Chapter 3

The Radiative Transfer code - OPTIM3D

Contents

3.1 The code

I developed a 3D radiative transfer code that I called OPTIM3D. I employed it to generate synthetic spectra and intensity maps in the snapshots of RHD simulations, taking into account the Doppler shifts caused by the convective motions. The radiation transfer is calculated in detail. Fig. 3.1 shows the flow-chart.

The code can use one-dimensional or three-dimensional models as input. The geometry is shown in Fig. 3.2. The models should contain the temperature, the density and the velocity at different atmospheric depth, for the one-dimensional models, and for all the grid points of the computational box.

Once the input simulation is read, OPTIM3D starts with the interpolation of the extinction coefficients into pre-calculated tables (the temperature/density points distribution is discussed in Sect. 3.2.1) with a double linear interpolation (see the same Sect.) for all the grid points of the input simulation and interpolation coefficients are stored.

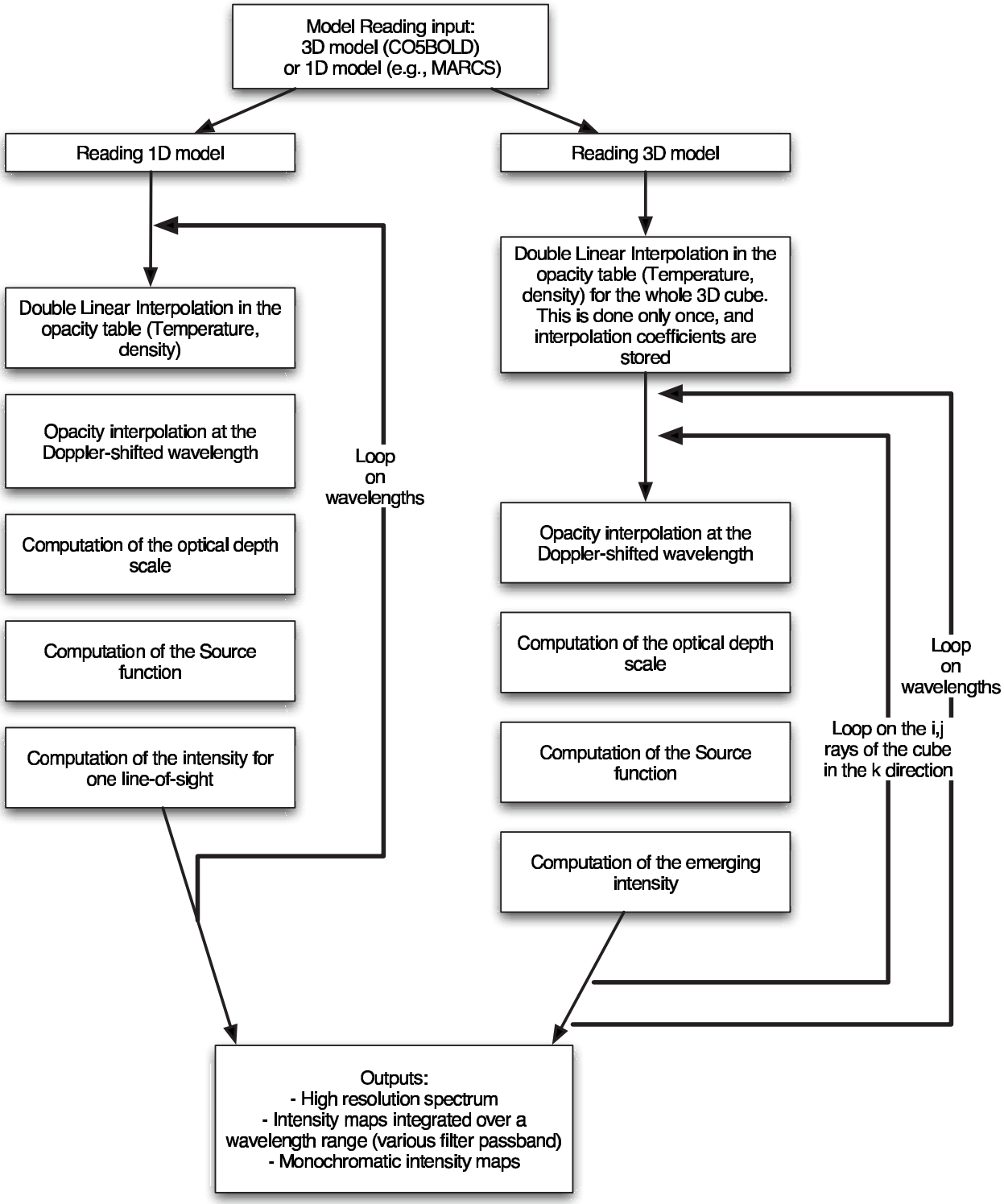

Figure 3.1: Schema of OPTIM3D

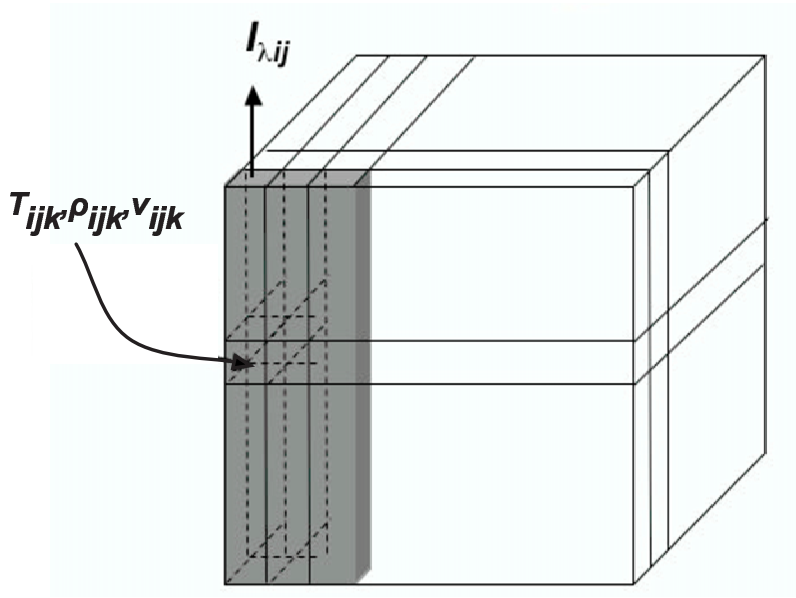

Figure 3.2: Geometry of the 3D radiative transfer code.

