Echelle spectra and the Ways Towards the VO Interoperability

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DAL2
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**FACULTY
OF INFORMATION
TECHNOLOGY
CTU IN PRAGUE**

Motivation

- 2000-2003 HEROS   pipeline by Stahl, Rivinius

- 2005 OES (low usage – hot stars not possible)

- 2006-2008 grant for proper merging of orders

  Result : total black magic

- Exoplanets in Ondrejov 2016 (Petr Kabath)

- OES - RV, Pucheros, PlatoSpec E152 La Silla

- PLATO ground support

- Interoperability of echelle spectra

DM Changes Request

3. Connect Points by Spectral Order
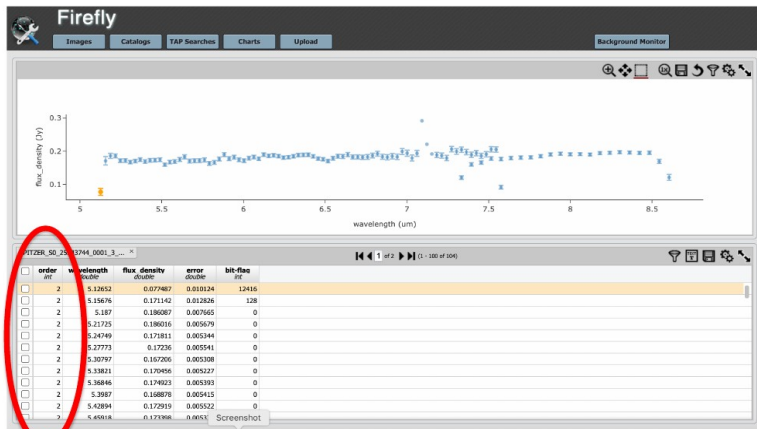
- Existing data model doesn't address order
- UCD="instr.order" does exist
- Natural to include order as a column in a single table

IVOA   9

Proposed Changes to SDM1.1 to Plot Spectral Orders

- 1-D spectra from Spitzer's Infrared Spectrograph have multiple spectral orders
  - Spectral orders can overlap in wavelength
  - Plotting a Spitzer spectrum without accounting for orders gives you a mess
- Option 1: Create separate tables for each order
  - Requires plotting multiple tables on one chart
  - Additional development requirement
- Option 2: Treat order as a column
  - Column-based plotting is common
  - UCD="instr.order" already exists
  - We propose column utype = spec:Spectrum.Data.SpectralAxis.Order
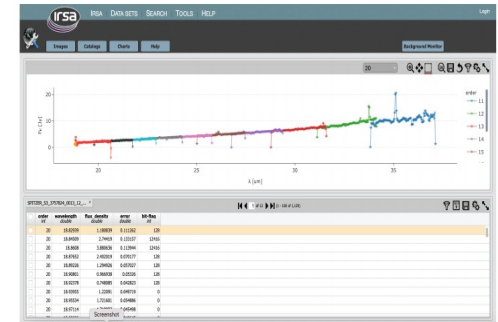
Firefly-based IRSA Viewer tool shows multi-order Spitzer spectrum as a chart (top) and a table (bottom). Both are interactive.

Since our proposed column utype for spectral orders has not yet been accepted by the IVOA, this implementation recognizes ipac:Spectrum.Data.SpectralAxis.Order

IVOA 5/26/21   10

Caltech

Vandana Desai 2020, 2021

P.S. Concerning the orders - it would be useful for echelle spectra as well and there are in fact two order numbers. One is the relative order counting from 1 (in IRAF it is called aperture number) and then there is an ABSOLUTE echelle order number - it is the real n where the echelle optics is working (number of wavelengths whic will fit the distance between two grooves on echelle grating. This absolute is important for checking the wavelength calibration etc ...
It sounds like those might even need distinct UCDs.

PS. Yes, IMHO the echelle spectra were abandoned in SSA and SDM for years (I tried it to push it since 2009 or so ..
BM: Very interested to see echelle spectra supported too. We have a lot of archival echelle spectra taken with the AAT (e.g. UCLES). Petr's note about the orders for a check on wavelength calibration are spot on. Reduction pipelines can sometimes misidentify orders, resulting in order-scale wavelength shifts that are quite bad, so it's useful to be able to pick up on those.

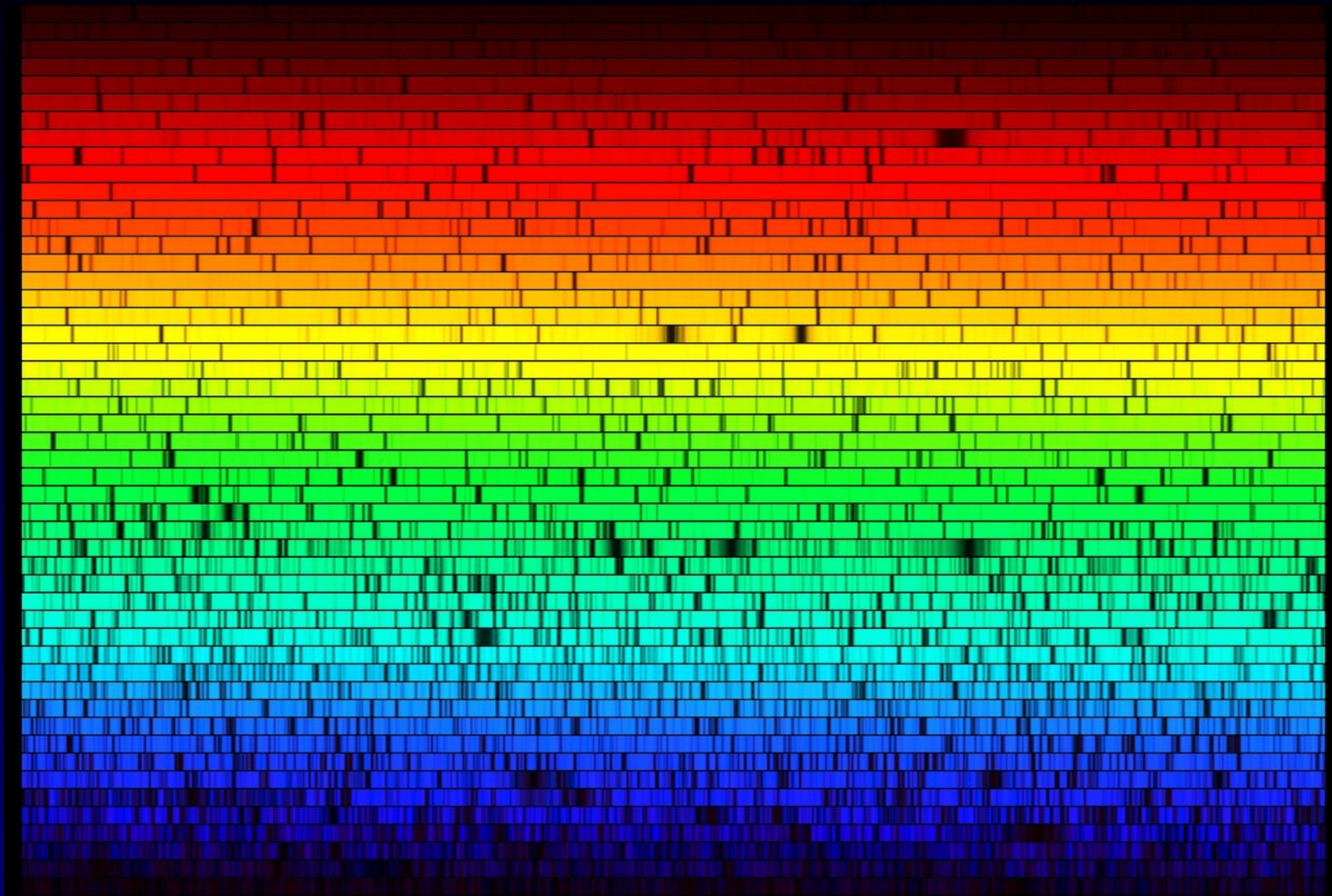Škoda 2021 - introducing *absorder, relorder* in discussion Etherpad

