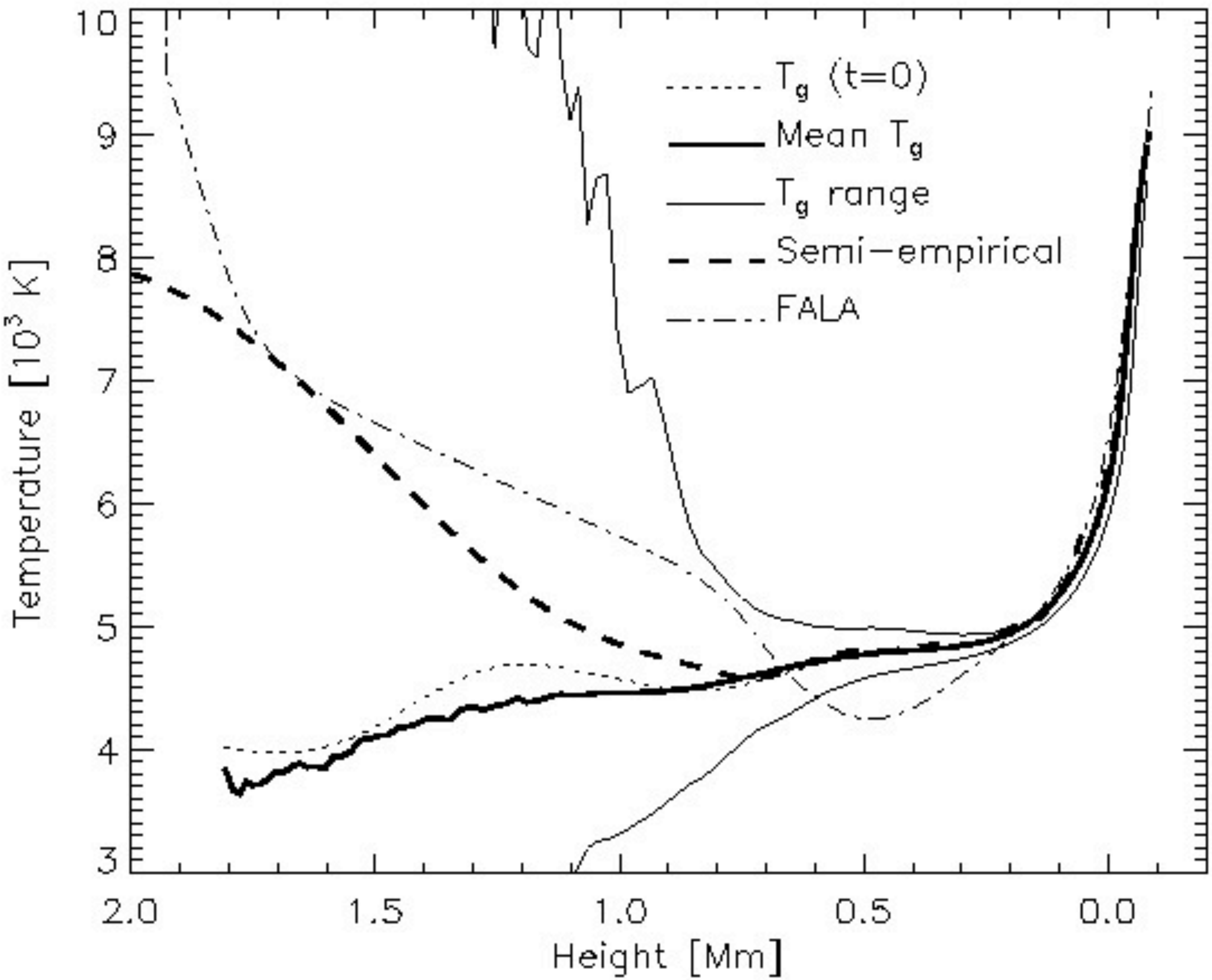
Dorfi & Drury, 1987, Jou. Comp. Phys. 69, 175

Continuum intensity

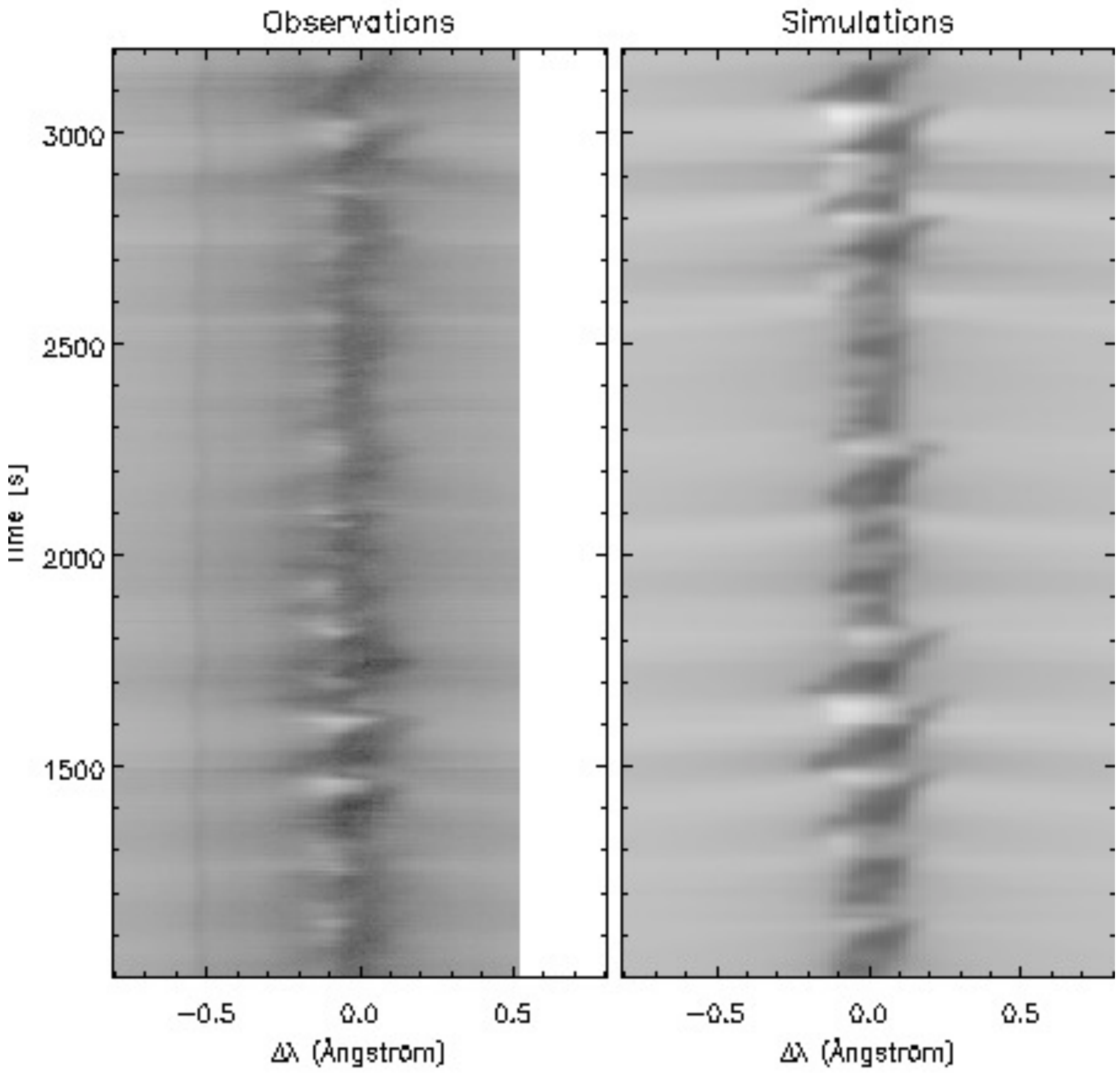


Intensity (solid) non-local. Source function (dotted) decoupled from Planck function (dashed). Intensity varies a lot less than local Planck function at tau=1

“Mean” temperature



Ca II H-line intensity



Ca II H-line formation

We rewrite the contribution function to intensity

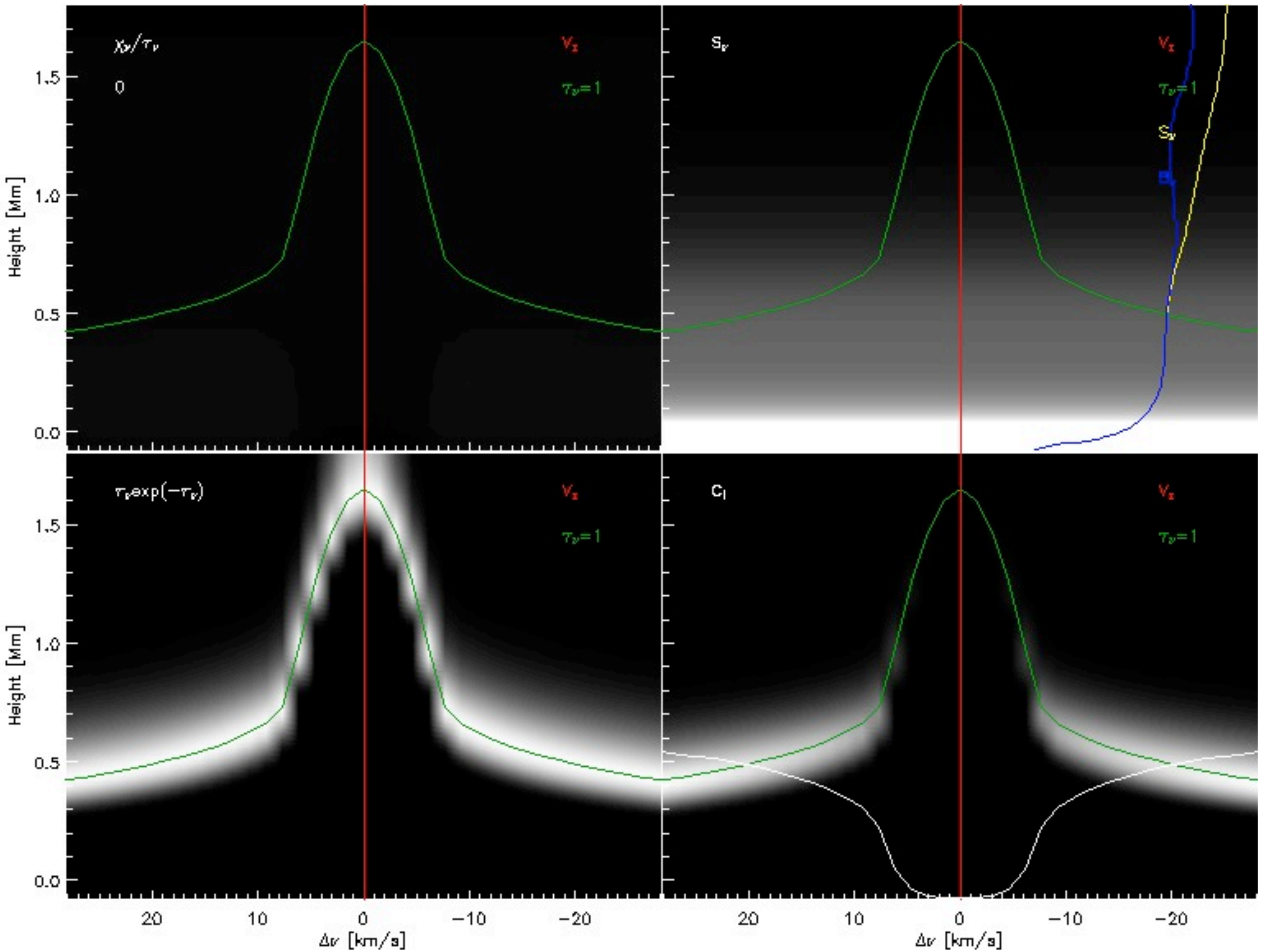
$$C_I(z) = \frac{1}{\mu} S_\nu(\tau_\nu) e^{-\tau_\nu/\mu} \chi_\nu$$

as

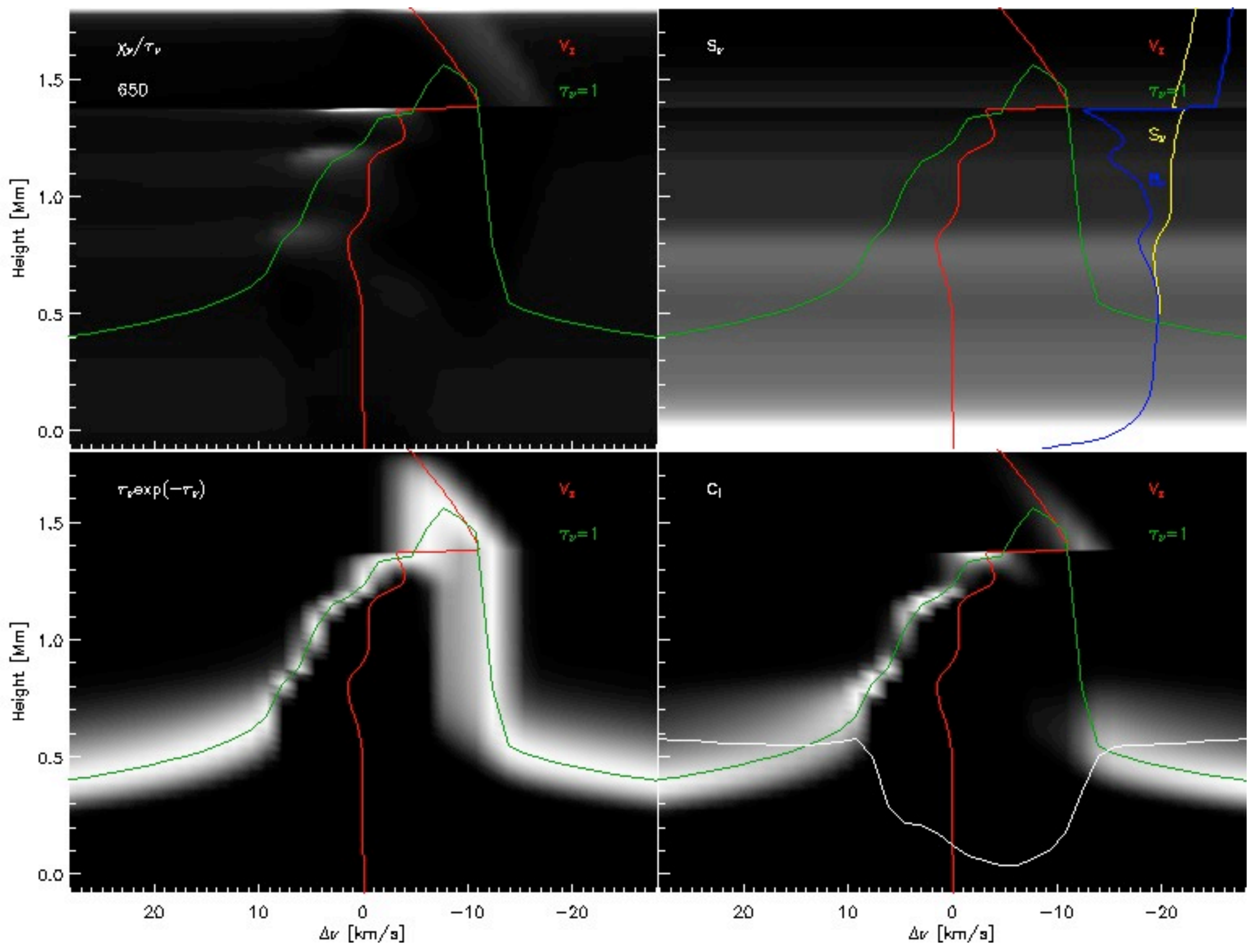
$$C_I(z, \mu = 1) = S_\nu(\tau_\nu) \tau_\nu e^{-\tau_\nu/\mu} \frac{\chi_\nu}{\tau_\nu}$$

and show separately the three factors:

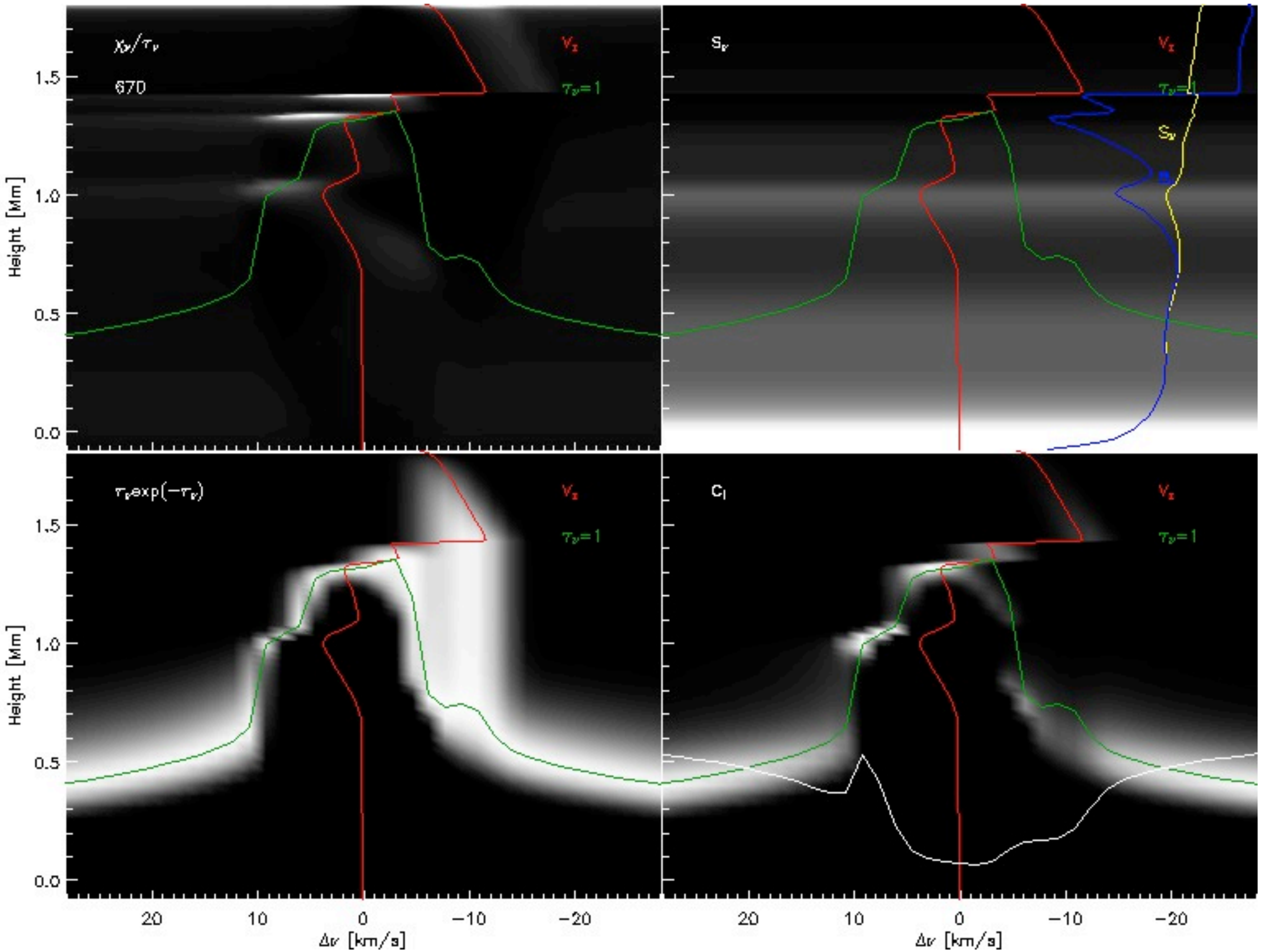
$$\frac{\chi_\nu}{\tau_\nu}, \quad S_\nu(\tau_\nu), \quad \tau_\nu e^{-\tau_\nu/\mu}$$



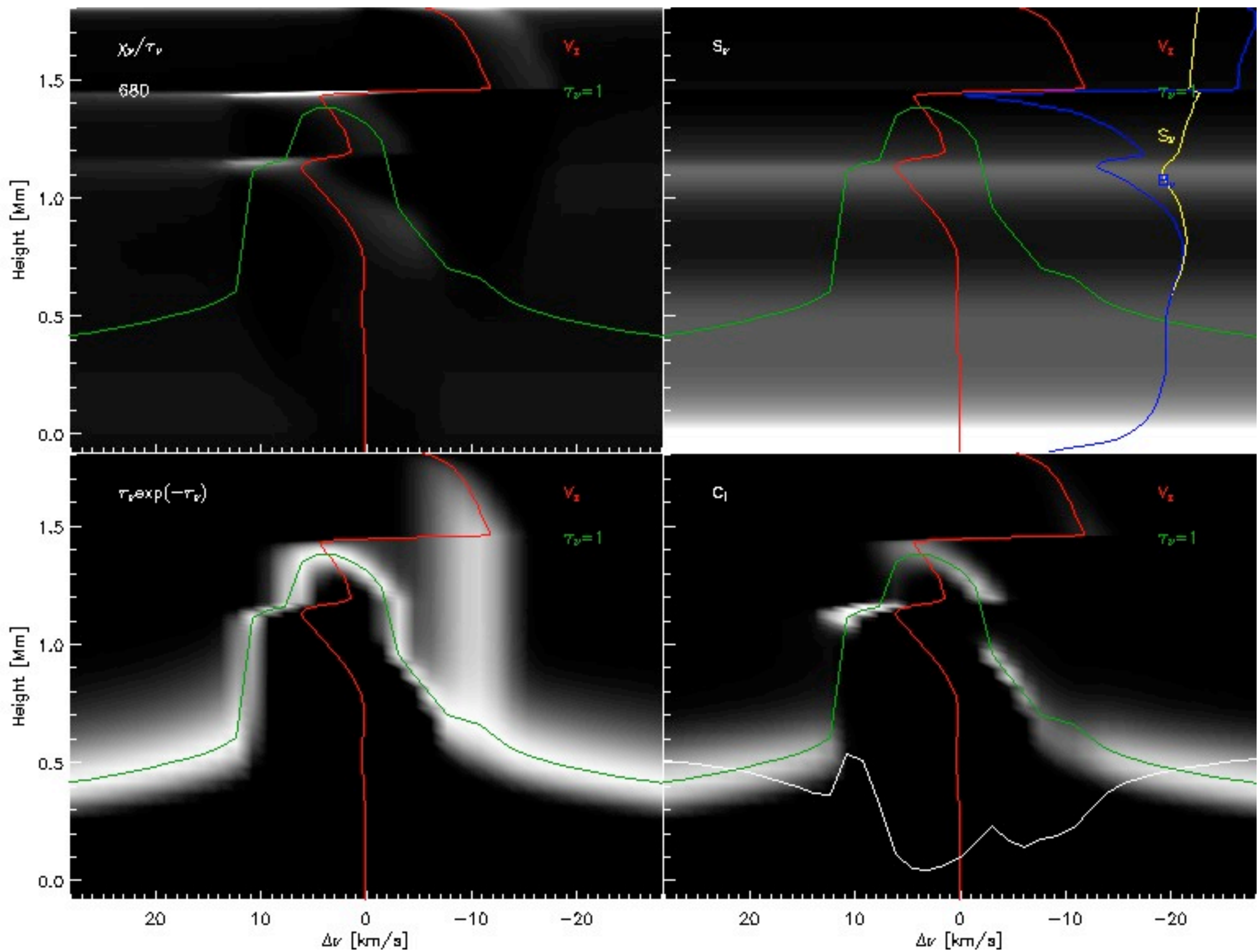
χν/τν
0
Vz
τν=1
Sν
Vz
τν=1
Sν
Bν
τνexp(−τν)
Vz
τν=1
CI
Vz
τν=1
Height [Mm]
Δν [km/s]



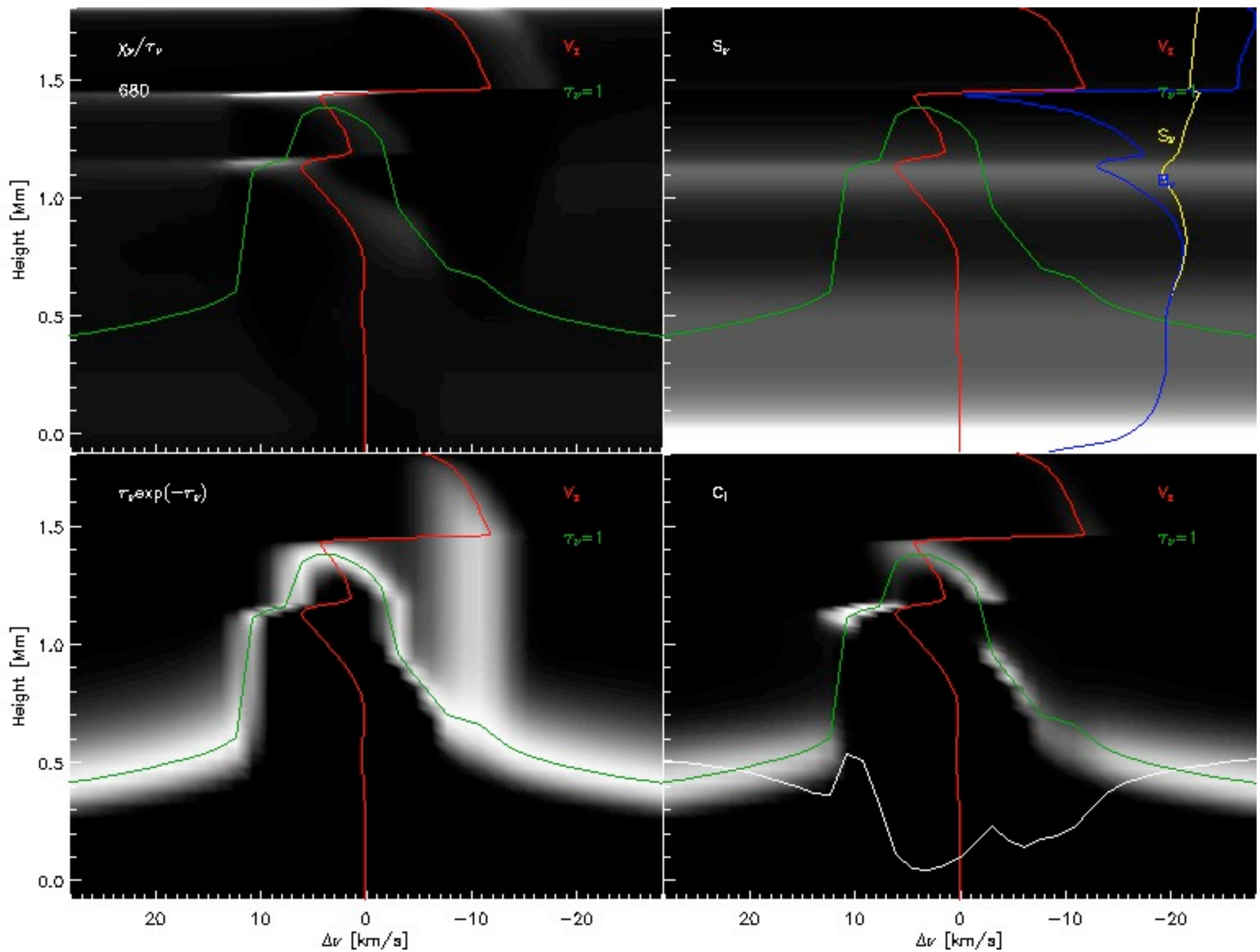
χ_ν/τ_ν
650
v_z
τ_ν=1
S_ν
v_z
τ_ν=1
S_ν
$\tau_\nu\exp(-\tau_\nu)$
v_z
τ_ν=1
c_I
v_z
τ_ν=1
Height [Mm]
Height [Mm]
0.0
0.5
1.0
1.5
20
10
0
−10
−20
$\Delta\nu$ [km/s]
$\Delta\nu$ [km/s]



χν/τν
670
Sν
τνexp(−τν)
CI
vz
τν=1
Height [Mm]
Δν [km/s]



χ_ν/τ_ν
680
S_ν
$\tau_\nu \exp(-\tau_\nu)$
C_I
v_z
$\tau_\nu=1$
S_ν
B_ν
Height [Mm]
$\Delta\nu$ [km/s]



The asymmetry of the CaII H-line (H2V bright grains) is caused by high opacity and small overlying opacity at the H2V wavelength at the location of the shock.

BIFROST

Hansteen 2004, Hansteen, Carlsson, Gudiksen 2007, Sykora, Hansteen, Carlsson 2008, Gudiksen et al 2011

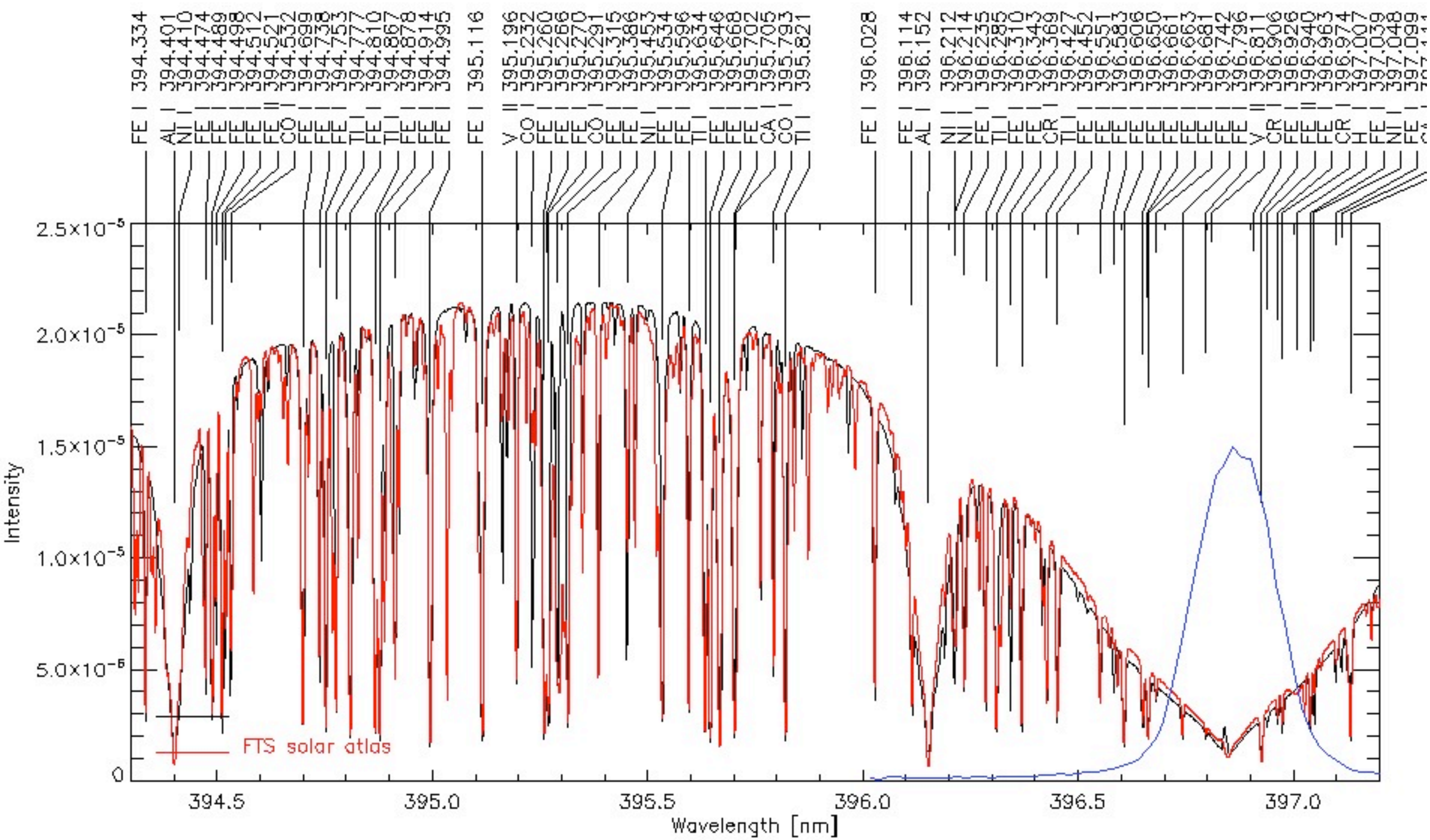
- 6th order scheme, with "artificial viscosity/diffusion"
- Open vertical boundaries, horizontally periodic
- Possible to introduce field through bottom boundary

- "Realistic" EOS
- Detailed radiative transfer along 48 rays
  - Multi group opacities (4 bins) with scattering
- NLTE radiative losses in the chromosphere, optically thin in corona

