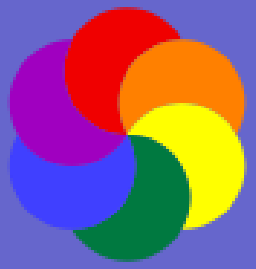
Introduction in iSpec



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What is iSpec?

- **iSpec: Integrated Spectroscopic Framework** for spectral analysis
- Author: Sergi Blanco-Cuaresma

- Determination of astrophysical parameters such as effective temperature, surface gravity, metallicity and individual abundances based on synthetic spectra fitting or equivalent widths measurements

- Works in conjunction with several radiative transfer codes:
  - **SPECTRUM** (R. O. Gray)
  - **Turbospectrum** (B. Plez)
  - **SME** (Valenti & Piskunov)
  - **MOOG** (C. Sneden)
  - **SYNTHE/WIDTH9** (R. Kurucz/Atmos port)

Instalation procedures

- iSpec can be downloaded from http://www.blancocuaresma.com/s/
- distributed under the terms of the GNU Affero General Public License (open source license), except the radiative transfer codes
- to install iSpec, use:
  - the virtual machine with all iSpec dependencies already included (i.e. python packages and compilers), ready-to-use for any platform (MacOS, Windows, Linux and Solaris), before this must install VirtualBox package (free software),
  - the source code in GNU/Linux and OSX.

follow the instructions from the on-line manual depending on the kind of installation you want to do!!!

Basics in using visual interface

- The visual interface is launched by double clicking "iSpec.command" or executing in a terminal located in iSpec's directory:

```
./iSpec.command
```

- Opening spectra, saving images and spectra, etc.

  Operations are executed only on the active spectrum!

- Spectra file formats:

1. FITS files ---> 1-D FITS file with *CDELT*/*CRVAL* values in the header and fluxes or FITS files containing a table where columns are wavelength, fluxes and optionally errors
2. Text files with *tab* as column delimiter and 3 columns (wavelength, flux and error):

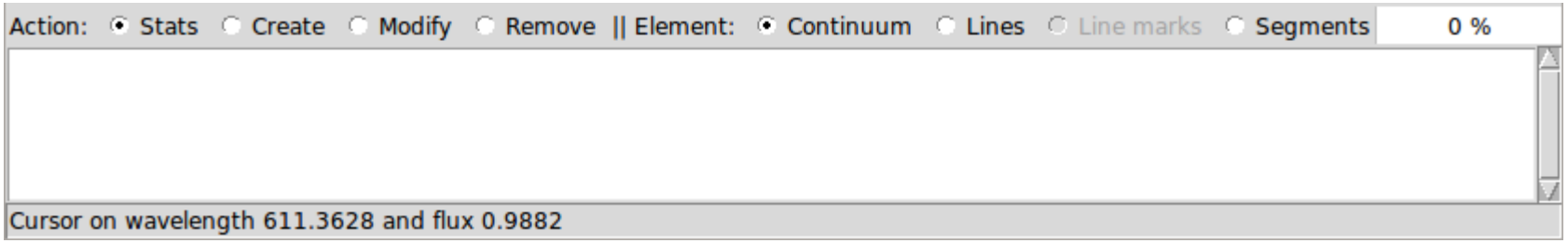
```
waveobs         flux            err
370.000000000 1.26095742505 1.53596736433
370.001897436 1.22468868618 1.55692475754
370.003794872 1.18323884263 1.47304952231
370.005692308 1.16766911881 1.49393329036
```

- Exploring spectra

Regions used in iSpec

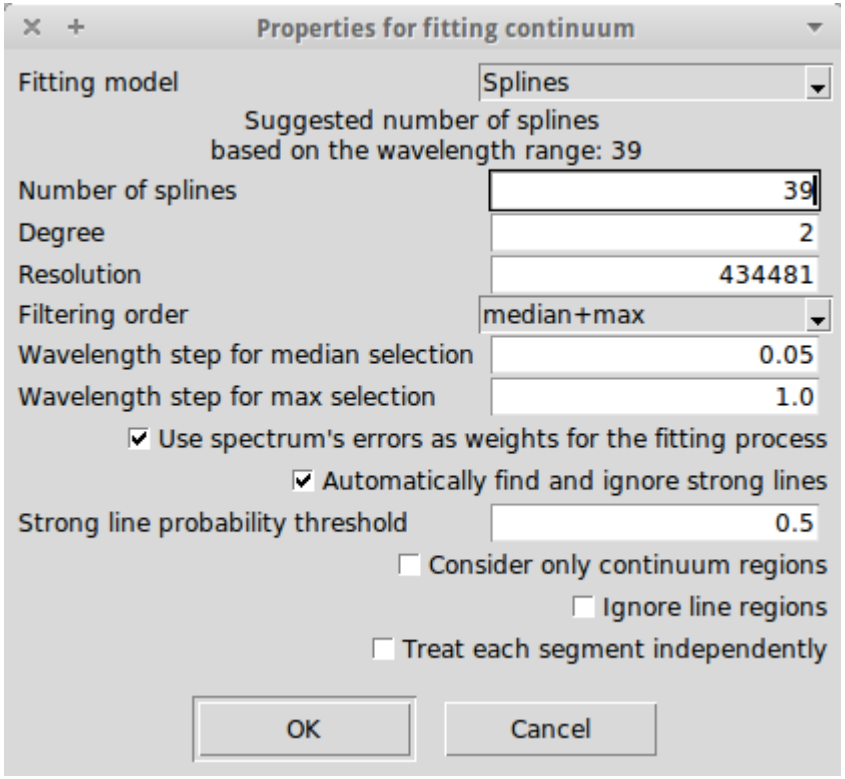
- **Continuum**: used for fitting the (pseudo-)continuum (instead of using the whole spectrum).
- **Line masks**: used for gaussian fitting (e.g. equivalent width measurements) and/or atmospheric parameters/abundance determination.
- **Segments**: used mainly for atmospheric parameters/abundance determination. The synthetic spectrum is going to be computed only for the spectral ranges inside segments, thus they should include all the line masks. It saves computation time, avoiding to compute the whole synthetic spectra.

