A hands-on lesson on classical spectroscopic methods

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Stellar spectroscopy and Astrophysical parametrisation from Gaia to Large Spectroscopic surveys, 21-23 September 2021

Outline

- How to create a synthetic spectrum
- How to derive atmospheric parameters with spectral synthesis (T_{eff}, $\log g$, [M/H], vmic, vmac, vsini)
- How to derive chemical abundances with spectral synthesis
- How to derive atmospheric parameters from the EW of iron (T_{eff}, $\log g$, [Fe/H], vmic)
- Examples

What's on the market?

Synthesis (with EW analysis)	Equivalent Width	Machine Learning
iSpec (Blanco-Cuaresma+ 2014)	FAMA (Magrini+ 2013)	The Cannon (Ness+ 2015)
fasma (Tsantaki+ 2018)	ARES+MOOG (Sousa+ 2008)	The Payne (Ting+ 2019)
SME (Piskunov+ 2017)	GALA (Mucciarelli+ 2013)	NN for RAVE (Guiglion+ 2020)
BACCHUS (Masseron+ 2016)	StePar (Tabernero+ 2019)	ML for APOGEE (Garcia-Dias+ 2018)
...	...	...

There are also hybrid methods: e.g. SP_Ace (Boeche+ 2016), MATISSE (Recio-Blanco+ 2006)

Differences on:

- analysis methods
- model atmosphere physics
- time consumption
- atomic line data
- a few publicly available (and fewer user friendly)
- many, many more ...

Choose your package depending on the specific problem (e.g. spectral type, rotation, resolution)

1. How to create a synthetic spectrum

1. How to get the flux at the top of the photosphere

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- Model atmosphere
  - MARCS (LTE, plane parallel/spherical geometry): cool stars
  - Kurucz (LTE, plane parallel): extended grid
  - TLUSTY (non-LTE, plane parallel): hot stars
- Line data: wavelengths, excitation potentials, oscillator strengths, broadening parameters
  - Vienna Atomic Line Database (VALD)
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- Radiative solver
  - MOOG
  - Turbospectrum
- Convolution with rotation kernels (vmac, vsini) & instrumental resolution

Let's create a Sun!