This is done only once for the first wavelength.
Afterwards, the extinction coefficient, that includes all absorption and scattering, is linearly interpolated at the Doppler-shifted wavelength (the wavelength resolution in the table is discussed in Sect. 3.2.2) and eventually the optical depth is calculated.

The intensity emerging at the surface along a rays is

$$\mathrm{I}(0) = \mathrm{I}(\tau)\,\mathrm{e}^{-\tau} + \int_0^{\tau} \mathrm{S}(\mathrm{t})\,\mathrm{e}^{-\mathrm{t}}\mathrm{dt} \tag{3.1}$$

where I is the intensity, τ is the maximum optical depth and S is the source function (here, at LTE ($\mathrm{S}_\lambda = \mathrm{B}_\lambda(\mathrm{T}_{\mathrm{ijk}})$, the Planck function at the temperature $\mathrm{T}_{\mathrm{ijk}}$, Fig 3.2). If the source function can be approximated by a polynomial of degree n in t, it is possible to evaluate the integral 3.1 exactly (when $\tau \to \infty$) using a Gauss-Laguerre quadrature of order n. I use such a quadrature with order n=9 provided by N. Piskunov. The weight and the abscissa are reported in Tab. 3.1. The source function is linearly interpolated at the required abscissae, as spline interpolation introduce unwanted oscillations with even S(t)<0.

This operation is done for every rays in the computational box and for all the wavelengths required.

3.2 Opacity tables

To reduce the computing time, the extinction coefficient is pre-tabulated as a function of the temperature, density and wavelength with the solar composition (Asplund et al.

Table 3.1: Gauss-Laguerre quadrature weights and abscissa

abscissae	weights
0.137793470540	3.08441115765E-01
0.729454549503	4.01119929155E-01
1.808342901740	2.18068287612E-01
3.401433697855	6.20874560987E-02
5.552496140064	9.50151697518E-03
8.330152746764	7.53008388588E-04
11.843785837900	2.82592334960E-05
16.279257831378	4.24931398496E-07
21.996585811981	1.83956482398E-09

2006). The extinction coefficient contains all the absorption and scattering.
The opacity tables are generated with MARCS (Gustafsson et al. 1975, Plez et al. 1992 and Gustafsson et al. 2008) and they take into account millions of molecular and atomic lines. For the atomic lines the VALD database (Piskunov et al. 1995) has been used. For the molecular lines, the source data is reported in Tab. 3.2 extracted from Gustafsson et al. (2008). For more details please refer to (Gustafsson et al. 2008, p. 6). The tables have been constructed with no micro-turbulence.

The opacity tables that I generate are of two types: one with the continuum opacities and one with the continuum+line opacities.

3.2.1 Temperature and density distribution

The temperature and density distribution used in the opacity tables covers the temperature and density range of RHD simulations in the outer layers (Fig. 2.10). In particular, the typical range of temperature and density used to produce the opacity tables is reported in Fig. 3.3. In this table (top right panel in Fig. 3.5) there are 51 temperature points: 30000., 22000., 18000., 15000., 13750., 12500., 11250., 10000., 9200., 8400., 7800., 7200., 6750., 6300., 5950., 5600., 5200., 4800., 4600., 4400., 4200., 4000., 3850., 3700., 3600., 3500., 3400., 3300., 3200., 3100., 3000., 2950., 2900., 2800., 2700., 2600., 2500., 2400., 2300., 2200., 2100., 2000., 1900., 1800., 1700., 1600., 1500., 1400., 1300., 1200., 1100. K.
And there are 25 density points, in logarithm: -20.,-19.5,-19.,-18.5,-18.,-17.5,-17.,-16.5,-16.,-15.5, -15.,-14.5,-14.,-13.5,-13.,-12.5,-12.,-11.5,-11.,-10.5,-10., -9.5,-9.,-8.,-7.

Table 3.2: Source of data for molecular line opacities

Species	Reference
HCN vib-rot	Harris et al. (2002)
H_2O	Barber et al. (2006)
C_2 Phillips, Swan, ballik-Ramsay	(1971, priv. comm.)
C_3	Jorgensen et al. (1989)
C_2H_2	Jorgensen (1989)
CH vib-rot	Jorgensen et al. (1996)
CH A-X, B-X, C-X	Plez et al. 2008 (in preparation)
CN A-X, B-X	Plez (unpublished)
CO vib-rot	Goorvitch (1994)
CO A-X	Kurucz (1995)
CaH A-X, B-X	Plez (unpublished)
FeH $F^4\Delta$-$X^4\Delta$	Plez (unpublished)
MgH A-X, B'-X	Kurucz (1995)
NH A-X	Kurucz (1995)
OH vir-rot	Goldman et al. (1998)
OH A-X	Kurucz (1995)
SiH A-X	Kurucz (1995)
SiO vib-rot	Langhoff & Bauschlicher (1993)
TiO $\alpha, \beta, \gamma', \delta, \varepsilon, \phi$,	
$E^3\Pi$-$B^3\Pi$,$a^1\Delta$-$f^1\Delta$	Plez (1998)
VO A-X, B-X, C-X	Plez (unpublished)
ZrO $B^1\Pi$-$A^1\Delta$,$B^1\Pi$-$X^1\Sigma$,	
$C^1\Sigma$-$X^1\Sigma$, $E^1\Phi$-$A^1\Delta$,	
$b^3\Pi$-$a^3\Delta$, $d^3\Phi$-$a^3\Delta$,	
$e^3\Pi$-$a^3\Delta$, $f^3\Delta$-$a^3\Delta$	Plez et al. (2003)