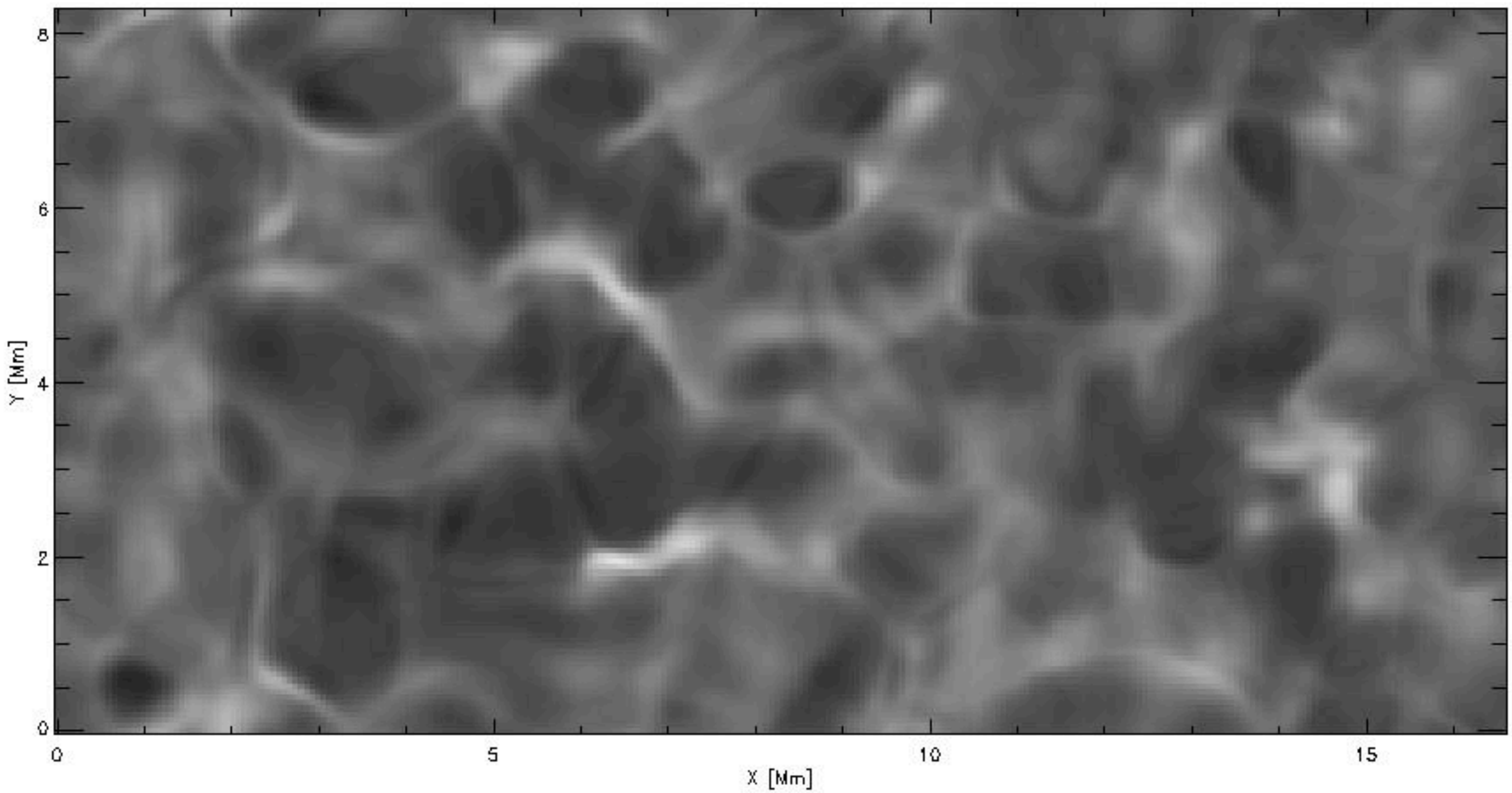
- Conduction along field lines
  - Operator split and solved by using multi grid method