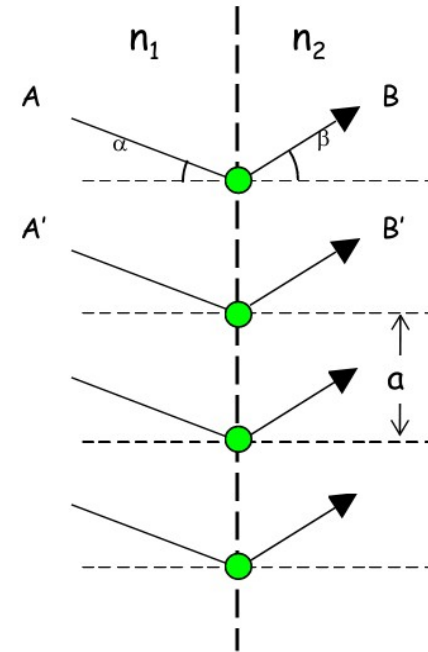# Spitzer IRS High Resolution Mode
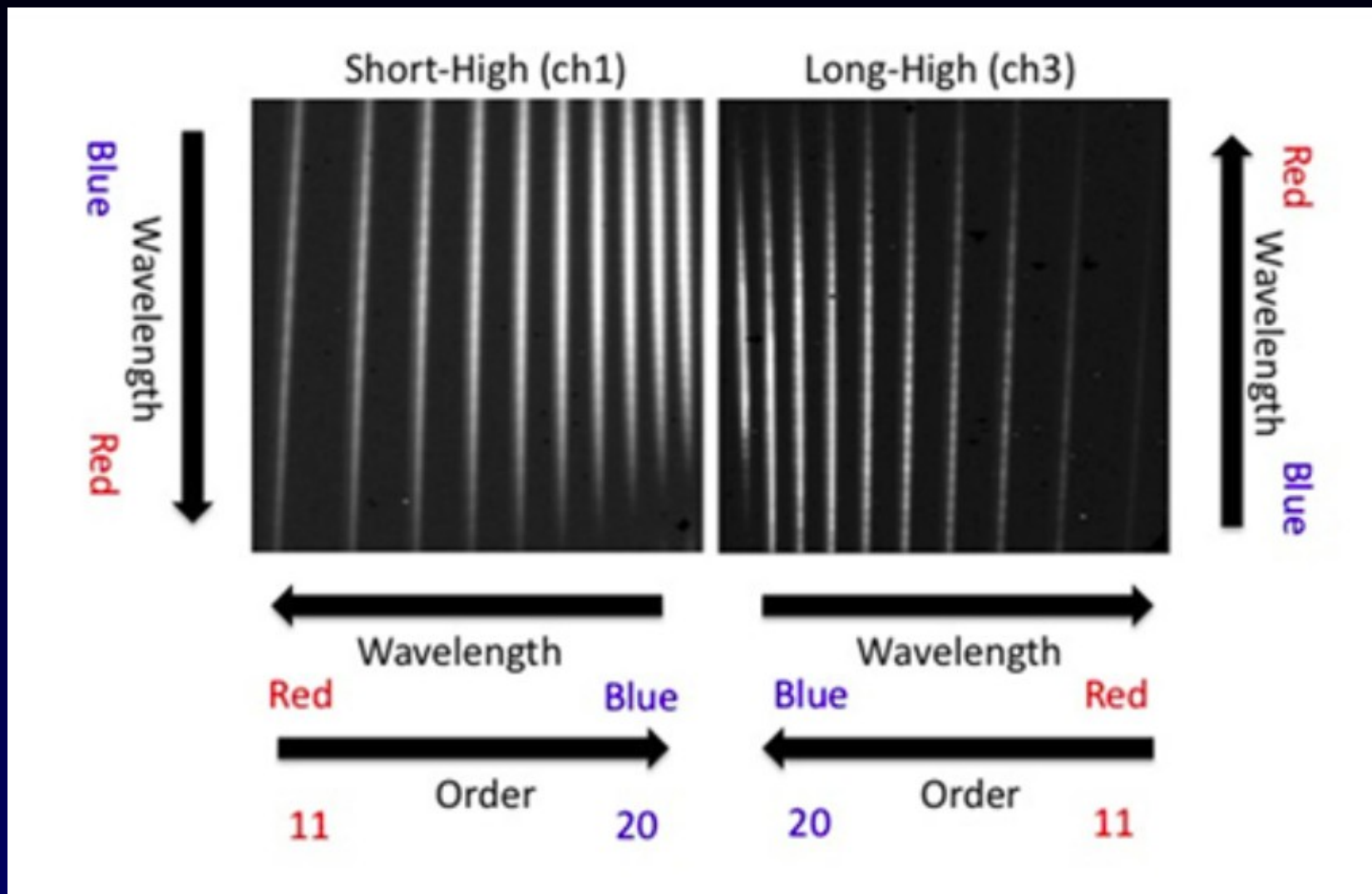
Atlas of Arcturus – 1D Normalized
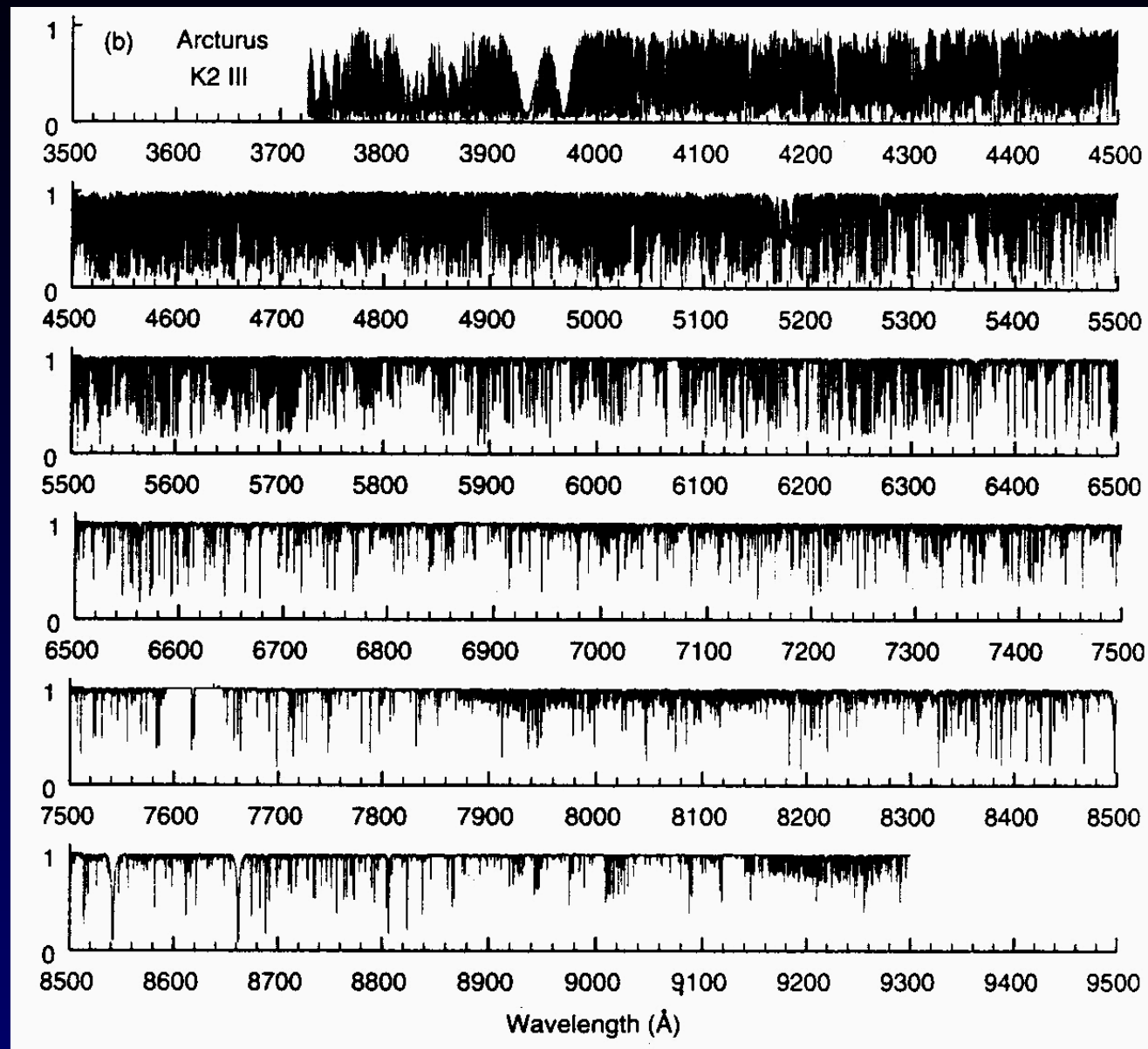
Spectrum of Arcturus (pixel-order)

KPNO NOIRLab

Grating Equation

- Interference condition:

$\Rightarrow$ *path difference between AB and A'B'*

- Grating equation:

$$mp\lambda = n_1 \sin\alpha + n_2 \sin\beta \quad \text{where} \quad \rho = \frac{1}{a}$$

Note the *m* is the spectrum (interference) order

High order – high dispersion   R ~ m*N (no of rules in beam)

Èchelle – stairway in French - coarse grooves   (big steps)
HARPS 31.6/mm

Echellette – normal grating in 1st , 2nd order …. e.g. 833 /mm

Definition of Orders

Appendix A ESPRESSO Spectral Format

Table 7 and Table 8 describe the spectral format recorded by each of the detectors, as provided by the ESPRESSO ETC. For each order number, from left to right, the wavelength of the central column, the free spectral range (FSR) size, the minimum and maximum wavelengths, the order starting and ending wavelengths and size, and the template spectra (TS) range, are given.

When comparing the ETC output with DRS products, be aware that the order numbering is different:

- *interference orders vs numbered orders on the detector*: while ETC numbers the orders using the physical interference orders m, the DRS products have their orders numbered from 1, starting from the bluest one;

- *single orders versus double orders in **singleHR** and **singleUHR***: while the ETC considers interference orders, the DRS products contain the two individual orders imaged on the detector for each of the interference order (see Sect. 3.3 for details). As such, the S/N reported by the ETC corresponds to the quadratic sum of the two orders in the DRS products.

Orders Define Geometry

Multiple orders

- Many orders to cover desired $\lambda\lambda$: *Free spectral range* $\Delta\lambda = \lambda/m$

- Orders lie on top of each other: $\lambda(m) = \lambda(n) \times (n/m)$

- Solution:
  - use narrow passband filter to isolate one order at a time
 - cross-disperse to fill detector with many orders at once

Cross-dispersion ↑

555
500
454
417
385
357
333
312

10 — 555
11
12
13
14
15
16 — 333

312   300

Primary dispersion →
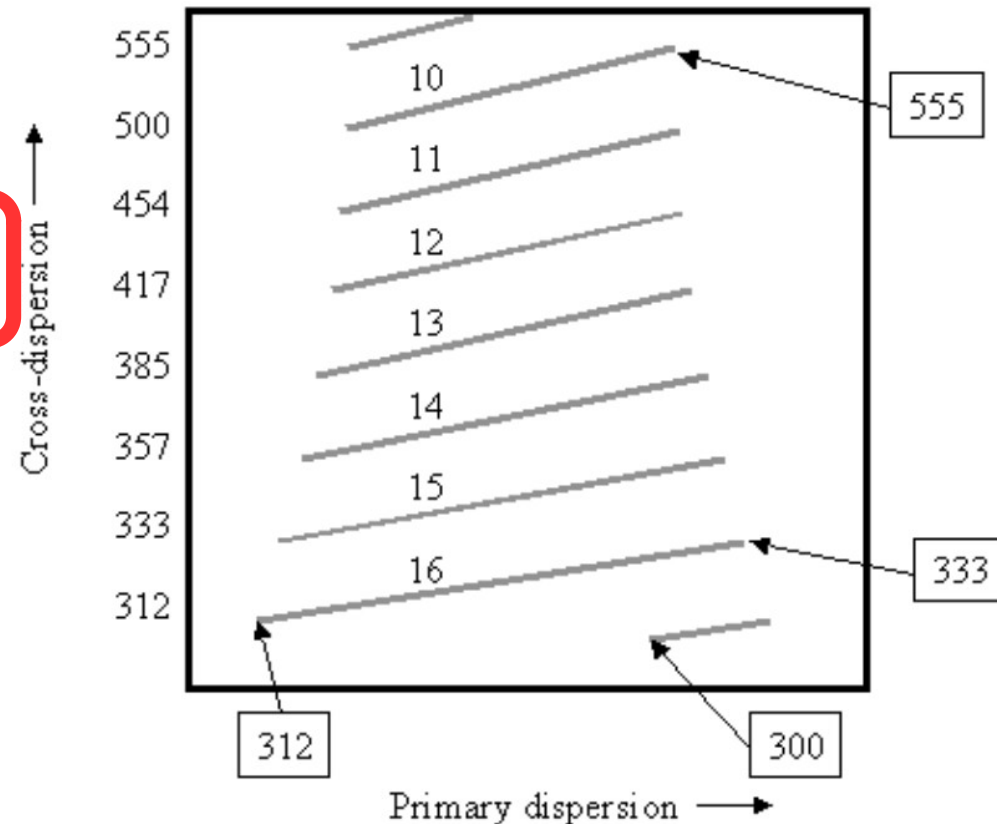
Cross dispersion may use prisms or low dispersion grating