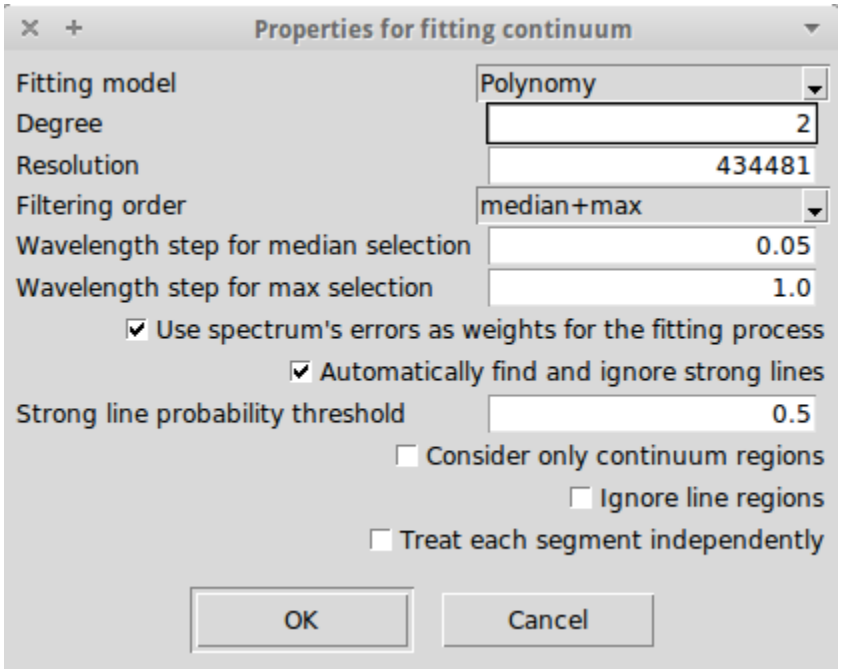
- For creating, modifying or removing regions, an action and an element should be selected:



Continuum fitting

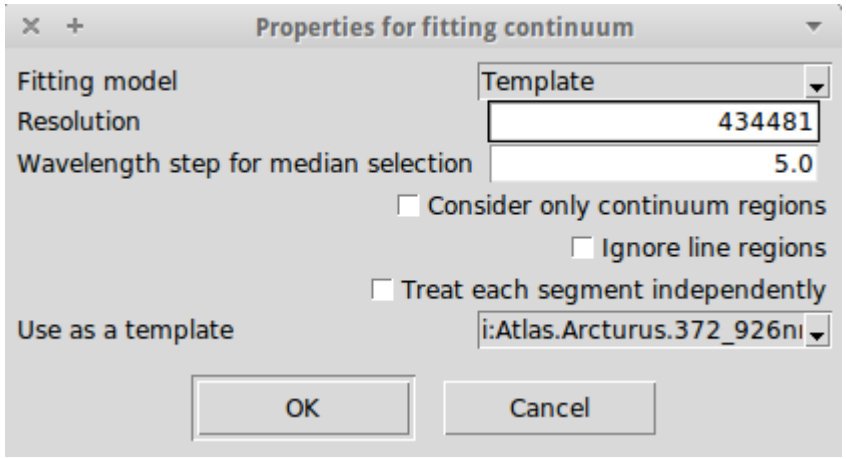
- Splines and polynomy

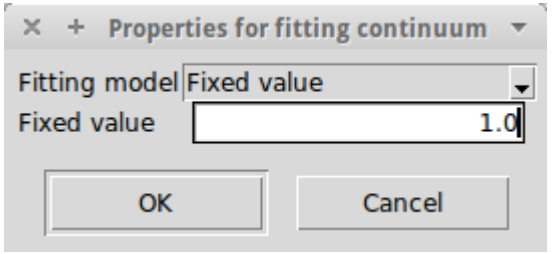




Continuum fitting

- Template or fixed value

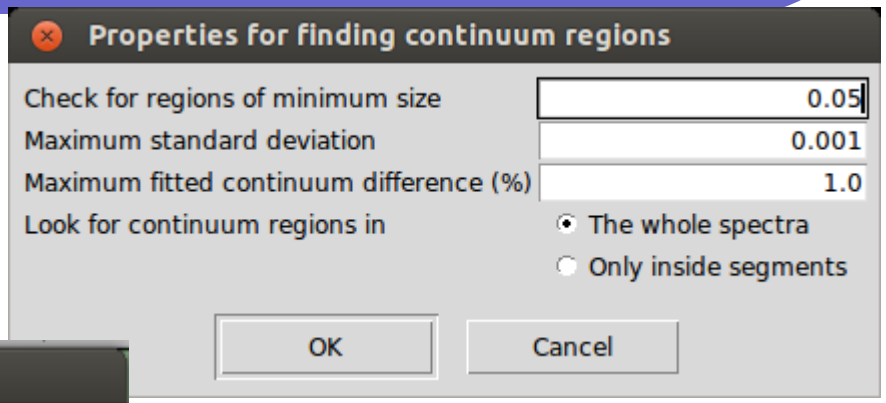


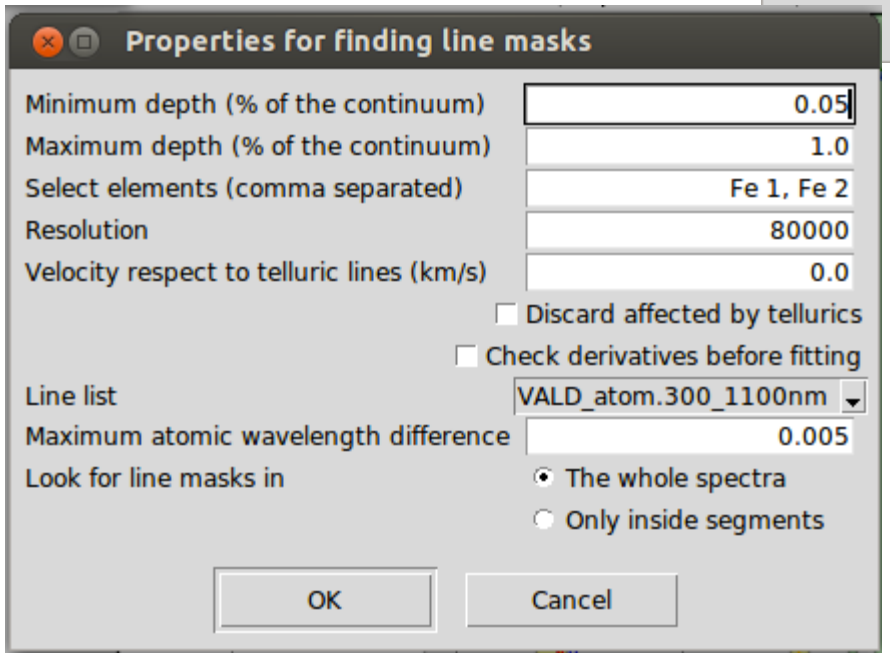


- After fitting don't forget to normalize the continuum!

Automatic finding of the regions

Automatic continuum regions

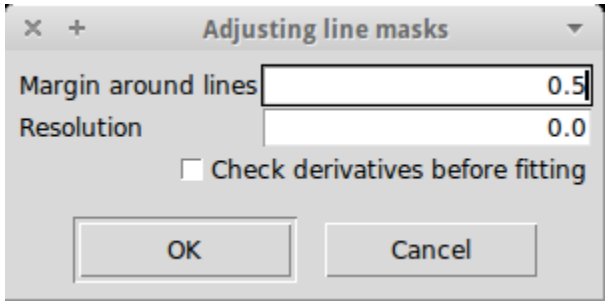




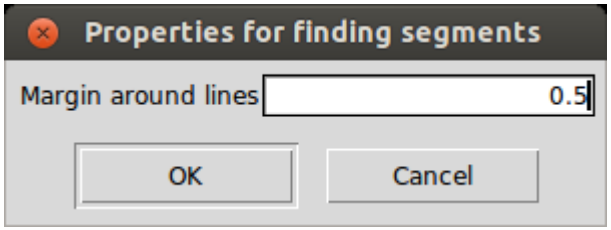
Automatic line masks

Automatic finding of the regions

Adjust line masks

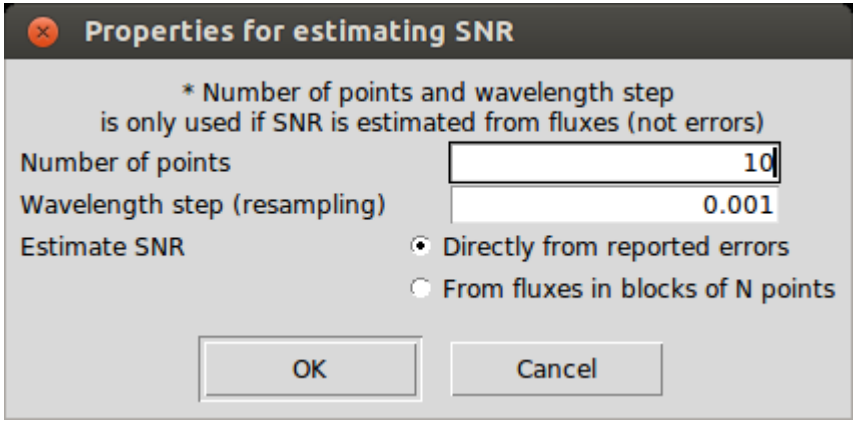


Create segments around line masks



Signal-to-Noise Ratio

- Signal-to-Noise ratio (S/N) can be estimated from:
  - errors: S/N is calculated by using the flux divided by the reported errors in the spectrum. This is the best way to calculate the S/N if the errors are present.
  - fluxes: the whole spectrum is checked, resampling and taking *N* by *N* measurements, calculating the S/N for each one and finally selecting the mean S/N as the global S/N. This estimation is influenced also by the stellar type.