- Time dependent Hydrogen ionization
- Generalized Ohm's Law

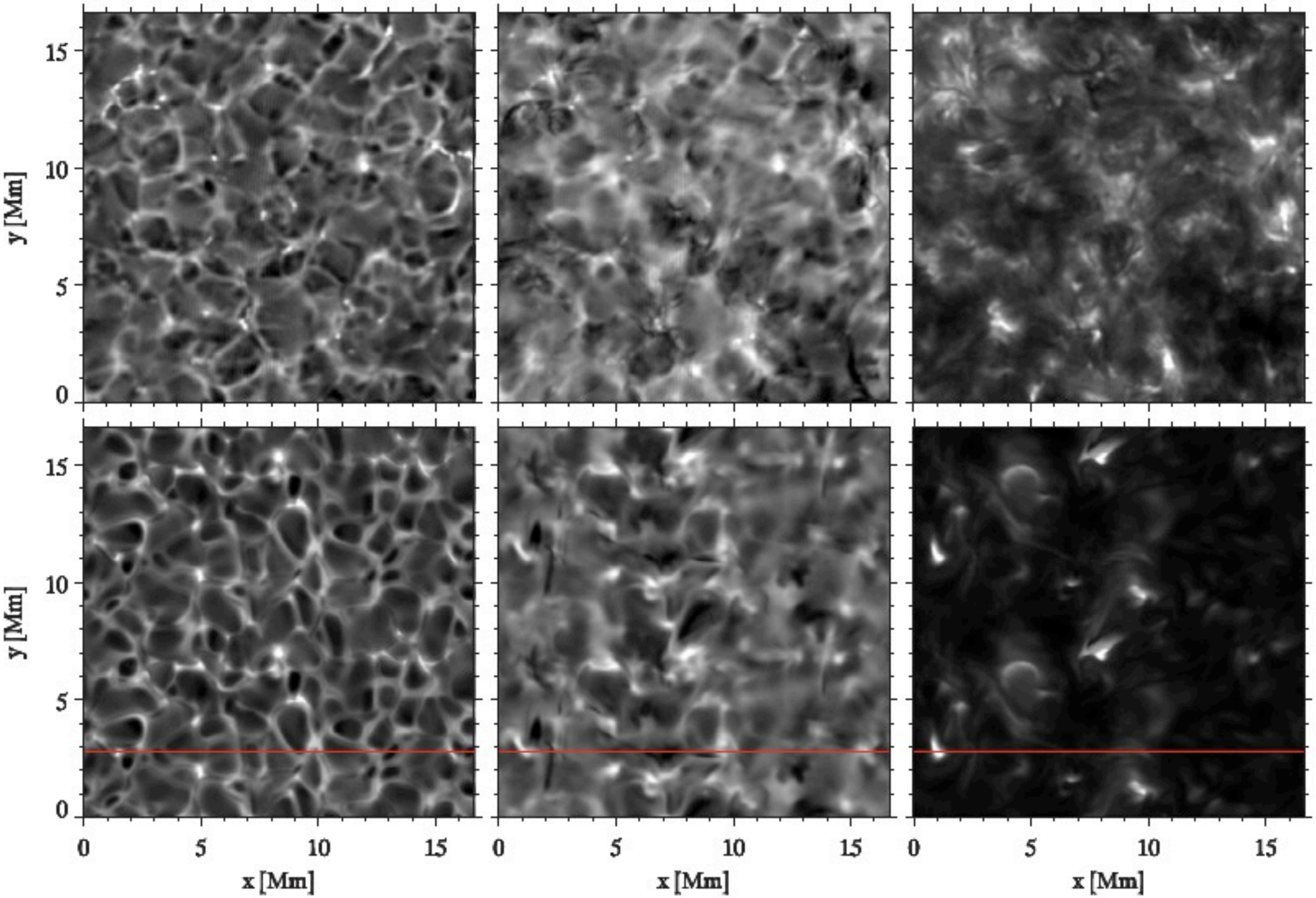
- non-LTE Ca-II, column by column



Simulation seen with Hinode Ca-H filter

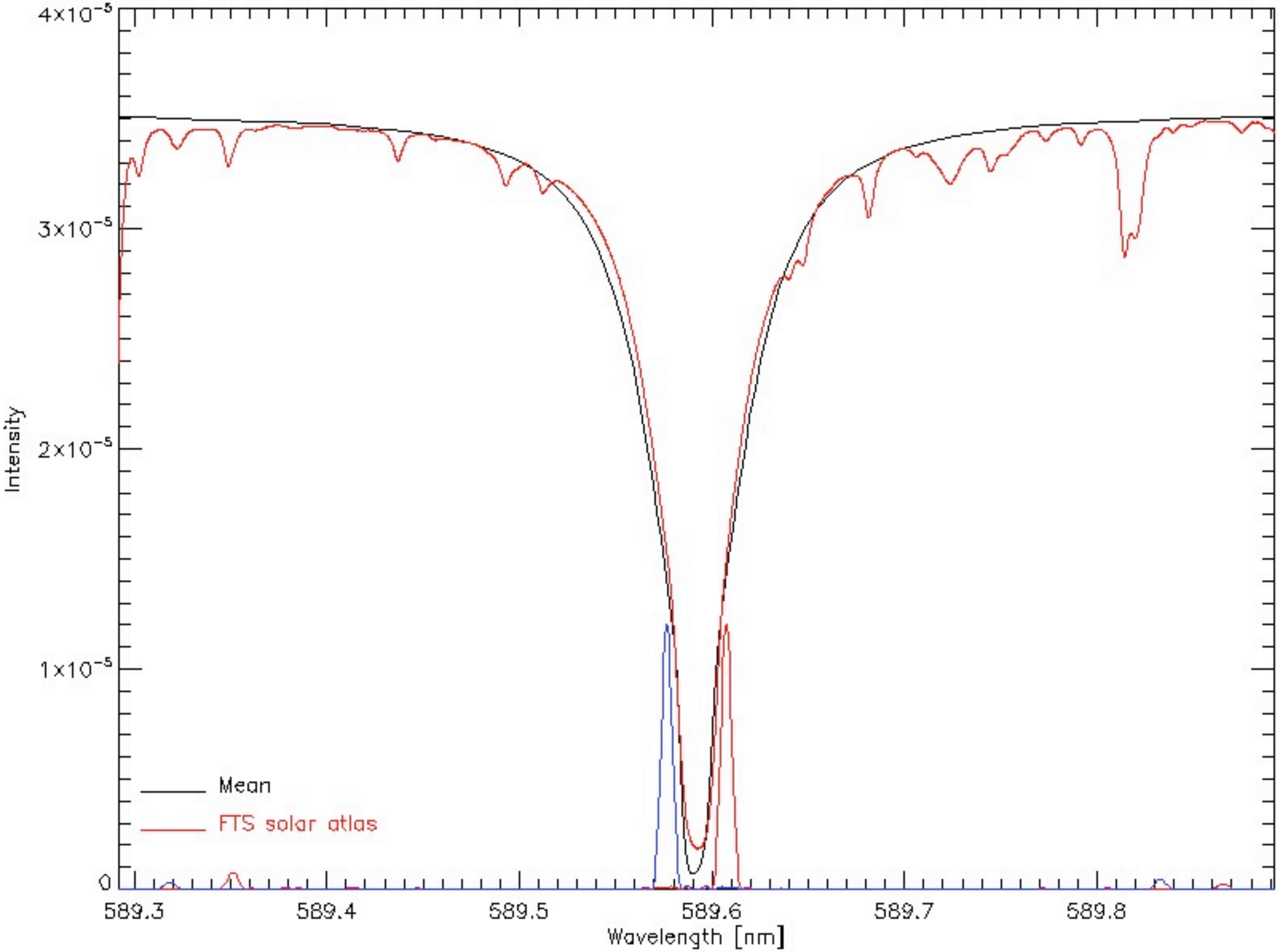


3D NLTE: Ca II 8542



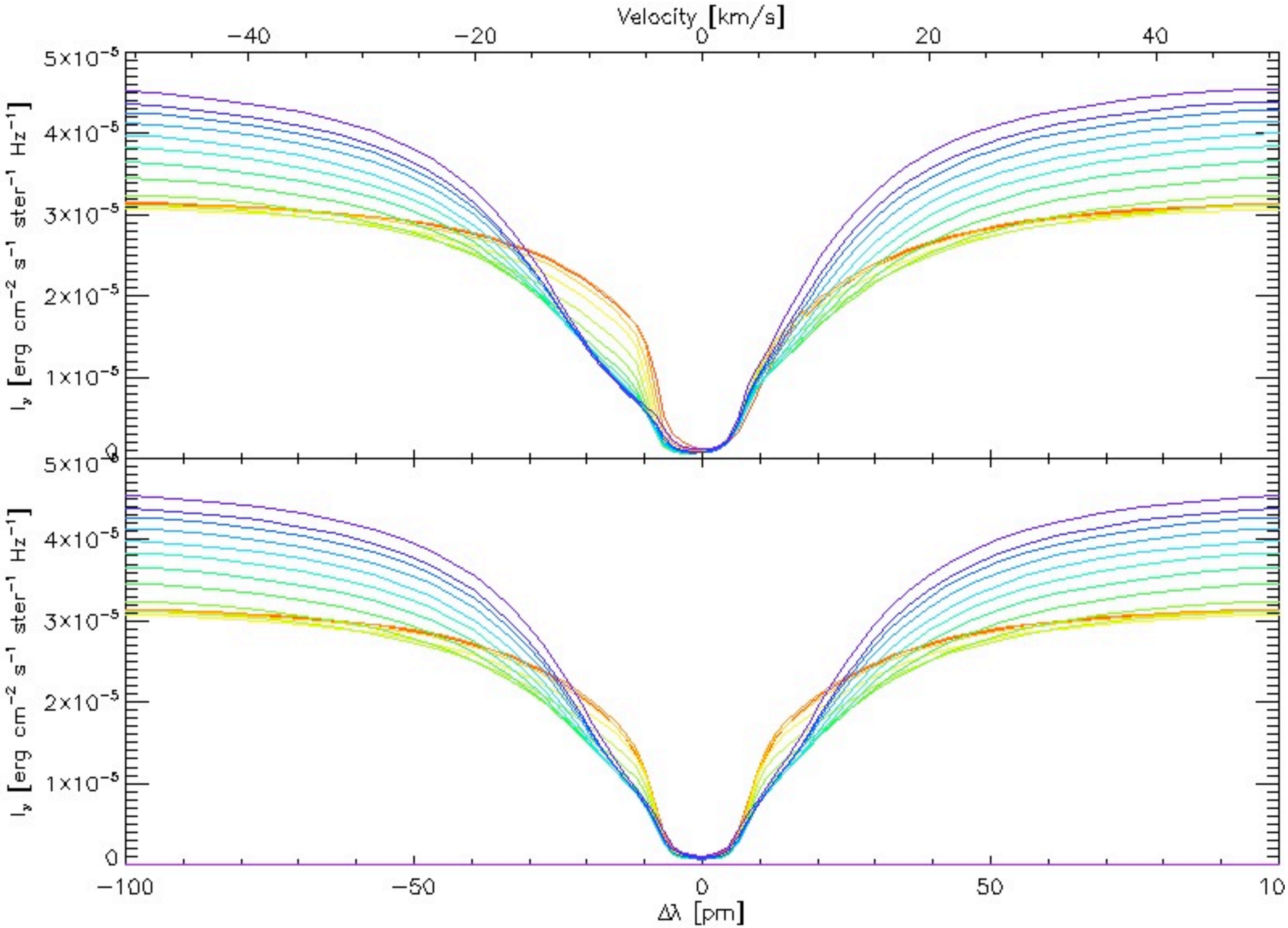
Leenaarts et al 2009: ApJ 694,L128

Na D



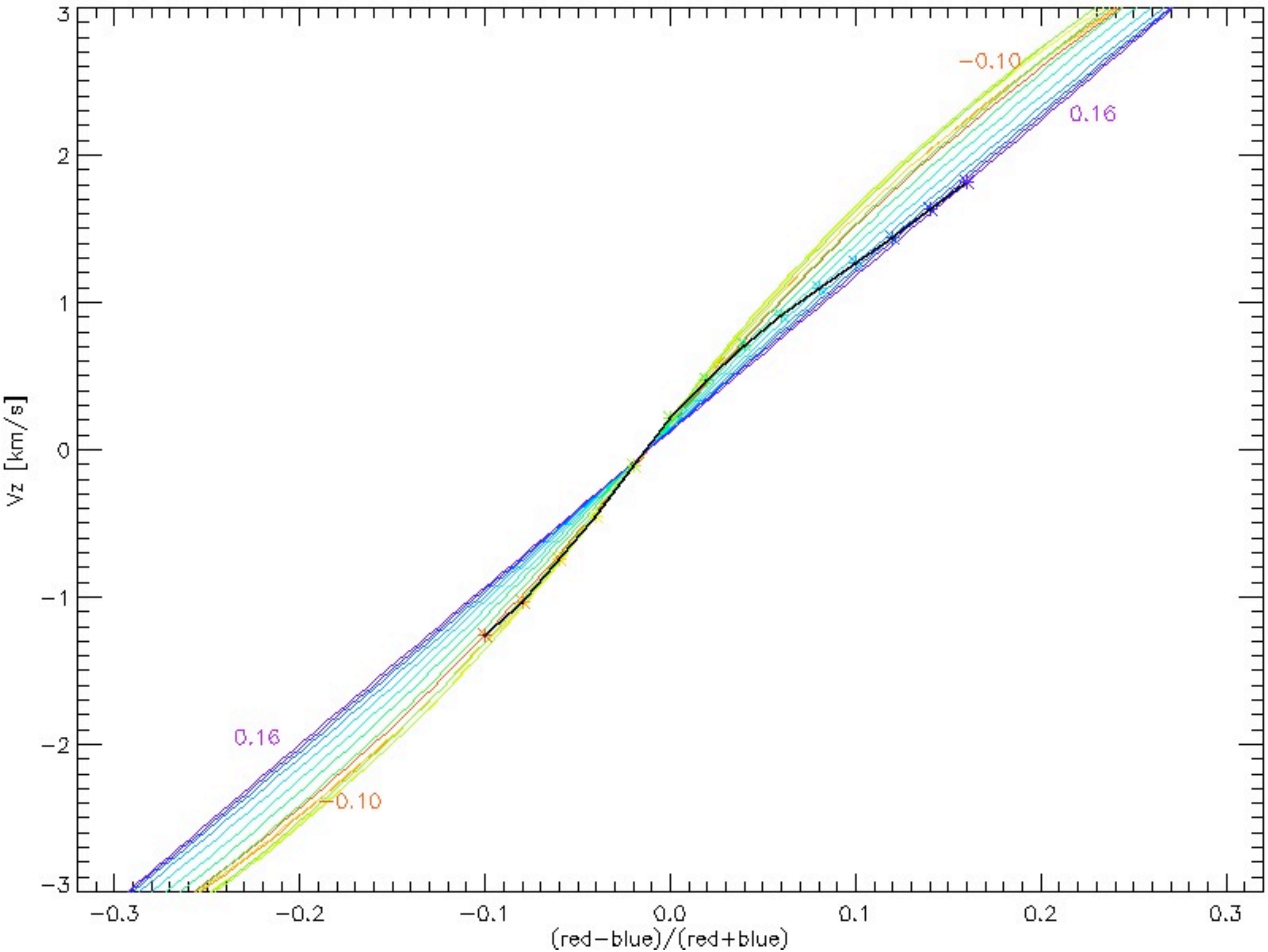
4×10⁻⁵
3×10⁻⁵
2×10⁻⁵
1×10⁻⁵
0
Intensity
589.3
589.4
589.5
589.6
589.7
589.8
Wavelength [nm]
Mean
FTS solar atlas

Na D

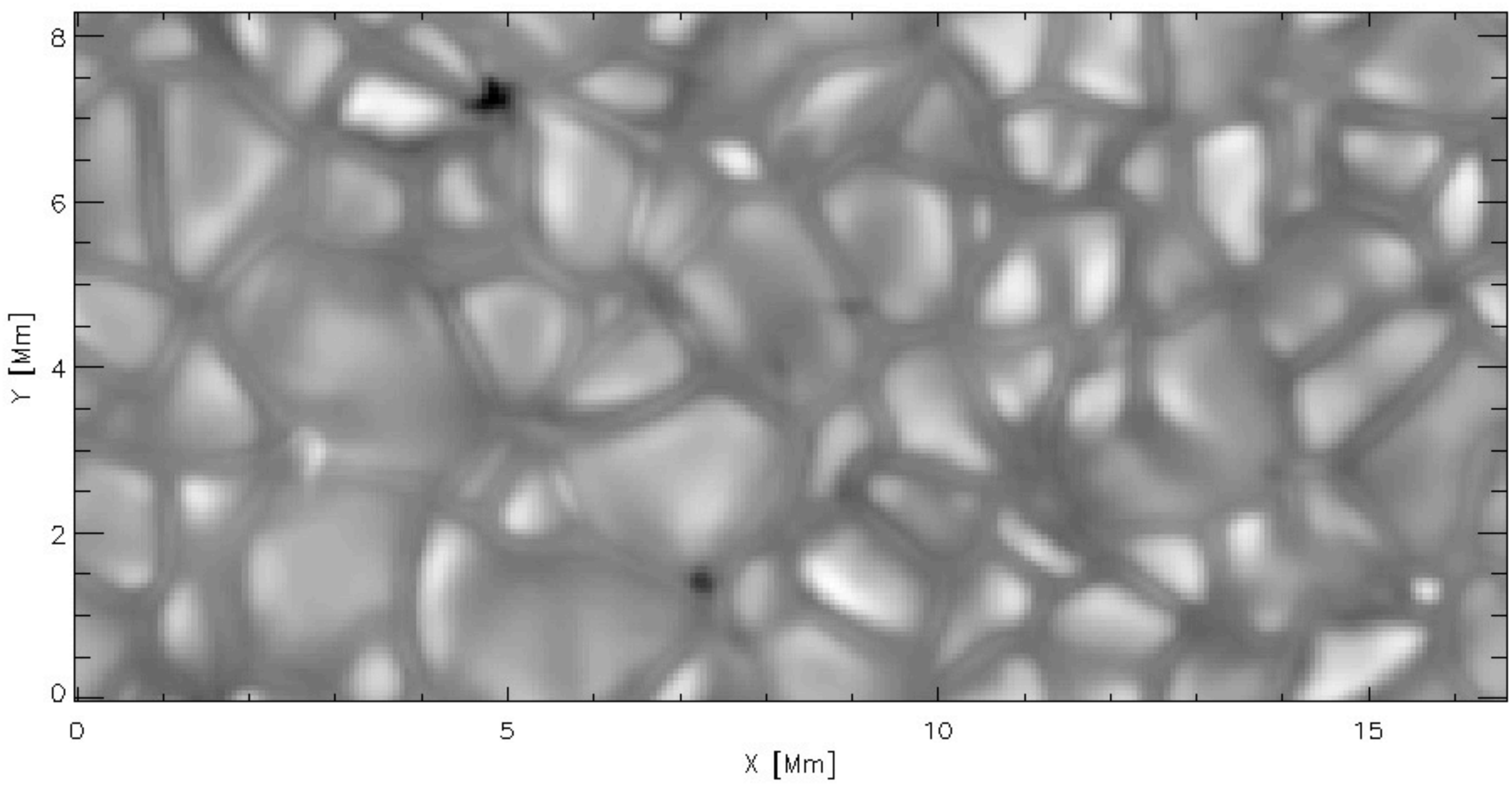


Velocity [km/s]
−40
−20
0
20
40
5×10⁻⁵
4×10⁻⁵
3×10⁻⁵
2×10⁻⁵
1×10⁻⁵
0
I_ν [erg cm⁻² s⁻¹ ster⁻¹ Hz⁻¹]
−100
−50
0
50
10
Δλ [pm]