Need for Cross-Dispersion

The èchelle cross-dispersed spectrograph

- No shadowing, very high orders (100+), high dispersion
- Order overlap avoided by cross-dispersion
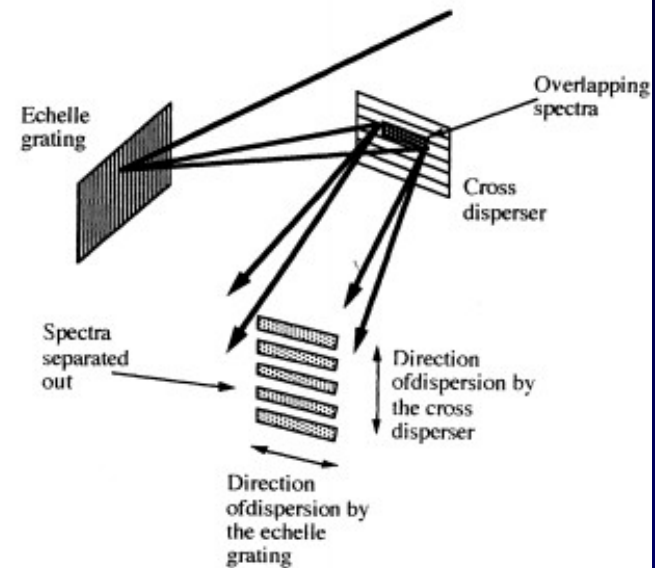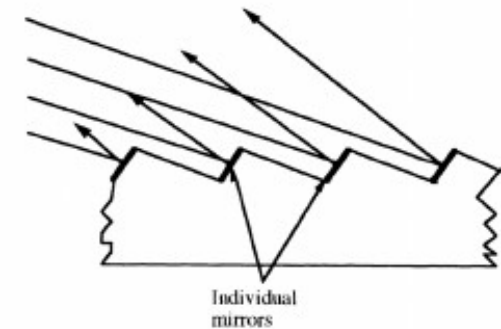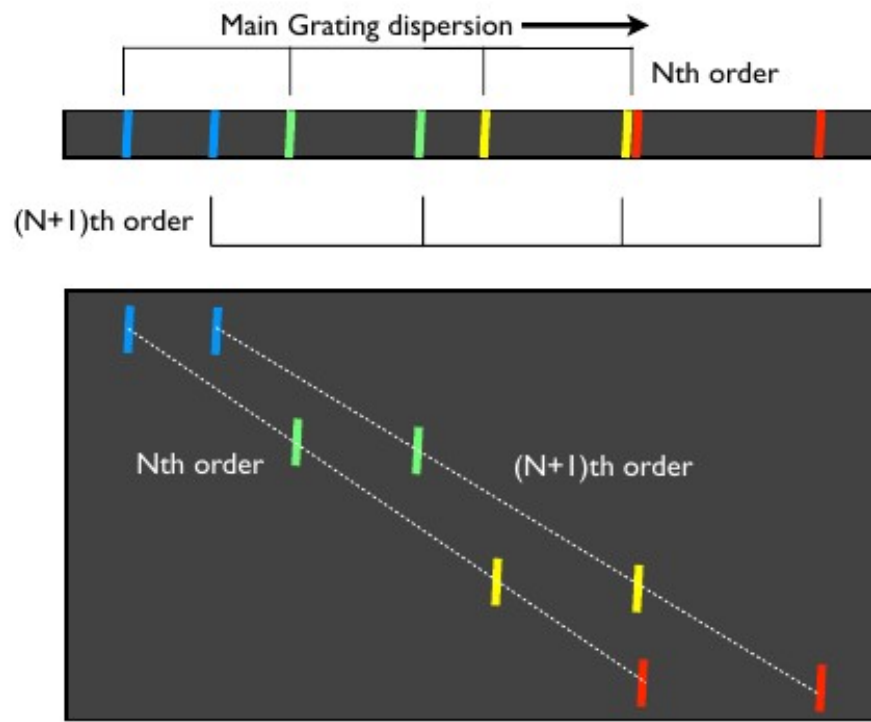
Cross-Disperser Type
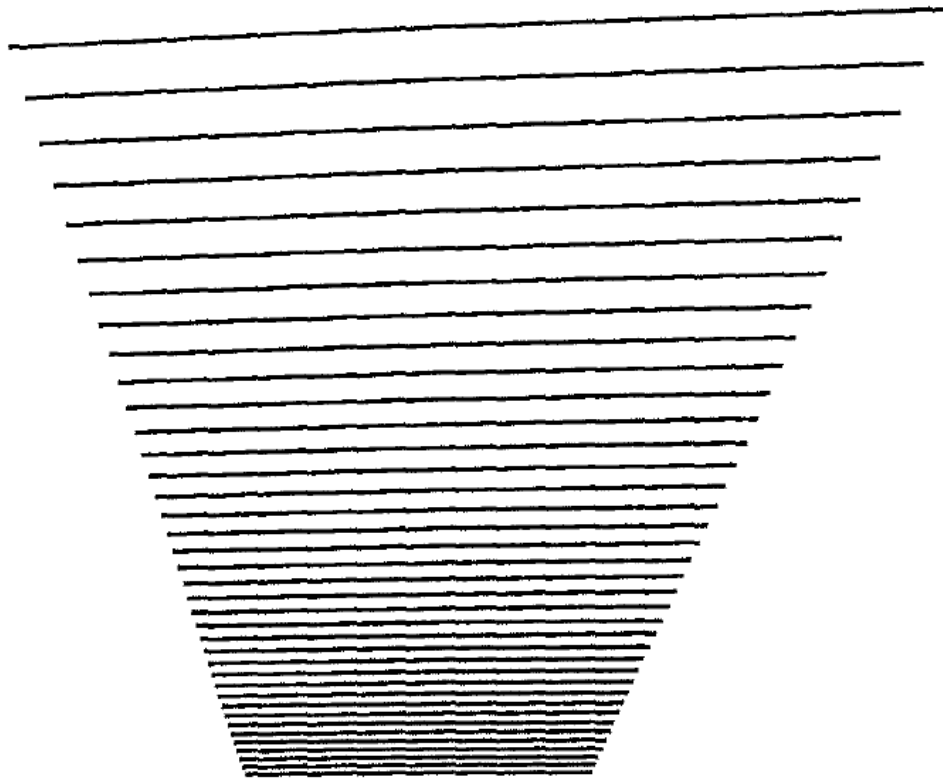
(a) Grating cross dispersion
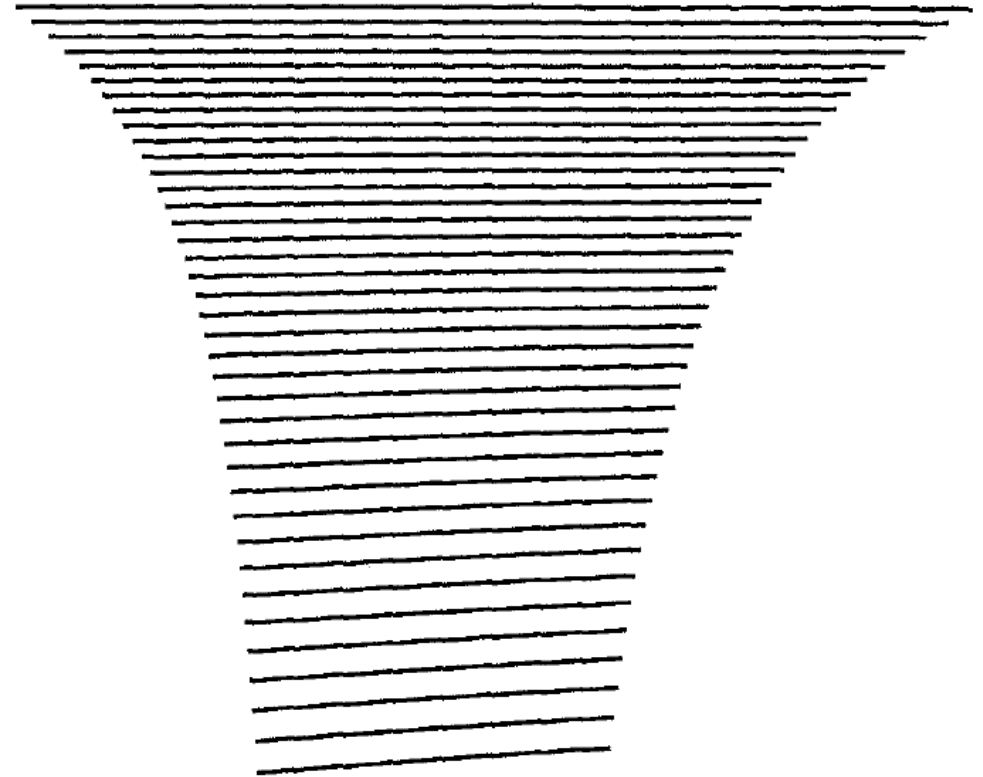
(b) Prism cross dispersion

Barnes 2005   Design study of HERCULES at NZ

OES – Balmer Series
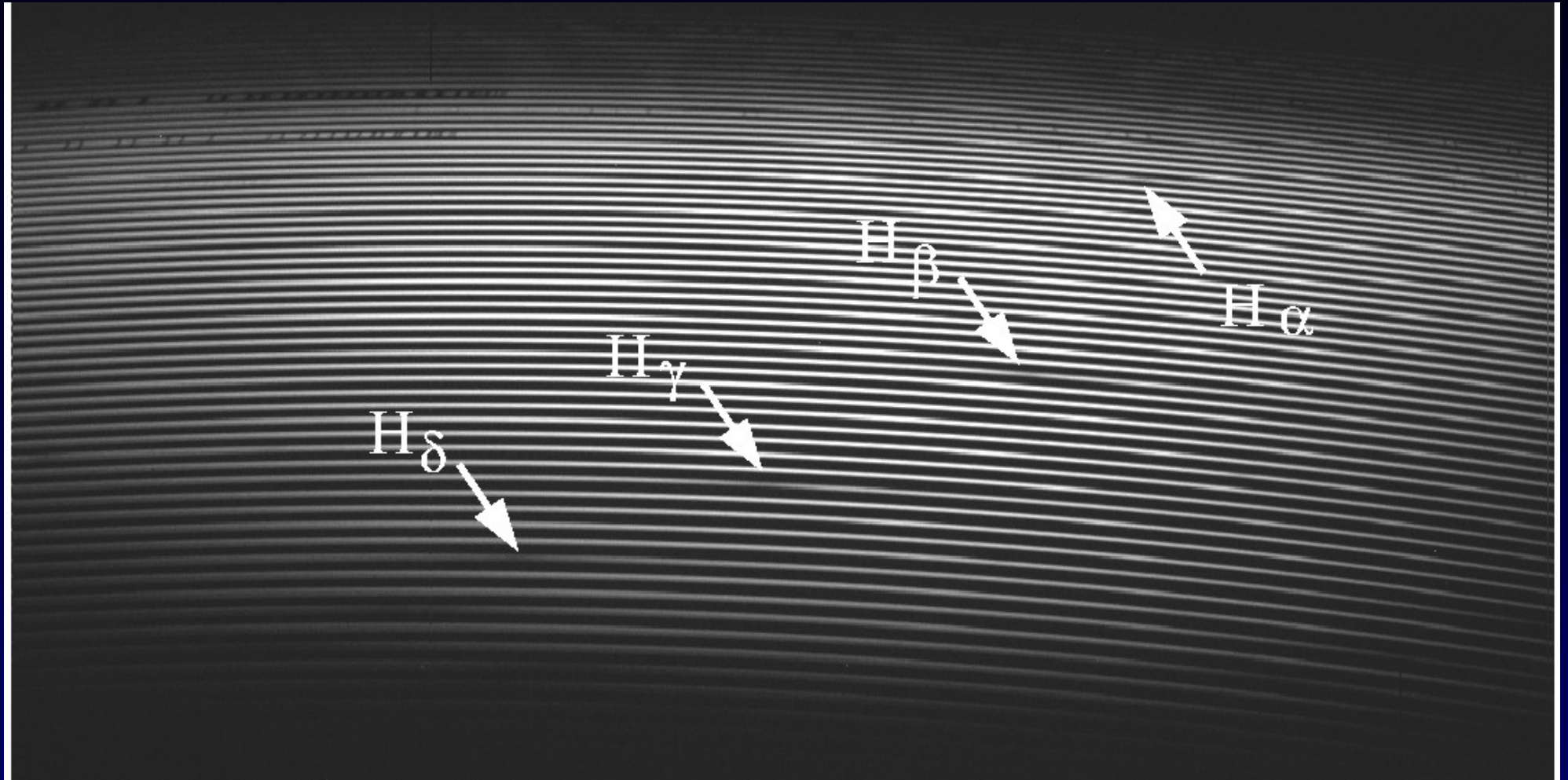
Repeating Comp Structures