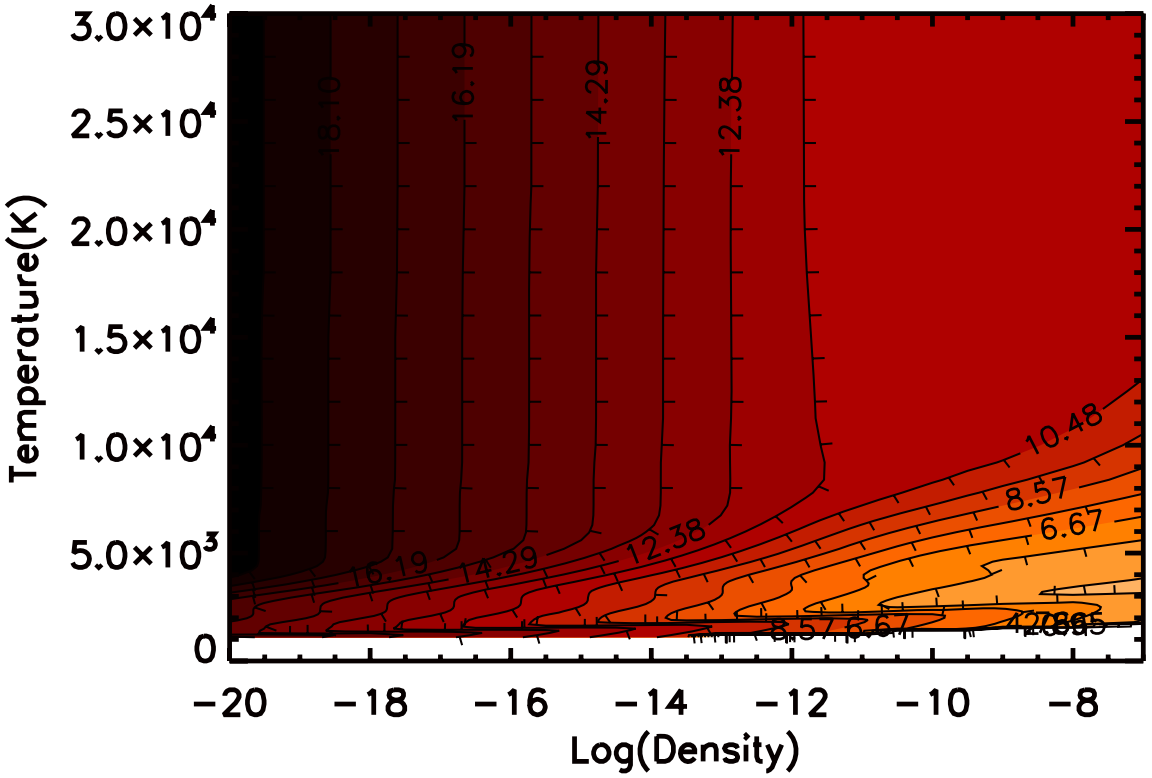

Figure 3.3: Logarithmic contour plot of the continuum+lines opacity divided by the density at 1.6 μm for the opacity table described in the text. Bright areas correspond to higher opacities.

In order to outline the temperature and density sample distribution, Fig. 3.4 displays some cuts in the table. I have chosen some characteristic temperatures and densities across the atmosphere for two different wavelength in the visible and in the H band. The crosses represents the temperature and the density points in the opacity table. While the density distribution is equally sampled over the whole range, there are more temperature points lower temperature (T<5000) and less at higher temperature (see Fig. 3.5, top-right panel). As a consequence, I give more weight to the atmospheric layers where the spectral line and the continuum form. In the Figure (top row), it is visible that the opacities in the optical and in the H band have a strong peak at lower temperatures that corresponds mostly to the contribution of TiO (optical) and H_2O (H band). In the deepest atmospheric layers, HI absorptions, excited by higher temperature, dominates.

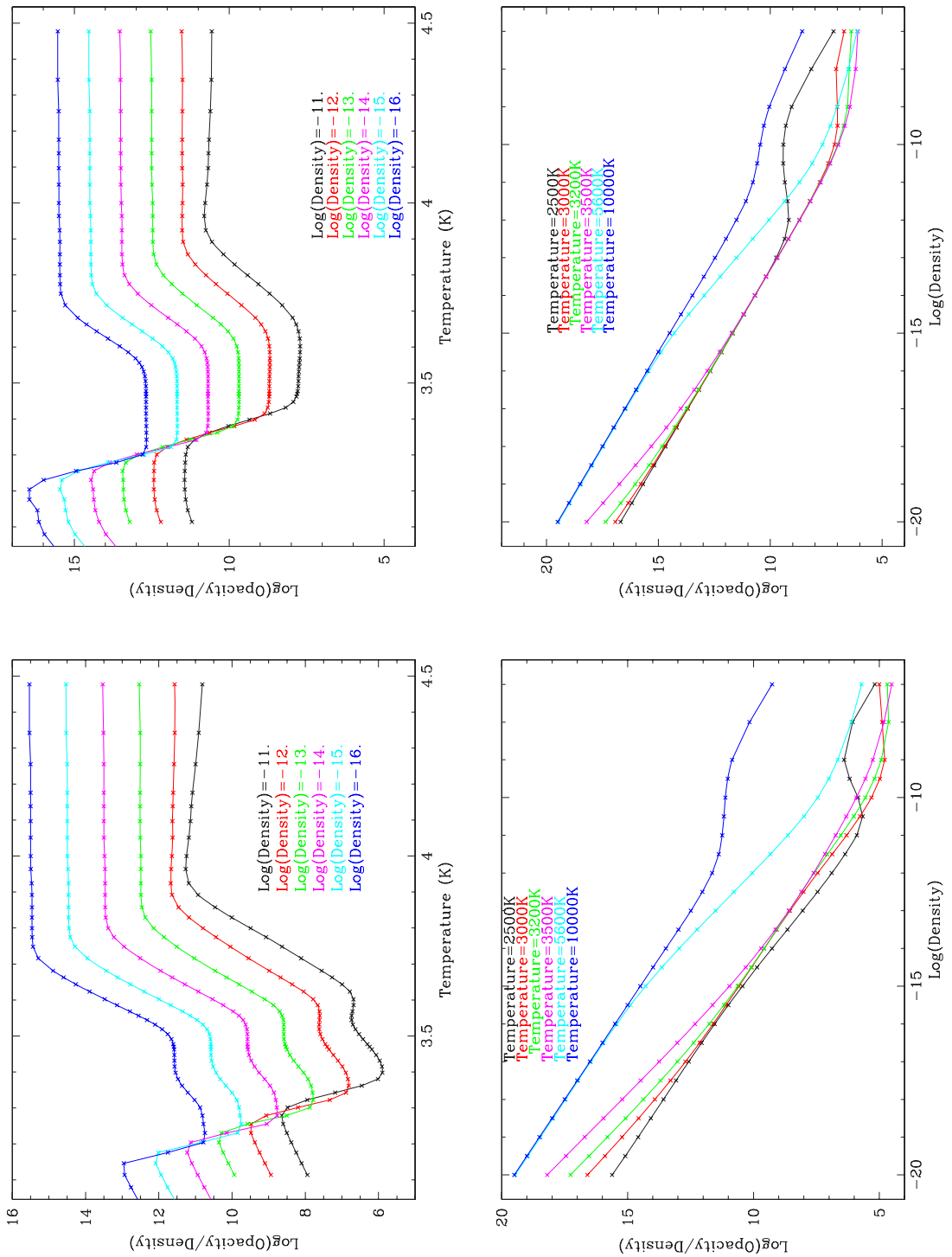

Figure 3.4: *Left column:* continuum+line logarithmic opacity versus the temperature for some characteristic value of the density in the H band at 1.6 μm. *Right column:* The same in the optical at 5000 Å.