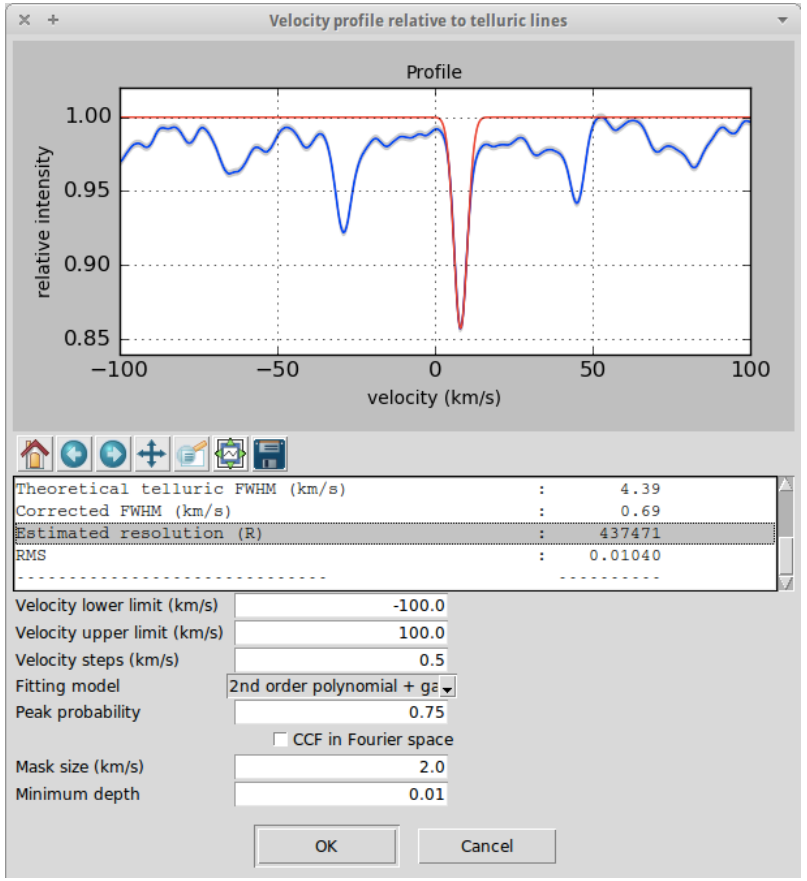


- Errors estimation based on S/N
- Add noise to spectrum fluxes

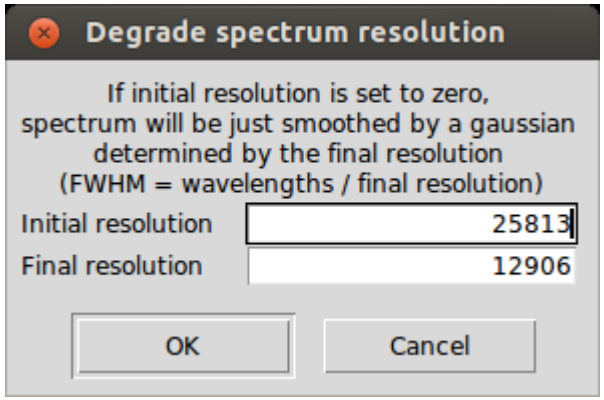
Spectral resolution

- Resolution can be estimated based on the FWHM of the telluric lines:

$$R = \frac{c}{(FWHM_{telluric} - FWHM_{theoretical})}$$

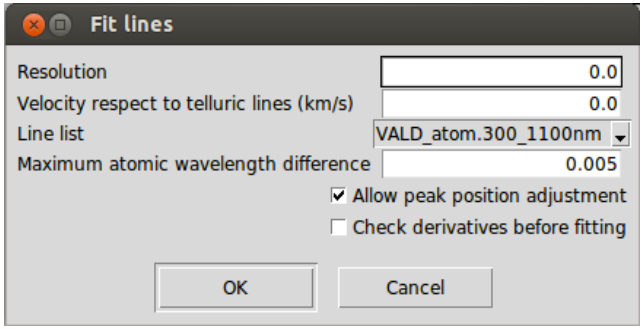


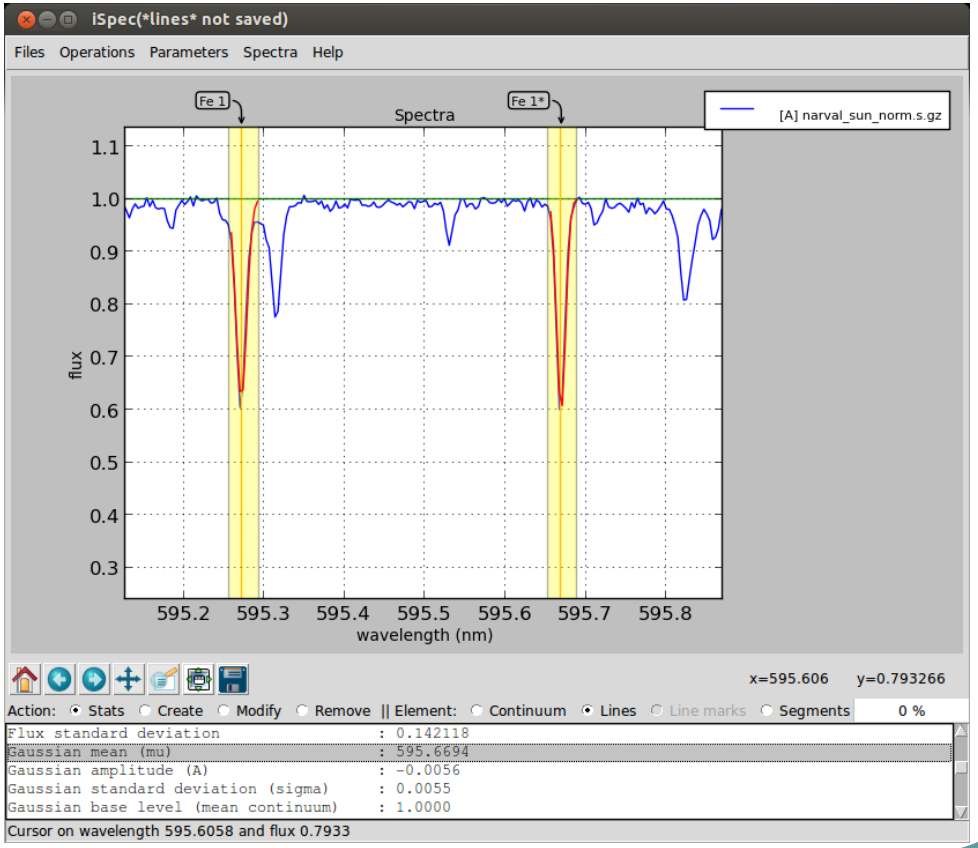
- Resolution degradation:



Absorption lines fitting

- For each defined line masks, a Gaussian can be fitted. It requires that the spectrum is corrected by its radial velocity and fitted continuum. The velocity respect to the telluric lines should also have been previously calculated.





Other useful operations

- Wavelength range reduction

- Apply mathematical expression

the wavelength, fluxes and error values of the active spectrum can be modified by applying many mathematical expressions

- Fluxes and errors cleaning

useful to remove cosmics although it should be used carefully since it would remove also emission lines

- Clean telluric regions

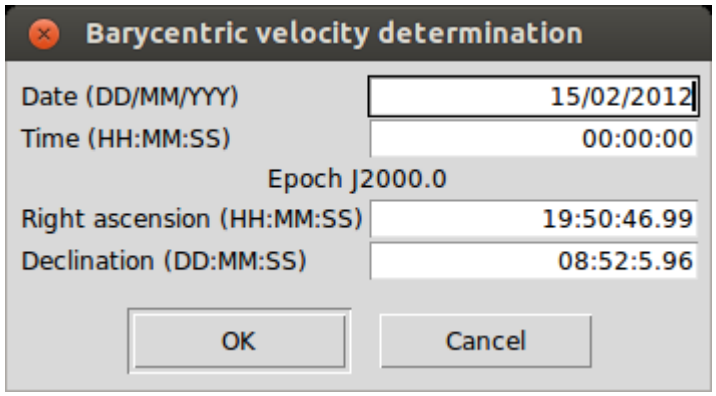
useful when the spectrum is going to be used as a template for measuring the radial velocity of another spectrum

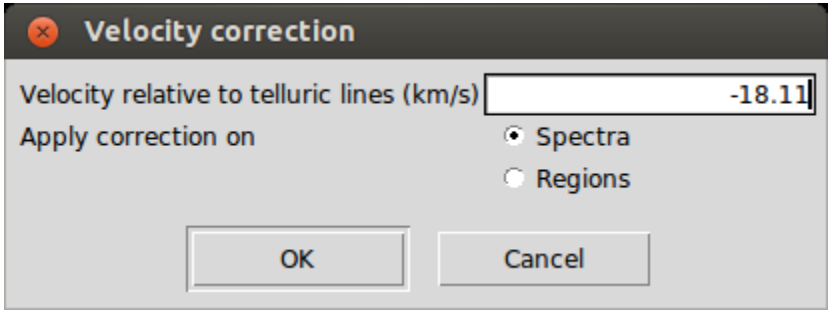
- Spectrum resampling

- Spectra combination

Barycentric and radial velocity determination

- The observed spectra can be corrected and transformed to the solar barycentric reference frame