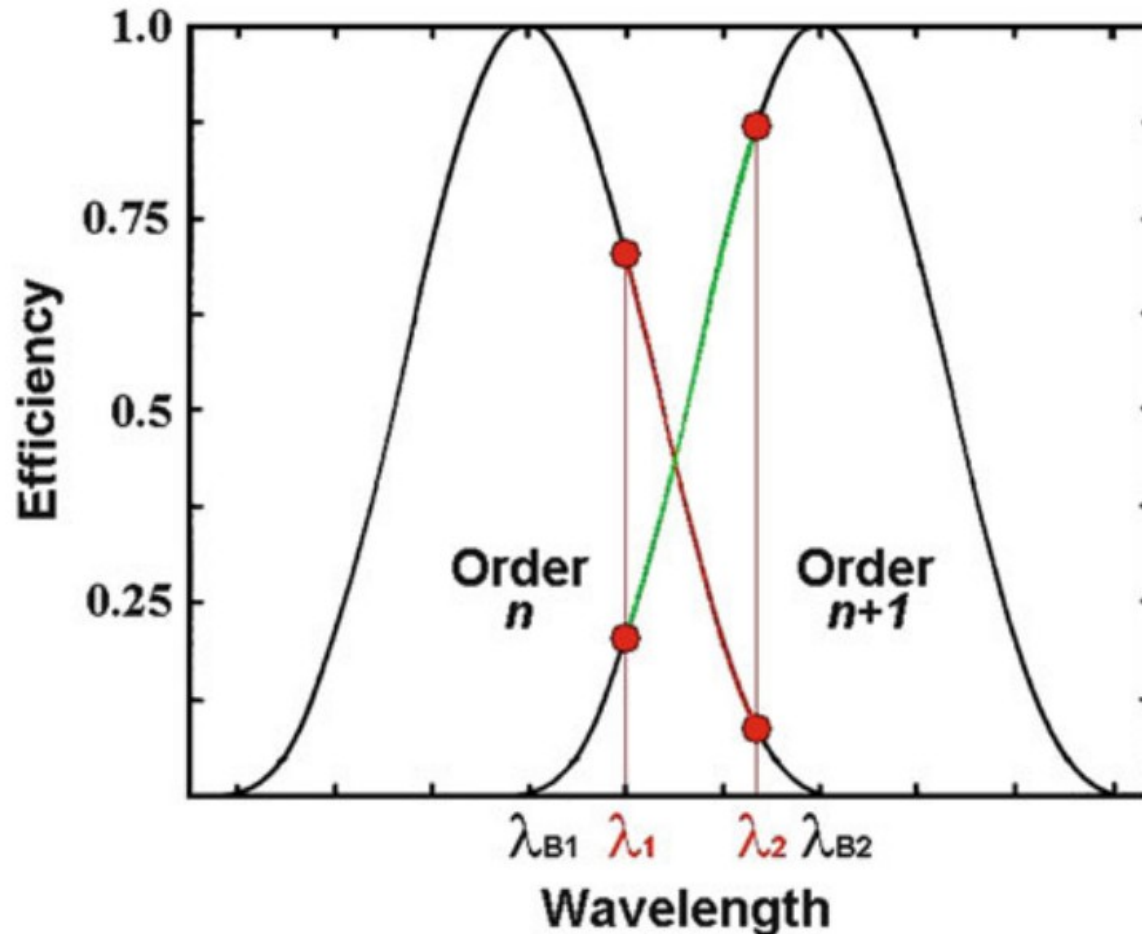OES – Miroslav Šlechta

Blazed Grating Intensity

Solution: Blazed Grating
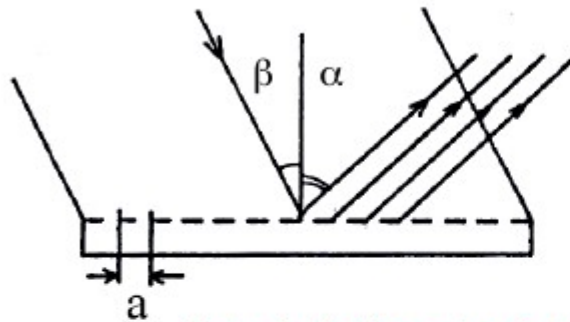
Single-slit diffraction envelope for blazed grating
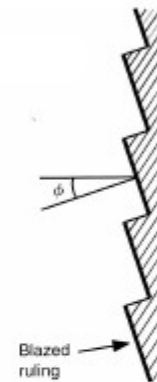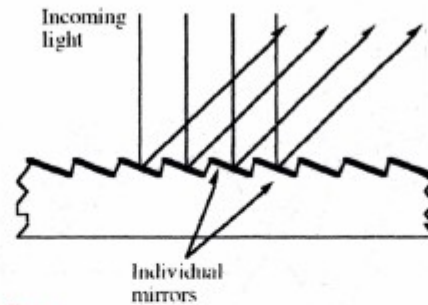
$$I(\beta) = \left[\frac{\sin\{(\pi b/\lambda)[\sin(\alpha + \phi) + \sin(\beta + \phi)]\}}{(\pi b/\lambda)[\sin(\alpha + \phi) + \sin(\beta + \phi)]} \right]^2$$
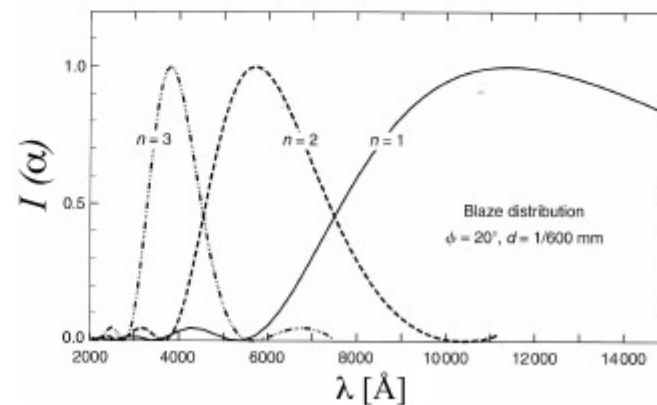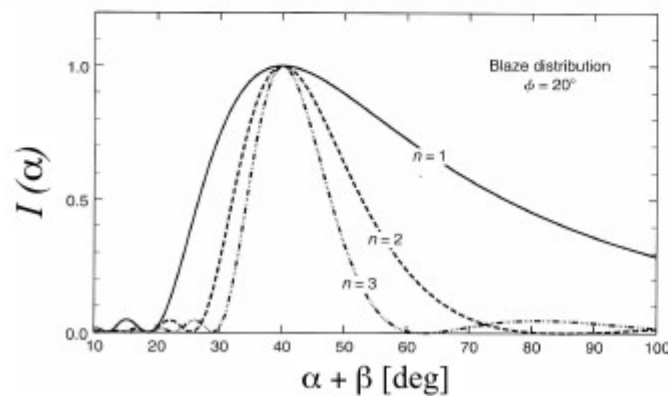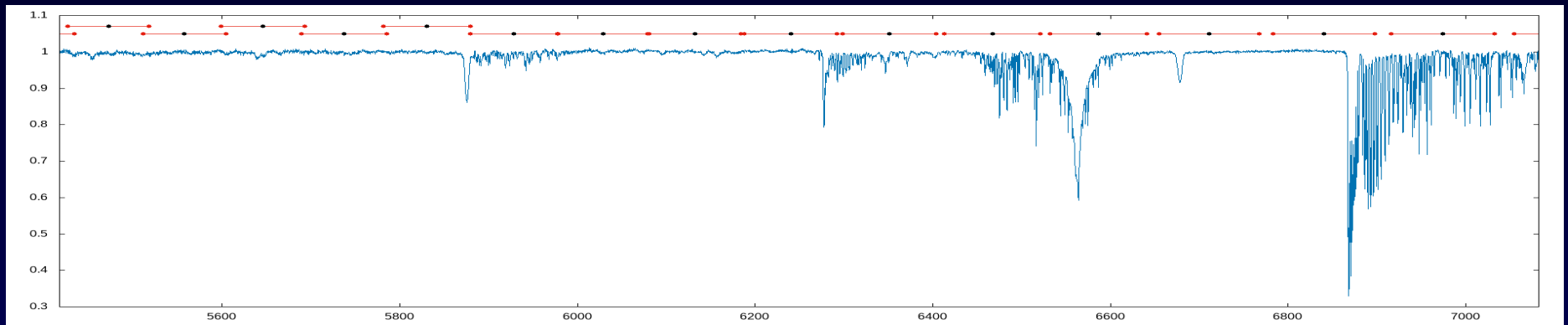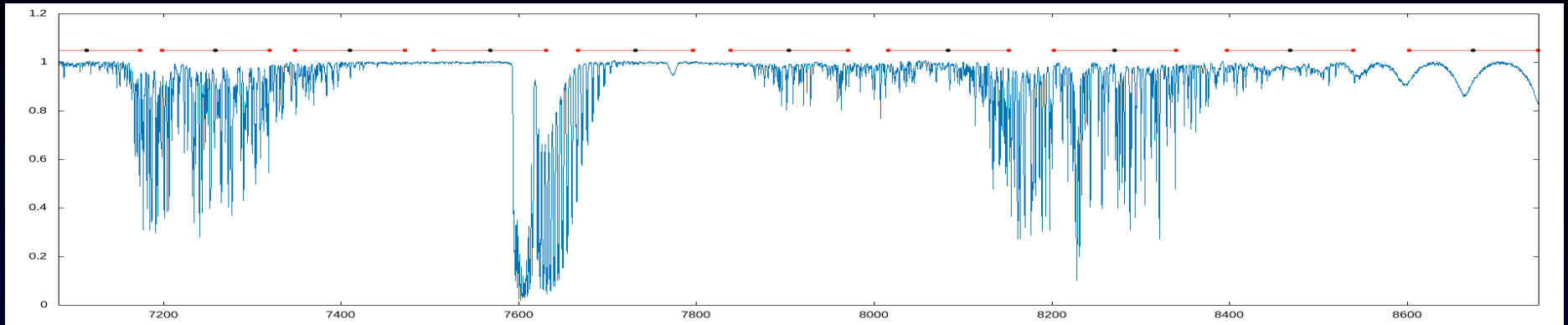
Overlapping Orders

