Inversion of Stokes profiles with SIR

Luis R. Bellot Rubio
Instituto de Astrofísica de Andalucía

Basilio Ruiz Cobo
Instituto de Astrofísica de Canarias

Version 4, 2017 February 20

SIR is distributed freely without any guarantee that it will work in your particular problem. Although you can use the code on your own, we STRONGLY recommend you to contact us for guidance during the first application of SIR to real observations.

If you find SIR useful for your work, you are kindly requested to include the following two references in your papers:

- Bellot Rubio, L.R. 2003, Inversion of Stokes profiles with SIR, (Freiburg: Kiepenheuer-Institut für Sonnenphysik)
- Ruiz Cobo, B., & del Toro Iniesta, J.C. 1992, ApJ, 398, 375

Contents

Chapter 1

Introduction

The present chapter gives an overview of SIR. It also describes in some detail the spectral synthesis calculations performed by the code and the inversion algorithm. The chapter contains material that is not directly related to the use of the program. If you are not interested in knowing how SIR works internally, read section 1.1 below and skip the remainder of the chapter. If you are not familiar with the concept of *nodes*, you must read section 1.3 as well.

1.1 General information

SIR (Stokes Inversion based on Response functions) is a package for the synthesis and inversion of spectral lines formed in the presence of magnetic fields. The code takes into account the Zeeman-induced polarization of the light and deals with all four Stokes parameters (I, Q, U, V) of any electric dipole transition and atomic species. SIR was developed for the automated analysis of solar spectra under LTE conditions.

In synthesis mode, the program calculates the Stokes spectra[1] emerging from any specified model atmosphere which may consist of up to two different components (either magnetized or nonmagnetized). This is done by solving numerically the radiative transfer equation (RTE) for polarized light. SIR handles in a straightforward manner the particular case in which no magnetic fields exist. Hence, it is also of interest for integrating the scalar RTE.

In inversion mode, SIR fits any combination of observed Stokes parameters for any arbitrary number of spectral lines. To this end, an initial (user-provided) model atmosphere is iteratively modified until the synthetic Stokes profiles match the observed ones. This process yields the thermal, dynamic and magnetic structure of the atmosphere in which the observed profiles were formed.

Spectral synthesis is carried out by means of a fast and accurate Hermitian integration of the RTE (Bellot Rubio, Ruiz Cobo & Collados 1998). This technique significantly improves the speed of other well-known methods (DELO, fourth order Runge-Kutta, etc). The opacity routines of Wittmann (1974) are used for the computation of absorption coefficients.

[1] By Stokes spectra or Stokes profiles we mean the dependence of I, Q, U and V on wavelength.

The inversion module of SIR implements a Marquardt nonlinear least-squares algorithm (Press et al. 1986) for the minimization of the differences between the observed and synthetic Stokes spectra. Marquardt's method translates the nonlinear problem into a linear one, the solution of which is carried out by means of a modified singular value decomposition (SVD) algorithm (Ruiz Cobo & del Toro Iniesta 1992). From a mathematical point of view, the modified SVD method implemented in SIR can be viewed as a regularization technique. Knowledge of the partial derivatives of the Stokes parameters with respect to the various atmospheric parameters, the so-called *response functions* (RFs), is crucial for the success of the inversion. Thus, the synthesis module of SIR calculates all the necessary RFs. Further details on RFs can be found in Ruiz Cobo & del Toro Iniesta (1994).

The performance of SIR has been quantified by Westendorp Plaza et al. (1998), who compared the behavior of SIR and the Milne-Eddington inversion technique of Skumanich & Lites (1992) in various numerical experiments. SIR has been successfully applied to the study of different solar structures observed in polarized light, such as sunspots (Collados et al. 1994; Westendorp Plaza et al. 1997a,b,c) and unresolved magnetic elements (Bellot Rubio et al. 1999), and for non-polarized light to structures such as penumbrae (del Toro Iniesta, Tarbell & Ruiz Cobo 1994), solar granulation (Ruiz Cobo et al. 1995, 1996; Rodríguez Hidalgo, Ruiz Cobo & Collados 1996), and solar oscillations (Ruiz Cobo, Rodríguez Hidalgo, & Collados 1997). In these analyses, model atmospheres were retrieved from the observed Stokes spectra.

SIR was introduced by Ruiz Cobo & del Toro Iniesta in 1992. Since then, the code has been extended to make it capable of dealing with a variety of different situations. As a result, the following programs are now available:

- A code for the inversion of Stokes profiles emerging from unresolved magnetic elements. It implements the geometry and constraints of the thin flux tube scenario for the analysis of active regions outside sunspots (Bellot Rubio, Ruiz Cobo & Collados 1998).
- A code for non LTE inversion of Stokes spectra (Socas-Navarro, Ruiz Cobo & Trujillo Bueno 1998).
- MISS (Multi line Inversion of Stellar Spectra; Allende Prieto, Ruiz Cobo & García López 1998). This code is intended to fit observed stellar spectra, so fluxes rather than specific intensities are used.

This manual describes in detail the various algorithms behind SIR. It also explains how to use SIR efficiently. SIR has been prepared to run under default conditions, so previous experience is not required. For best performance, however, the user is expected to get acquainted with the various options allowed by the program. Although completely automated, the inversion of Stokes spectra with SIR requires some human intervention. Indeed, the user is expected to find the optimum inversion conditions for the particular application of SIR at hand. This usually requires several trial runs of the program.

1.2 The synthesis module

1.2.1 Spectral synthesis

Spectral synthesis is carried out by solving the radiative transfer equation for Zeeman split lines

$$\frac{\mathrm{d}\boldsymbol{I}(\tau_5)}{\mathrm{d}\tau_5} = \mathsf{K}(\tau_5)\,[\boldsymbol{I}(\tau_5) - \boldsymbol{S}(\tau_5)]\,,$$

where τ_5 represents the continuum optical depth at 5000 Å along the line of sight (hereafter LOS), K is the total absorption matrix (a 4×4 matrix describing the absorption properties of the atmosphere), and $\boldsymbol{S} = (S_I, S_Q, S_U, S_V)^\dagger$ the source function vector. Since LTE conditions are assumed, the source function vector is given by $\boldsymbol{S} = (B_\nu[T], 0, 0, 0)^\dagger$, with $B_\nu[T]$ the Planck's function at the local temperature T.

Except for the numerical integration of the RTE, the derivatives entering the calculation of the RFs, and the routines for hydrostatic equilibrium, the synthesis module of SIR is based on the code by Wittmann (1974). The evaluation of K and $\boldsymbol{S}$ is made under the assumption of local thermodynamic equilibrium (LTE). The atomic populations are then computed by means of the Saha and Boltzmann equations. It is implied that

1. The magnetic field is strong and no quantum interferences between Zeeman sublevels exist.

2. Collisional rates are high enough, so the various sublevels corresponding to the same energy level are equally populated.

3. The frequency and direction of photons scattered by an atom are independent on the frequency and direction of the incoming photons (*complete redistribution on scattering*).

The physical parameters needed to compute K are specified in the model atmosphere, which need to be discretized in an equally spaced logarithmic scale of the continuum optical depth at 5000 Å. At each grid point, the temperature, electron pressure, microturbulence, magnetic field strength, azimuth and inclination of the magnetic field vector, and LOS velocity are specified. The model atmosphere is completed with a set of depth-independent parameters: macroturbulent velocity, stray light contamination and filling factor (for two component atmospheres).

The particularly simple expressions adopted by the elements of K for Zeeman-line transfer and electric dipole transitions can be found, e.g., in Rees (1987). Magnetooptical effects leading to linear and circular birefringence are fully considered. The continuum absorption coefficient k_c is evaluated for a given wavelength, temperature and electron pressure by taking into account contributions from H, He, H^-, He^-, H_2^-, H_2^+, C, Mg, and Na, as well as Rayleigh scattering by H, H_2 and He, and Thomson scattering by free electrons (see Wittmann 1974). Other atomic and molecular line opacity sources, which are neglected in the present version of SIR, can be included in a straightforward manner.

By default (if electronic pressure is not a free parameter) SIR assumes hydrostatic equilibrium. After each iteration step, the electron pressures of the already perturbed model

atmosphere are put into hydrostatic equilibrium by using the equation of state of an ideal gas with variable mean molecular weight to take into account the partial ionization of the various atomic elements. Gas pressures are computed from temperatures and electron pressures on the assumptions of LTE and chemical equilibrium. In this process, the partial pressures of H, H^+, H^-, H_2, H_2^+ and other 83 elements are determined following the strategy outlined by Mihalas (1967). At present, the only molecules considered for the calculation of gas pressures are H_2 and H_2^+, but up to 91 other molecules can be included quite straightforwardly (Wittmann 1974).