I have checked the impact of the temperature and density distribution of the tables on the spectral synthesis using a MARCS model (T_{eff}=3500K, log(g)=-0.5, microturbulence=2km/s, solar metallicity) and computing a spectrum with Turbospectrum (Plez et al. 1993, Alvarez & Plez 1998 and further improvements by B. Plez) and OPTIM3D. For this test I use a double linear interpolation in the opacity tables.

Fig. 3.6 displays two spectral region: the optical (top row) and the H band (bottom row). In both cases, the synthetic spectrum computed with Turbospectrum is in red, the black line corresponds to an opacity table with 29 temperature points and 18 density points (29x18), the blue line to an opacity table with 51 temperature points and 25 density points (51x25) and the green line to an opacity table with 61 temperature points and 25 density points (61x25).
The difference between the opacity tables are reported in Fig. 3.5. The 29x18 table is coarser than the other two, both in density and temperature points. Tables 51x25 and 61x25 differs only in temperature points, the latter has more points in the region between 2600 and ∼3850 (where the spectral line and continuum form) where I added some temperature points, changing the temperature step to 50K.

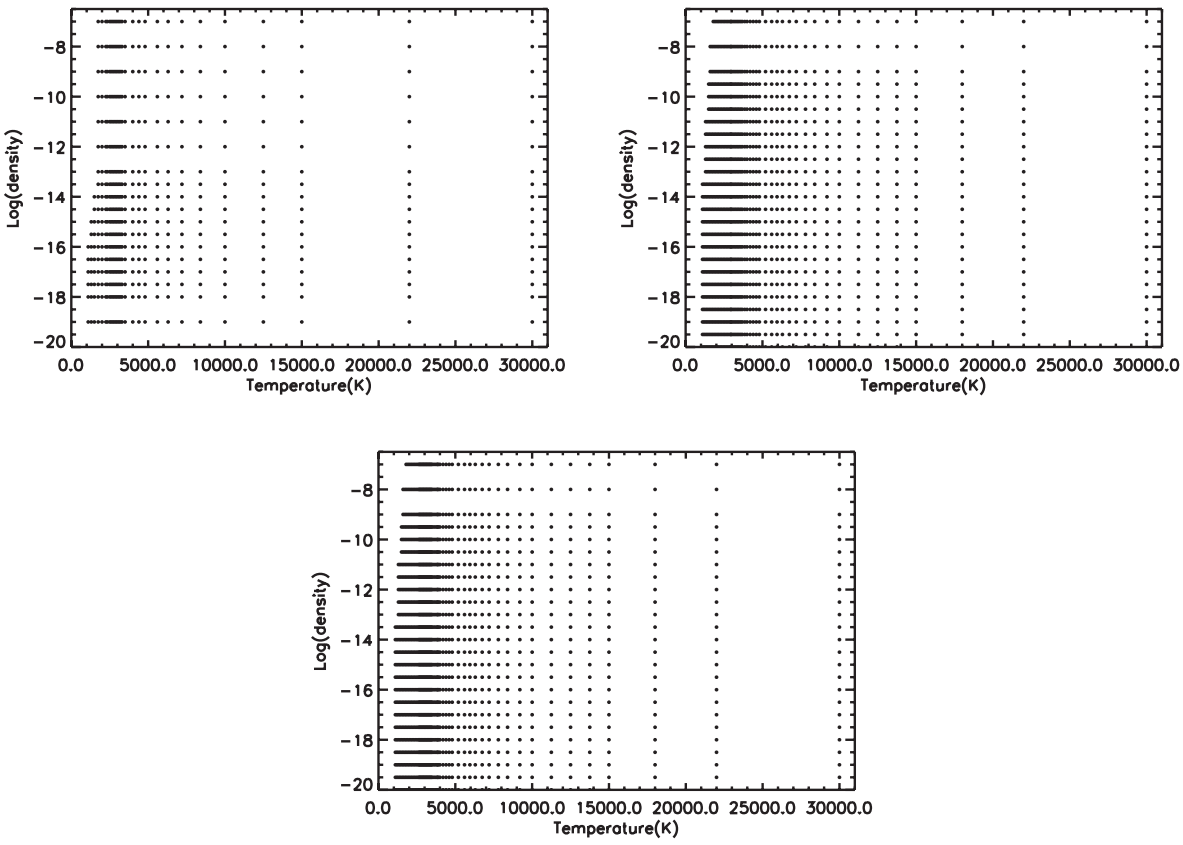

Figure 3.5: Temperature and density points distribution in three opacity tables with 29 temperature points and 18 density points (top left panel), with 51 temperature points and 25 density points (top right panel) and with 61 temperature points and 25 density points (bottom panel).

Fig. 3.6 shows that increasing the number of temperature and density points in the tables weakens the differences between the Turbospectrum and OPTIM3D for this MARCS model. In the visible region of the spectrum, the relative difference with respect to Turbospectrum is about $\sim 14\%$ for the opacity table with 25x18 points and then it decreases down to $\sim 8\%$ for the 51x25, and finally $\sim 5\%$ for the 61x25 table. In the H band regions, the differences are lower than 3.5%.
The size of the opacity tables depend on the number of temperature and density points (plus the wavelength resolution, Sect. 3.2.2). Since the opacity tables need to cover a wavelength range as large as possible for the high resolution spectral synthesis, I have chosen to use the 51 temperature/25 density points distribution.