Fig. 5.15 Sketch of the efficiencies in two adjacent orders. Identical wavelength intervals in the orders are indicated in *red* and *green*. Both wavelengths λ_1 and λ_2 are imaged in the two orders n and $n+1$. The two blaze peaks of the orders are positioned at λ_{B_1} and λ_{B_2}
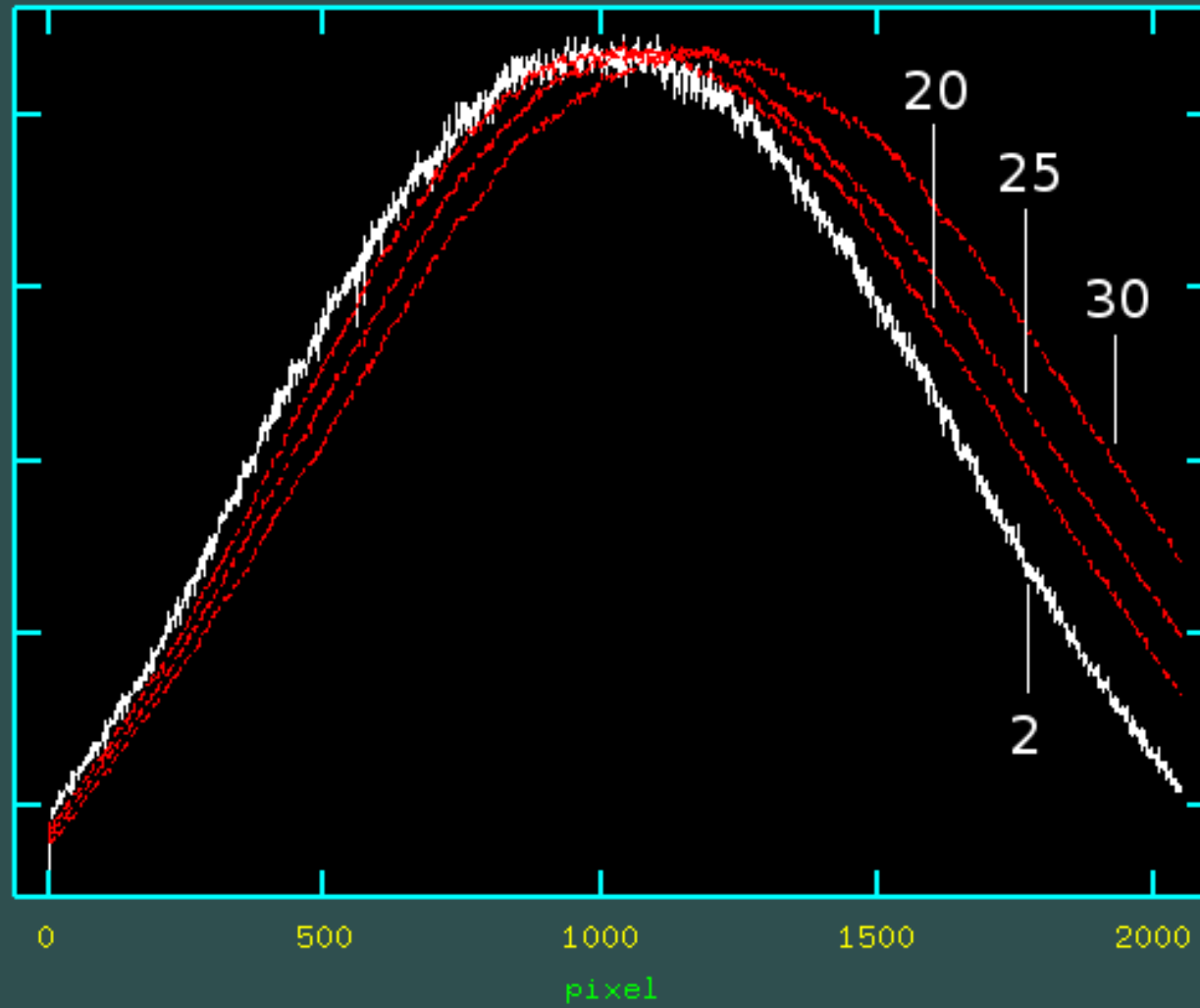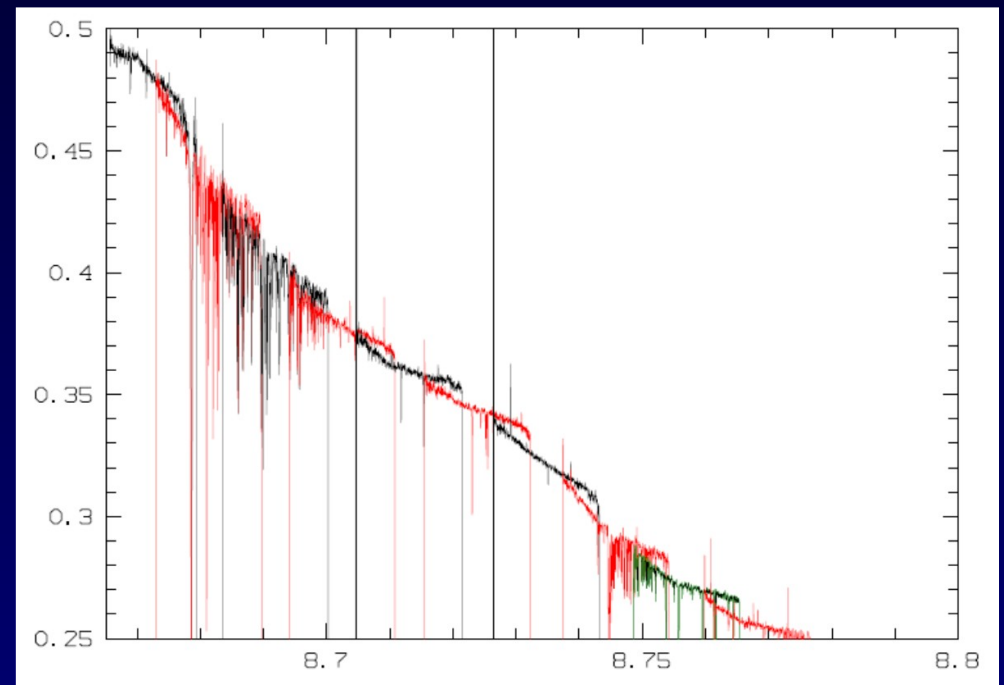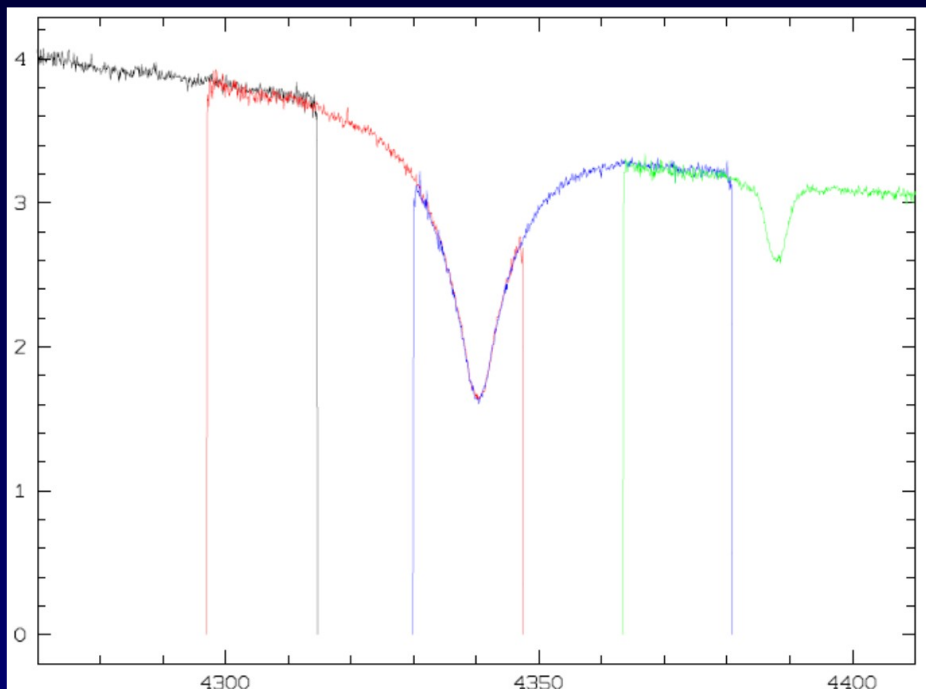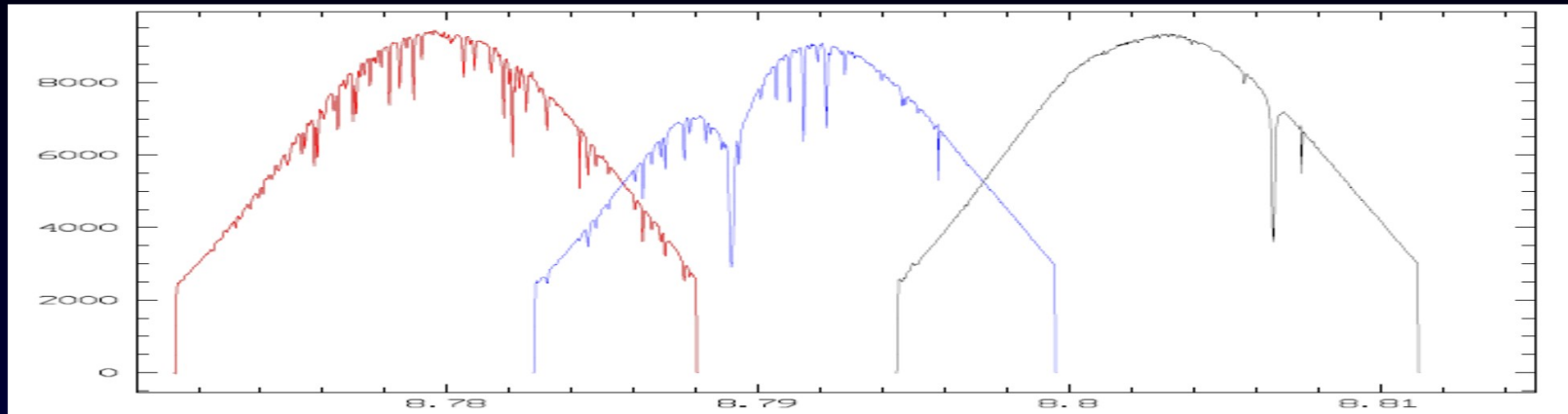
OES Echelle Spectra - Gaps
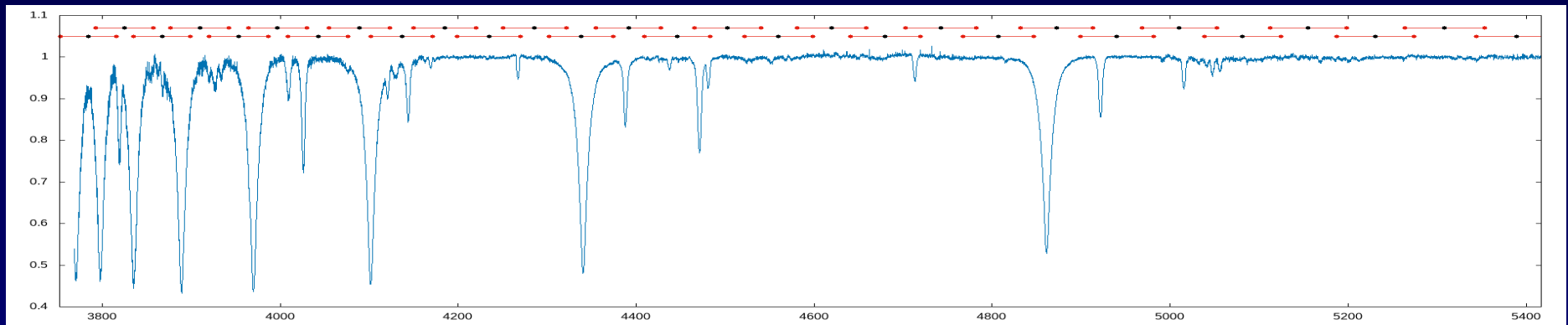
M. Šlechta Montage of spectra from CCD700 single order spectrograph, Perek 2m