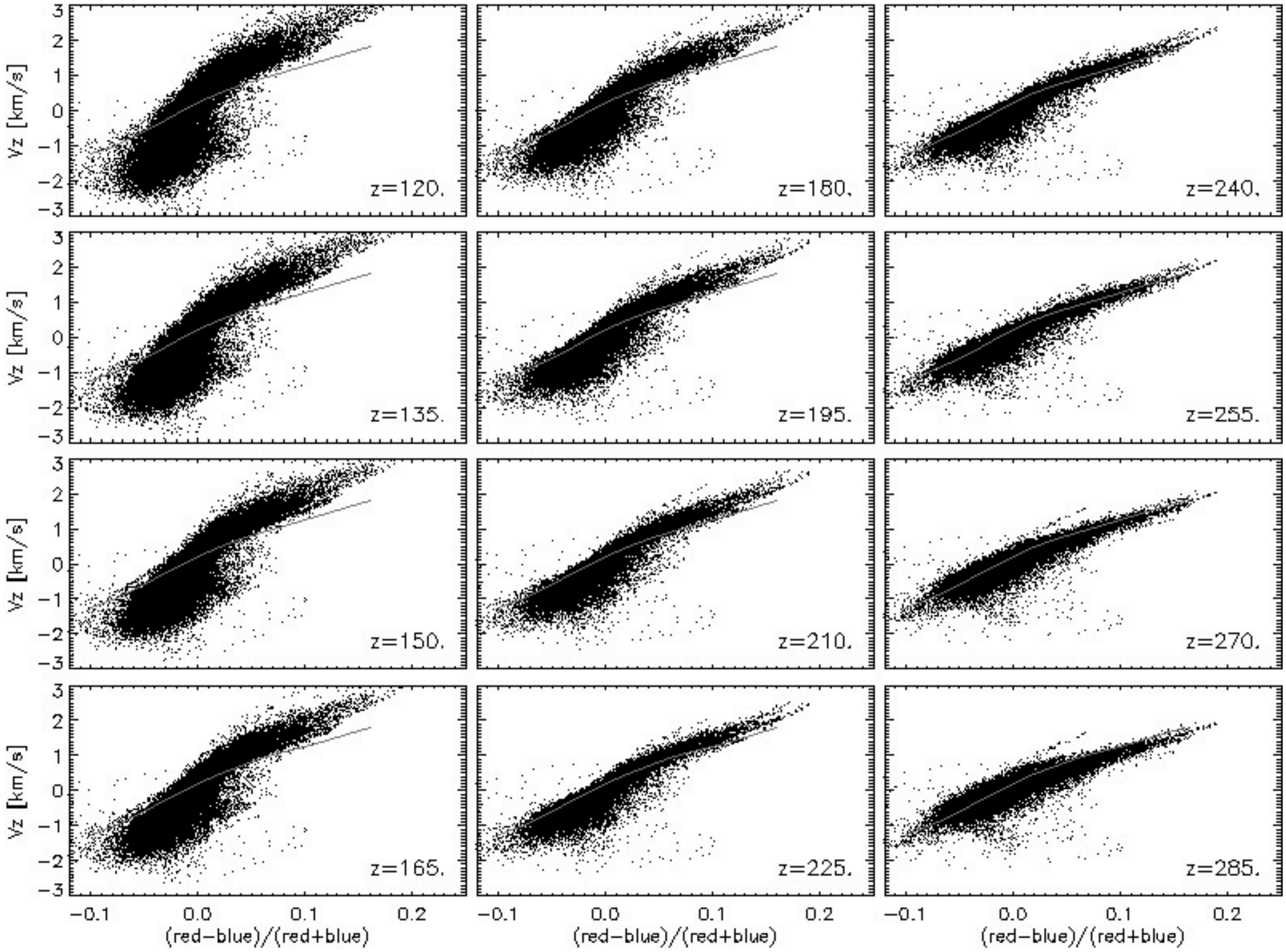
Calibration curve



Na D synthetic Dopplergram

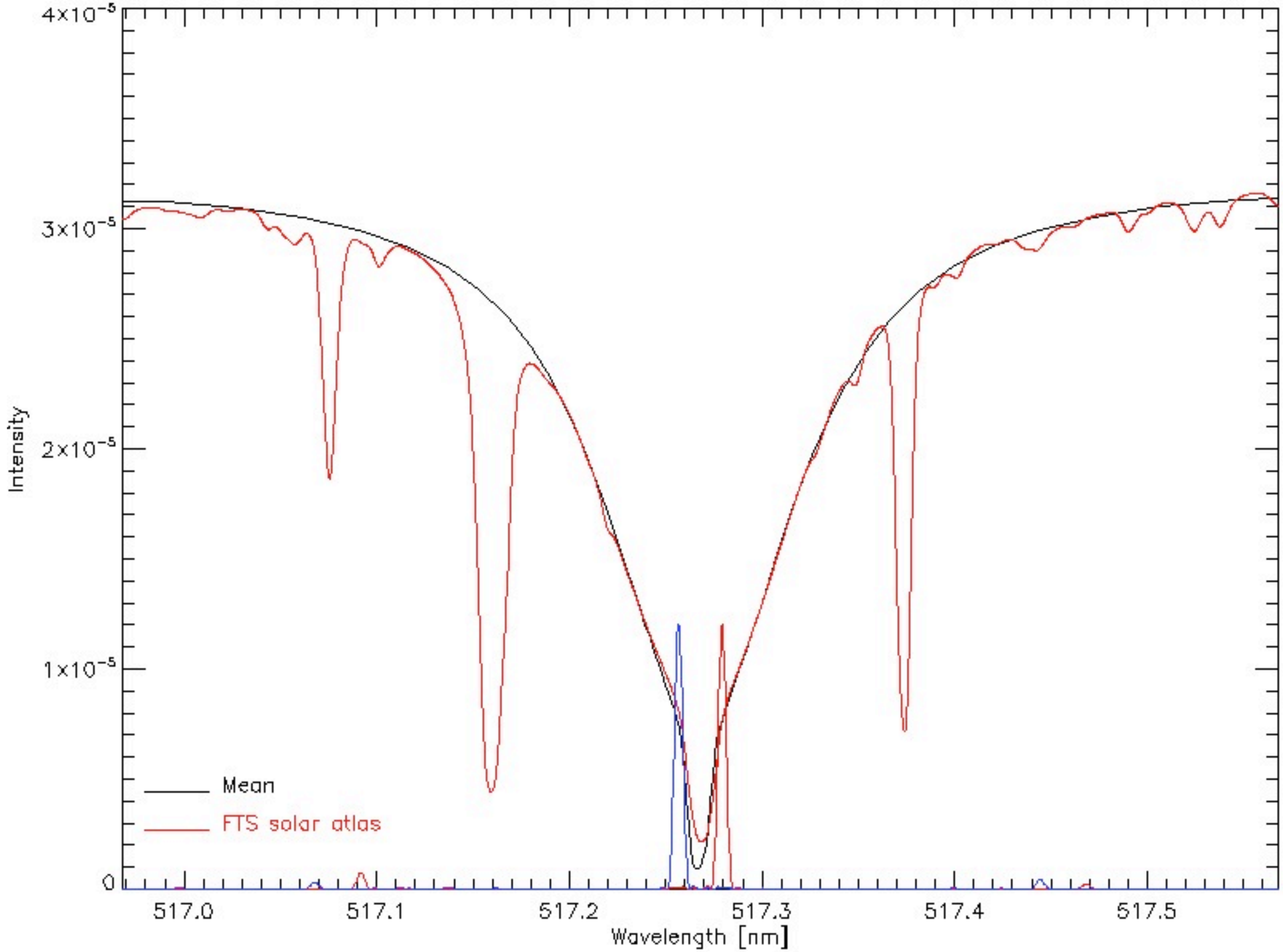


Na D



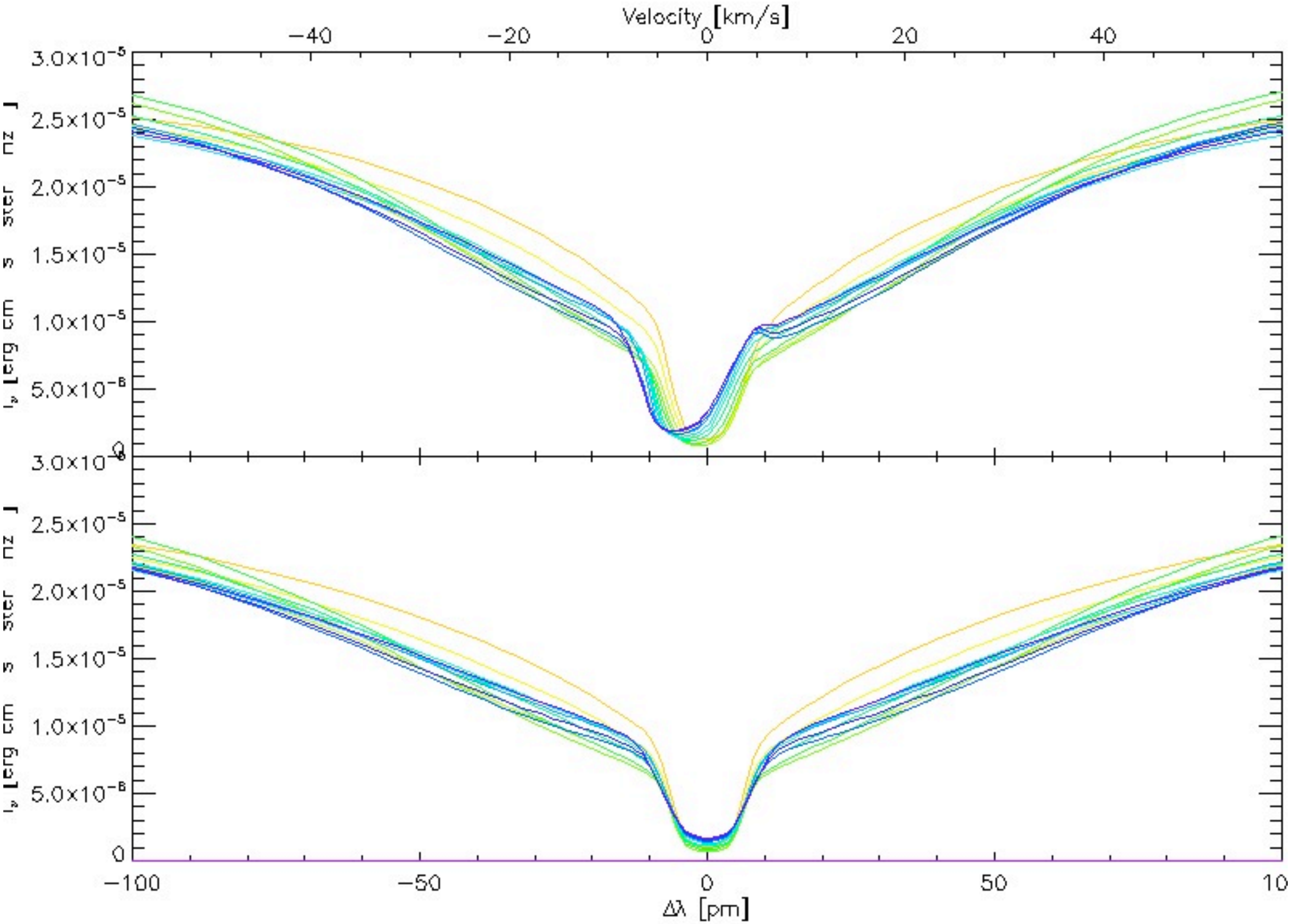
Vz [km/s]
(red−blue)/(red+blue)
z=120.
z=135.
z=150.
z=165.
z=180.
z=195.
z=210.
z=225.
z=240.
z=255.
z=270.
z=285.

Mg b

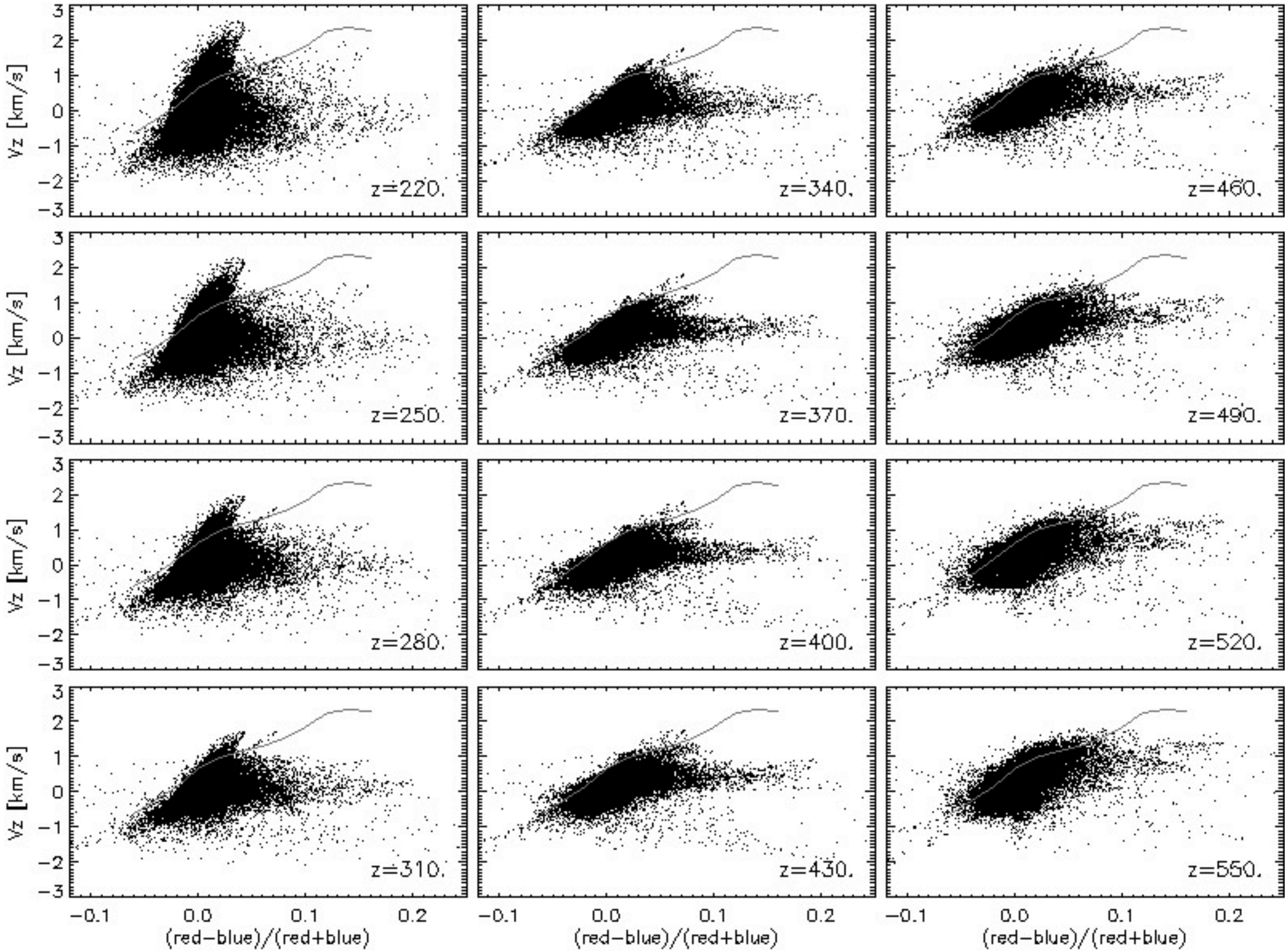


4×10⁻⁵
3×10⁻⁵
2×10⁻⁵
1×10⁻⁵
0
Intensity
517.0
517.1
517.2
517.3
517.4
517.5
Wavelength [nm]
Mean
FTS solar atlas

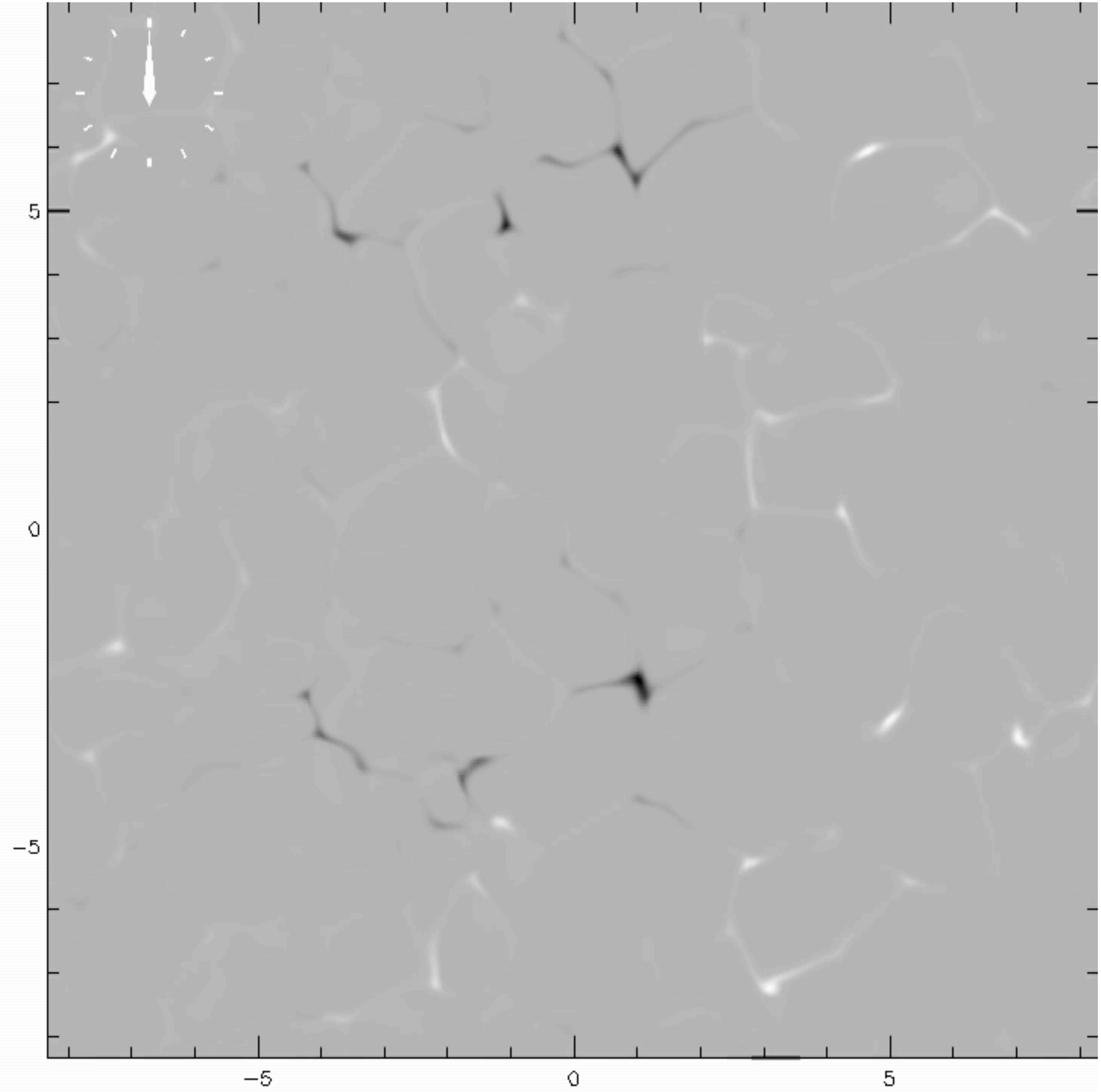
Mg b


Velocity [km/s]
−40
−20
0
20
40
3.0x10⁻⁵
2.5x10⁻⁵
2.0x10⁻⁵
1.5x10⁻⁵
1.0x10⁻⁵
5.0x10⁻⁶
0
−100
−50
0
50
10
Δλ [pm]