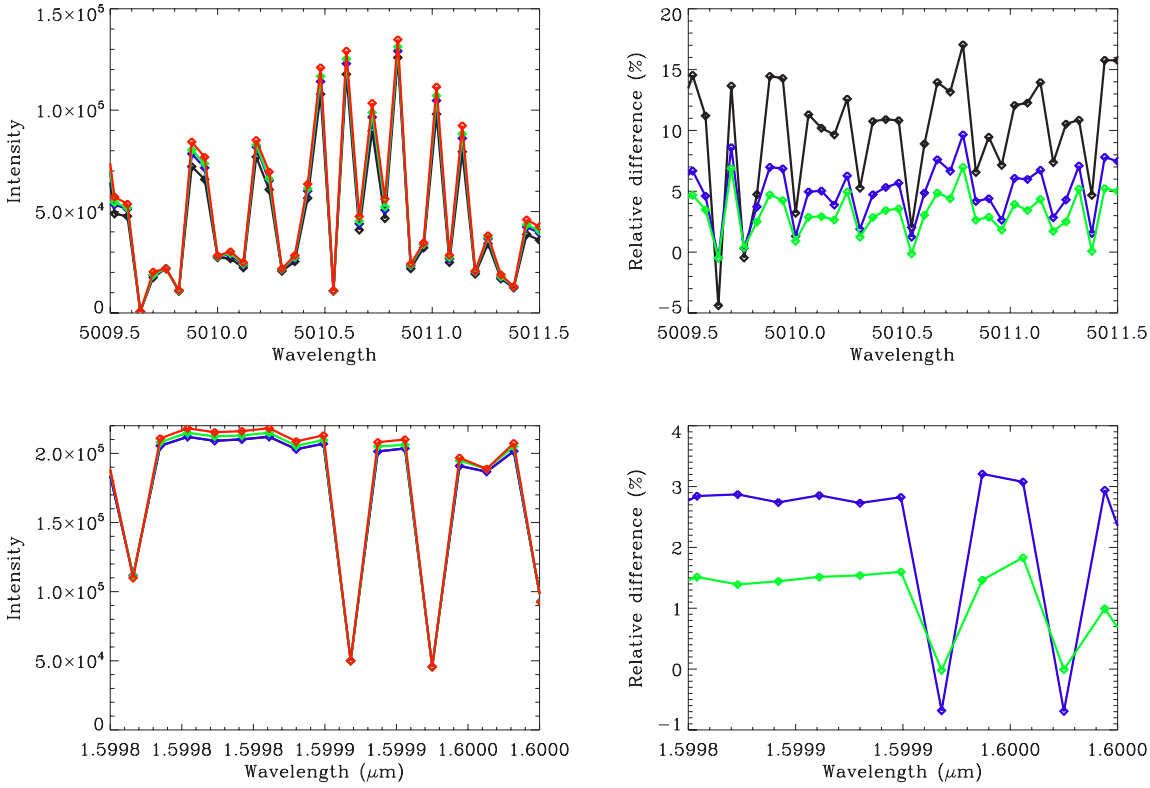

Figure 3.6: Test on the temperature and density distribution in the opacity tables in two different regions of the spectrum (Top row visible, bottom row H band). *Left column:* red line is the spectrum of a MARCS model (T_{eff}=3500K, log(g)=-0.5, microturbulence=2km/s, solar metellicity) computed with Turbospectrum. The black line is the resulting spectrum computed with OPTIM3D using an opacity table with 29 temperature points and 18 density points, blue line with an opacity table with 51 temperature points and 25 density points and green line with 61 temperature points and 25 density points. The resolution for the calculation is v=3.6 km/s and the calculated points are marked by diamonds. *Right panel:* relative difference between spectra computed with OPTIM3D and Turbospectrum with respect to Turbospectrum (colors have the same meaning as for left column).

Once read the temperature and density structure from the RHD simulation, OPTIM3D interpolates into the opacity tables. In order to test the fastest and most adapted interpolation, I have used the one-dimensional MARCS model and the spectral synthesis code Turbospectrum to compare with my OPTIM3D code. In Turbospectrum, the opacity is calculated on the fly and no interpolations are done in tables. Thus, I have compared the emerging intensity computed with the "exact" opacities (Turbospectrum) with the intensity obtained by the interpolated opacities (OPTIM3D).
The one-dimensional MARCS model used has T_{eff}=3500K, surface gravity=-0.5, microturbulence=2 km/s and solar metallicity. Fig. 3.7 shows that using the cubic spline interpolation, the synthetic spectra of OPTIM3D (black line in left panel) and Turbuspectrum (red dashed line in left panel) are close. The relative difference with respect to Turbospectrum is about 5% with peaks at 8% close to the continuum (at 5009.7 Å) and to the strong absorption line (at 5010.8 Å).

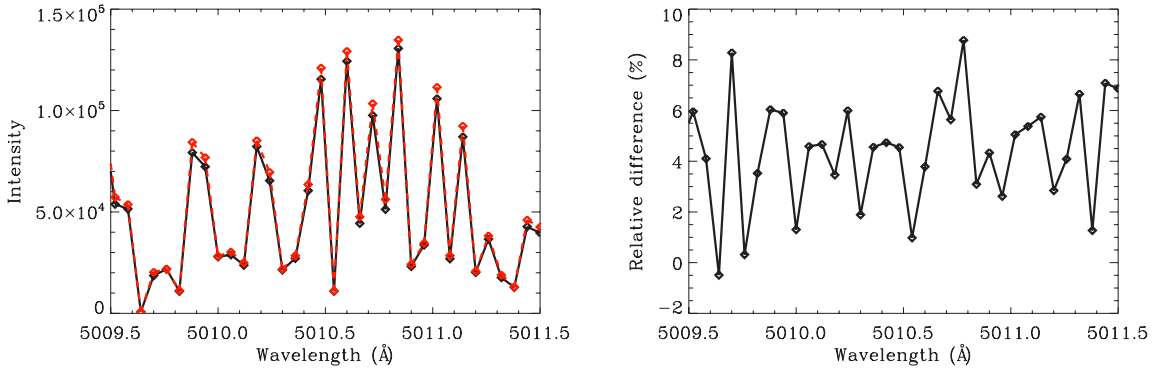

Figure 3.7: Test on the interpolation in the opacity tables with 51 temperature points and 25 density points. *Left panel:* red dashed line is the spectrum of a MARCS model (T_{eff}=3500K, log(g)=-0.5, microturbulence=2km/s, solar metellicity) computed with Turbospectrum and black line with OPTIM3D. The resolution for the calculation is v=3.6 km/s and the calculated points are marked by diamonds. *Right panel:* relative difference with respect to the spectrum computed with Turbospectrum.