OES Blaze shift

Šlechta

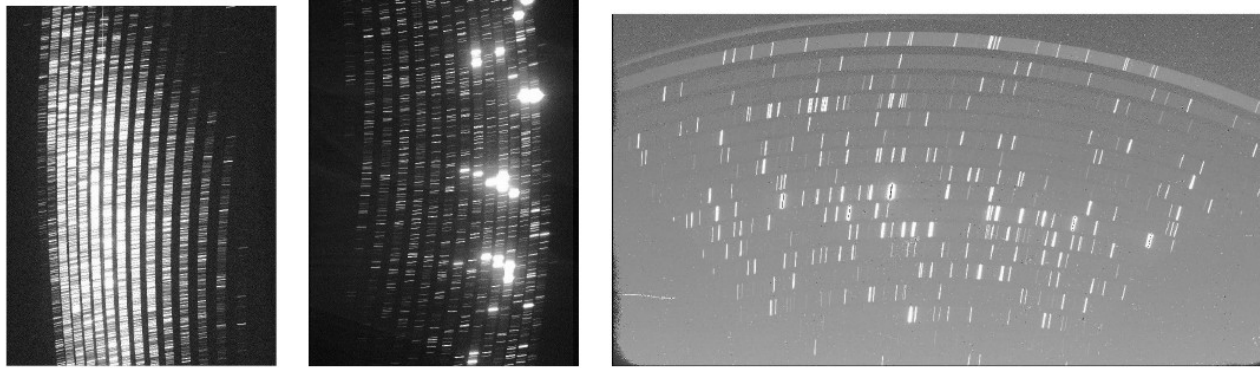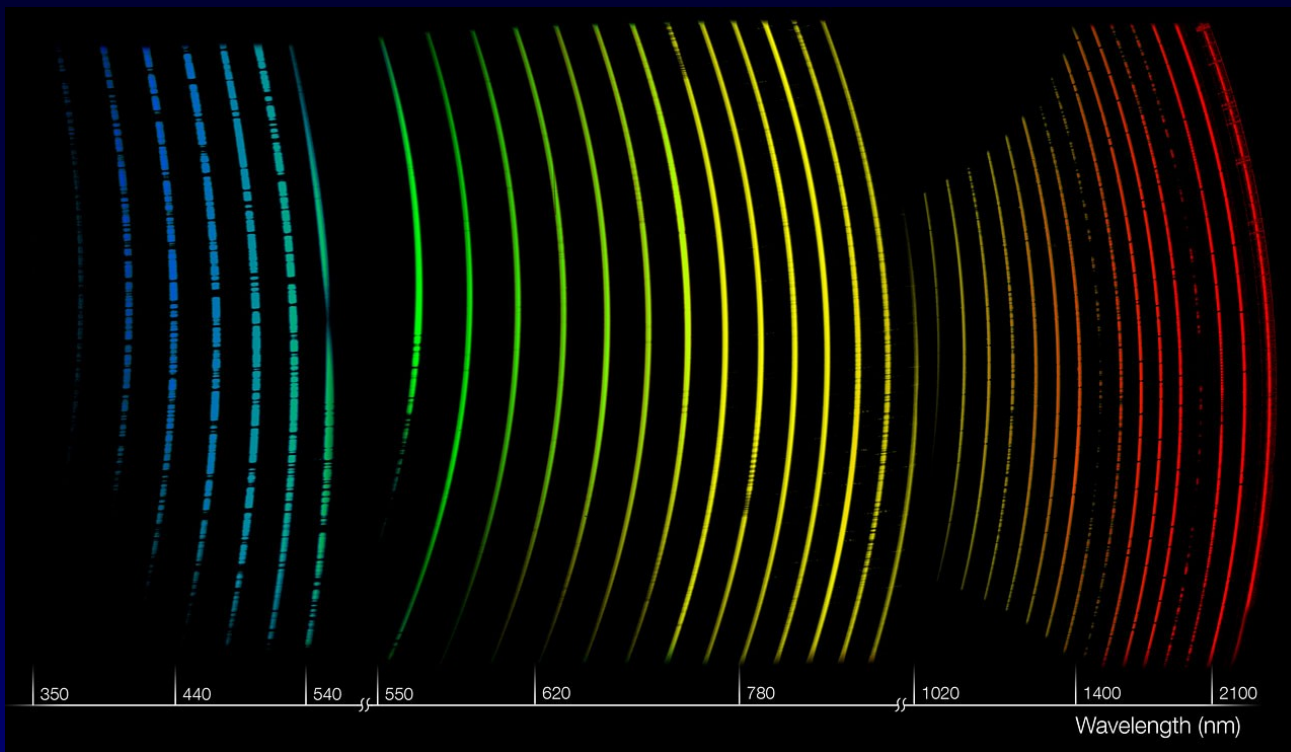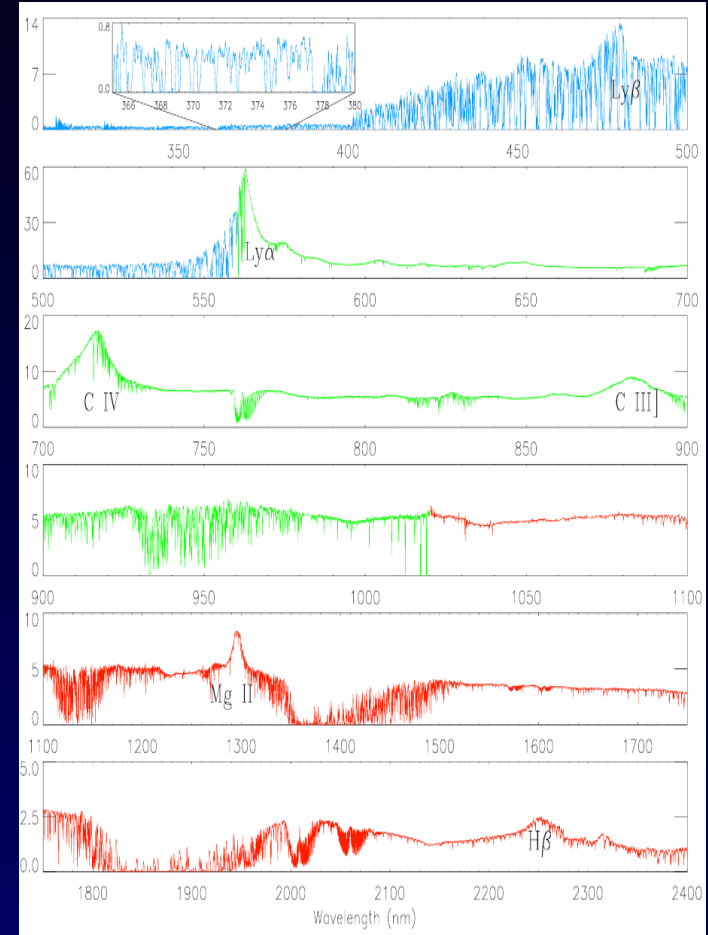# Echelle Spectra Problems in Hot Stars

ESO X-Shooter

Figure 1. This image displays left to right the XSH UVB, VIS and NIR spectral formats with different image scales.

2936-24807 A,
R ~9100,17400,11300
0.5arcsec slit

Modigliani et al. 2010

High-z QSO
Vernet et al. 2011

HARPS-S

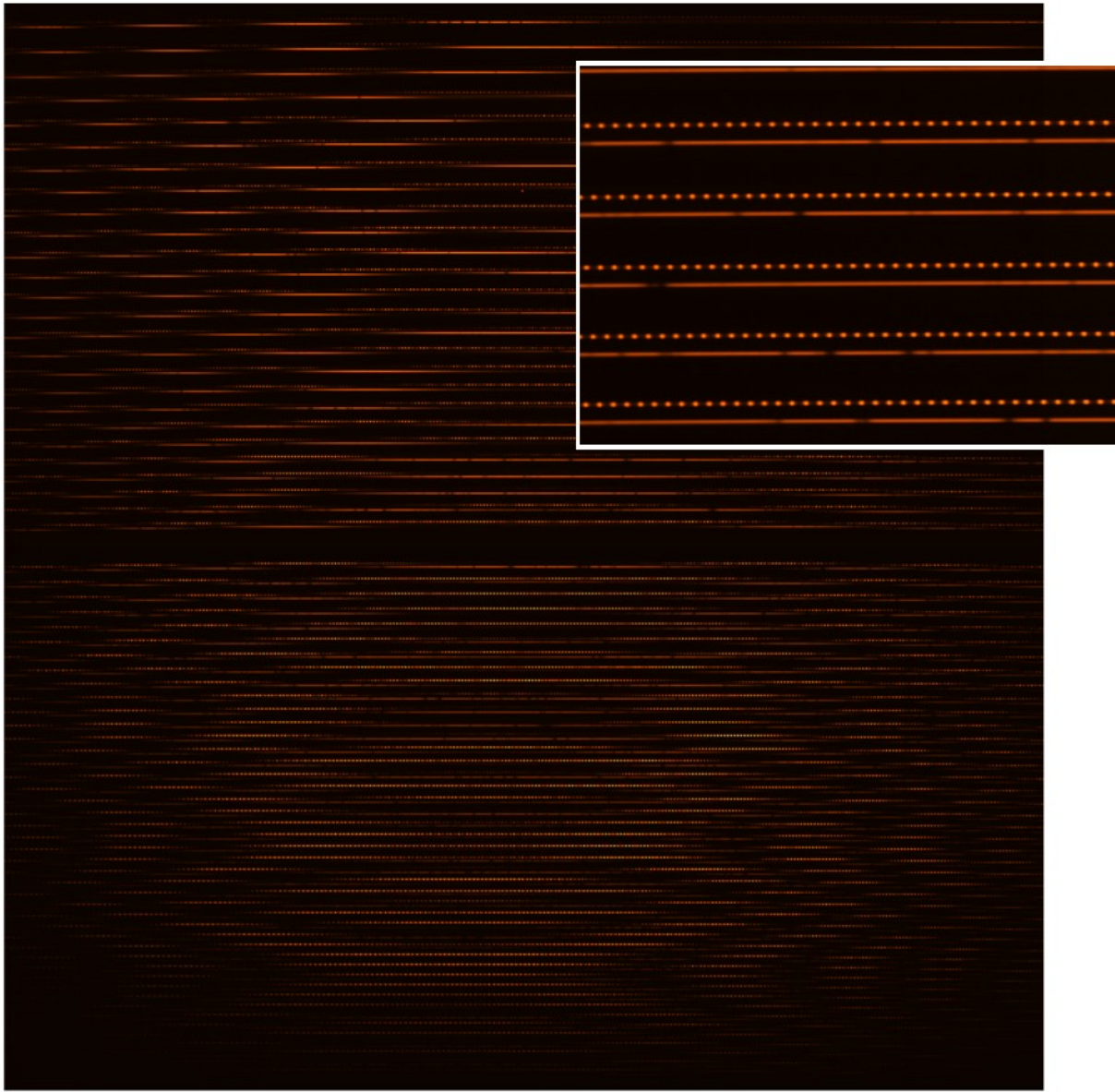71 orders (89-161) – 115 not

3780-6910 A

R~115000

dRV~3m/s

4096 Pix * 71 orders
~290 000 points in 1D
spectrum

HARPS-N

Order N°	Central wavelength [Å]	Total spectral range Δλ [Å]
89	6880.8	75.9
90	6804.4	75.1
91	6729.7	74.3
156	3951.6	43.4
157	3926.3	43.1
158	3901.3	42.8

Cosentino et al. 2012

HARPS-N Pipeline

Cosentino et al. 2012 — The final product is just a number (RV in given time)