Barycentric and radial velocity determination

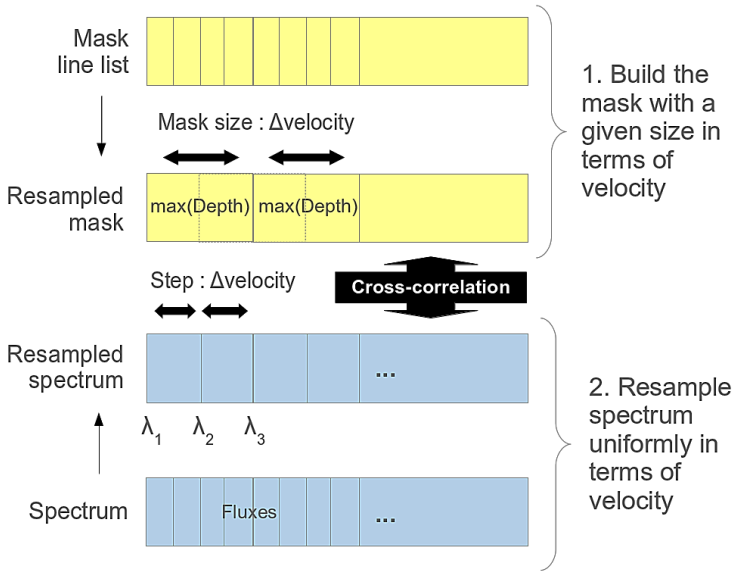
- The velocity profile can be determined relative to three different references:
  - **Atomic data**: useful for determining the radial velocity of a star, when the barycentric velocity due to the earth orbit has been already corrected
  - **Telluric lines**: for identifying the position of the telluric lines (thus these regions can be ignored) or for evaluating if a given spectrum has already been corrected by the barycentric velocity (if not, the output velocity will be zero)
  - **Template**: Any loaded spectrum or an internal synthetic one can be used for determining the relative radial velocity

- The cross-corelation algorithm is used to compute the RV:

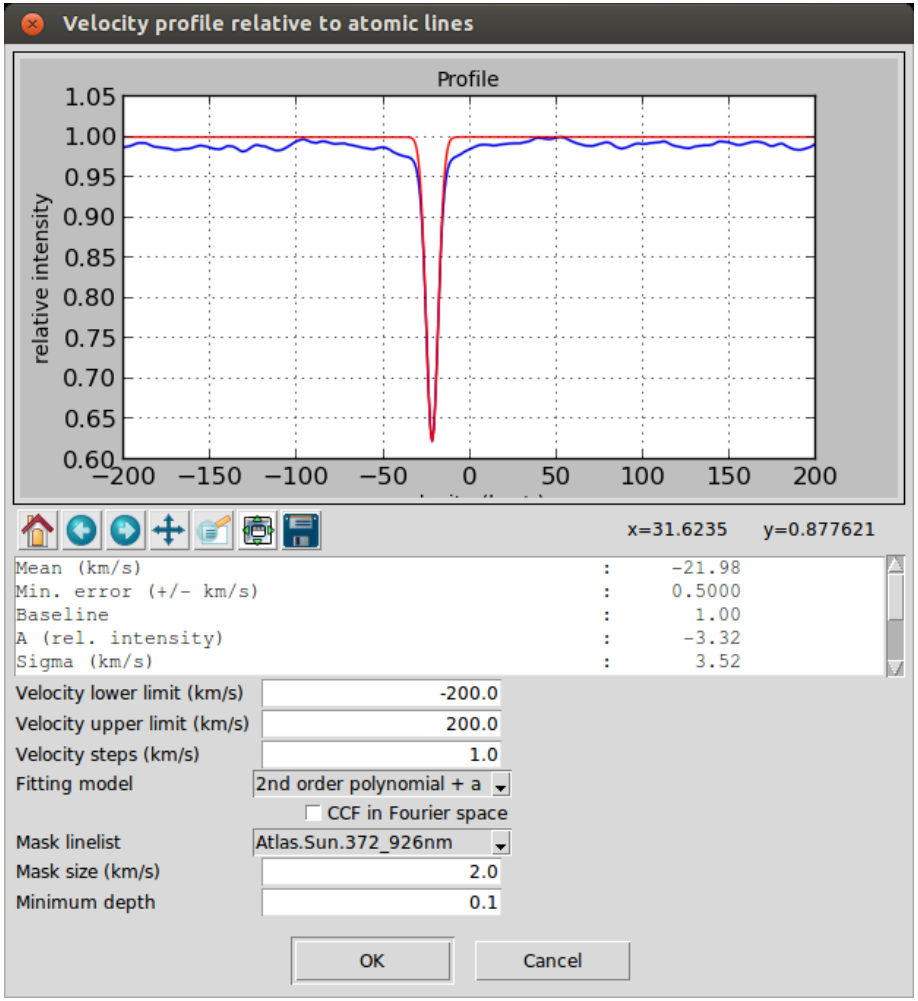
$$C(v) = \sum_{lines} \sum_{pix} p(pix, v) \cdot flux(pix)$$

p – template function (depends on the spectral type of the star)