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```
MARCS
Teff= 5777   log g= 4.44
NTAU        72
 5.37932065E-04    3784.6 1.511E+01 2.446E+09 2.514E-04 7.508E-02 1.000E+05
 7.04358347E-04    3806.3 1.977E+01 3.157E+09 2.912E-04 7.989E-02 1.000E+05
 8.97001104E-04    3827.9 2.516E+01 3.968E+09 3.352E-04 8.275E-02 1.000E+05
 1.12114053E-03    3851.2 3.142E+01 4.901E+09 3.842E-04 8.394E-02 1.000E+05
 1.38277017E-03    3875.6 3.870E+01 5.981E+09 4.386E-04 8.400E-02 1.000E+05
 1.68900324E-03    3900.3 4.721E+01 7.234E+09 4.997E-04 8.346E-02 1.000E+05
 2.04821557E-03    3925.3 5.719E+01 8.692E+09 5.679E-04 8.253E-02 1.000E+05
 2.47003418E-03    3949.9 6.890E+01 1.038E+10 6.458E-04 8.133E-02 1.000E+05
 2.96503163E-03    3974.2 8.262E+01 1.236E+10 7.349E-04 8.009E-02 1.000E+05
 3.54549590E-03    3998.0 9.867E+01 1.465E+10 8.366E-04 7.892E-02 1.000E+05
 4.22616872E-03    4021.5 1.175E+02 1.730E+10 9.519E-04 7.791E-02 1.000E+05
 5.02375022E-03    4044.4 1.396E+02 2.040E+10 1.084E-03 7.737E-02 1.000E+05
 5.95691999E-03    4067.1 1.654E+02 2.398E+10 1.237E-03 7.732E-02 1.000E+05
 7.04850982E-03    4089.7 1.956E+02 2.813E+10 1.410E-03 7.757E-02 1.000E+05
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 1.60229445E-02    4208.0 4.433E+02 6.148E+10 2.713E-03 8.042E-02 1.000E+05
 1.88238605E-02    4233.4 5.205E+02 7.172E+10 3.098E-03 8.141E-02 1.000E+05
 2.20936211E-02    4259.5 6.108E+02 8.362E+10 3.541E-03 8.256E-02 1.000E+05
 2.59125342E-02    4286.4 7.161E+02 9.748E+10 4.041E-03 8.357E-02 1.000E+05
 3.03761432E-02    4313.9 8.391E+02 1.136E+11 4.612E-03 8.454E-02 1.000E+05
 3.55924653E-02    4342.2 9.830E+02 1.323E+11 5.264E-03 8.543E-02 1.000E+05
 4.16892557E-02    4370.9 1.151E+03 1.540E+11 6.005E-03 8.627E-02 1.000E+05
 4.88128382E-02    4399.9 1.347E+03 1.794E+11 6.856E-03 8.738E-02 1.000E+05
 5.71301126E-02    4429.1 1.577E+03 2.087E+11 7.832E-03 8.883E-02 1.000E+05
 6.68354590E-02    4458.4 1.844E+03 2.429E+11 8.953E-03 9.065E-02 1.000E+05
 7.81644639E-02    4487.8 2.156E+03 2.824E+11 1.022E-02 9.268E-02 1.000E+05
 9.13940125E-02    4517.2 2.521E+03 3.284E+11 1.168E-02 9.520E-02 1.000E+05
 1.06839751E-01    4546.4 2.946E+03 3.818E+11 1.334E-02 9.809E-02 1.000E+05
 1.24881981E-01    4575.8 3.443E+03 4.437E+11 1.522E-02 1.014E-01 1.000E+05
 1.45962545E-01    4604.8 4.025E+03 5.156E+11 1.738E-02 1.056E-01 1.000E+05
```

Let's create a Sun!

Caution: Spectral synthesis is model dependent!

- Stellar atmospheric parameters (5777, 4.44, 0.0, 1.0)
- Model atmosphere
    - MARCS (LTE, plane parallel/spherical geometry): cool stars

+ optical depth at standard wavelengths
+ temperature in K
+ number density of free electrons
+ number density of all other particles

= Calculate the radiative transfer equation → Flux

```
MARCS
Teff= 5777   log g= 4.44
NTAU        72
 5.37932065E-04   3784.6 1.511E+01 2.446E+09 2.514E-04 7.508E-02 1.000E+05
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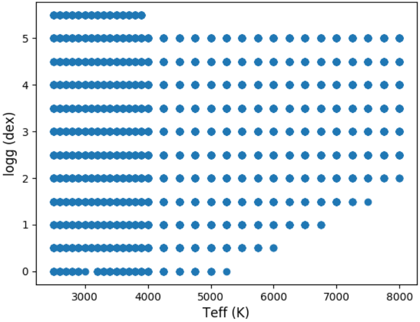

Interpolation within the grids in needed
(e.g. scipy.interpolate.griddata)

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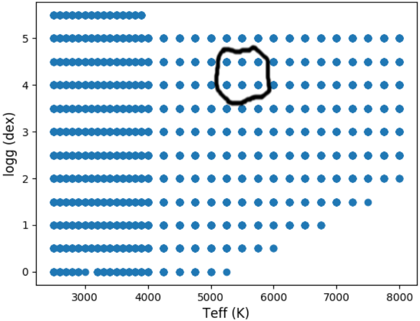