The synthesis is carried out under the assumption that the predominant broadening mechanisms are van der Waals broadening Γ_6 and radiation broadening $\Gamma_{\rm rad}$. Stark broadening is neglected. Unsöld (1955) theory is employed in the computation of Γ_6, but the possibility of enhancing this coefficient is left open to correct deviations of the theory (see Wittmann 1974 for details). Thus, Γ_6 can be multiplied by a user-specified enhancement factor E that is usually in the range 1-3. SIR can handle different enhancement factors for the different spectral lines (see section 3.3.4).

Once K and $\boldsymbol{S}$ have been calculated, SIR solves the RTE by means of an Hermitian algorithm (Bellot Rubio, Ruiz Cobo & Collados 1998). This new strategy was developed to accelerate the solution of the RTE provided by the DELO method (Rees, Murphy & Durrant 1986). The Hermitian algorithm is based on the Taylor expansion of the Stokes vector to fourth order in optical depth. It provides an approximation to the evolution operator at no extra cost, which is crucial for the calculation of response functions. The main advantages of the Hermitian method are accuracy and speed.

The synthesis module of SIR is capable of dealing with blends. It is possible, for example, to synthesize the Stokes profiles of a particular spectral line by including the contribution of nearby lines. This is achieved by adding, at every wavelength, the absorption matrices of the different contributing atomic transitions.

The various steps through which SIR calculates simulated Stokes spectra are:

1. The files containing the model atmosphere and the atomic parameters of the lines to be synthesized are read.

2. The RTE is integrated numerically for the wavelengths specified in a wavelength grid file. If the atmosphere consists of two different components, the Stokes spectra emerging from each component, $\boldsymbol{I}_1(\lambda)$ and $\boldsymbol{I}_2(\lambda)$, are computed individually and then mixed according to their filling factors f_1 and f_2, with $f_1 + f_2 = 1$. In this case, the emergent Stokes spectrum is
$$\boldsymbol{I} = f_1\,\boldsymbol{I}_1 + f_2\,\boldsymbol{I}_2,$$

3. The same height-independent macroturbulent velocity $v_{\rm mac}$ is assumed for all spectral lines. The effect of the macroturbulence is simulated by convolving $\boldsymbol{I}$ with a gaussian
$$M(\lambda - \lambda_0, v_{\rm mac}) = \frac{1}{\sqrt{2\pi}\,\sigma} {\rm e}^{-\frac{(\lambda-\lambda_0)^2}{2\sigma^2}},$$

where $\sigma \equiv \lambda_0 v_{\rm mac}/c$, λ_0 is the central wavelength of the transition and c is the speed of light. Additionally, the macroturbulent-broadened profiles ($\boldsymbol{I}^* = \boldsymbol{I} * M$) may be convolved with the PSF of the spectrograph if it is available.

4. The last step in simulating the observed profiles $\boldsymbol{I}_{\rm obs}$ is to add a user-provided stray light spectrum $\boldsymbol{I}_{\rm str}$ that contributes a fraction α to $\boldsymbol{I}_{\rm obs}$:

$$\boldsymbol{I}_{\rm obs} = (1-\alpha)\,\boldsymbol{I}^* + \alpha \boldsymbol{I}_{\rm str}.$$

1.2.2 Response functions

Response functions (RFs) to the various atmospheric parameters $x(\tau)$, $\boldsymbol{R}_x(\lambda,\tau)$, are calculated at every optical depth and wavelength according to the formula

$$\boldsymbol{R}_x(\tau) = \mathsf{O}(0,\tau)\left\{\mathsf{K}(\tau)\frac{\partial \boldsymbol{S}(\tau)}{\partial x} - \frac{\partial \mathsf{K}(\tau)}{\partial x}\left[\boldsymbol{I}(\tau)-\boldsymbol{S}(\tau)\right]\right\},$$

where $\mathsf{O}(0,\tau)$ represents the evolution operator from τ to the surface. By definition, the modification of the emergent Stokes spectrum $\delta\boldsymbol{I}(\lambda)$ after perturbations $\delta x(\tau)$ of the atmospheric parameter x at optical depth τ is given by

$$\delta\boldsymbol{I}(\lambda) = \int_0^\infty \boldsymbol{R}_x(\lambda,\tau)\,\delta x(\tau)\,{\rm d}\tau. \tag{1.1}$$

If a nonzero macroturbulence is used to synthesize the emergent Stokes spectrum, all the RFs have to be convolved with M as well. The same applies if the spectrograph profile is taken into account.

1.3 The inversion module

The inversion of Stokes profiles proceeds by minimizing a merit function which is the sum of the squared differences between observed and synthetic data weighted by the uncertainties of the observations and by some factors w_{ki}^2. The merit function is defined as

$$\chi^2 \equiv \frac{1}{\nu}\sum_{k=1}^{4}\sum_{i=1}^{M}\left[I_k^{\rm obs}(\lambda_i) - I_k^{\rm syn}(\lambda_i)\right]^2 \frac{w_{ki}^2}{\sigma_{ki}^2}, \tag{1.2}$$

where index $k = 1,\ldots,4$ samples the 4-component vectors containing the observed (obs) and synthetic (syn) Stokes profiles, $i = 1,\ldots,M$ sample the wavelengths at which the spectrum has been measured, ν is the number of degrees of freedom (i.e., the number of observables minus the number of parameters to be inverted) and σ_{ki} are the uncertainties of the observations. SIR automatically adjusts the factors w_{ki}^2 so as to give the same relative weight to the Stokes parameters of different spectral lines, independently of their amplitudes. The user may specify that more weight is to be assigned to a particular Stokes parameter. For example, more weight could be desired for Stokes V when analyzing magnetic regions. Subsection 3.3.1 explains in detail how to vary the relative weights of the various Stokes parameters.

By default, SIR assumes that the uncertainties σ_{ki} are all equal to a constant value σ given by the signal-to-noise ratio of the observations. However, σ_{ki} is set to 10^{15} for points in the observed profiles that will **not** be considered for inversion. This option is useful, for example, when the intensity profiles are contaminated by blends of solar or terrestrial origin, but the corresponding polarization profiles (Q, U and V) are not. In this case, one may invert the whole Q, U and V profiles and the portion of the intensity profile that is not contaminated with blends by simply replacing the undesired intensities by -1.0 in the file containing the observed spectrum (see Section 3.3.1 for more details). When SIR finds values smaller than -1.0 for any of the Stokes parameters, the corresponding σ_{ki} are set to 10^{15}, the consequence being that such data points are not taken into account in the fit.