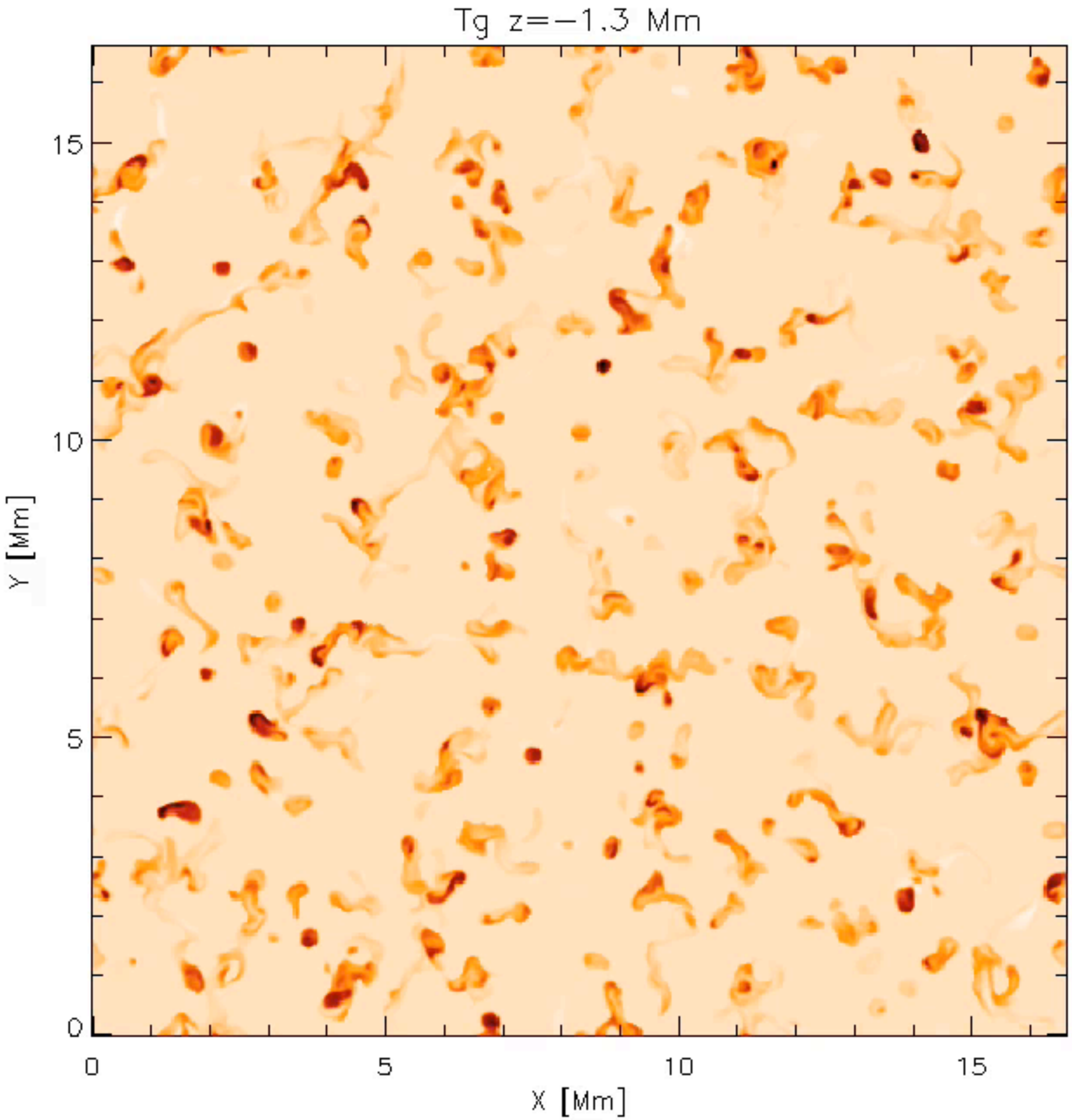
Mg b

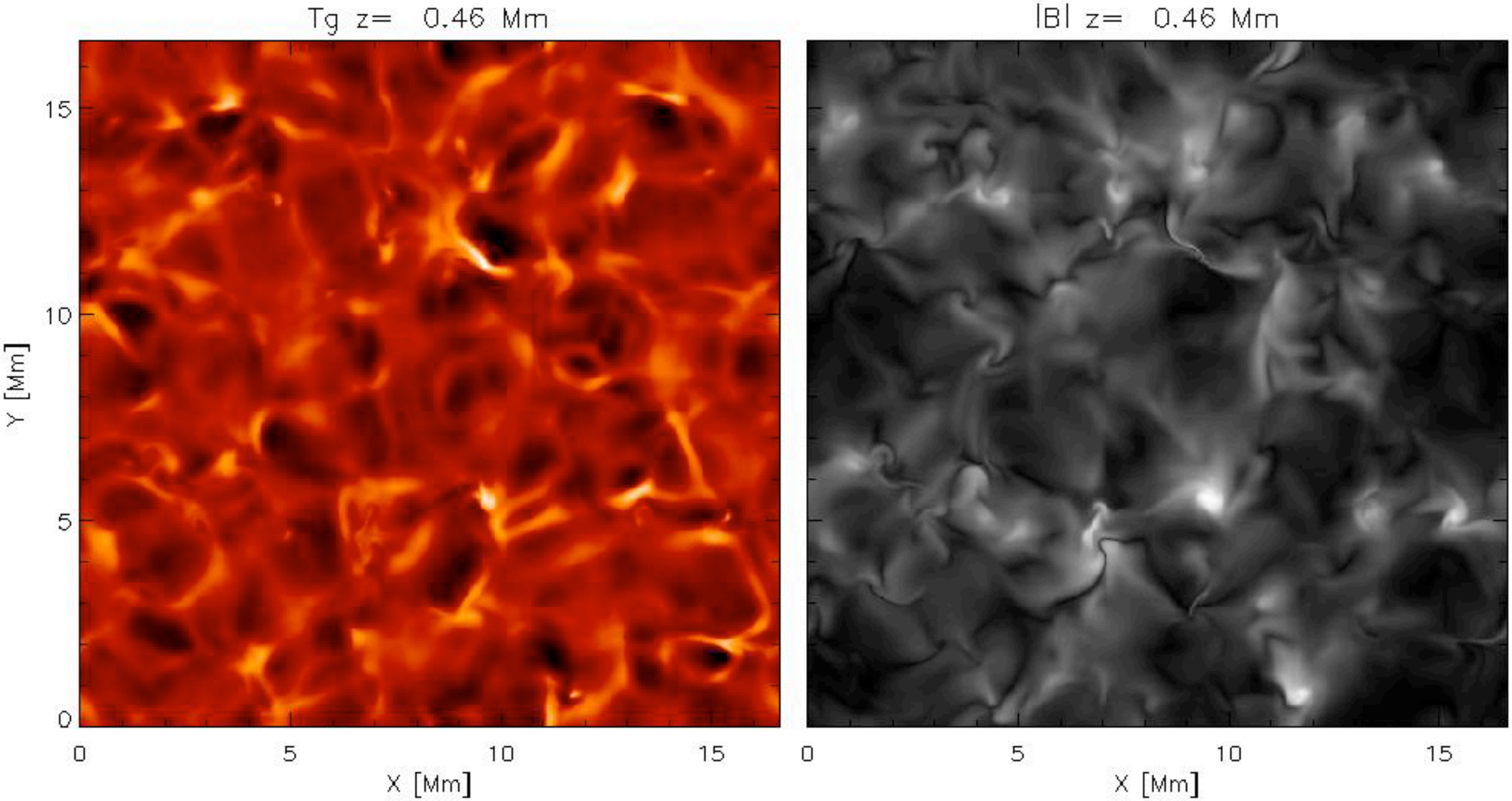


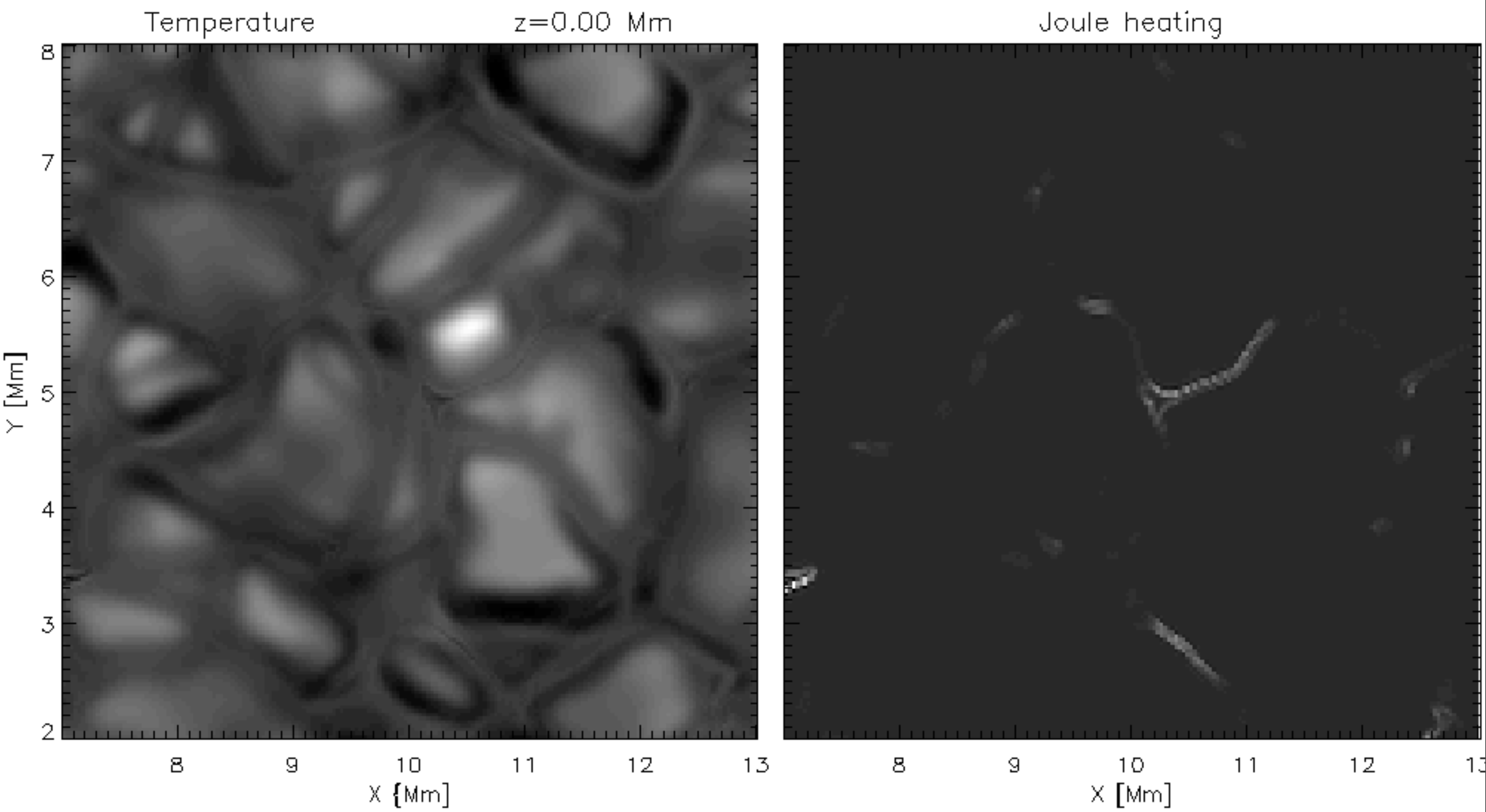
Vz [km/s]
z=220.
z=250.
z=280.
z=310.
z=340.
z=370.
z=400.
z=430.
z=460.
z=490.
z=520.
z=550.
(red−blue)/(red+blue)

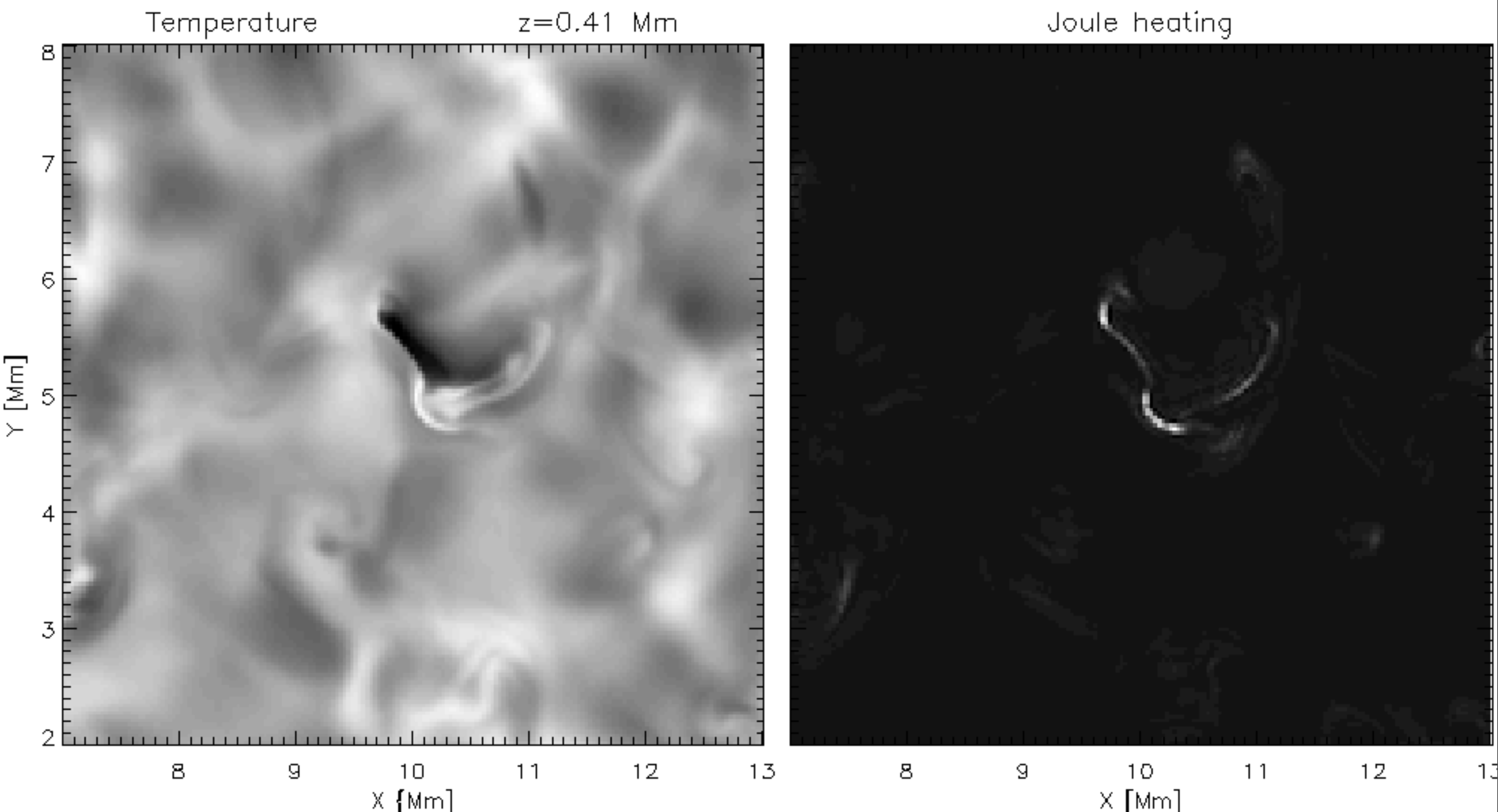


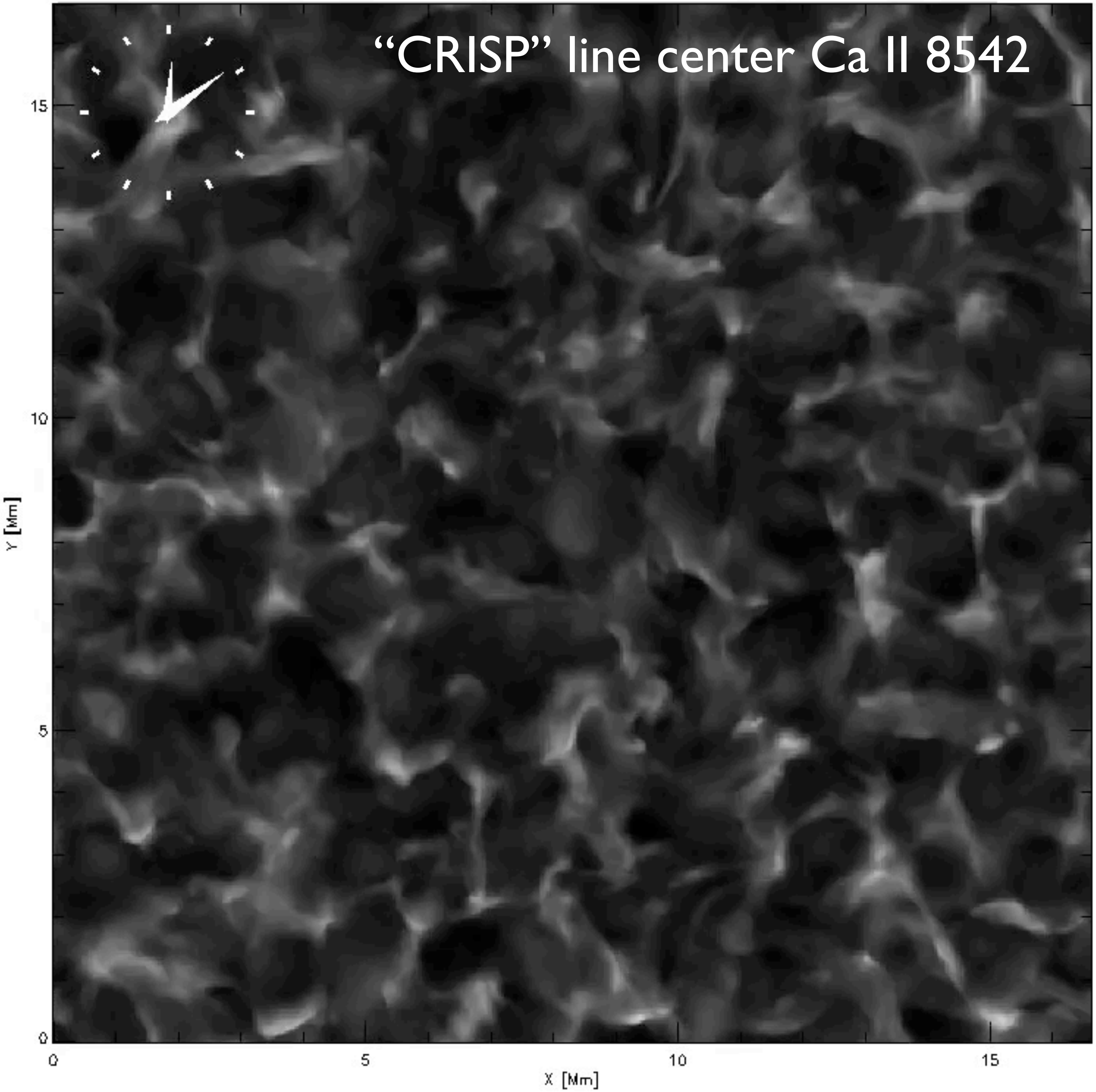
5
0
−5
−5
0
5


Tg z=−1.3 Mm
Y [Mm]
X [Mm]
0
5
10
15

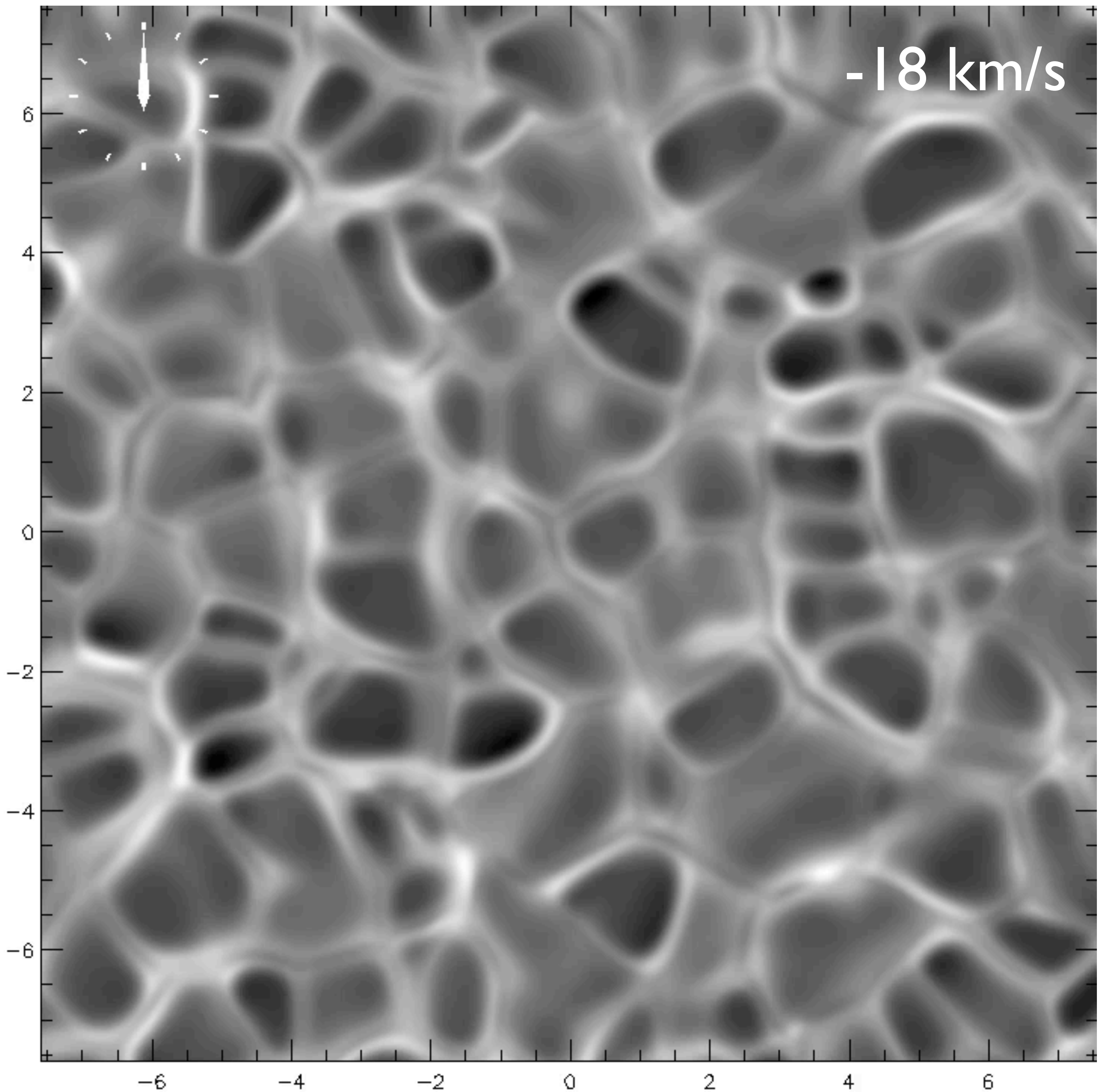

Tg z= 0.46 Mm
|B| z= 0.46 Mm
Y [Mm]
0
5
10
15
X [Mm]
0
5
10
15
X [Mm]
0
5
10
15


Temperature
z=0.00 Mm
Joule heating
Y [Mm]
X {Mm]
X [Mm]
8
7
6
5
4
3
2
8
9
10
11
12
13