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# Wavelength	ele	EP	loggf	vdwaals	Do
5339.188	20.1	8.44	-0.075	-7.196	nan
5339.416	26.0	4.43	-2.146	-7.51	nan
5339.526	27.0	4.23	-0.377	-7.51	nan
5339.937	26.0	3.27	-0.609	-7.221	nan
5340.189	26.0	4.29	-2.229	-7.52	nan
5340.447	24.0	3.44	-0.724	-7.262	nan
5340.666	22.0	0.82	-3.174	-7.65	nan
5341.033	26.0	1.61	-1.717	-7.68	nan
5341.053	25.0	2.11	-5.671	-7.74	nan
5341.070	21.0	1.94	3.341	0	nan
5341.327	27.0	4.15	-0.424	-7.51	nan
5341.489	22.0	3.06	-0.760	-7.58	nan
5341.524	58.1	0.67	-5.088	0	nan
5342.701	27.0	4.02	0.578	-7.51	nan
5342.958	21.0	0.00	-2.439	-6.11	nan
5342.969	19.0	1.61	-1.795	0	nan
5343.380	27.0	4.03	0.024	-7.51	nan
5343.438	26.0	4.37	-0.806	-7.51	nan

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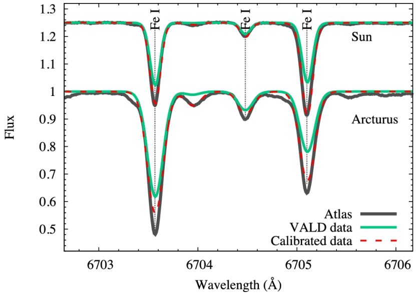

Tsantaki+ 2018

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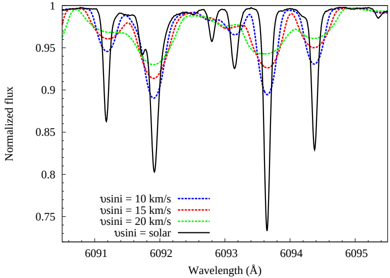

Caution on rotation

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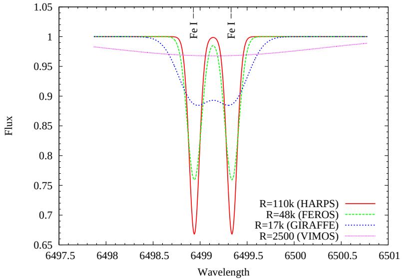

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  astropy: pyasl.rotBroad, pyasl.instrBroadGaussFast

Let's create a Sun!

Putting everything together

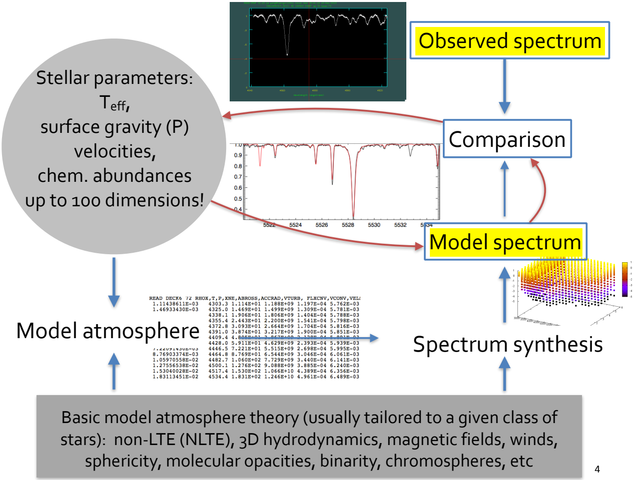
python-based spectral synthesis package:
`github.com/MariaTsantaki/FASMA-synthesis`
yalm configuration file

*config1.yml

```yaml
star1:
    linelist: FASMA-synthesis/FASMA/rawLinelist/linelist.lst
    teff: 5777
    logg: 4.44
    feh: 0.00
    vt: 1.0
    vmac: 3.21
    vsini: 1.90
    model: marcs
    save: False
    plot: True
    plot_res: False
    intervals_file: FASMA-synthesis/FASMA/rawLinelist/intervals.lst
    snr: null
    resolution: 115000
```

Questions?