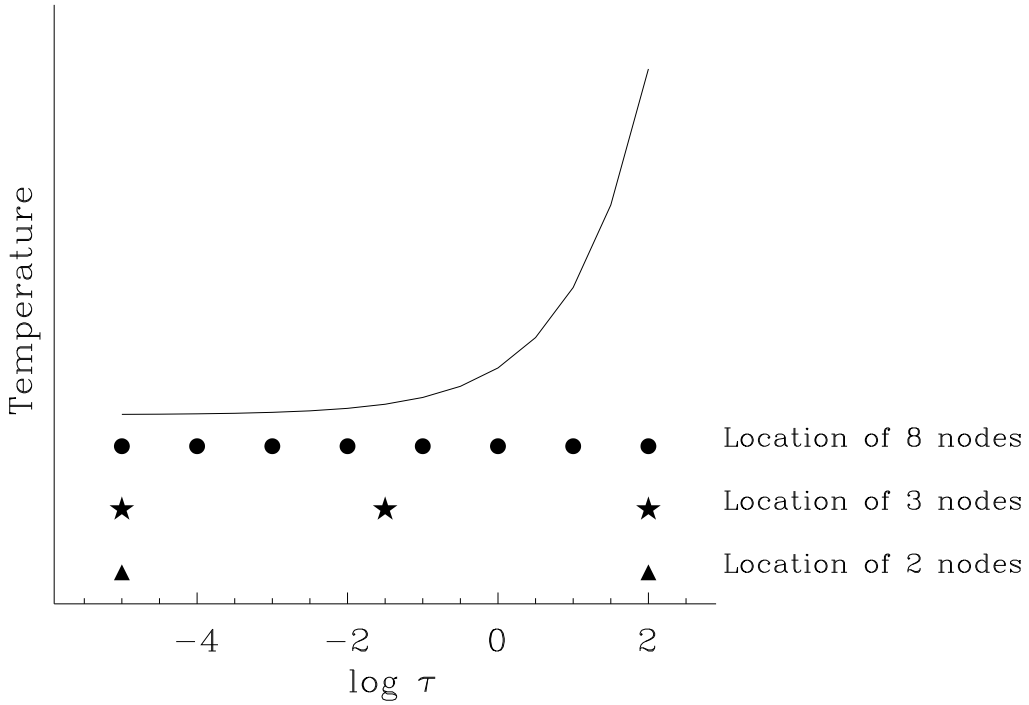

Figure 1.1: Schematic explanation of how the nodes are chosen. The particular case of temperature (T) is considered. The atmosphere is discretized in the logarithmically evenly spaced grid shown in the x–axis, the step size being $\Delta\log\tau = 0.5$ in this particular example. The optical depths at which perturbations of the temperature will be sought are determined by the number of nodes selected. If the user specifies two nodes, perturbations of T at $\log\tau = -5.0$ and $\log\tau = 2.0$ will be found. With three nodes, perturbations will be found at $\log\tau = -5.0$, $\log\tau = -1.5$ and $\log\tau = 2.0$. The same scheme applies with a larger number of nodes. Note that five nodes cannot be used here because there are no sufficient spatial points in the grid to produce an even distribution of the nodes through the whole atmosphere.

The minimization of Eq. (1.2) is carried out iteratively by modifying an initial user-

provided model atmosphere. This process yields the perturbations of the guess atmosphere required for the synthetic spectrum to match the observed one. However, the minimization of χ^2 is complex because $\boldsymbol{I}^{\rm syn}$ depends nonlinearly on the various atmospheric parameters. To handle this problem, SIR implements a Marquardt algorithm (Press et al. 1986). Marquardt makes use of the derivatives of χ^2 with respect to the model parameters. It turns out that these derivatives can be expressed in terms of RFs (Ruiz Cobo & del Toro Iniesta 1992), which explains the relevance of the RFs for the inversion.

In order to reduce the number of free parameters, the perturbations of the depth-dependent physical quantities characterizing the initial guess model atmosphere are calculated only for a few grid points (called *nodes*) of the spatial grid in which the atmosphere is discretized. For each physical quantity (e.g., temperature, LOS velocity, etc), the atmosphere is represented by a different set of nodes. The perturbations of the various parameters in all the remaining grid points are approximated by linear or cubic-spline interpolation of the perturbations at the nodes.

Figure 1.1 explains in more detail the concept of nodes introduced by SIR. Once the number of nodes has been specified for a given physical quantity, the code locates the optical depths at which perturbations will be sought. If only one node is allowed, the perturbation suggested by Marquardt is added to the values of the physical quantity under consideration at all heights (i.e., its depth stratification is modified by a constant perturbation). With two nodes, the perturbations at the nodes are interpolated linearly to the whole atmosphere. With three nodes, either linear or parabolic interpolation is used. With four or more nodes, linear or cubic-spline interpolation is applied. Sect. 3.2 explains how to select one or other type of interpolation.

SIR allows the user to specify the number of nodes for each physical quantity. Note that the number of free parameters equals the sum of the number of nodes adopted for the various physical quantities. The set of iterations carried out without modifying the number of nodes is called a *cycle*. Usually, SIR needs two or three cycles to arrive at the final solution. In each iteration cycle, the number of free parameters is normally increased to permit more flexibility to the solution.

1.3.1 Error estimation

For the computation of errors in the retrieved parameters we follow a simple physical argument. According to Eq. (1.2), the weighted squared difference between the observed and synthetic spectra can be written as

$$\sum_{i,k} \delta I_{ki}^2 \frac{w_{ki}^2}{\sigma_i^2} = \nu \chi^2, \tag{1.3}$$

with $\delta I_{ki} \equiv I_k^{\rm obs}(\lambda_i) - I_k^{\rm syn}(\lambda_i)$. Now assume that m model parameters are to be inverted, each one being responsible of a fractional part $1/m$ of the observed differences δI_{ki}^2. With these hypotheses we can find a set of perturbations $\delta x(\tau)$ to the original parameters that

minimize χ^2. Using the definition of the RFs (see Eq. 1.1) we have

$$\frac{\delta I_{ki}}{\sqrt{m}} = R_{x,k}(\lambda_i, \tau)\delta x(\tau)\Delta\tau, \tag{1.4}$$

and so

$$\sigma^2_{x(\tau)} \equiv [\delta x(\tau)]^2 = \frac{\nu\chi^2}{m(\Delta\tau)^2 \ \sum_{i,k} R^2_{x,k}(\lambda_i, \tau) \ w^2_{ki}/\sigma^2_i}. \tag{1.5}$$

We have implicitly assumed that all model parameters are independent, so changes in a given parameter do not influence the remaining ones. Indeed, Monte Carlo simulations have demonstrated that the actual uncertainties are well represented by Eq. (1.5). As it might have been expected, uncertainties $\sigma_{x(\tau)}$ are proportional to the inverse of the RF to changes in $x(\tau)$. Therefore, parameters that have little influence on the emergent Stokes spectrum show the largest uncertainties. This is the case for most parameters outside the region where the spectral lines used are formed.

Chapter 2

Installing and running SIR

This chapter provides a brief guide for getting and installing SIR. To date, the program has been run successfully in Sun and Alpha workstations. More platforms are expected to be added to the list in the near future.

2.1 Where to get the program

The latest version of SIR (16 February 2017) is in:

https://github.com/brc/SIR

where you will find the `sir.tar` file. This file contains the following directories:

- `default`. This subdirectory keeps default files.
- `idl`. Several IDL procedures for visualizing model atmospheres and Stokes profiles. There are also some utilities for extracting observed profiles from the IDL FTS spectral atlas.
- `manual`. This subdirectory contains the present manual.
- `models`. Here you will find some standard model atmospheres which may be of use in real inversions. A number of utilities for modifying these models or others are provided as well.
- `program`. This subdirectory keeps the source programs and the macros needed to compile SIR.
- `test`. This subdirectory contains a particular inversion intended to test the degree of success of the installation.

- `Barklem`. Several files to evaluate collisional (pressure) broadening parameters α and σ resulting from the quantum mechanical theory of Anstee, Barklem, and O'Mara. It includes a file with a large list of spectral lines and the original Barklem program `widthcom`.

You may also obtain the `sir.tar` file by sending an email to `brc@iac.es` or to `lbellot@iaa.es`.

2.2 How to install the program

To install the program, create a directory called `sir` in your home directory, copy the `sir.tar` file to that directory and type

```
tar xvf sir.tar
```

The files will be extracted with their original path names. This will create the directories mentioned above.

Now you have to compile and link the various subroutines. To this end, move to the directory `~/sir/program`. There you will find a `Makefile` which will do the job:

`make` compiles every routine and updates the resulting object file in the SIR library (`libreria.a`).

`make` by default compiles and links sir.x using `ifort` compiler.

`make fc=gfortran` compiles and links sir.x using `gfortran` compiler.

The executable file is available under the name `sir.x`.

2.3 Optimizing SIR at installation time

SIR has been prepared to minimize the CPU and memory usage of the machine. If you want to take advantage of this capability when dealing with a particular problem, you should (re)compile all the routines to specify the appropriate array dimensions to be used for the particular application of SIR at hand.

In the `~/sir/program` directory there is a file called `PARAMETER` which provides the values of the following parameters at compilation time:

- `kt`: Maximum number of spatial points in the grid used to discretize the model atmosphere.
- `kn`: Maximum number of nodes allowed for each of the depth-dependent physical quantities. By definition, `kn` $\leq$ `kt`.
- `kl`: Number of spectral lines (including blends) to be inverted.

- `kld`: Total number of wavelength samples.

At installation, the `PARAMETER` file provides the following default values: `kt` = 64, `kn` = 64, `kl` = 100 and `kld` = 600. Note that, whenever you change any of these array dimensions, the whole set of routines must be compiled again (with `compileall`) and linked (with `linkprog sir`).

