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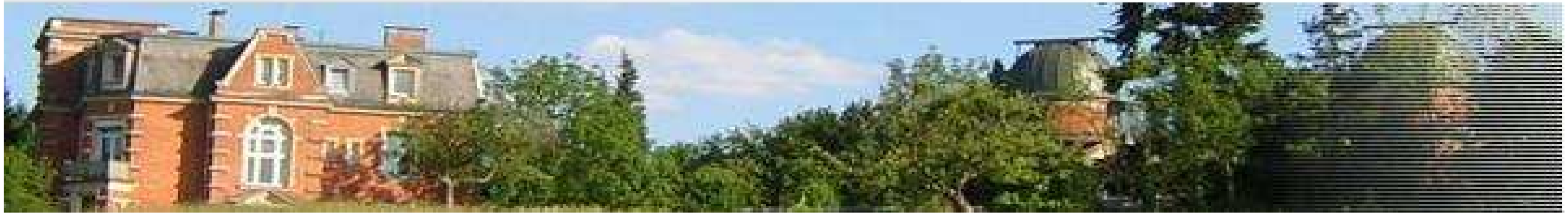


DETAIL/SURFACE

Exercises

N. Przybilla

Non-LTE line-formation calculations with DETAIL & SURFACE

I) Directory Structure (in **group**)

DETSURF

atmospheres	atmospheric structures in DETAIL format
atomic_data	atomic input data for Exercise 2
exercises	exercise material (pdf)
input	DETAIL/SURFACE control files
runs	working directory

II) Exercise 1: Invoking DETAIL & SURFACE

Task: run DETAIL & SURFACE

enter **runs**

sample control files are

DETAIL_input_bss_vega
SURFACE_input_bss_vega

log O/H+12=8.53

data required by DETAIL to solve SE and RT for

- O I model atom similar to one by Baschek, Scholz & Sedlmayr, A&A, 55, 375 (1977) **BSS**
- model atmosphere for Vega adopted from Kurucz' homepage

and by SURFACE to calculate emergent flux using

- NLTE level populations
- refined line-broadening

```
detail < control_file > output
```

- requires possibly auxiliary files,
  e.g. photoionization cross-sections
- **output**: detailed information, required for
  e.g. model atom verification or physical interpretation
  → previous discussion
- NLTE level populations: **fort.7**

```
surface < control_file > output
```

- requires possibly auxiliary files, e.g. broadening tables
- **output**: detailed information, as above

  → previous discussion
- physical flux: **fort.7**
- rectified flux: **fort.70**

Comments

- last call of ABUNDANCE sets values for calculation
- abundances are normalised to H+He !!!
- BABS: $b_i = n_i/n_i^{LTE}$ (Zwaan) else $b_i = \frac{n_i/n_i^{LTE}}{n_C/n_C^{LTE}}$ (Menzel)
- convergence criterion: $\Delta n/n \sim 10^{-4}$
- inner boundary condition: LTE ($b_i=1$) → $\tau_{Ross} \sim 100$-200 sufficient
- error handling by DETAIL/SURFACE - but: user mistakes possible
- user has to provide the correct **ODF file** via `ln -sf ~/DETSURF/ODF/xyz ODF`
- meaningful renaming of output files recommended

verify your output by comparing with **~/DETSURF/solutions**: **vega*bss***

III) Exercise 2: O I model atom

log O/H+12=8.53

Task:
construction of a simple model atom for O I,
similar to that of Carlsson & Judge, ApJ, 402, 344 (1993) **CJ**

- energy levels up to n=4 shall be considered, i.e. also excited singlet and triplet states, with more up-to-date transition data
- all required data to be found in **atomic_data** preformatted for use with DETAIL & SURFACE
- use **DETAIL_input_bss_vega** and **SURFACE_input_bss_vega** (in **runs**) and the DETAIL/SURFACE manual for guidance
- calculate NLTE populations with DETAIL (check convergence!) & emergent flux with SURFACE for the Vega model

verify your results by comparing with **~/DETSURF/solutions/vega*cj***, sample input files in **~/DETSURF/solutions/input**: **DETAIL_input_cj_vega**, **SURFACE_input_cj_vega**