2. How to derive stellar parameters



Credit to M. Bergemann

2. How to derive stellar parameters

Pre-process the observed spectrum

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- input format (fits, dat)

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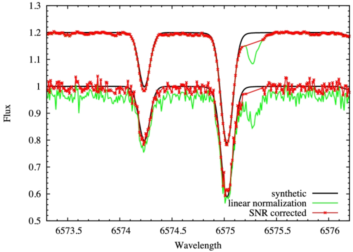

Minimization process

Pre-process the observed spectrum

- input format (fits, dat)
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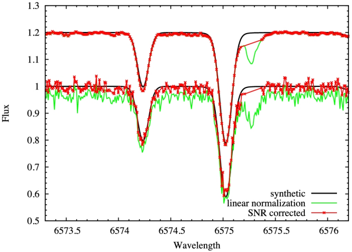
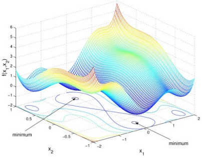
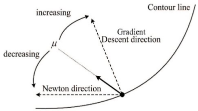


Minimization process

- χ^2 minimization (`mpfit`, Levenberg-Marquardt)





Credit B. Asadi

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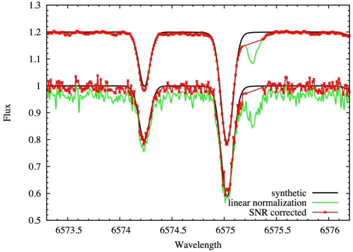
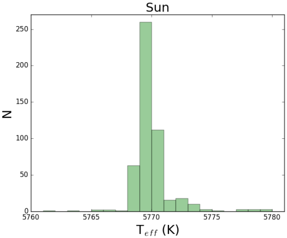


Minimization process

- χ^2 minimization (`mpfit`, Levenberg-Marquardt)
- initial conditions



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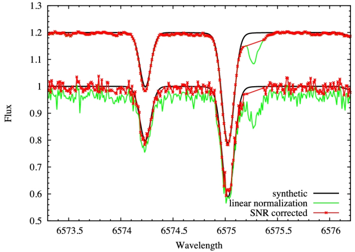

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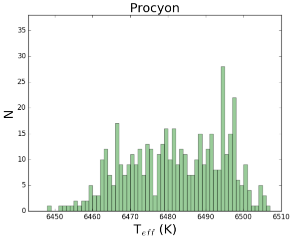

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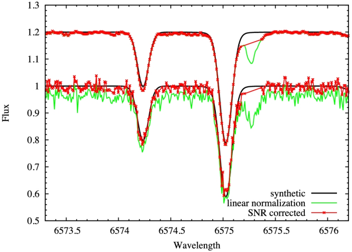

Minimization process

- χ^2 minimization (`mpfit`, Levenberg-Marquardt)
- initial conditions
- refine minimization options

- clean for bad/missing lines
- vmic: T_{eff}, $\log g$, [Fe/H] (Tsantaki+ 2013, Mortier+ 2013)
- vmac: T_{eff} (Valenti+ 2005)

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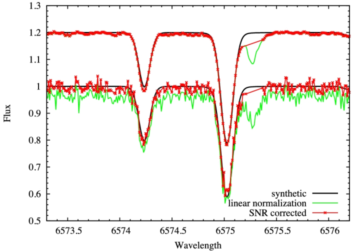

Minimization process

- χ^2 minimization (`mpfit`, Levenberg-Marquardt)
- initial conditions
- refine minimization options
- fixed parameters

- log g: seismic, trigonometric
- vmic: T_{eff}, log g, [Fe/H] (Tsantaki+ 2013, Mortier+ 2013)
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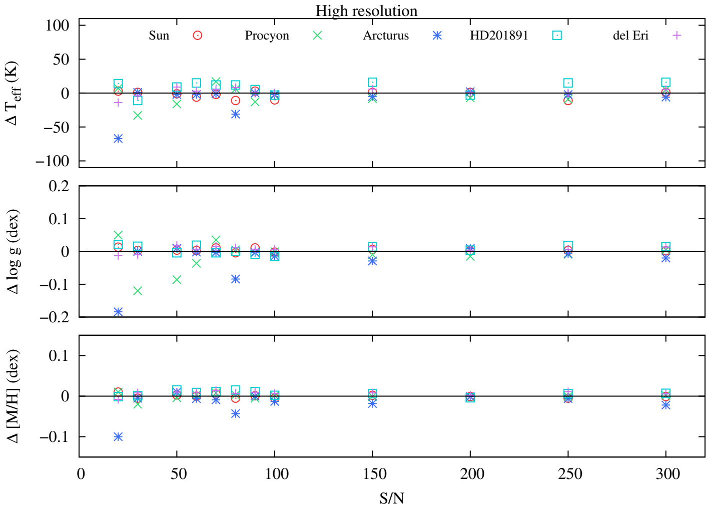
2. How to derive stellar parameters