2.4 Running SIR

Once SIR has been properly installed, it can be run by typing either

```
sir.x
```

or

```
echo sir.trol | sir.x
```

The second form is used to directly provide the code with the name of the control file (`sir.trol`, in this example). If the first command is issued, the program will ask for the name of the control file right after having been called up. In order to run SIR without having to specify where the `sir.x` program resides, it is advisable that the directory `~/sir/program` be included in the user's path. This can be done by adding the following sentences to the `.cshrc` file in the home directory

```
set SIRpath = ( ~/sir/program/ )
set path = ($path $SIRpath)
```

At present, SIR inverts one single set of Stokes spectra per program call. If time series or two-dimensional maps of Stokes spectra are to be analyzed, the user may write very simple Unix scripts to run SIR repeatedly without having to invoke the program for each of the individual spectra. An example of such an script will be given in Section 3.5.

2.5 Checking the installation

The `~/sir/test` directory contains the results of a particular inversion which may be used to test the behavior of the code in other machines. To this end, run SIR from that directory by typing `echo sir.trol | sir.x` and compare the temperatures in the resulting model atmospheres (called `guess_1.mod`, `guess_2.mod` and `guess_3.mod`) with those in the test model atmospheres `test_1.mod`, `test_2.mod` and `test_3.mod`.

If everything is correct, the differences between the temperatures in the test models and the model atmospheres resulting from the inversion should be small (differences of up to 200-500 K may be present in the very deep and upper layers; such differences are absolutely normal). If this is not the case, the models will differ significantly, revealing that the compiler

does not behave as expected. Should this occur, please contact lbellot@kis.uni-freiburg.de or brc@iac.es.

Normally, malfunctioning of the code is produced by the way the compiler handles local variables upon re-entering a given subroutine. SIR was developed using a compiler that does *not* initialize to zero the local variables whenever a subroutine is reentered (i.e., the variables from the previous call are kept), but other compilers do, causing the program to crash.

Chapter 3

Fundamentals of operation

In the following, the various input/output files used by SIR are described in detail. Some useful hints are also given.

3.1 Introduction

Major efforts have been made to ensure that SIR will detect and report the errors caused by improper use of established formats and/or typos in the input files. In addition, we have tried to make SIR as user-friendly as possible, in the sense that the human interaction with the program has been reduced to a minimum. However, SIR cannot be regarded as a black box that once fed with the observations will produce good results. Indeed, some (crucial) intervention is expected from the user, namely the selection of the optimum number of nodes. The success of the inversion critically depends on the experience of the user, so playing with the code is highly recommended before inverting real observations. We also advise you to contact us for guidance during the first applications. Our feedback will be important for you to be sure that SIR is being used in the proper way.

SIR receives information via the input files described in this chapter. At present, to change the conditions under which the inversion is carried out, the user has to edit these files by hand and stick to the rules given below to prevent errors from occurring. Work is currently being done to develop a window interface to SIR which will be used to control the various options without having to modify any file by hand.

3.2 The control file

SIR uses the files and performs the operations specified in the control file. Control files are recognized by the extension `.trol`.

Control files have 42 lines that must be ordered as in the example of Table 4.1. Each line is divided in three parts. The first one extends until the colon mark (:). The second extends from the colon to the exclamation mark (!). The third one goes from the exclamation mark

Table 3.1: Example of a control file

```
Number of cycles                  (*) : 3              ! (0=synthesis)
Observed profiles                 (*) : profiles.per
Stray light file                      : stray.per      ! (none=no stray light contam)
PSF file                              : psf.dat        ! (none=no convolution with PSF)
Wavelength grid file              (s) : grid.grid      ! (none=automatic selection)
Atomic parameter file                 : LINEAS         ! (none=DEFAULT LINES file)
Abundance file                        : THEVENIN       ! (none=DEFAULT ABUNDANCES file)
Initial guess model 1             (*) : guess1.mod
Initial guess model 2                 : guess2.mod
Weight for Stokes I                  :1                ! (DEFAULT=1; 0=not inverted)
Weight for Stokes Q                  :1                ! (DEFAULT=1; 0=not inverted)
Weight for Stokes U                  :1                ! (DEFAULT=1; 0=not inverted)
Weight for Stokes V                 :10                ! (DEFAULT=1; 0=not inverted)
AUTOMATIC SELECT. OF NODES?           :                ! (DEFAULT=0=no; 1=yes)
Nodes for temperature 1               : 1,5,10,12
Nodes for electr. press. 1            :
Nodes for microturb. 1                : 0,1
Nodes for magnetic field 1            : 1
Nodes for LOS velocity 1              :
Nodes for gamma 1                     :
Nodes for phi 1                       :
Invert macroturbulence 1?             : 1              ! (0 or blank=no, 1=yes)
Nodes for temperature 2               :
Nodes for electr. press. 2            :
Nodes for microturb. 2                :
Nodes for magnetic field 2            :
Nodes for LOS velocity 2              :
Nodes for gamma 2                     :
Nodes for phi 2                       :
Invert macroturbulence 2?             :                ! (0 or blank=no, 1=yes)
Invert filling factor?                :                ! (0 or blank=no, 1=yes)
Invert stray light factor?            : 1              ! (0 or blank=no, 1=yes)
mu=cos (theta)                        :                ! (DEFAULT: mu=1.)
Estimated S/N for I                   : 200            ! (DEFAULT: 1000)
Continuum contrast                    :                ! (DEFAULT: not used)
Tolerance for SVD                     :                ! (DEFAULT value: 1e-4)
Initial diagonal element              :                ! (DEFAULT value: 1.e-3)
Splines/Linear Interpolation          :                ! (0 or blank=splines, 1=linear)
Gas pressure at surface 1             :                ! (0 or blank=Pe boundary cond.)
Gas pressure at surface 2             :                ! (0 or blank=Pe boundary cond.)
Magnetic pressure term?               :                ! (0 or blank=no, 1=yes)
NLTE Departures filename              :                ! blank= LTE (Ej. depart_6494.dat')
```

to the end of the line. These three parts contain the name of the field, the information to be used by SIR, and comments or additional explanations for the user, respectively. SIR ignores all what is written in the line after the exclamation mark.

The first line in the control file specifies the number of cycles of the inversion (i.e., how many times the number of nodes is going to change). The following eight lines provide SIR with the names of several input files. Full paths (up to 300 characters) can be used here. The remaining lines specify details of the inversion.

The information required by SIR is contained in the second part of each line. More than one file name or numerical value can appear there, *always separated by commas*. At the beginning of each iteration cycle, SIR will read the appropriate name or number in the sequence. For example, the sequence `1,5,10,12` in the field `Nodes for temperature 1` in Table 4.1 instructs SIR to use one node for the first cycle, 5 nodes for the second, and 10 nodes for the third cycle. Note that only three cycles will be performed (as specified in the first line of the file), so the last number in the sequence (12) is not used. In much the same way, *every* line of the control file may contain different variables to be used in the corresponding iteration cycle.

Many lines in the control file may be left blank, in which case SIR will adopt *default* values for the relevant parameters. Other lines, however, need to be filled with the appropriate information. For convenience, these lines are marked with an asterisk (*) before the colon. In synthesis mode, providing the information for lines marked with (s) before the colon is **mandatory**.

Taking the control file of Table 4.1 as an example, we now briefly discuss the exact meaning of the different entries:

- `Number of cycles`. Compulsory. This parameter indicates the number of iteration cycles to be carried out. In our example, SIR is forced to perform three cycles. For synthesis of Stokes spectra (without inversion), the number of cycles should be set to zero. If the number of cycles is -1, response functions will be computed and saved to disk.

- `Observed profiles`. Compulsory. This is the name of the file containing the observed profiles (in inversion mode) or the name of the file where the synthesized profiles will be stored (in synthesis mode).

- `Stray light file`. Name of the file containing the stray light intensity profile ($\boldsymbol{I}_{\rm str}$). If no name is specified, the synthetic profiles will be computed with $\alpha = 0$ (i.e., no stray light contamination). The wavelengths of the stray light profile must coincide with those in the observed profiles, otherwise an error message will be issued and the program will abort.

- `PSF file`. Name of the file containing the spectrograph profile. If no name is specified, the synthetic profiles are not convolved with the PSF of the spectrograph.

- `Wavelength grid file`. Compulsory in synthesis mode, optional otherwise. This is the name of the file specifying the wavelengths at which the profiles are known. In

inversion mode, the wavelengths can be read from the profiles themselves, so there is no need to specify any wavelength grid. However, this file must be used when blended lines are desired (see below).