IV) Exercise 3: NLTE line-formation with DETAIL & SURFACE

Task: a) NLTE calculations for 3 model atoms for O I
for Vega and a Vega-like supergiant
b) comparison with LTE
c) determination of NLTE abundance ‘corrections‘
d) NLTE & LTE profiles @ same W_λ
e) physical interpretation

- 3rd O I model atom to be used: **PBBKV**
  Przybilla, Butler, Becker, Kudritzki & Venn, A&A, 359, 1085 (2000)

  control files are in **input**: ***pbbkv***

  there, also additional control files for the SG can be found
  - copy these to **runs**

Grotrian diagrams

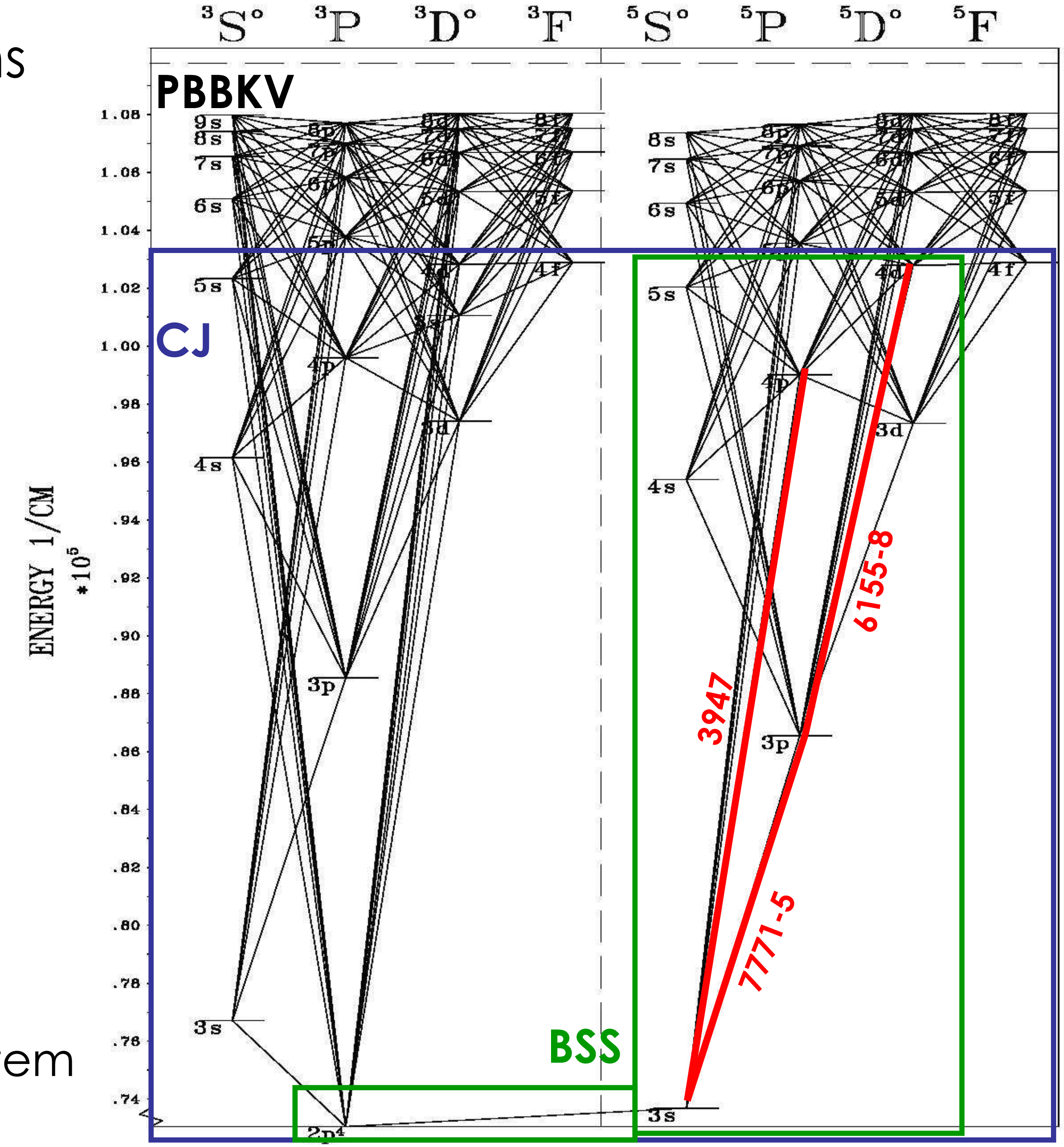
model atoms

PBBKV

CJ

BSS

increasing complexity



+ singlet spin system

3a) NLTE calculations for 3 O I model atoms

- run all control files to generate 6 emergent NLTE fluxes
  check for convergence – use 120 iterations for **CJ** & **PBBKV**