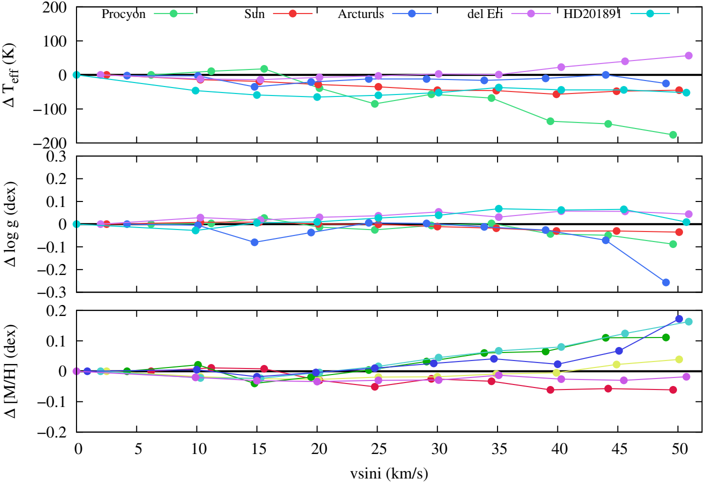
Error analysis



(Tsantaki+ 2014)

2. How to derive stellar parameters

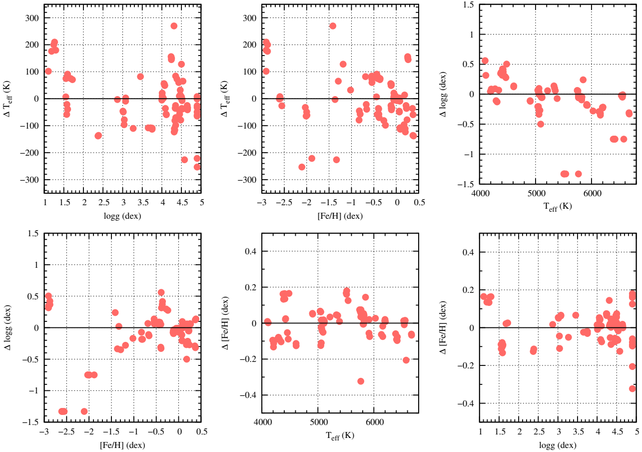
Error analysis



(Tsantaki+ 2014)

2. How to derive stellar parameters

Error analysis



Correlations in parameters with the benchmark values (Tsantaki+ 2014)

2. How to derive stellar parameters

Putting everything together!

*config2.yml

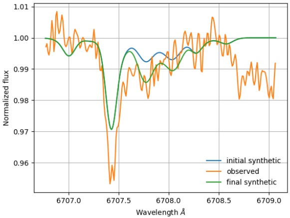
```yaml
star1:
    linelist: FASMA-synthesis/FASMA/rawLinelist/linelist.lst
    teff: 5777
    logg: 4.44
    feh: 0.0
    vt: 1.0
    vmac: 3.21
    vsini: 1.90
    model: marcs
    save: False
    element: False
    fix_teff: False
    fix_logg: False
    fix_feh: False
    fix_vt: True
    fix_vmac: True
    fix_vsini: False
    plot: True
    plot_res: False
    damping: 1
    minimize: True
    refine: refine
    observations: FASMA-synthesis/FASMA/spectra/Sun_HARPS.fits
    intervals_file: FASMA-synthesis/FASMA/rawLinelist/intervals.lst
    snr: null
    resolution: 115000
```

Questions?