- `Atomic parameter file`. Name of the file containing the atomic data for the spectral lines considered. If no name is specified, SIR will look for the default `LINES` file in the ∼`/sir/default/` directory.

- `Abundance file`. Name of the file containing the abundances of the various chemical species in the solar atmosphere. If no name is specified, the default `ABUNDANCES` file in the ∼`/sir/default` directory will be used. We normally use the THEVENIN abundance file.

- `Initial guess model 1`. Compulsory. This is the name of the model atmosphere to be used for synthesis (if in synthesis mode) or the name of the initial guess model (if in inversion mode). The format of this file is explained in Section 3.3.6. In our example, the starting model is called `guess1.mod`. The improved model resulting from the first iteration cycle will be called `guess1_1.mod`, and will be read as the initial guess model for the second iteration cycle. After this new cycle, the improved model is `guess1_2.mod`, and so on. An inversion run may be started with an initial guess model called `model_4.mod`, for instance. In this case, SIR will take care of updating the subindex whenever an iteration cycle has finished. Thus, the improved model resulting from the first cycle will be called `model_5.mod`.

- `Initial guess model 2`. Same as above, but only if a two-component model atmosphere is being used. The name of the initial guess model for the second component does not need to coincide with that of the first component. Thus, for instance, one might start the inversion with an initial second component called `model2_7.mod`. The number of depth points in model 2 must coincide with that in model 1. Otherwise, the program is aborted.

- `Weights for Stokes I, Q, U and V`. These parameters indicate the relative weight of Stokes I, Q, U and V in the χ^2 merit function. In the example of Table 4.1, Stokes V is given ten times more weight than Stokes I, Q and U. If no weight is specified, a default weight equal to unity will be assigned. Zero weights imply that the corresponding Stokes parameters will not be inverted.

- `AUTOMATIC SELECT. OF NODES?` If this parameter is set to zero (the default), the user must specify by hand the number of nodes to be used for each physical quantity in all the iteration cycles.

  If this parameter is set to one, then an algorithm automatically will select such a number of nodes for every parameter in each iteration. The algorithm is based on the quest for the roots or zeros of the partial derivative of χ^2 with respect to each parameter. See del Toro Iniesta & Ruiz Cobo, 2016) for a detailled description. Obviously, as the derivative depends on the observational data, it is influenced by noise and, consequently, spurious zeros should be eliminated. Consequently, the algorithm determines the number of

nodes after looking for positive relative maxima, and negative relative minima, larger in absolute value than a given threshold.

In case the automatic selection of nodes mode is chosen, the user must specify by hand the maximum number of nodes to be used for each physical quantity in all the iteration cycles. A * symbol means that the maximum number of nodes is the number of optical depths, and, consequently, the algorithm can select any number of nodes. Obviously leaving blank or null the maximum number of nodes means that the corresponding parameter is not inverted.

- `Nodes for the various atmospheric parameters in models 1 and 2.`

  `-Manual Selection of nodes.`

  The following eighteen fields specify **the number of nodes** to be used in each iteration cycle (only if manual selection of nodes has been chosen). Consider the following example from our control file in Table 4.1:

```
AUTOMATIC SELECT. OF NODES?   : 0
Nodes for temperature 1       : 1,5,10
Nodes for electron pressure 1 :
Nodes for microturbulence 1   : 0,1
Nodes for magnetic field 1    : 1
```

  In the first cycle, temperature will be given one node, microturbulence zero nodes, and magnetic field one node. In the second cycle, temperature is given 5 nodes, microturbulence one node and magnetic field one node. In the last cycle (the third one), ten nodes will be used for temperature and one for microturbulence and magnetic field, respectively.

  In most of the cases (for instance when we are inverting only Fe I lines) the electron pressure sholdn't be inverted, since there is no sufficient information in the profiles to estimate it reliably. In this case the pressure are determined from the tempearture stratification solving the Hydorstatic equilibrium equation.

  Note that some physical parameters are considered to be height-independent, so that they can be given only zero or one node. These include macroturbulence, filling factor and stray light factor.

  `-Automatic Selection of nodes.`

  In this case the following eighteen fields specify **the maximum number of nodes** to be used in each iteration cycle, i.e., the algorithm will determine the suitable number of nodes for each quantity, but that number will be always lower than the value specified here. Consider the following example in which a manual selection of nodes is specified for the first cycle, and an authomatic one for cycles 2 and 3:

```
AUTOMATIC SELECT. OF NODES?   : 0,1
Nodes for temperature 1       : 2,5,*
Nodes for electron pressure 1 :
Nodes for microturbulence 1   : 0,1
Nodes for magnetic field 1    : 1,2,5
```

In the first cycle, the number of nodes is specified by input of the following lines, i.e. 2 nodes for temperature, microturbulence zero nodes, and magnetic field one node. In the second cycle, the algorithm can select a maximum of 5 nodes for temperature, one node for microturbulence and a maximum of 2 nodes for magnetic field. In the last cycle (the third one), the algorithm can select for temperature any number of nodes (limitted only by the number of optical depths of the model), one node for microturbulence and a maximum of 5 nodes for magnetic field.

- `mu=cos(theta)`. This is the value of the cosine of the heliocentric angle θ of the observations. Default value is 1 (profiles emerging from disk center). In the present version of SIR, the model atmospheres are always considered to be **along the line of sight**, i.e., the optical depths refer to the line of sight, not to the local vertical. If you specify a value for μ different from 1, nothing will change except that the hydrostatic equilibrium calculation will be done correctly (along the vertical, not along the line of sight).

- `Estimated S/N for I`. This parameter serves to scale the χ^2 merit function (in fact, it determines the uncertainties σ of the observations). When the actual S/N ratio of the observed profiles (measured in the continuum intensity) is provided, the χ^2 values returned by the code are the true ones. The default value is 1000. The specific value adopted for this parameter does not influence the inversion itself.

- `Continuum contrast`. When a model atmosphere consisting of two components is used, it is possible to include in the fit the continuum contrast as a new observable. This value is defined as $I_{c,1}/I_{c,2}$, where $I_{c,i}$ stands for the continuum intensity emerging from model i. The default is not to use this constraint.

- `Tolerance for SVD.` This parameter (called ε hereafter) is used by the modified Singular Value Decomposition (SVD) method to invert the Hessian matrix appearing in Marquardt's algorithm. The Hessian matrix contains the second-order derivatives of χ^2 with respect to the free model parameters. The SVD method diagonalizes the Hessian matrix and sets to zero the *inverse* of those diagonal elements being smaller than the product of ε and the maximum diagonal element. Thus, ε eliminates singularities or quasi-singularities in the Hessian matrix. When ε is very small, say 10^{-5}, only the real singularities will be eliminated and the diagonal matrix will still contain small elements. This will result in very good fits, but at the expense of possibly retrieving oscillating or abruptly changing stratifications of the physical parameters. When ε is large, say 0.1 or 0.01, many diagonal elements are eliminated. This produces a loss of information which translates into rather smooth stratifications and fits that cannot reproduce the observations.

  Because of these reasons, reasonable values for ε are 10^{-3}–10^{-4}. For noisy profiles, one may prefer using large values of ε. For high S/N ratio profiles or cycles with very few free parameters (two nodes at most), one should use small values of ε (of the order of 10^{-4} or smaller). On the other hand, if no convergence is achieved from the very beginning, one may try to increase ε before changing the initial guess model.

  The default value of ε is 10^{-4}.

- `Initial diagonal element`. It is typically of the order of 10. The diagonal element (hereafter λ) is used by the Marquardt's algorithm to vary smoothly from the steepest descent method (to be preferred far from the minimum of χ^2) to the Hessian method (which should be used close to the minimum). Large values of λ imply that the steepest descent method is being used. The value of λ is modified continuously by SIR. After successful iterations (within a given iteration cycle), SIR decreases λ by a factor 10. Unsuccessful iterations increase the value of λ by a factor 10. For initial guess models differing wildly from the actual model, the initial λ should be set to a high value (say, 100 or 1000). For initial models close to the actual one, λ can be set to a small value (say, 0.1 or 0.01). The convergence of SIR is faster the smaller the value of λ.

- `Splines/Linear Interpolation`. Set this parameter to 0 if you want to interpolate the perturbations to the guess atmosphere by means of cubic splines. Use 1 if you want to have linear interpolation in between nodes. Cubic splines will produce smoother stratifications of the physical parameters, but they may lead to unrealistic oscillations, especially in the upper atmospheric layers. Linear interpolation is preferable in certain cases, although the stratifications will look more discontinuous.