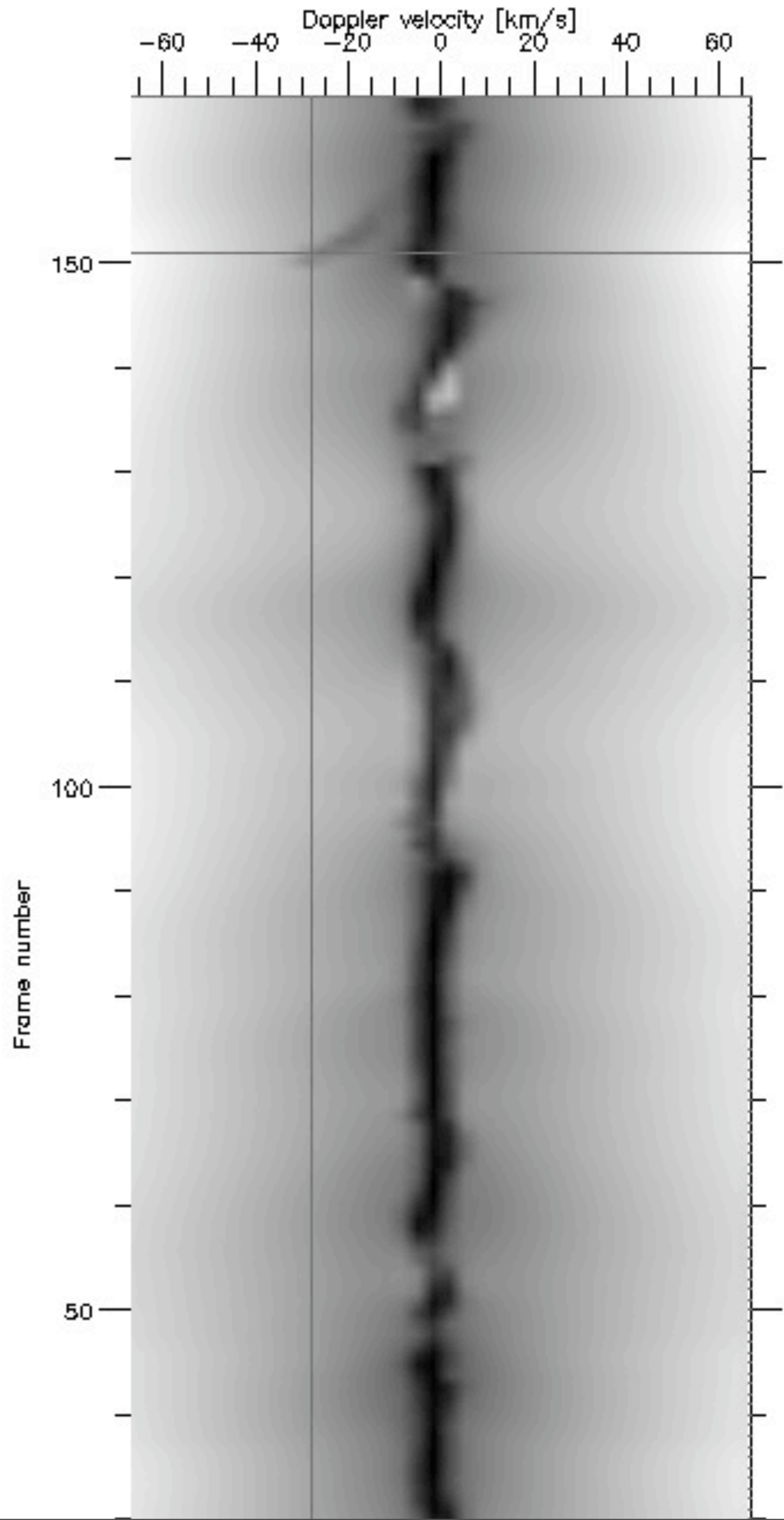

Temperature
z=0.41 Mm
Joule heating
Y [Mm]
X {Mm]
X [Mm]
8
7
6
5
4
3
2
8
9
10
11
12
13

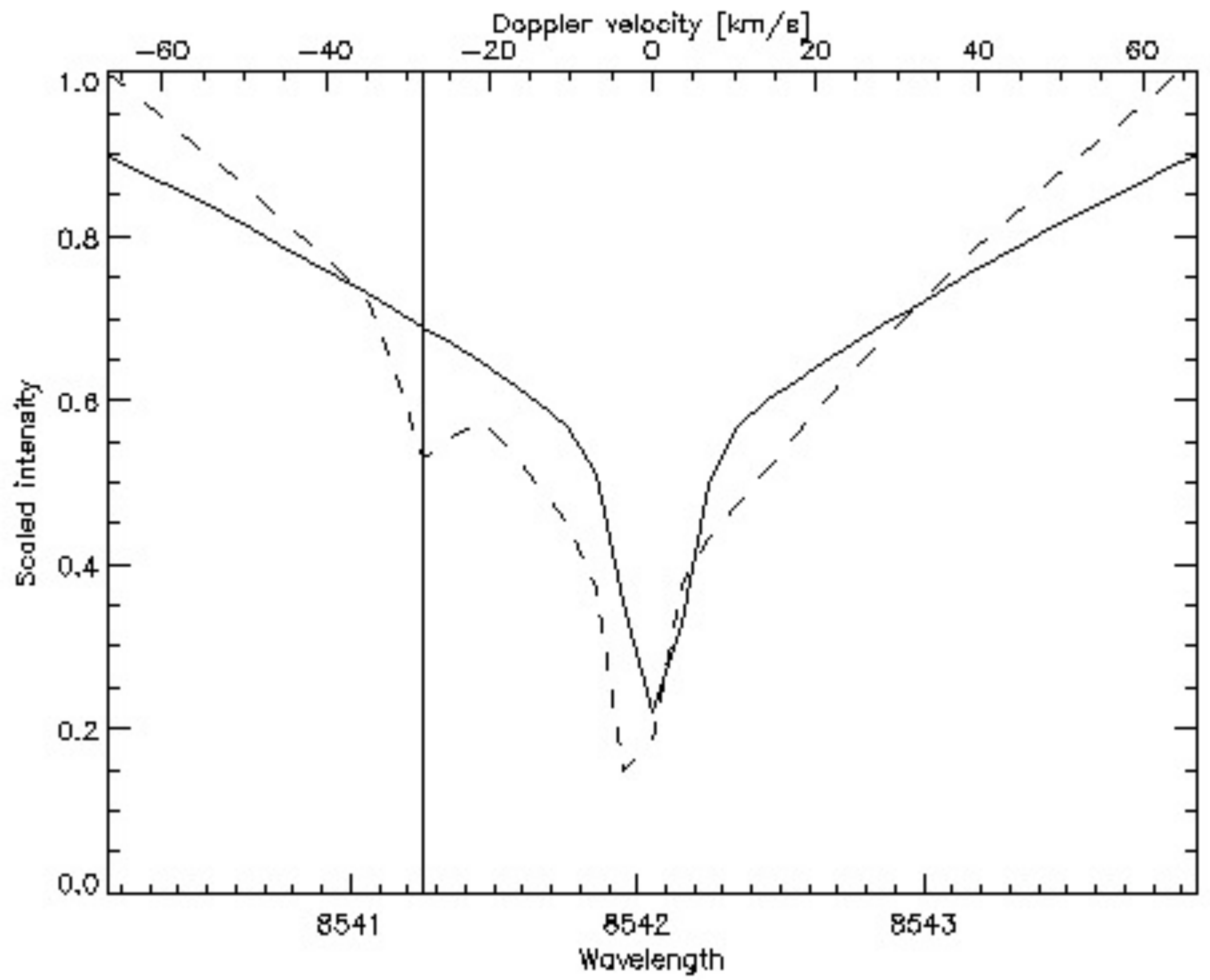


“CRISP” line center Ca II 8542
15
10
5
0
Y [Mm]
0
5
10
15
X [Mm]