I have also tested how the relative difference between the two codes behave increasing the number of temperature points. Using the same distributions as in Fig. 3.5 (opacity table with 61 temperature points and 25 density points). Fig. 3.8 shows the results. The relative difference is now lower than 8%. The spline interpolation in the opacity tables reduces the relative difference between the Turbospectrum and OPTIM3D. However, it may introduce unwanted oscillation in RHD global simulations (see Sect. 3.1) and it is too costly for the whole RHD computational cube (see example with a local model Sect. 3.3). Thus, I have chosen to use the double linear interpolation described above.

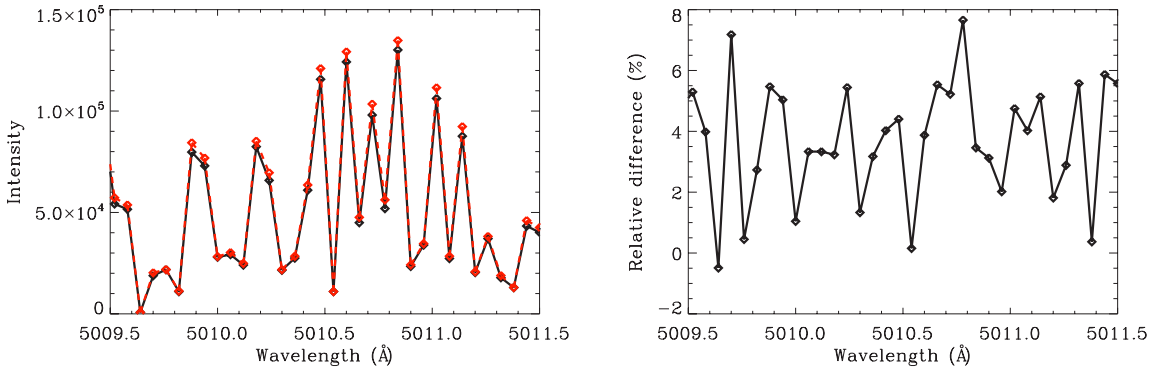

Figure 3.8: Test on the interpolation in the opacity tables with 61 temperature points and 25 density points. *Left panel:* red dashed line is the spectrum of a MARCS model (T_{eff}=3500K, log(g)=-0.5, microturbulence=2km/s, solar metellicity) computed with Turbospectrum and black line with OPTIM3D. The resolution for the calculation is v=0.3 km/s and the calculated points are marked by diamonds. *Right panel:* relative difference with respect to the spectrum computed with Turbospectrum.

3.2.2 Spectral resolution of the tables

In order to assure a correct description of the line profile I have to set a spectral resolution high enough in the opacity tables. This is important because OPTIM3D interpolates also at the Doppler shifted wavelength. In order to have a first estimation the spectral resolution of the tables, I consider, for instance, a turbulent velocity equal to ξ=2 km/s (a typical value for the microturbulence). Usually, the thermal motions are smaller than turbulent ones and the FWHM of a spectral line is approximatively

$$\mathrm{FWHM} \simeq 2\sqrt{2\log 2}\Delta\lambda_{\mathrm{Doppler}} = 2.35 \cdot \Delta\lambda_{\mathrm{Doppler}} = 4.7 \text{ km/s} \tag{3.2}$$

and the resolution needed is

$$\mathrm{Resolution} = \frac{\mathrm{c}}{\mathrm{FWHM}/2} = \frac{300000 * 2}{4.7} \sim 130000 \tag{3.3}$$

To ensure an accurate interpolation, I chose a resolution bigger than the estimation above: 500000 (v=0.6 km/s) for the continum+line opacity tables and 50000 (v=6 km/s) for the continuum opacity tables.
Fig. 3.9 displays the relative difference between a spectrum computed using continuum+line opacity tables with a resolution of v=0.6 km/s, a resolution of v=1 km/s (black) and v=1.5 km/s (red) in the optical region. As input model, I have use a snapshot of the RHD simulation st35gm03n07 (Tab. 4.1). The resolution for the calculation is v=0.3 km/s. I chose a resolution for the calculation higher than the spectral resolution of the tables in order to see the impact of the interpolation. The relative difference between the two highest resolution is lower than 1%. Opacity tables with larger spectral resolution become too big in term of disk space.

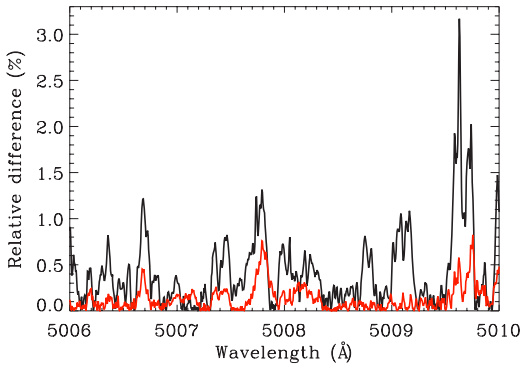

Figure 3.9: Relative difference between a spectrum computed using opacity tables with a resolution of v=0.6 km/s and opacity tables with a resolution of v=1km/s (red) and v=1.5 km/s (black). The resolution for the calculation is v=0.3 km/s.

3.3 Comparison with Linfor3D

Linfor3D (Cayrel et al. 2007 for the Non-LTE version and http://www.aip.de/~mst/Linfor3D/linfor_3D_manual.pdf for the LTE version) is used for the spectral synthesis of the RHD simulations in the local configurations (Sect. 2.2.1) and it computes line and continuous opacity on the fly. The code accounts for the Doppler shifts. The line depression is computed from the continuum (reverse transfer equation). In order to cross-check the resulting spectra from OPTIM3D and Linfor3D, I modified my code to work on local models. As OPTIM3D computes the intensity along the line of sight, the corresponding outgoing intensity of a local model is the one coming out from the center of the stellar disk.
First, I created an "artificial" line list (Tab. 3.3) with three iron lines (with increasing strength) centered at a laboratory wavelength equal to 5500 Å.

Table 3.3: Artificial FeI lines

Wavelength (Å)	Excitation potential (eV)	$\log(gf)$
5500.000	2.000	-7.000
5500.000	2.000	-6.500
5500.000	2.000	-6.000

Then, I generated the opacity tables based only on this list and using the same abundances as in Linfor3D calculations. Eventually, I computed the spectra (with a resolution of v=0.16 km/s) around the central value of the lines without microtubulence, using a local model with T_{eff}=3700 K and surface gravity equal to 1. Hans-Gunther Ludwig did the same with Linfor3D.