- `Gas pressure at surface 1 and 2`. These values specify the gas pressure at the uppermost grid point. They influence the calculation of hydrostatic equilibrium. If no number is given, the electron pressure of the starting model at the uppermost layer is used as initial value for hydrostatic equilibrium.

3.3 Description of the input files

Some input files may contain a header where important information (e.g., the meaning of the different columns) can be written by the user. Such a header cannot exceeds 20 lines and should end with a line of the form `-----` having at least 10 characters. In the descriptions below, we will indicate which files admit headers.

3.3.1 Profile files

These files contain the observed Stokes spectra, the stray light profile or the synthesized spectra, and are given the extension `.per`. It is important to keep this naming convention in order for the auxiliary IDL plotting routines to be able to recognize them.

A valid profile file has six columns which give the four Stokes parameters emerging from one single pixel as a function of wavelength. The meaning of these columns is as follows:

- **First column:** It contains an index with which the spectral line is identified. These indices will be looked for in the atomic parameter file afterwards.

- **Second column:** $\Delta\lambda$, i.e., observed minus line central wavelength in mÅ. Accurate **laboratory** central wavelengths have to be used in order for the inversion code to be able to derive absolute velocities.

- **Third to sixth columns:** The corresponding Stokes parameters I/I_c, Q/I_c, U/I_c and V/I_c, respectively, measured at $\Delta\lambda$. I_c represents the continuum intensity of the quiet sun **at disk center**. To normalize the profiles actually observed, one may use the average continuum of the intensity profiles emerging from pixels where no significant polarization signal exists. This will give the quiet sun continuum intensity at the heliocentric angle of the observations. The continuum intensity at disk center is then found by multiplying this value by the corresponding limb-darkening factor.

  The profiles resulting from a spectral synthesis are already normalized to the quiet sun continuum at disk center (assumed to be that resulting from the Harvard Smithsonian Reference Atmosphere)

  Since $Q \propto \cos 2\psi$ and $U \propto \sin 2\psi$, where ψ stands for the azimuth of the magnetic field vector, Q reaches its maximum and $U = 0$ when $\psi = 0$. The coordinate system to which Q and U refer is determined by the polarimeter.

All the spectral lines should be given an index, but they do not need to be ordered according to this index in the profile files.

To instruct SIR not to fit any of the Stokes parameters in a given wavelength range, it suffices to write negative numbers (e.g., -10) in the corresponding rows of the profile file. In this way, sections of Stokes I heavily blended by unknown lines can be removed from the fit while still keeping the other Stokes parameters. When SIR finds Stokes I, Q, U or V values smaller than -1 in the profile file, it assigns infinite uncertainties to those measurements, effectively eliminating them from the fit.

Negative values of Stokes I, Q, U and V must also be used to extend the wavelength range of the spectral lines **to ensure that the convolution of the profiles with the instrumental profile and the macroturbulence is done correctly**.

3.3.2 PSF file

This file contains the instrumental profile of the spectrograph or filtergraph, determined either empirically or theoretically. SIR calculates the Fourier transforms of the instrumental and the synthetic Stokes profiles and multiplies them. The product in Fourier space is equivalent to a convolution in wavelength space, so the convolved synthetic profiles are recovered by transforming back to wavelength space.

PSF files have two columns. The first one give $\Delta\lambda$ (in mÅ) and the second the value of the instrumental profile at that $\Delta\lambda$.

3.3.3 Wavelength grid files

In synthesis mode, or if blends are to be considered, a wavelength grid must be specified. The wavelength grid file may contain a header and is given the extension `.grid`.

The wavelength grid file contains four columns as follows:

Line and blends indices (in this order)	:	Initial lambda (mA)	Step (mA)	Final lambda (mA)
1,4	:	-400,	20,	400
2	:	-400,	20,	400
3	:	-400,	20,	400

The columns are separated by a colon and two commas, respectively. The first column contains the index of the line to be synthesized (which will be looked for in the file containing the atomic parameters), or the index of a line appearing in the profile files. If a given line is to be blended with other lines, the indices of these lines should be written after the index of the first line separated by commas. Note that the number of lines plus blends cannot exceed `kl`. In the example above, the line 1 is to be blended with the line 4, while the lines 2 and 3 are not blended.

The remaining columns specify the spectral range to be synthesized. The second column gives the initial $\Delta\lambda$, the third column the step, and the fourth column the final $\Delta\lambda$, expressed in mÅ.

The ordering of the lines in the wavelength grid file does not need to be the same as in the profile files.

3.3.4 Atomic parameter file

This file contains the atomic parameters of the transitions to be considered. It may possess a header. There is a default atomic parameter file called `LINES` in the `~/sir/default/` directory.

Valid atomic parameter files have eigth columns as follows:

Line=Ion	Wavelength	E	Exc.Pot	log(gf)	Transition	α	σ
2=FE 1	6301.5012	1.0	3.654	-0.75	5P 2.0- 5D 2.0	0.243	2.3520e-14
3=FE 1	6302.4936	1.0	3.686	-1.236	5P 1.0- 5D 0.0	0.240	2.3976e-14
4=FE 1	5576.0888	1.0	3.428	-0.910	7D 1.0- 7D 0.0	0.232	2.3912e-14

The first column gives the index with which the line is identified in the profile and the wavelength grid files. The index is separated by a `=` sign from the atomic symbol of the element. To specify the atomic element, capital or lower case letters may be used (but do not mix them!). For iron, either `FE` or `XX` can be employed. The ionization stage is specified by a number: 1 means neutral atom, and 2 singly ionized atom. At present, SIR can handle only the two first ionization stages.

The second column specifies the (laboratory) central wavelength of the transition (in Å). The third column gives the enhancement factor to the van der Waals coefficient Γ_6. The fourth and fifth columns give the excitation potential of the lower level (in eV) and the logarithm of the multiplicity of the level times the oscillator strength, respectively. The sixth column specifies the atomic transition. The transition is used only if magnetic fields are present, since it determines the number and strength of the various Zeeman components,

but it is always necessary to avoid error messages. In the absence of magnetic fields, you do not need to know the exact transition to be able to synthesize or invert the corresponding intensity spectrum, so if you do not have it, use any valid transition to fill the sixth column. Finally, the last two columns specify the collisional broadening parameters α and σ resulting from the quantum mechanical theory of Anstee, Barklem, and O'Mara. σ is expressed in cm^2. If these parameters are zero, the classical Unsöld (1955) formula is used (together with the enhancement factor mentioned above) for the calculation of the damping factor.

3.3.5 Abundance file

This file contains the abundances A_x of the various chemical species x, defined as $A_x = 12 + \log[x]/[\mathrm{H}]$. It may possess a header. A default abundance file called `ABUNDANCES` is in the `~/sir/default/` directory and contains the abundances listed by Anders & Grevesse (1989). There is also an abundance file called `THEVENIN` which gives the abundances quoted by Thévenin (1989; see the file header for bibliographic references).

Valid abundance files have two columns. The first one indicates the atomic number, and the second the abundance in the logarithmic scale already mentioned.

3.3.6 Model atmosphere files

These files specify the various physical quantities characterizing the model atmospheres, either those employed as initial guess models or those resulting from the inversion. They are identified with the extension `.mod`. Several standard model atmospheres can be found in the `~/sir/model` directory.

Valid model atmosphere files have a first line with three numbers written in free format. These numbers indicate the macroturbulent velocity (in km s^{-1}), the filling factor (ranging from 0 to 1), and the stray light contamination (in percent), respectively.

After the first row, n_τ lines follow. There are eleven columns providing the logarithm of the **line-of-sight** continuum optical depth at 5000 Å, the temperature (in K), the electron pressure (in dyn cm^{-2}), the microturbulent velocity (in cm s^{-1}), the magnetic field strength (in G), the line-of-sight velocity (in cm s^{-1}), the inclination and azimuth of the magnetic field vector (in deg), the geometrical height (in cm), the gas density (in g cm^{-1}), and the gas pressure (in dyn cm^{-2}), respectively. The inclination γ of the magnetic field vector is measured with respect to the line of sight, and ranges from 0 to 180 degrees (these values corresponding to longitudinal fields pointing to and away from the observer, respectively). The azimuth ψ is reckoned from the direction where Q is maximum and $U = 0$ (which is defined by the polarimeter), and increases counterclockwise as seen by the observer. The azimuth varies between 0 and 360 degrees. Negative inclinations should be avoided.