3. How to derive chemical abundances

- Overall metallicity ([M/H]) is derived from all the elements in a region
- Individual chemical abundances ([El/H]) are derived for a specific element

- Create a synthetic spectrum of a known star (T_{eff}, $\log g$, [M/H], vmic, vmac, vsini) of the specific species
- $[El/H]$ is the only free parameter
- χ^2 minimization → best-fit value
- Select from: Li, Na, Mg, Al, Si, Ca, Sc, Ti, V, Cr, Mn, and Ni



e.g. Lithium

3. How to derive chemical abundances

Putting all together!

```
star1:
    linelist: FASMA-synthesis/FASMA/rawLinelist/linelist_elements.lst
    teff: 5777
    logg: 4.44
    feh: 0.0
    vt: 1.0
    vmac: 3.21
    vsini: 1.90
    model: marcs
    save: False
    element: Li
    plot: True
    plot_res: False
    damping: 1
    minimize: True
    observations: FASMA-synthesis/FASMA/spectra/Sun_HARPS.fits
    intervals_file: FASMA-synthesis/FASMA/rawLinelist/intervals_elements.lst
    snr: null
    resolution: 115000
```

Questions?

5. The Equivalent Width method

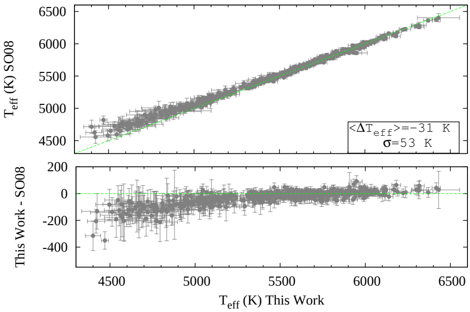
Ingredients:

- Line list of neutral (FeI) and ionized species (FeII)
- EW measurements (IRAF, daospec, ARES)
- Calculate [Fe/H] from the curve of growth
- Model atmospheres (MARCS, Kurucz)
- *excitation* balance of FeI lines → T_{eff}
  ionization balance of FeI and FeII lines → $\log g$

5. The Equivalent Width method

Ingredients:

- Line list of Fe isolated lines

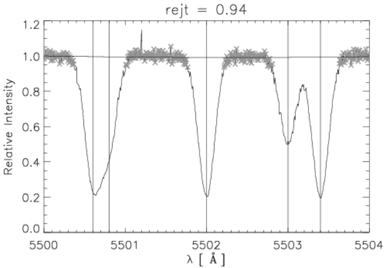


- EW measurements (IRAF, daospec, ARES)
- Calculate [Fe/H] from the curve of growth
- Model atmospheres (MARCS, Kurucz)
- *excitation* balance of FeI lines → T_{eff}
  ionization balance of FeI and FeII lines → $\log g$

5. The Equivalent Width method

Ingredients:

- Line list of Fe isolated lines
- EW measurements with ARES



- Calculate [Fe/H] from the curve of growth
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- *excitation* balance of FeI lines → T_{eff}
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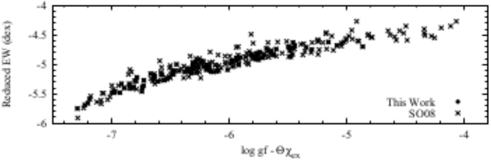
5. The Equivalent Width method

Ingredients:

- Line list of Fe isolated lines
- EW measurements with ARES
- Calculate [Fe/H] from the curve of growth: MOOG+MARCS



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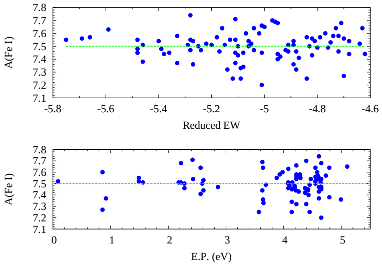


Fe I = Fe II

- Microturbulence:
A(FeI) vs reduced EW (=$\log EW/\lambda$)