3.3.1 Spectra

Fig. 3.10 shows the resulting spectra. The colored curves corresponds to the spectral lines calculated with OPTIM3D, while the black curves with Linfor3D. The differences are less than 3% and larger in the wings. This is satisfactory for the analysis developed in this work (the uncertainty on the observed cross correlation function is 1-2 km/s, Josselin & Plez 2007) because OPTIM3D, as it is structured, is useful for calculating large portion of the spectra taking into account millions of molecular and atomic lines, while Linfor3D is more accurate when only one or few lines are computed. OPTIM3D uses pre-tabulated opacities with a finite number of points: 51 temperature points and 25 density points and a wavelength resolution $\lambda/\Delta\lambda$=500000 (v=0.6 km/s), while the resolution used in comparison is $\lambda/\Delta\lambda$ ∼1800000 (v=0.16 km/s, the resolution used for Linfor3D calculations). The interpolation in the opacity table could be the cause of the difference between the codes.

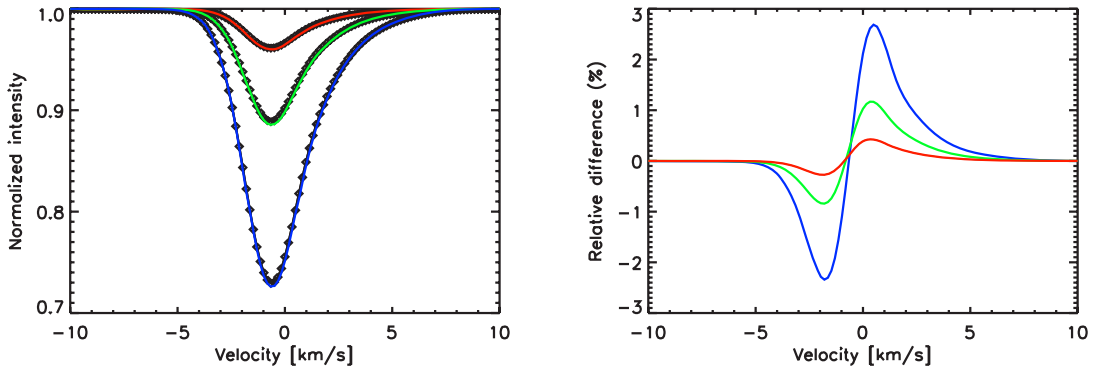

Figure 3.10: Cross-check OPTIM3D and Linfor3D - spectra. *Left panel:* colored spectral lines are computed with OPTIM3D and the black curves corresponds to the spectral line computed with Linfor3D. The resolution for the calculation is v=0.16 km/s. *Right panel:* Relative difference between the two codes with respect to Linfor3D. The colors corresponds to the three different spectral lines.

In order to determine the source of the discrepancy, I have computed the same RHD model using a spline interpolation for temperature and density in the opacity tables. This has increased enormously the CPU time (from 1.2 s/wavelength to 240 s/wavelength). Fig. 3.11 shows that now the relative difference are lower than 0.2%. Thus, the fact that OPTIM3D has to interpolate into opacity tables is the main source of the differences between the two codes.
The conclusion is that when only one line is computed for high performing abundances determination, Linfor3D is better because it avoids the interpolations into opacity tables. On the other side, when I have to compute a large range of wavelength taking into account millions of molecular and atomic lines simultaneously and I need to do it fast, OPTIM3D (with a double linear interpolation in the opacity tables) is a good choice.

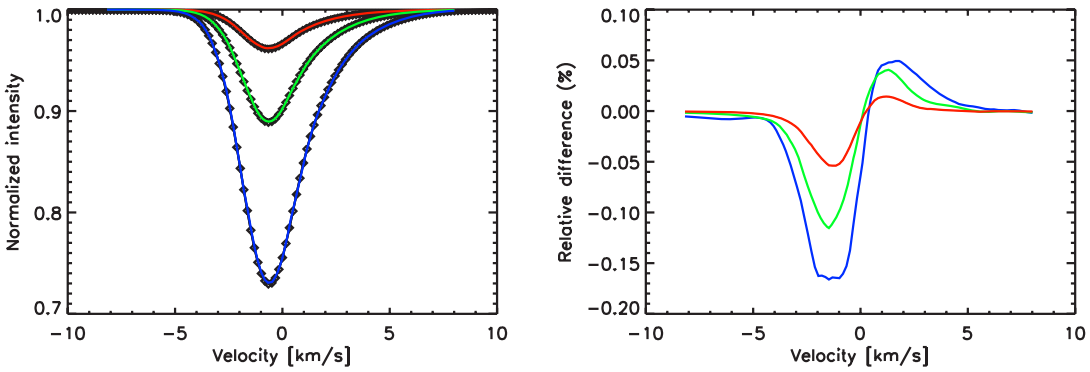

Figure 3.11: Same as in Fig. 3.10, but this time for spectra computed with OPTIM3D I have used a spline interpolation in the opacity tables.

3.3.2 Continuum intensity

I compared also the continuum intensity. The intensity maps look pretty similar (Fig. 3.12, top panel). The improvement of the spline interpolation in the opacity tables is also noticeable here. The relative difference of the continuum intensity derived from OPTIM3D using a double linear interpolation is lower than 2% (bottom left panel), while the same calculation with the spline interpolation is lower than 1.5% (bottom right panel). The remaining uncertainty is probably due still to the interpolations. I recall that I have done the calculation of these artificial lines using the same abundances as in Linfor3D. This is important because the continuum opacity at this wavelength is strongly dependent on the H^- opacity ($\sim$ 95% of the total continuum opacity at 5500Å), and some metals (e.g., Fe, K, Na, Ti, Si, Ca, Mg) are important electron donors. Slightly changes (0.05 dex) in the abundances affect the resulting continuum intensity.