The model atmospheres must run from larger to smaller optical depths, otherwise an error message will be issued. If two components are used, the optical depths of the two models must coincide. In this case, it is also necessary that the sum of the two filling factors provided in the first line of the files be equal to unity. If not, SIR will adopt the filling factor of the first component (f_1) to calculate the corresponding filling factor of the second component as

$f_2 = 1 - f_1$.

In synthesis mode, the optical depths that specify the model atmosphere do not need to be equally spaced. This feature can be used, for example, to deal with abrupt changes of the physical quantities along the line of sight. Numerical integrations of Heaviside-like functions, as would be the elements of the absorption matrix if very step gradients of the physical quantities exist, are often innacurate. One way to overcome this problem is to improve the sampling of the atmosphere around the optical depth where the jump of the physical quantity takes place. This results in more accurate integrations, but requires non-equally spaced grids.

In inversion mode, the optical depths must be equally spaced, since the nodes are evenly distributed through the whole atmosphere. When constructing a given model atmosphere, it is important to make sure that the number of depth points, `ntau`, permits the selection of a wide set of nodes. This is possible if `ntau` $-$ 1 has a large number of divisors. Adequate values of `ntau` are, for example, 13, 25, 37 and 49.

For an accurate integration of the radiative transfer equation, spacings of the order of 0.1 in the logarithm of the optical depth are recommended. Spacings larger than 0.5 may lead to inaccurate integrations. Spacings smaller than, say, 0.05 does not imply greater precision (except for Heaviside-like stratifications) but increase the computation time. Typically, the depth grid should extend from 1.0 to -4.0 for photospheric lines and from 1.0 to -6.0 for chromospheric lines.

3.4 Output files

SIR generates files containing the retrieved model atmospheres, the synthetic Stokes spectra emerging from these atmospheres and the errors of the various parameters determined.

The Stokes profiles emerging from the retrieved model atmosphere are stored in a file whose name is identical to that of the model file except that the extension is changed from `.mod` to `.per`. For example, the file `guess_2.per` contains the Stokes spectra emerging from the model `guess_2.mod`.

The errors (uncertainties) in the retrieved parameters are written to files having the same structure as model files. Instead of physical quantities, however, error files contain the uncertainties of the retrieved parameters. Note that the errors are computed only at the location of the nodes and then interpolated to the whole atmosphere. The name of the error file is identical to that of the file containing the model to which it refers, except that the extension is changed from `.mod` to `.err`.

In addition, a log file is generated. This log file, whose name is identical to that of the control file except that the extension is changed from `.trol` to `.log`, keeps all the information printed on the computer screen at execution time.

If SIR is working on a synthesis mode (number of cycles equal to zero) it writes a `[profile].per` file, taking the filename from the `Observed profiles` input name in the `.trol` file.

If the number of cycles is set to -1, SIR will evaluate the Response Function for those

Table 3.2: Example of a generic control file for the inversion of a large number of individual profiles

```
Number of cycles      (*) : 3            ! (0=synthesis)
Observed profiles     (*) : profile.per
Stray light file          : stray.per    ! (none=no stray light contam)
Initial guess model 1 (*) : guess.mod
Initial guess model 2     :
```

paremeters having a non zero nuber of nodes. In order to save memory inside the code, only up to 2 simultaneously RF can be evaluated for a model, i.e., if we want to evaluate, for instance, the response function for temperature, magnetic field and velocity, we should first set the number of nodes of temperature and magnetic field to a non zero number and set to zero the nodes of the other variables. Later we will set to zero the temperature and magnetic field and to a non-zero value the velociy and run again the code. The output filenames (for an input model `[model].mod`) will be `[model].rt` for temperature, `[model].rpe` for electronic presure, `[model].rmic` for microturbulence, `[model].rh` for magnetic field strength, `[model].rvz` for line of sight velocity, `[model].rinc` for inclination, `[model].raz` for azimuth, and `[model].rmac` for macroturbulence. In order to read these files an IDL procedure (see 4.1.1) can be used.

3.5 Inverting a large number of profiles automatically

When a large number of individual profiles are to be inverted, the user has to modify the control file to change the name of the file containing the observed spectra and, possibly, other inversion options. This can be done manually, but for large datasets a script is desirable.

The idea is to copy all the individual profiles to a generic file whose name actually appears in the control file. The inversion code will write the resulting model atmospheres in generic files which must be renamed after the inversion of one set of spectra in order to avoid losing them.

Imagine, for instance, that you wish to invert ten different Stokes spectra stored in files named `profile_i.per`, where `i` varies between 1 and 10. Each inversion consists of three iterative cycles, in which the number of nodes is kept constant. The relevant part of the control file to be used is displayed in Table 3.2. Note that the observed spectra are stored in the generic file called `profile.per`. The initial guess model is named `guess.mod`. The models resulting from the three inversion cycles will be called `guess_1.mod`, `guess_2.mod` and `guess_3.mod`.

The following Unix script can be used to invert automatically all the Stokes spectra:

```
#!  /bin/csh
if (!(-e sir.log)) then
     touch sir.log
endif
```

```
set per='.per'
set one='_1.mod'
set two='_2.mod'
set three='_3.mod'
set i=1

while ($i <= 10)
     cp profile$i$per profile.per

     echo ' ' >> sir.log
     echo '****************** Start ***************' >> sir.log
     time cat sir.trol >> sir.log
     echo sir.trol | ~/sir/program/sir.x
     echo ' ' >> sir.log
     echo 'Total time:'  >> sir.log
     time >> sir.log
     echo '****************** End ******************' >> sir.log

     cp guess_1.mod guess$i$one
     cp guess_2.mod guess$i$two
     cp guess_3.mod guess$i$three

 i += 1
end
```

In this particular example, the models resulting from the inversion of `profile_3.per` would be called `guess3_1.mod`, `guess3_2.mod` and `guess3_3.mod`, and so on.

Chapter 4

Additional programs

4.1 IDL programs

The following programs are in the ∼/sir/idl directory.

4.1.1 Reading & Writing SIR format

`read_model.pro` and `write_model.pro` read and write model files [model].mod

`read_profile.pro` and `write_profile.pro` read and write profile files [profile].per

`read_RF.pro` reads Response Function files [model].rt for temperature, [model].rpe for electronic presure, [model].rmic for microturbulence, [model].rh for magnetic field strength, [model].rvz for line of sight velocity, [model].rinc for inclination, [model].raz for azimuth, and [model].rmac for macroturbulence, all of then for the 4 Stokes parameters evaluated in models containing a non null magnetic field.

`read_RF_nomag.pro` reads Response Function files [model].rft, [model].rpe, [model].rmic, and [model].rmac, only for the Stokes I evaluated in models without magnetic field.

4.1.2 Sensitivity region.

We define 'the sensitivity region of a model to perturbations of a physical quantity' as the optical depth range at which the perturbation of a physical quantity produces a change of a Stokes parameter larger than the noise.

`sensitivity.pro` allows to evaluate the sensitivity region of a model to perturbations of a physical quantity. It uses the observed and synthetic profiles (because it uses the miss-fit as an estimation of the noise) together with the Response function evaluated for the corresponding physical quantity.

4.1.3 Graphics2

This IDL program was written to visualize the Stokes profiles and model atmospheres resulting from SIR. It is invoked within IDL by typing `graphics2`. `graphics2` uses a file called `scales` which sets the axes of the different plots. The scaling is automatic, but can be optimized manually. The `scales` file should be in the `~/sir/idl` directory.

You are advised to add `~/sir/idl` to the IDL path to avoid having to give the full path of the `graphics2` program every time it is used.

4.1.4 FTSIDL

The FTSIDL routine allows the extraction of individual spectral lines from the FTS atlas provided by the KIS IDL library. This atlas gives the intensity spectrum of the quiet sun at disk center as measured with the Fourier Transform Spectrometer at the McMacth-Pierce telescope on Kitt Peak. FTSIDL produces files containing the profiles and the corresponding wavelength grids ready to be used by SIR.

FTSIDL extracts the spectral lines specified in a user-provided atomic parameter file called `LINESFTS`. This file must *not* contain a header. FTSIDL is invoked by typing

IDL> `ftsidl,arg_1,arg_2`

where `arg_1` and `arg_2` specify the number of lines which will be extracted. `arg_1` gives the position in the `LINESFTS` file of the first spectral line to be extracted. The argument `arg_2` indicates the position occupied in the the `LINESFTS` file by the last spectral line to be extracted.

