





Spectroscopic Data Systems (SDS):

PEPSI Data Reduction User Manual

Version 1.0 – January 30, 2020





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1 Revision history

Issue	Date	Changes	Responsible
V1.0	22.01.2020	First issue	II

2 About this document

This document outlines Image Processing and Data Analysis Facilities of the Spectroscopic Data Systems (SDS) software package.





3 Introduction

The data reduction pipeline is running on the PEPSI data reduction server and processing all incoming images without user interaction.

In order to start the program, type sds 2 to open FITS Image Browser, or sds 1 to open FITS Spectrum Browser (by typing sds 12 opens them both). The command sds 3 open FITS Table Browser to operate with FITS Binary Tables.





4 FITS Image Browser

Images in the current directory are all shown in the browser table and any image can be selected with the table bar and displayed by pressing Enter.



Figure 1: The FITS Image Browser table (left) with the Image Browser Display (right).





4.1 Image Browser Tools Menu

Bias subtraction	
Definition of orders	
Tune order definition	
Copy echelle orders	
Standard extraction	
Optimal extraction	
Wavelength calibration	Alt-W
Apply wavelength solution	
Merge std slices	
Merge opt slices	
Image for each slice	
Stop application	
Continuum fit	Alt-C
Filters	
Frequency spectrum	
🕅 Math on images	
Image processing	

- Bias subtraction in Sec.4.2
- Definition of orders uses calibration tracing flat field spectra made for each slice separately to define traces for each order and every slice with a 3D polynomial fit. Creates polynomial fit files with extension trace. The échelle order numbers can be assigned with Alt-F9 from the Image Display located in its Tools menu.
- Tune order definition fits existing order definition from tracing flats to the selected image (e.g. science or flat field image) to remove any offsets between them.
- Copy echelle order copies order definition from tracing flat to any selected image by creating a FITS record TRACE with the tracing file name in it (with extension trace). In case of PEPSI context it also adds the slicer suffix SXS, SXT, DXT, or DXS to the keyword. The tracing flat has to be tagged as Included with Alt-Ins and the target images tagged as Marked with Ins keys.
- Standard extraction integrates the flux for each slice and all orders without cosmic spices elimination. Creates image with extension std.
- Optimal extraction integrates the flux for each slice and all orders with cosmic spices elimination by constructing a spatial profile image from the flux distribution in cross-dispersion direction with the subsequent fit to the raw data. Creates resulting image with extension opt and spp for the spatial profile.
- Wavelength calibration in $\mathrm{Sec.4.3}$
- Apply wavelength solution creates a wavelength calibrated image with the wavelength solution taken from the ThAr image. The calibration image has to be tagged as Included with Alt-Ins and the target images tagged as Marked with Ins keys.
- Merge std slices creates image (mrg) with slices merged into a single order with the wavelength scale of the central slice. In this mode the flux and its variances are co-added from the rebinned pixels.
- Merge opt slices the same as before but in this mode the flux is averaged with weights as the inverse variance of the rebinned pixels.
- Image for each slice creates separate images for each slice separately. The slice number is added to the resulting image name.
- Stop application allows to stop some lengthy processing procedures without dialog window, e.g. order definition or optimal extraction.
- Continuum fit in Sec.??
- Filters in Sec.??
- Frequency spectrum in Sec.??
- Math on images in $\mathrm{Sec.4.4}$
- Image Processing in Sec.4.5





4.2 Bias subtraction

Columns	Rows								
Prescan: 0	Prescan: 0								
CCD pixels: 2048	CCD pixels: 2048								
Subtract bias: 🗹	Subtract bias:								
Spline: 5	Spline: 5								
Sigma clipping: 1	Sigma clipping: 1 🙀								
Swap pixels: 🗌	Swap pixels: 🗌								
Trim image: 🗌	Trim image: 🗌								
First pixels: 0	First pixels: 0								
Last pixels: 0	Last pixels: 0 🕅								
Use FITS keywords: 🗹	Transpose image: 🗌								
Keep bias overscan: 🗌	Show images:								
Convert to photons: 🗹 Variance estimation: 🗹	File extension: bss								
Project: pepsi.bias									
Start	op Close								

The bias subtraction uses the original raw images with extension fits and is a part of the Image Processing pipeline. In order to validate bias subtraction settings as well for testing or development purposes it can be opened from Tools menu of the Image Browser.

- □ **Prescan** and **CCD pixels** defines CCD prescan width and the number of CCD pixels after which the overscan starts: applicable only to a single amplifier CCD device.
- \checkmark Subtract bias tells whether the bias over scan shall be subtracted in columns and/or rows.
- $\hfill\square$ Spline defines the spline smoothing factor to smooth and subtract overscan.
- \Box Sigma clipping defines the statistical level at which the spikes in the bias overscan are be rejected.
- \checkmark Swap pixels tells to swap each column or row in the image: applicable only to a single amplifier CCD device.
- ✓ Trim image enables skipping the number of columns or rows at the beginning and the end of the image: applicable only to a single amplifier CCD device.
- \checkmark Use FITS keywords tells to use FITS header TRIMSEC keyword to trim the resulting unbiased CCD image.
- ✓ Keep bias overscan enables to keep bias overscan in the image after bias subtraction with no image trimming applicable: this is useful for testing and development.
- ✓ Convert to photons allows to convert ADUs to photoelectrons according to the CCD gain factor (e/ADU) given in the FITS header. For a single amplifier CCD it uses GAIN FITS keyword and for the mosaic CCD it uses indexed GAIN1, GAIN2... keywords.
- \checkmark Variance estimation allows to create additional image section in the FITS file where the variances for each pixel are stored. The variance is estimated with the CCD gain factor and the readout noise obtained from the bias overscan. In case the image is not converted to photoelectrons, the variance is estimated in Eds.
- ✓ Transpose image tells to swap CCD columns and rows.
- \checkmark Show images allows to display resulting images as processed.
- \Box File extension specifies the file extension for the resulting image.
- **Project** opens the File Selector window to choose another project file. All parameters of this application can be saved into a specific project file and retrieved any time later.
- **Start** starts processing a single or selected images.
- **Stop** interrupts the processing sequence.
- Close closes the dialog window.