$flux$ – spectrum fluxes



Barycentric and radial velocity determination

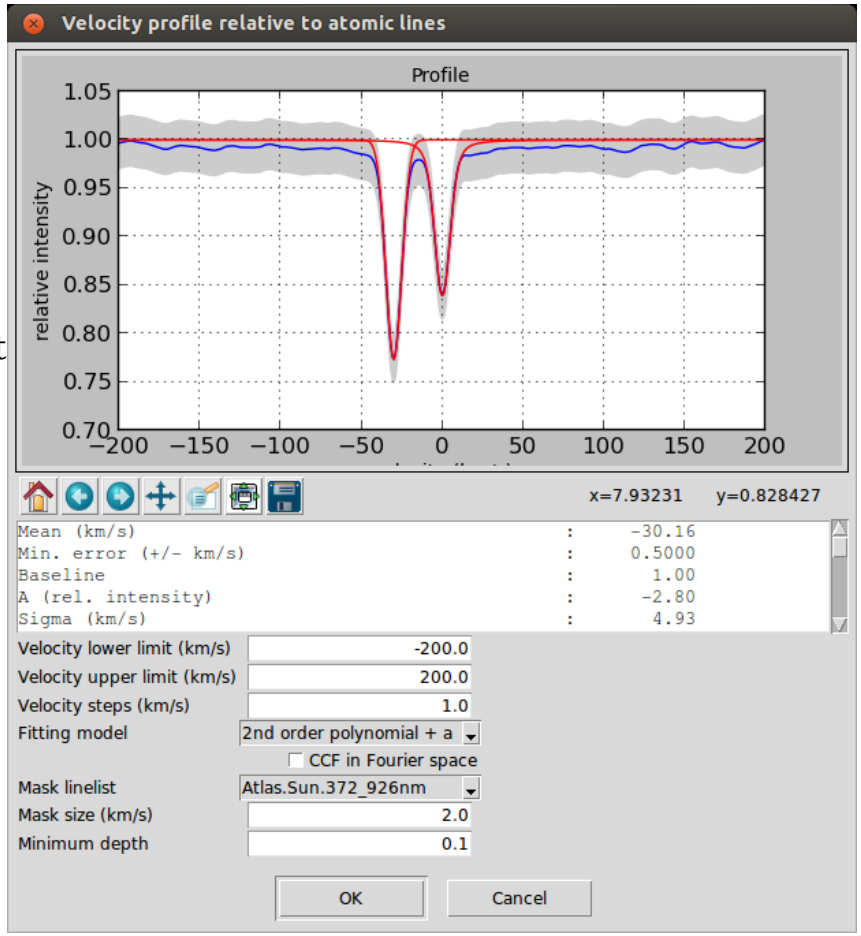


Identification of spectroscopic binaries

- The velocity determination function relative to atomic data can be used to identify spectroscopic binaries:

- iSpec automatically detect outlier peaks in the velocity profile in order to detect spectroscopic binaries and fit more than one Gaussian/Voigt

- Two examples for:
  HD 5516
  HD 85503



Synthetic spectra computation

What do we need to compute synthetic spectrum?

- Radiative transfer code:
  - SPECTRUM
  - Turbospectrum
  - SME
  - MOOG
  - SYNTHE/WIDTH9

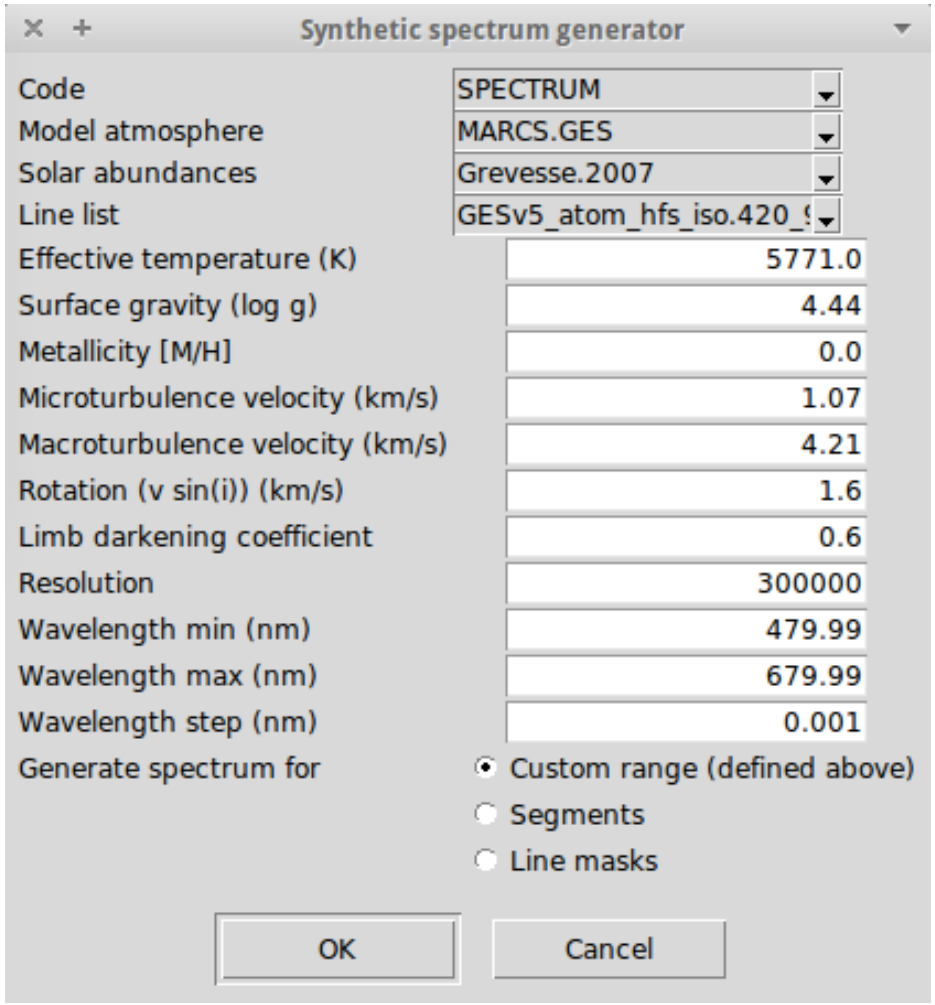
- Atomic line list with laboratory parameters:
  - **VALD**: two line lists extracted from the VALD database with a wavelength range:
    - from 300 to 1100 nm
    - from 1100 to 24000 nm
  - **GES** line list: they are used in the Gaia-ESO Survey. It covers the wavelength range from 420 to 920 nm:
    - With hyperfine structure (HFS) and isotopes (recommended)
    - Without HFS and isotopes