Each file produced by FTSIDL contains a single spectral line whose index in `LINESFTS` serves to construct its name. For example, line 4 in `LINESFTS` will be written in the file `idl4.per`.

4.2 Fortran 77 programs

The following programs are in the `~/sir/model` directory. They should be compiled using the scripts and libraries found in the `~/sir/program` directory.

4.2.1 `modelador3.x`

This program modifies a specified model atmosphere file in several ways:

1. It allows the user to change the spacing of the spatial depth grid, as well as the stratification of the different physical parameters according to the formula

$$x_{\rm new} = a + b\, x_{\rm old} + c\, \log \tau_5,$$

where $x_{\rm new}$ and $x_{\rm old}$ are the new and old physical parameters, respectively. The user must provide the constants a, b, and c. In this way, the stratification of a given parameter can be modified by adding a constant (a), by multiplying the old stratification by a factor b, and/or by introducing a gradient dependent on $\log \tau_5$.

2. Reevaluates and overwrites the geometrical heights scale (nineth column) from the optical depts scale, temperature and electronic pressure taking or not into account de hydrostatic equilibrium. The $z = 0$ km level is set at the point where $\tau_5 = 1$.

3. Reevaluates and overwrites the optical depth scale from the geometrical heights, temperature and electronic pressure.

4. Puts a given atmosphere in hydrostatic equilibrium. Note that the initial models used by SIR are ussually (default option) in hydrostatic equilibrium, so it is convenient to run this program option before invoking SIR.

5. Evaluates thermodinamical quantities from the input model. It generates an output file [model].th containing n_τ rows and 12 columns:

   column 1: $log\tau$: the logarithm of the line-of-sight continuum optical depth at 5000 Å. It is equal to the first column of [model].mod file.
   column 2: μ: mean molecular weight (dimensionless).
   column 3: n_e: electron density [cm^{-3}]
   column 4: n_H: Hydrogen density [cm^{-3}]
   column 5: n_{H+}: Proton density [cm^{-3}]
   column 6: Ionization degree (dimensionless).
   column 7: $\alpha = \left(\frac{d\ln\rho}{d\ln P}\right)_T$
   column 8: $\delta = -\left(\frac{d\ln\rho}{d\ln T}\right)_P$
   column 9: c_v: Specific heat at constant volume.
   column 10: c_p: Specific heat at constant pressure.
   column 11: c_s: Adiabatic sound speed [cm s^{-1}].
   column 12: $\nabla_{\rm ad} = \left(\frac{d\ln T}{d\ln P}\right)_S$: Adiabatic Nabla.

- modelador3.x uses the subrutines of SIR, and the sources can be found in ∼`/sir/program`
- It should be compiled using the Makefile:

  `make modelador3.x` by default it compiles and links modelador3.x using `ifort` compiler.

  `make fc=gfortran modelador3.x` compiles and links modelador3.x using `gfortran` compiler.

- To run modelador3.x: `echo model.mtrol | modelador3.x`
- An example of the file `model.mtrol` can be found in the subdirectory ∼`/sir/model`. A test example, including all the required files is in the subdirectory ∼`/sir/test`

Table 4.1: Example of a control file `[filename].mtrol`

Input Model?	(*) :	model_in.mod	!filenm input mod SIR format
Ouput Model?	(*) :	model_out.mod	!filenm output mod SIR format
New grid (tau1,taun,—step—)	:	1.2,-5,0.1	!none=default no modify
Degree of pol. used to interpol.	:		!none=default= 2
change from, to (ini &final indx)	:		!default 1,ntotal points of new grid
temp. (a+b*t+c*logtau) a,b,c?	:	200,1,0	!give a,b,c (default 0,1,0 = no modify)
elec.pres. (a+b*t+c*logtau) a,b,c?	:		!give a,b,c (default 0,1,0 = no modify)
microturb. (a+b*t+c*logtau) a,b,c?	:		!give a,b,c (default 0,1,0 = no modify)
magn. fld. (a+b*t+c*logtau) a,b,c?	:		!give a,b,c (default 0,1,0 = no modify)
LOS vel. (a+b*t+c*logtau) a,b,c?	:		!give a,b,c (default 0,1,0 = no modify)
gamma (a+b*t+c*logtau) a,b,c?	:		!give a,b,c (default 0,1,0 = no modify)
phi (a+b*t+c*logtau) a,b,c?	:		!give a,b,c (default 0,1,0 = no modify)
height z (a+b*t+c*logtau) a,b,c?	:		!give a,b,c (default 0,1,0 = no modify)
gas pres.(a+b*t+c*logtau) a,b,c?	:		!give a,b,c (default 0,1,0 = no modify)
density (a+b*t+c*logtau) a,b,c?	:		!give a,b,c (default 0,1,0 = no modify)
Hydrostatic Equilibrium (yes=1)	:	1	!none=default=0 no modify
Magnetic Pressure term? (yes=1)	:	1	!none=default=0 no included
tau,Pe $\rightarrow$ z,Pg(1) or z,Pg$\rightarrow$tau,Pe(2)	:		!default=1 from tau,Pe$\rightarrow$z,Pg(only in case non HE)
Abundance file?	:	ASPLUND	!ASPLUND, THEVENIN or ABUNDANCES
Cosine of theta (mu)	:		!none=default=1.
gas pressure @ surface (boundary)	:		!none=default=value of the input model, if < 0 it contains -ρ at surface

Bibliography

[1] Allende Prieto, C., Ruiz Cobo, B., & García López, R. 1998, ApJ, 502, 951

[2] Anders, E., & Grevesse, N. 1989, Geochimica et Cosmochimica Acta 53, 197

[3] Bellot Rubio, L.R., Ruiz Cobo, B., & Collados, M. 1998, ApJ 506

[4] Bellot Rubio, L.R., Ruiz Cobo, B., & Collados, M. 1999, A&A 341, 31

[5] Collados, M., Martínez Pillet, V., Ruiz Cobo, B., del Toro Iniesta, J.C., & Vázquez, M. 1994, A&A 291, 622

[6] Press, W.H., Flannery, B.P., Teukolsky, S.A., & Vetterling, W.T. 1986, Numerical Recipes (Cambridge: Cambridge University Press)

[7] Rees, D.E. 1987, in: Numerical Radiative Transfer, ed. W. Kalkofen, (Cambridge: Cambridge University Press), 213

[8] Rees, D.E., Murphy, G. A., & Durrant, C. J. 1989, ApJ 339, 1093

[9] Rodríguez Hidalgo, I., Ruiz Cobo, B., del Toro Iniesta, J.C., Collados, M., & Sánchez Almeida, J. 1995, in: JOSO Annual Report 1995, ed. M. Saniga, Astronomical Institute, Tatranská Lomnica (Slovakia).

[10] Ruiz Cobo, B., & del Toro Iniesta, J.C. 1992, ApJ 398, 375

[11] Ruiz Cobo, B., & del Toro Iniesta J.C. 1994, A&A 283, 129

[12] Ruiz Cobo, B., Rodríguez Hidalgo, I., & Collados M. 1997, ApJ 488, 462

[13] Skumanich, A., & Lites, B.W. 1987, ApJ 332, 473

[14] Socas-Navarro, H., Ruiz Cobo, B., & Trujillo Bueno, J. 1998, ApJ, 507, 470

[1989] Thévenin F., 1989, A&AS 77, 137

[15] del Toro Iniesta, J.C., Tarbell, T.D., & Ruiz Cobo, B. 1994, ApJ 436, 400

[16] del Toro Iniesta, J.C., & Ruiz Cobo, B. 2016, Living Rev. Sol. Phys. 13, 4

[17] Westendorp Plaza, C., del Toro Iniesta, J.C., Ruiz Cobo, B., Martínez Pillet, V., Lites, B.W., & Skumanich, A. 1998, ApJ 494, 453

[18] Westendorp Plaza, C., del Toro Iniesta, J.C., Ruiz Cobo, B., Martínez Pillet, V., Lites, B.W., & Skumanich, A. 1997, in: Advances in the physics of sunspots, eds. B. Schmieder, J.C. del Toro Iniesta & M. Vázquez (Proc. First ASPE, ASP Conf. Ser. 118), Astronomical Society of the Pacific, 202

[19] Wittmann, A. 1974, Solar Phys. 35, 11