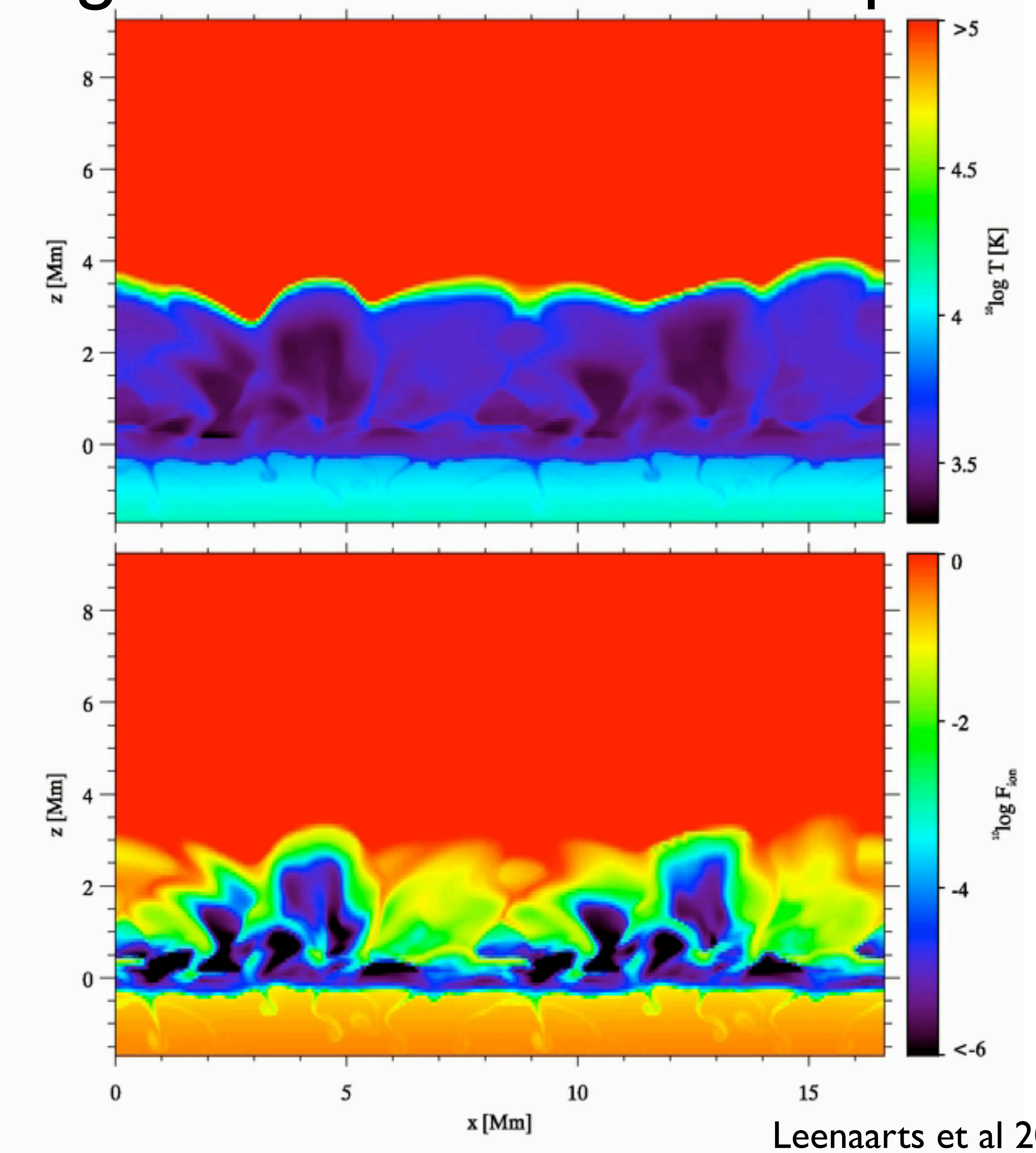

-18 km/s
6
4
2
0
−2
−4
−6
−6
−4
−2
0
2
4
6

Diagnostics

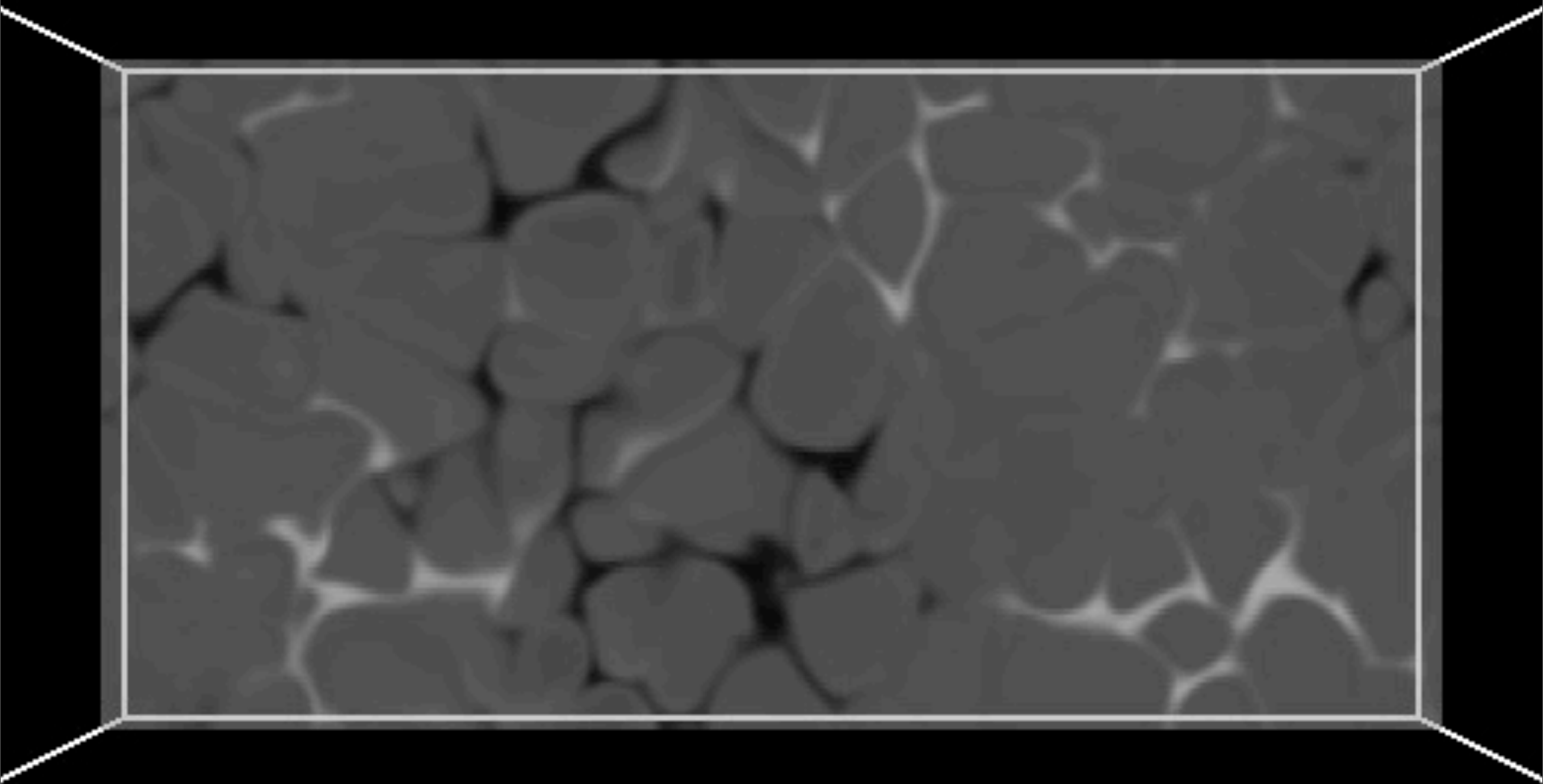


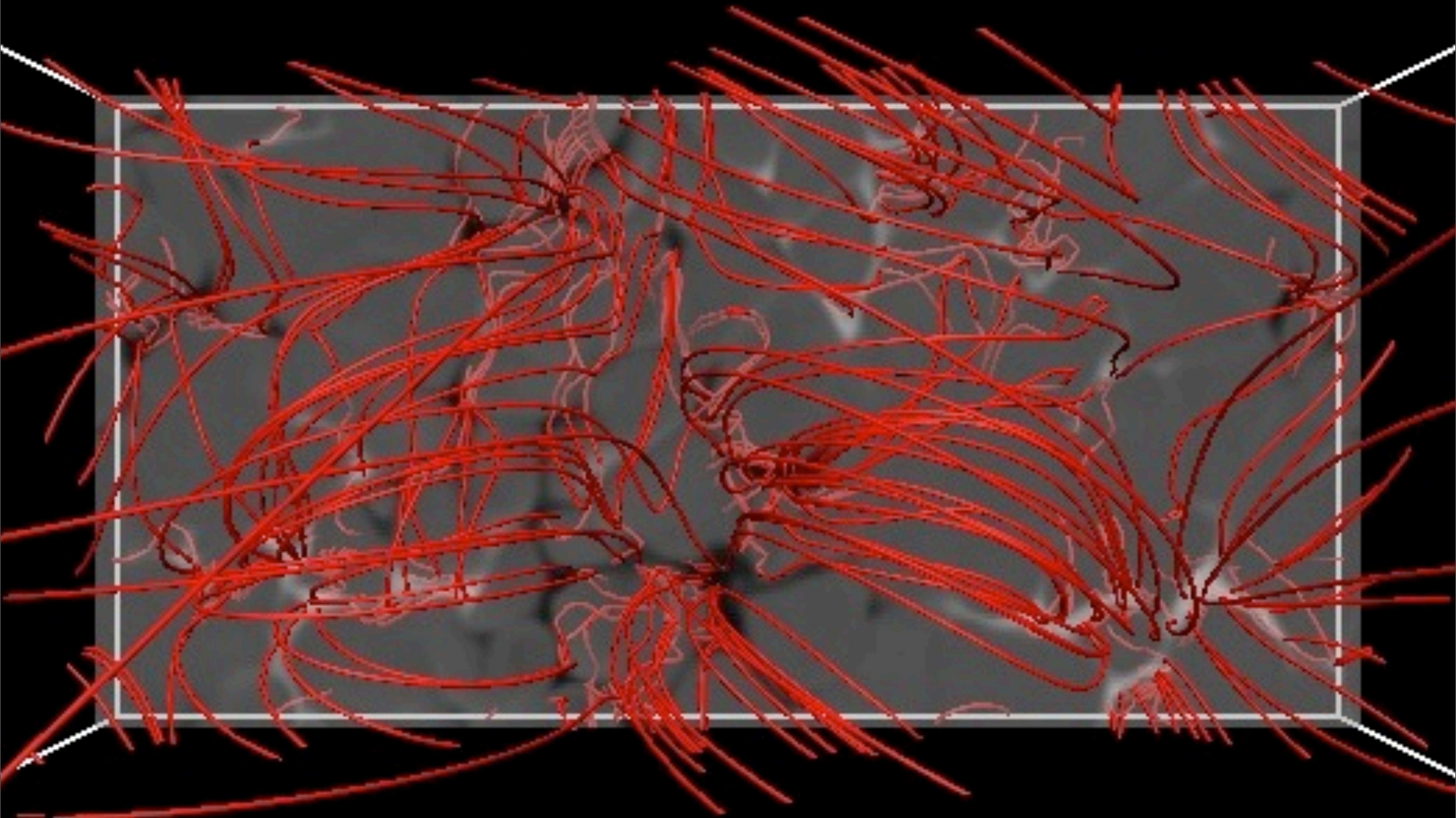


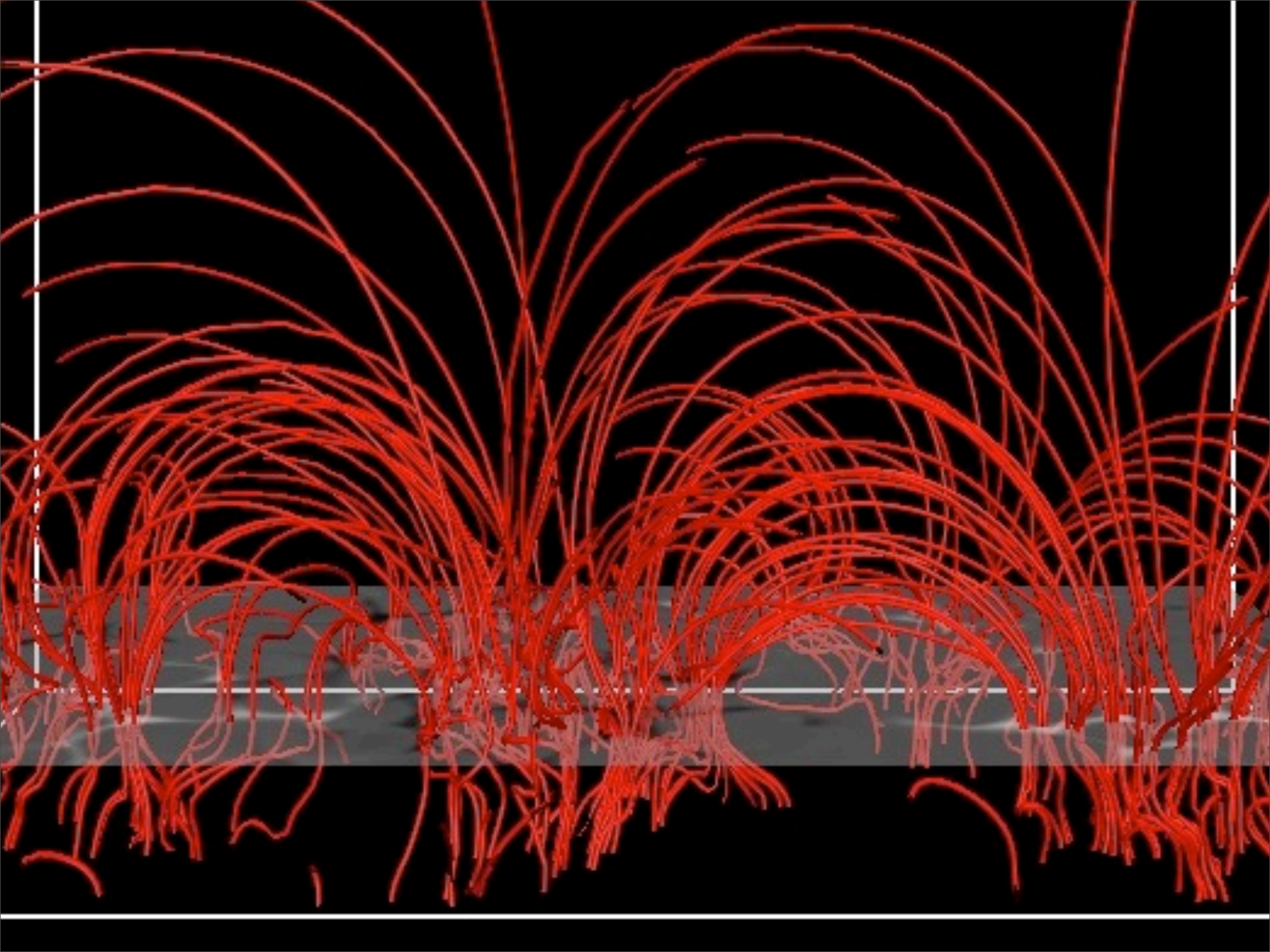
Hydrogen ionization out of equilibrium

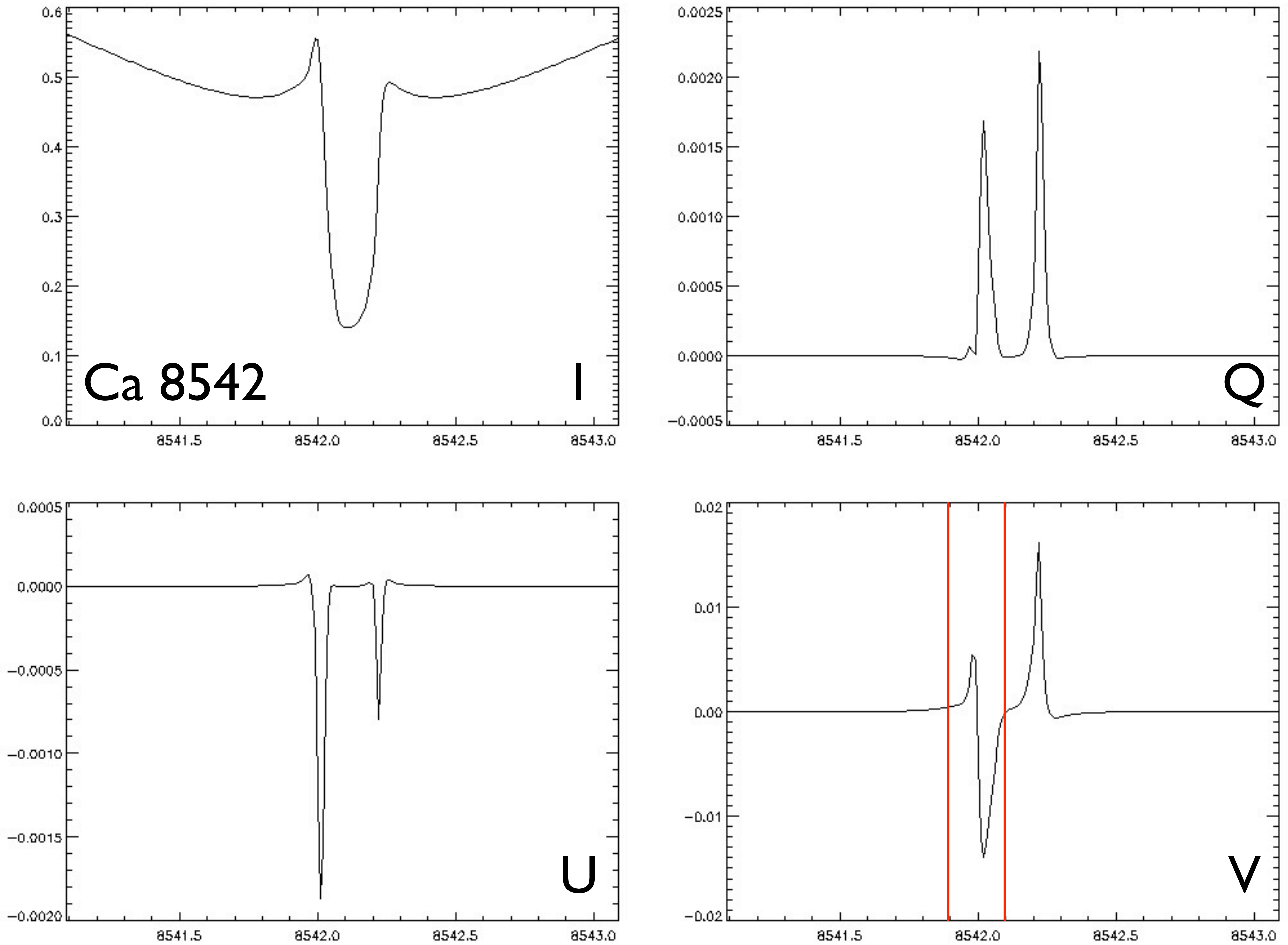


Leenaarts et al 2007: A&A 473, 625

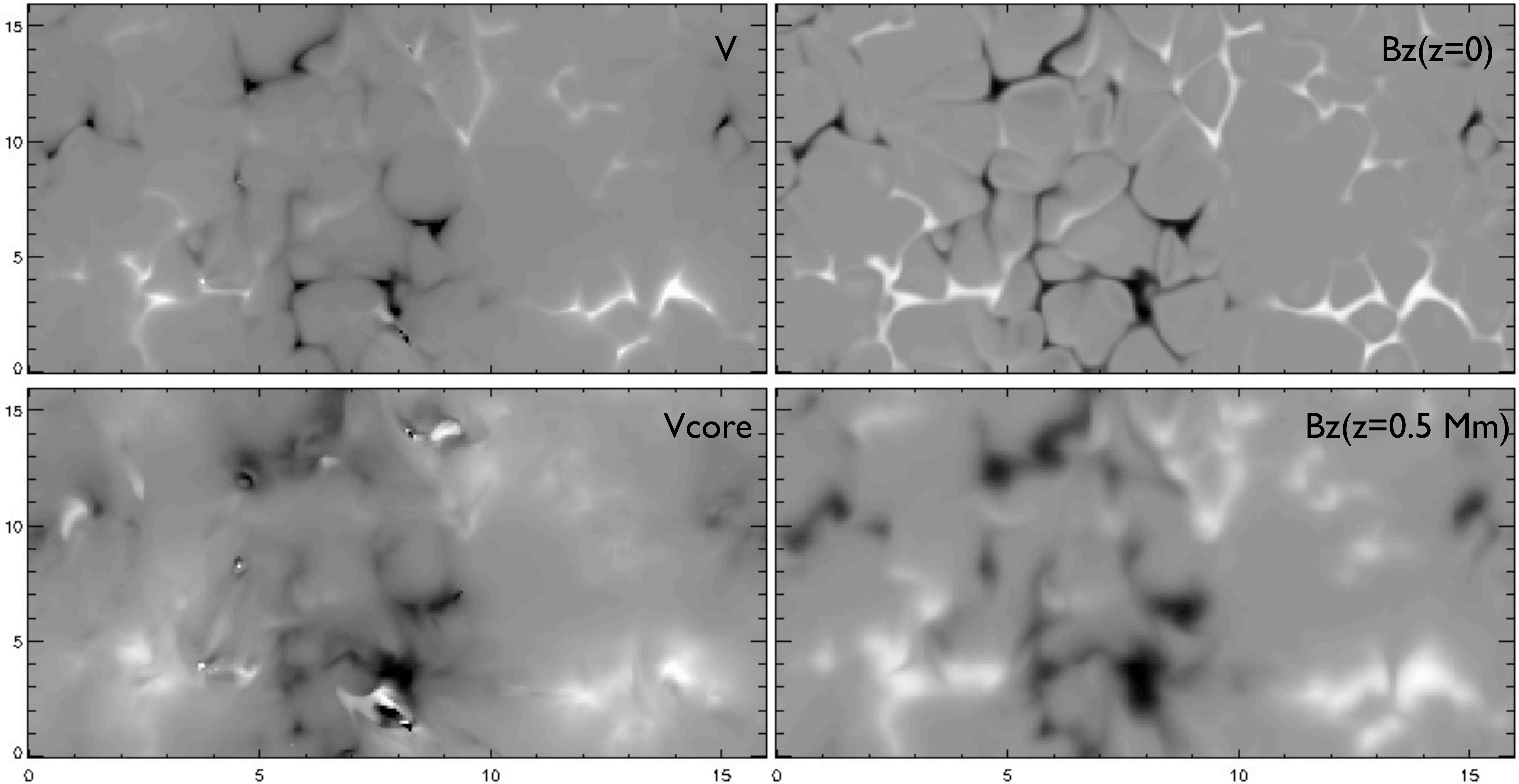







Ca 8542
I
Q
U
V
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
−0.0005
0.0005
0.0000
−0.0005
−0.0010
−0.0015
−0.0020
0.02
0.01
0.00
−0.01
−0.02
8541.5
8542.0
8542.5
8543.0

Ca 8542



Jaime de la Cruz Rodrigues et al