- compare NLTE line profiles

  O I $\lambda\lambda$3947
  O I $\lambda\lambda$6155-8
  O I $\lambda\lambda$7771-5

  from **BSS**, **CJ** & **PBBKV** model atoms for Vega & SG
  use `nlteplots_fl`

- your interpretation?

Intermezzo: Visualisation with the Fawlty Language

If you are familiar with IDL, you will feel at home. Note that FL is a project under development, so don‘t expect any functionality beyond the most basic. There is no manual for FL at present.

invoke the FL by: `fl` exit via: `exit`

- reading of SURFACE **fort.70** (**fort.7**) files:

  `read_surf_fl,‘filename‘,lambda,flux`

- plotting of flux vs. lambda:

  `plot,lambda,flux,xr=[7771,7776],yr=[0.1,1.05],xsty=1,ysty=1`

  useful keywords: `xtitle=‘ ‘,ytitle=‘ ‘,charsize=1.0,lin=1`

- overplotting:

  `oplot,lambda2,flux2`

- text output in plot:

  `xyouts,xcoordinate,ycoordinate,‘ ‘`

- standard display is screen window
- Postscript output generated by:

  `set_plot,'ps'` `set_plot,'x'` recovers screen display

- file names set by:

  `device,filename='   '` `device,/close` closes file

- recompiling routine:

  `.run routine_name`

- plotting of NLTE profiles in 3a) by:

  `nlteplots_fl` edit filenames in **runs/nlteplots_fl.pro**

- comparison of NLTE and LTE profiles in 3b) by:

  `lteplots_fl` edit filenames in **runs/lteplots_fl.pro**

  both generate 2 PS files

- reading atmospheric structure (in DETAIL format):

```
read_st_fl,‘filename‘,m,t,na,ne
```

m: mass scale
t: temperature
na: number density of heavy particles
ne: number density of electrons

- logarithmic plotting:

```
plot,alog10(m),t
```

- reading NLTE populations & departure coefficients (DETAIL **output** file)

```
read_pops_fl,‘filename‘,n,b,lab
```

n: NLTE level populations
b: departure coefficients
lab: labels of levels

- plotting departure coefficients in 3e) by:

```
departures_fl
```

edit filenames in **runs/departures_fl.pro**

generates PS file

3b) Comparison with LTE

- copy SURFACE control files **input/*LTE*** to **runs**
- run all control files to generate 6 emergent LTE fluxes for same abundance log O/H+12=8.53
- compare LTE with NLTE line profiles for

  O I $\lambda\lambda$3947
  O I $\lambda\lambda$6155-8
  O I $\lambda\lambda$7771-5

  from **PBBKV** model atom for Vega & SG
  use `lteplots_fl`

- your interpretation?

3c) Determination of NLTE abundance ‘corrections‘

- due to time constraints no practical work here

- procedure:
  - construct LTE curve-of-growth W_λ=f(O abundance)
  - find abundance at which W_λ^{NLTE} is reproduced
  - difference of NLTE and LTE abundance

    → **NLTE abundance ‘correction‘**

- schematically for 2 lines in Vega & SG

3d) NLTE & LTE profiles @ same W_λ

- calculate LTE emergent fluxes for

log O/H=8.56 & 9.11 (Vega)
log O/H=8.72 & 10.10 (SG)

→ reproduce W_λ^{NLTE}(log O/H=8.53)for O I λ6158 and O I λ7771

- compare LTE line profiles for O I λ6158 and O I λ7771 with NLTE line profiles for log O/H=8.53 (**PBBKV** model) in Vega and SG

- your interpretation?

3e) Physical interpretation: a first step

- plot departure coefficients b_i for strategic levels

  O I ground state
  O I 3s $^5S^o$, 3p ^5P, 4d $^5D^o$
  O II ground state

  as a function of log m for Vega & SG
  use `departures_fl`

- your interpretation?