- Solar abundances taken from different authors and publications

Synthetic spectra computation

- Grids of model atmospheres:
  - **MARCS** GES/APOGEE models (plane-parallel + spherical)
    - Effective temperatures (Teff): [2500, 2600, 2700, 2800, 2900, 3000, 3100, 3200, 3300, 3400, 3500, 3600, 3700, 3800, 3900, 4000, 4250, 4500, 4750, 5000, 5250, 5500, 5750, 6000, 6250, 6500, 6750, 7000, 7250, 7500, 7750, 8000] K
    - Gravities (Logg): [0.0, 0.5, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0, 4.5, 5.0] dex
    - Metallicities ([M/H]): [-5.00 , -4.00 , -3.00 , -2.50, -2.00 , -1.50, -1.00 , -0.70, -0.50, -0.20, 0.00 , 0.20, 0.50, 0.70, 1.00] dex
    - Standard abundance composition, with α–enhancement elements;
  - **ATLAS9** Kurucz/Castelli/APOGEE/Kirby models (plane-parallel)
    - Effective temperatures (Teff): [3500, 3750, 4000, 4250, 4500, 4750, 5000, 5250, 5500, 5750, 6000, 6250, 6500, 6750, 7000, 7250, 7500, 7750, 8000, 8250, 8500, 8750] K
    - Gravities (Logg):[0.0, 0.5, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0, 4.5, 5.0] dex
    - Metallicities ([M/H]): [-5.00, -4.50, -4.00, -3.50, -3.00, -2.50, -2.00, -1.50, -1.00, -0.50, -0.30, -0.20, -0.10, 0.00, 0.10, 0.20, 0.30, 0.50, 1.00] dex
    - Standard abundances (no enhanced).

Synthetic spectra computation



iSpec uses linear interpolation with the previous models to compute theoretical spectra with any atmospheric parameters that fall inside the grids

Atmospheric parameters determination

1. Based on **synthetic spectral fitting technique** (minimization between observed spectrum and theoretical spectra computed on the fly)

- Required initial steps:
  - Initial atmospheric parameters
  - List of parameters that should be free (recommended: effective temperature, surface gravity, metallicity, microturbulence and resolution)
  - Line masks with the spectral regions that are going to be used in the computation, good line selection is required for a good determination of parameters, iSpec includes a line selection based on VALD and GES atomic line lists
  - Segments that cover one or more line masks (instead of the full spectrum, which would be slower)

Atmospheric parameters determination

2. Based on **equivalent width technique** (by using EWs from observed Fe absorption lines to derive Fe abundances)

- The assumption of LTE must be fulfilled:
  - Ionization balance ---> <Fe I> = <Fe II>
  - Excitation equilibrium ---> No trends on [Fe/H] vs. line excitation potential
  - Abundances not correlated with equivalent widths ---> No trends on [Fe/H] vs. EWs

- Required initial steps:
  - Load spectrum and the line masks (corresponding to Fe lines)
  - Fit the continuum
  - Fit the lines:
    - a Gaussian/Voigt profile will be fitted to determine the EW, central wavelength, etc.
    - a cross-match with the selected atomic data will be executed to assign atomic data for each line (it will be used to derive atmospheric parameters)

Chemical abundances analysis

1. Based on **synthetic spectral fitting technique** (minimization between observed spectrum and theoretical spectra computed on the fly)

- Required initial steps:
  - Determine the atmospheric parameters
  - Fix all the parameters except the "individual abundance" and select the element to be derived
  - Line masks corresponding a lines of the element we want to derive
  - Segments that cover one or more line masks (instead of the full spectrum, which would be slower)

Chemical abundances analysis

2. Based on **equivalent width technique** (by using EWs from observed absorption lines to derive element abundances)

- Required initial steps:
  - Load a spectrum and the line masks to be used in the analysis
  - Fit the continuum
  - Fit the lines:
    - a Gaussian/Voigt profile will be fitted to determine the EW, central wavelength, etc.
    - a cross-match with the selected atomic data will be executed to assign atomic data for each line
  - Specify the atmospheric parameters of the star

Python scripting in iSpec

- From visual interface the user can interact with the spectra and use different useful functionalities (good for learning and testing)
- But there are options and functionalities that can only be accessed via Python (recommended for complex scientific studies)
- Look into the file **„example.py”**