HARPS-S

Line Profile Variation - Spica

Si III 4552 A

SOFIN at NOT

Also FT on profiles

Dynamic Fourier Spectrum

Harrington et al. 2016
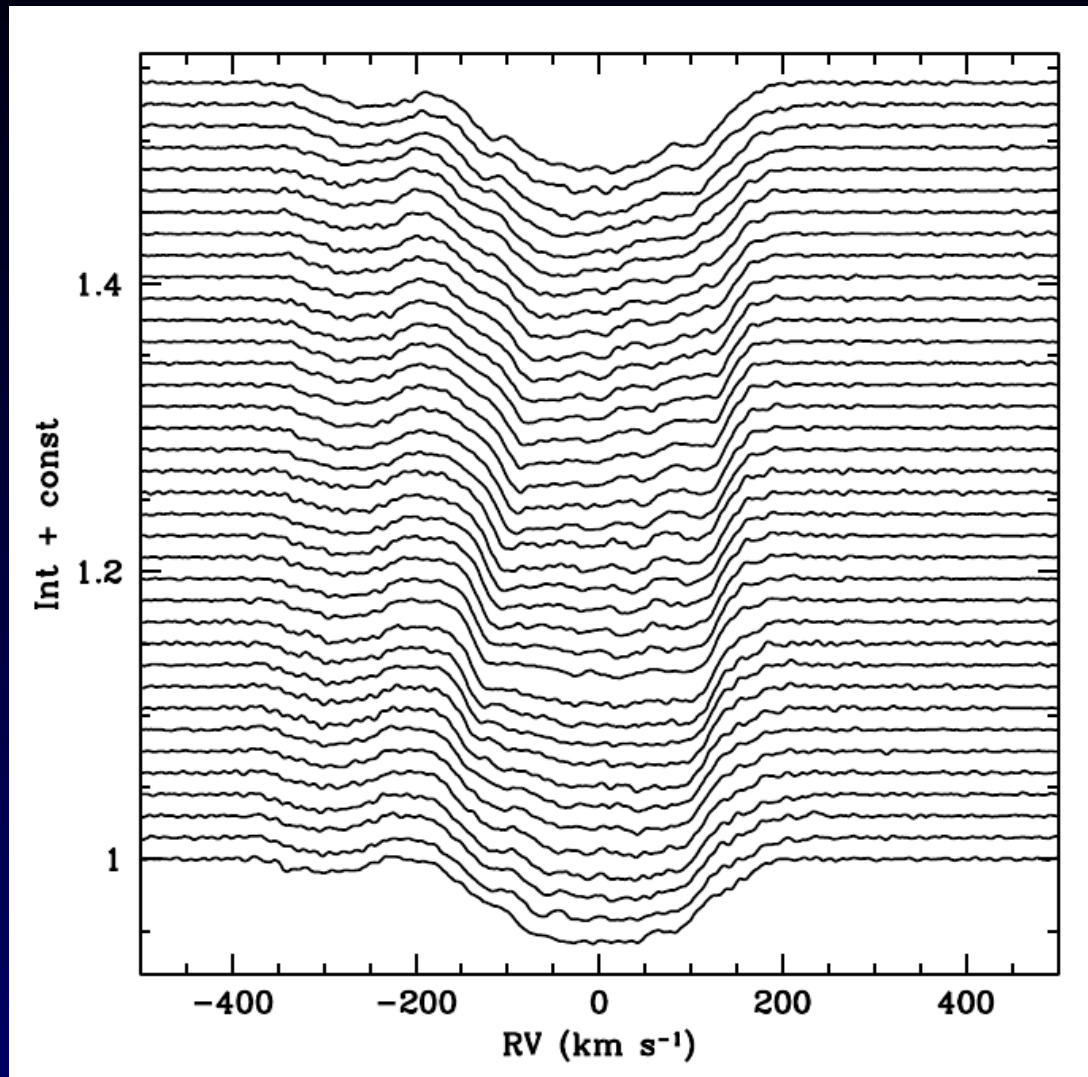
Pulsational LPV
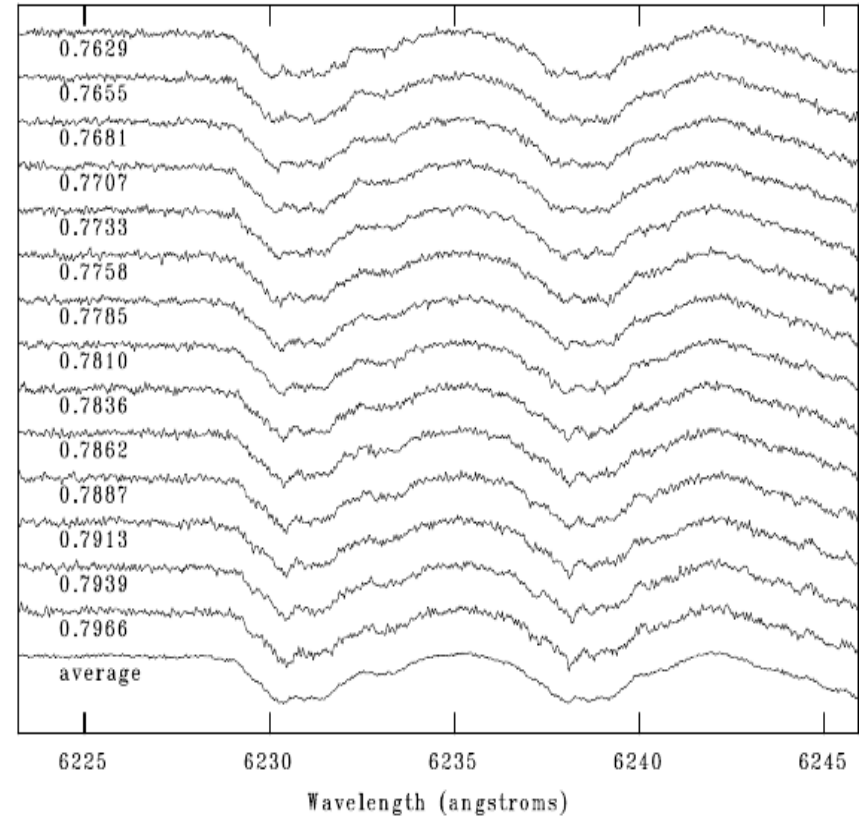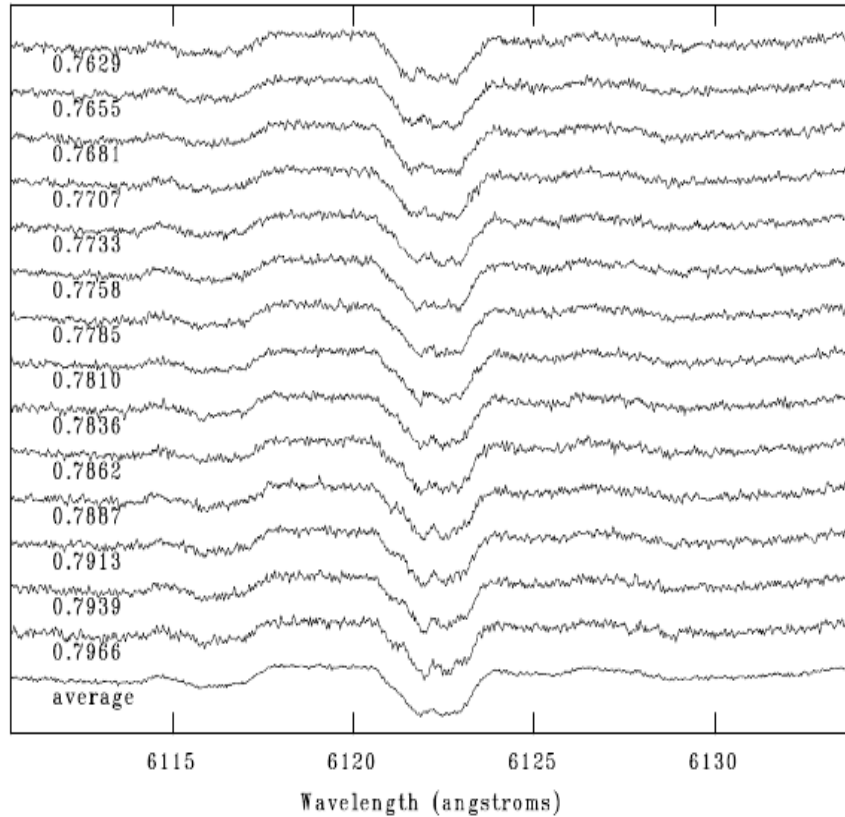
Figure 1. Spectral profile variability of Mn II 6122 Å, Fe I 6231 Å, and Fe II 6238 Å lines in the UVES spectra of HD 21190. Spectra are

Gonzales at al. 2018   HD 21190   δ Sct   star

Echelle spectrographs for precise RV

Figure 11. Radial velocity data phase-folded to the orbital periods of π Men b (top panel) and π Men c (bottom panel). The bottom panel shows all instruments except for ESPRESSO in gray. Each panel shows the RV data with the contribution from the other planet removed.

Exoplanets

Stars with narrow lines

No merging

Direct S2D

Huber et al. 2022

HARPS-S in SPLAT

2-d compound coordinate system
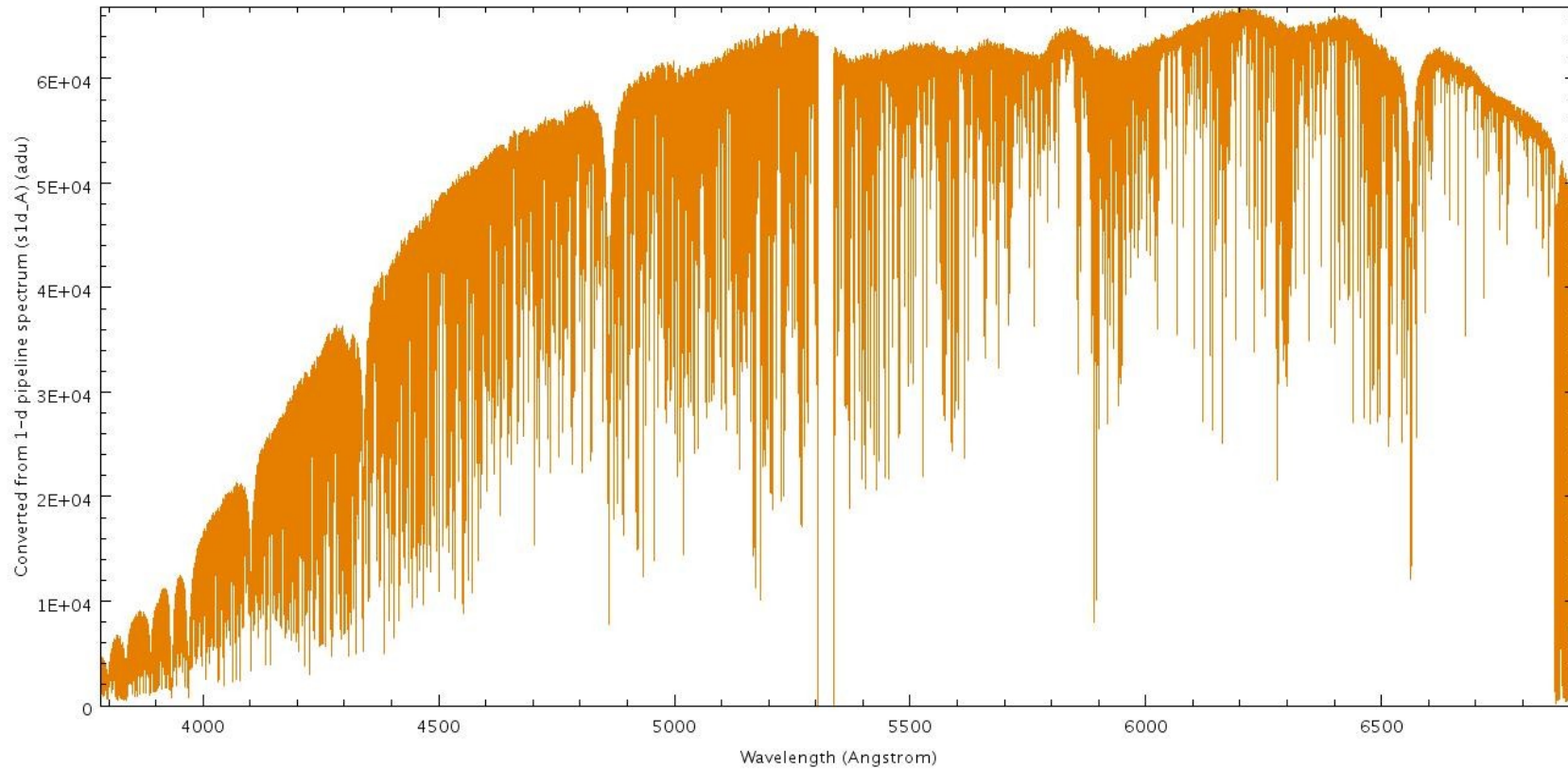
313138 points   Procyon