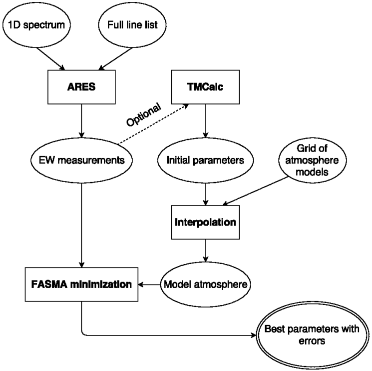
- $T_{\rm eff}$: Excitation Balance
All abundances from Fe should agree for all excitation potentials

- $\log g$: Ionization Balance
Average $\log A$ obtained from differing ionization stages must agree

5. The Equivalent Width method

Ingredients:

- EW measurements with ARES
- Calculate [Fe/H] from the curve of growth: MOOG+MARCS
- *excitation* balance of FeI lines → T_{eff}
  ionization balance of FeI and FeII lines → $\log g$



(Andreasen+ 2017)

5. The Equivalent Width method

Ingredients:

- EW measurements with ARES
- Calculate [Fe/H] from the curve of growth: MOOG+MARCS
- *excitation* balance of FeI lines → T_{eff}
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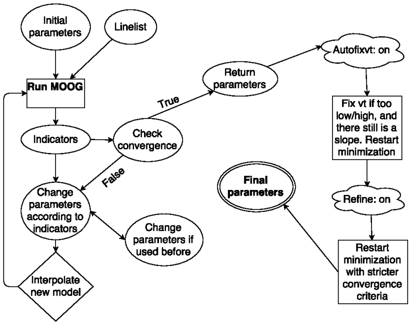
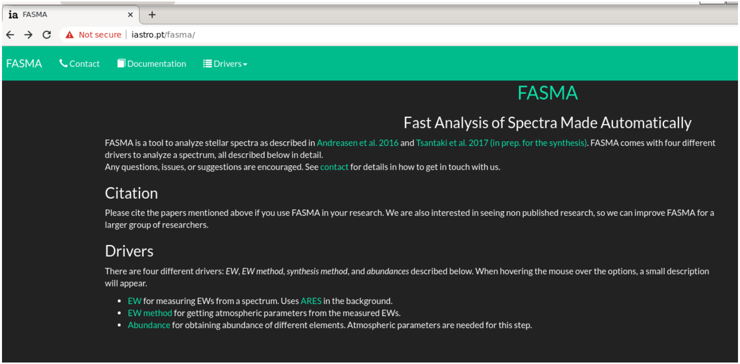


(Andreasen+ 2017)

5. The Equivalent Width method



`www.iastro.pt/fasma`

References

- Books
  - The Observation and Analysis of Stellar Photospheres, Gray D., Cambridge University Press, 2015
- Free packages for parameters
  - SME (Valenti+ 1996)
  - GALA (Mucciarelli+ 2013)
  - FAMA (Magrini+ 2013)
  - q2 (Ramirez+ 2014)
  - iSpec (Blanco-Cuaresma+ 2014)
  - fasma (Tsantaki+ 2018)
  - StePar (Tabernero+ 2019)
- Radiative transfer codes
  - MOOG (Sneden+ 1973)
  - SYNTHE (Kurucz+ 1981)
  - SPECTRUM (Gray+ 1992)
  - Turbospectrum (Plez+ 2012)
- Model atmospheres
  - Kurucz (Kurucz+ 1999)
  - PHOENIX (Hauschildt+ 1997)
  - MARCS (Gustafsson+ 2008)
- Atomic data / Line lists
  - NIST (Kramida+ 2020)
  - VALD (Ryabchikova+ 2015)
  - Kurucz (Kurucz 1995)
  - Surveys: Gaia-ESO, APOGEE
  - Specific for K-type (Tsantaki+ 2013)
  - Specific for M-type (Marfil+ 2021)
- Free packages for EWs
  - ARES (Sousa+ 2007)
  - DAOSPEC (Stenson+ 2008)
  - VoigtFit (Krogager+ 2018)

Finally remarks

Things conviniently neglected:

- Non-LTE
- 3D hydrodynamics
- magnetic fields
- winds
- sphericity
- molecules

Don't use the codes as black boxes. Be patient... astronomers are not programers.

8. Exercise

Your turn!