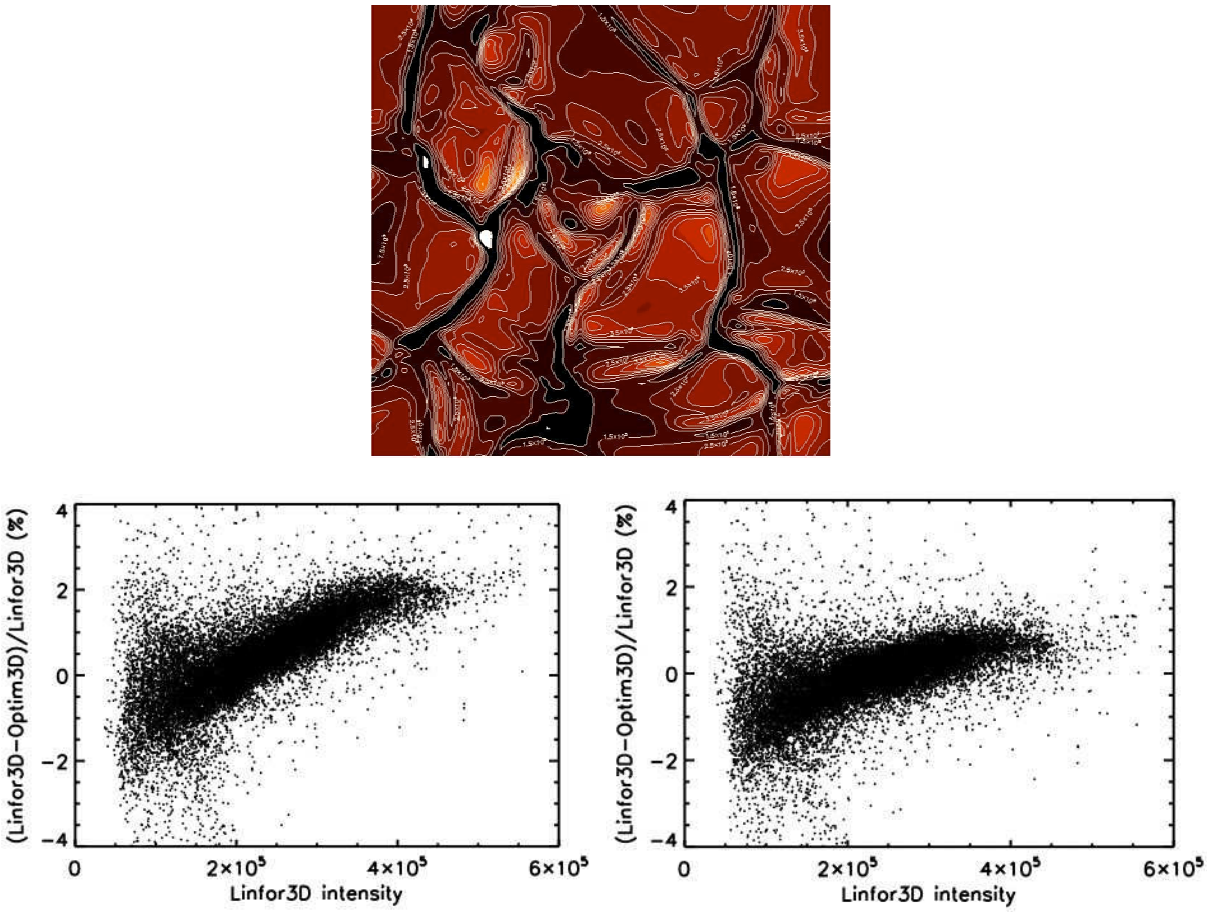

Figure 3.12: Comparison between OPTIM3D and Linfor3D - continuum intensity. *Top panel:* temperature color scale of the continuum intensity at 5500 Å computed with OPTIM3D, the white contour line is the Linfor3D continuum intensity. *Bottom left panel*: Scatter-plot of the relative difference of the continuum intensity, OPTIM3D has used a double linear interpolation in the opacity tables. *Bottom right panel*: same as in bottom left, but here OPTIM3D has used a spline interpolation in the opacity tables.

3.4 Optimization and CPU time

OPTIM3D in written in F77 with some routine in F90. In particular, this has been necessary to integrate OPTIM3D in the original spectral synthesis code (SPEC by Bernd Freytag) for CO^{5}BOLD models. SPEC is completely written in F90 (like CO^{5}BOLD) and it has the advantage to read directly the RHD models using the nomenclature and set up of CO^{5}BOLD. I decided then to include OPTIM3D in the SPEC structure in order to access to the simulations I need without any disk space-consuming conversion. The result is a shell structure (SPEC) aimed to read directly the models and an inner-core (OPTIM3D) aimed to compute the detailed radiation transport equation.
Up to now, OPTIM3D is not a parallel code. The jobs can run in parallel using wisely the shell script and the resource available; however, I plan to implement the parallelization.
As I have mentioned in Tab. 2.1, the RHD models are strongly CPU-demanding and this

depends on the resolution and the radiation transfer treatment (see Sect. 2.3.4). In this context, the radiation transport computation is also CPU-demanding. OPTIM3D has been compiled on different architecture:

1. Macintosh Xserve G5 DP with processor clock speed of 2.5 Ghz and 4 Gb of RAM memory (IBM-XLF Fortran compiler[10])
2. Macintosh Xeon 4 cores with processor clock speed of 2.66 GHz and 8 Gb of RAM memory (INTEL Fortran compiler[11])
3. Macintosh bi-Xeon 4 cores with processor clock speed of 3 GHz and 8 Gb of RAM memory (same compiler as above)
4. PC-Linux Xeon 4 cores with processor clock 3 GHz and 8 Gb of RAM memory (same compiler as above)

To give an idea of the CPU time needed, using the machine (2): to calculate a synthetic spectrum of 1000 Å at 6000 Å with a resolution of 100000 takes about 5.7 hours per snapshot (about 1.2 seconds per wavelength). Each model consists of $\sim$ 100 snapshots. For this reason, a large part of my PhD has been used to develop and optimize the code for high resolution RHD simulations. In Sect. 3.3, I have also tested the spline interpolation into the opacity tables, the CPU time grows enormously and the computation of a 100 wavelengths spectrum of a local RedGiant model takes 7h (4.2 min per wavelength[12]). Another point of concern is the optimization of the code. Enormous efforts have been done on the development of the code to speed the calculations up. The most evident implementations are: (i) the interpolation of the temperature and density points in the pre-tabulated opacity tables that is executed only once for all the computational cube; (ii) the Gauss-Laguerre quadrature; (iii) the asymptotic development of the exponential. Still, the exponentials constitute the larger part of the CPU time needed.

[10] http://www.nersc.gov/nusers/resources/software/ibm/xlf.html
[11] http://www.intel.com/cd/software/products/asmo-na/eng/282048.htm
[12] A more optimized algorithm for spline interpolation could be implemented.