1D Merges in SPLAT-VO
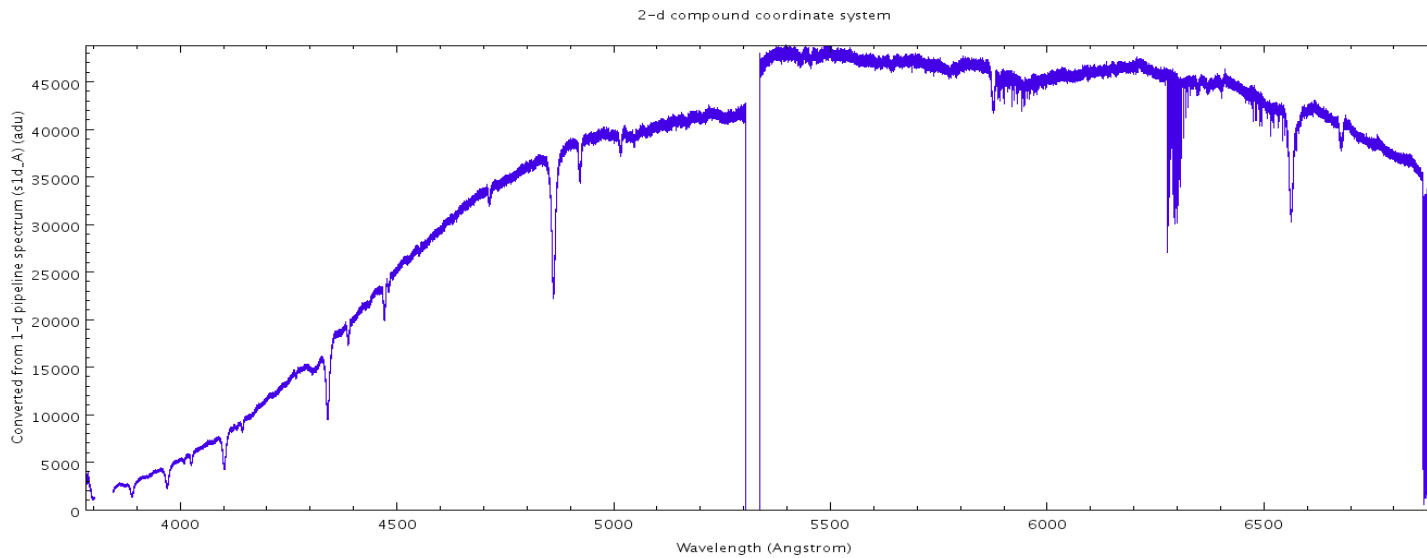
HARPS
unblazed
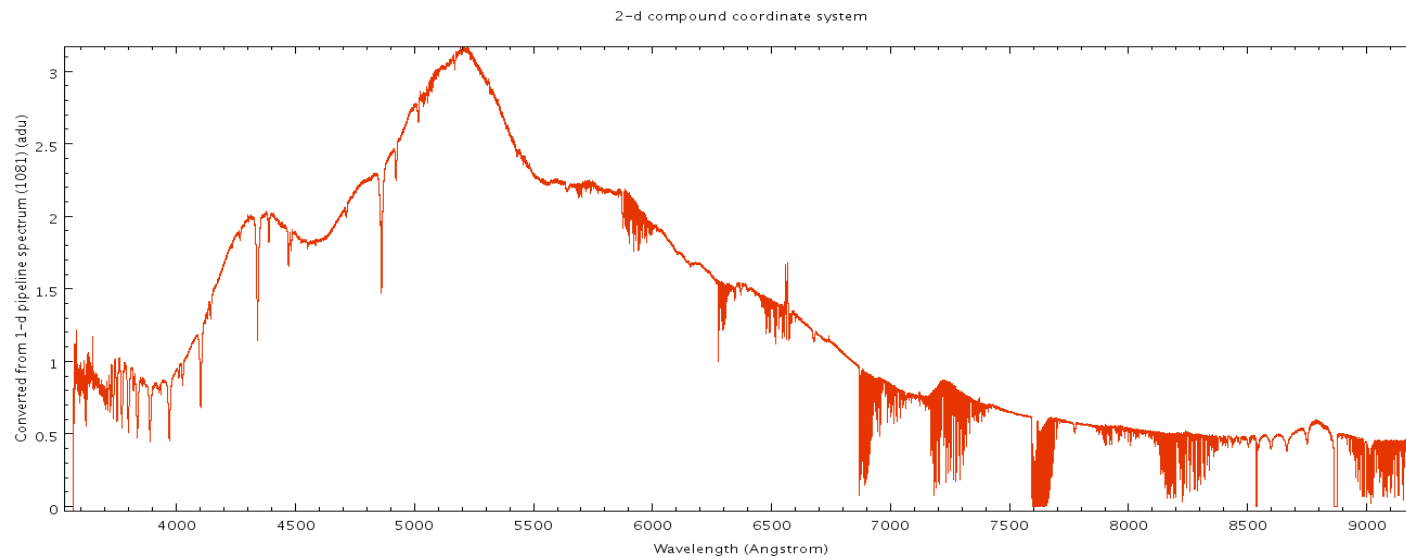
FEROS
pseudonormalized

Why Not Use 1D Order-Merged Spectra

Error propagation for S2D spectra is relatively straightforward since there is no resampling step in the process. Extracted pixels remain independent of each other.

S1D Spectra

The resampling process that is necessary to generate S1D spectra from S2D spectra inevitably introduces correlations between adjacent rebinned pixels in the S1D spectra. To calculate the errors on the S1D spectra one propagates errors in the usual way to the S1D

We note however that the existence of correlations makes the use of the S1D spectrum non-trivial for science purposes

In general, the use of the S2D spectrum is recommended whenever possible to avoid correlations between adjacent data points, which are unavoidable as soon as some resampling is performed.

The most important novelty of the code is the fact that non-rebinned reduced data are propagated throughout the analysis process alongside the standard rebinned spectrum obtained from coaddition. Tests on simulated absorption lines show that the results of line fitting performed on an ensemble of rebinned spectra do not follow a chi-squared distribution (Cupani et al., in prep). In fact, errors in the rebinned spectra are correlated across pixels and the degrees of freedom are ill-defined due to degeneration among the line parameters. The problem is avoided when using non-rebinned spectra; this is the only safe condition in which a chi-squared best-fitting test can be applied, and it will be first made available for quasar spectral analysis by the ESPRESSO DAS.

Cupani et al. 2016

Echelle Spectra Formats

- MANY

- Each order is one spectrum (BeSS)   - not seen easily

- Each order SEPARATED – different WCS + overlaps

- Tables CSV (Opera), FITS Binary tables

- FITS Pseudo image (CERES package)

  - Each line flux for 1 spectrum type (raw, unblazed, noise, normalized…

  - line 1 – wavelength array

IRAF *.ec files

Figure 4: Echelle Spectrum with Legendre Polynomial Function

```
WAT0_001= 'system=multispec'
WAT1_001= 'wtype=multispec label=Wavelength units=Angstroms'
WAT2_001= 'wtype=multispec spec1 = "1 113 2 4955.442888635351 0.05...
WAT2_002= '83 256 0. 23.22 31.27 1. 0. 2 4 1. 256. 4963.0163112090...
WAT2_003= '976664 -0.3191636898579552 -0.8169352858733255" spec2 =...
WAT2_004= '9.081188912082 0.06387049476832223 256 0. 46.09 58.44 1...
WAT2_005= '56. 5007.401409453303 8.555959076467951 -0.176732458267...
WAT2_006= '09935064388" spec3 = "3 111 2 5043.505764869474 0.07097...
WAT2_007= '256 0. 69.28 77.89 1. 0. 2 4 1. 256. 5052.586239197408 ...
WAT2_008= '271 -0.03173489817897474 -7.190562320405975E-4"
WCSDIM  =                      2
CTYPE1  = 'MULTISPE'
LTM1_1  =                     1.
CD1_1   =                     1.
CTYPE2  = 'MULTISPE'
LTM2_2  =                     1.
CD2_2   =                     1.
```

5.6 Pixel Array Dispersion Function

The parameters for the pixel array dispersion function consists of just the number of coordinates ncoords. Following this are the wavelengths at integer physical pixel coordinates starting with 1.

To evaluate a wavelength at some physical coordinate, not necessarily an integer, a linear interpolation is used between the nearest integer physical coordinates and the desired physical coordinate

Valdes 1988 , part of IRAF help, docs, specwcs.ps.Z
summary in ADASS 1993

If 1D Order Merging is Applied

- Resampling to common lambda grid (flux)

  Introduces always pixel correlations !!!
- Loosing lambda precision (1/3 pixels missing)
- Resampling to log lambda better (RV)
- High noise at the edges (must cut off)
- Unblazing by 1D flat or 2D flat – not ideal
- Undulating structures
- If corrected – wobbles on continuum
- Science precision is preferred (vs. visual)

VO Access of S2D

- S2D spectra - unblazed, unmerged
- Query by order   (absolute if possible)
  - If starts ~ 1 it is relative
- If pseudonormalized   (flux ~1.0)
  - FLUXCALIB=normalized ?
- For DM – keep pixels → Binary Tables
- For precise RV – preferred S2D - complete
- For line analysis - short cutouts (SODA)
  - SODA in lambda, log lambda or RV
  - Order (absolute /relative)

Vacuum vs. Air Wavelegths in SSAP

- Unsolved problem in SSAP (Škoda IVOA 2017, Shanghai)

- SSAP requires VACUUM wavelenght (e.g. STIS),

- But original files from ground mostly in AIR

- Astronomers remember air wavelenghts (in papers He4471 A)

- Are there metadata to specify the nature of spectrograph ?

     (is it in vacuum vessel, which part)

- Conversion not precise (only approximate formulae)

- Double conversion – RV precision lost !

www.as.utexas.edu/~hebe/apogee/docs/air_vacuum.pdf   Apogee technical note, Allende Prieto 2011

$$\frac{\lambda_0 - \lambda}{\lambda} = n - 1 = a + \frac{b1}{c1 - 1/\lambda_0^2} + \frac{b2}{c2 - 1/\lambda_0^2}$$ IAU resolution 1991

dard air is about 10^{-8} or roughly 3 m/s at 1.6 μm. Note that it is straightforward to go from vacuum to standard air wavelengths with Eq. 1, but the inverse process requires iteration since n is given as a function of vacuum wavelength.

Thank you