Since PEPSI uses a mosaic CCD with 16 amplifiers, the bias subtraction procedure uses AMPSEC (image region with prescan and overscan) and IMASEC (image region without extra-scans) FITS keywords for each amplifier. The relevant FITS keyword for the PEPSI CCD are shown as follows where the overscan in columns and rows is equal to 50 pixels.

EXTEND = MOSAIC =	T T		/ Extension is present / Image is CCD mosaic			
DETSIZE =	'[1:10560,1:10560]'		/ Detector size			
DETECTOR=	'STA1600LN'		/ STA Archon controller X12	2-F 1.0.1028		
AMPSEC1 =	'[1:1370,1:5330]'	/	Amplifier index section	AMPSEC9 = '[1:1370,5331:10660]'	/	Amplifier index section
IMASEC1 =	'[1:1320,1:5280]'	/	Image index section	IMASEC9 = '[1:1320,5381:10660]'	/	Image index section
AMPSEC2 =	'[1371:2740,1:5330]'	/	Amplifier index section	AMPSEC10= '[1371:2740,5331:10660]'	/	Amplifier index section
IMASEC2 =	'[1371:2690,1:5280]'	/	Image index section	IMASEC10= '[1371:2690,5381:10660]'	/	Image index section
AMPSEC3 =	'[2741:4110,1:5330]'	/	Amplifier index section	AMPSEC11= '[2741:4110,5331:10660]'	/	Amplifier index section
IMASEC3 =	'[2741:4060,1:5280]'	/	Image index section	IMASEC11= '[2741:4060,5381:10660]'	/	Image index section
AMPSEC4 =	'[4111:5480,1:5330]'	/	Amplifier index section	AMPSEC12= '[4111:5480,5331:10660]'	/	Amplifier index section
IMASEC4 =	'[4111:5430,1:5280]'	/	Image index section	IMASEC12= '[4111:5430,5381:10660]'	/	Image index section
AMPSEC5 =	'[5481:6850,1:5330]'	/	Amplifier index section	AMPSEC13= '[5481:6850,5331:10660]'	/	Amplifier index section
IMASEC5 =	'[5481:6800,1:5280]'	/	Image index section	IMASEC13= '[5481:6800,5381:10660]'	/	Image index section
AMPSEC6 =	'[6851:8220,1:5330]'	/	Amplifier index section	AMPSEC14= '[6851:8220,5331:10660]'	/	Amplifier index section
IMASEC6 =	'[6851:8170,1:5280]'	/	Image index section	IMASEC14= '[6851:8170,5381:10660]'	/	Image index section
AMPSEC7 =	'[8221:9590,1:5330]'	/	Amplifier index section	AMPSEC15= '[8221:9590,5331:10660]'	/	Amplifier index section
IMASEC7 =	'[8221:9540,1:5280]'	/	Image index section	IMASEC15= '[8221:9540,5381:10660]'	/	Image index section
AMPSEC8 =	'[9591:10960,1:5330]'	/	Amplifier index section	AMPSEC16= '[9591:10960,5331:10660]'	/	Amplifier index section
IMASEC8 =	'[9591:10910,1:5280]'	/	Image index section	IMASEC16= '[9591:10910,5381:10660]'	/	Image index section

The conversion to photoelectrons is done with GAIN FITS keywords for each amplifier, but the variance is estimated with the additional gain factor slope GAINS which provides the gain factor value at a given ADU number of the pixel. The readout noise measured from overscan of each amplifier is stored into the FITS header of the image and used for variance estimation.

GAIN1	=	1.550280	/ (CCD	amplifier	gain factor	in (e/ADU	GAINS1	=	0.662213	/	CCD	amplifier	gain	slope	times	65535
GAIN2	=	1.553919	/ (CCD	amplifier	gain factor	in (e/ADU	GAINS2	=	0.741984	/	CCD	amplifier	gain	slope	times	65535
GAIN3	=	1.559687	/ (CCD	amplifier	gain factor	in (e/ADU	GAINS3	=	0.631926	/	CCD	amplifier	gain	slope	times	65535
GAIN4	=	1.539479	/ (CCD	amplifier	gain factor	in (e/ADU	GAINS4	=	0.700027	/	CCD	amplifier	gain	slope	times	65535
GAIN5	=	1.562029	/ (CCD	amplifier	gain factor	in (e/ADU	GAINS5	=	0.645251	/	CCD	amplifier	gain	slope	times	65535
GAIN6	=	1.551208	/ (CCD	amplifier	gain factor	in (e/ADU	GAINS6	=	0.642080	/	CCD	amplifier	gain	slope	times	65535
GAIN7	=	1.558944	/ (CCD	amplifier	gain factor	in (e/ADU	GAINS7	=	0.657344	/	CCD	amplifier	gain	slope	times	65535
GAIN8	=	1.552657	/ (CCD	amplifier	gain factor	in (e/ADU	GAINS8	=	0.647146	/	CCD	amplifier	gain	slope	times	65535
GAIN9	=	1.522927	/ (CCD	amplifier	gain factor	in (e/ADU	GAINS9	=	0.603137	/	CCD	amplifier	gain	slope	times	65535
GAIN10	=	1.549798	/ (CCD	amplifier	gain factor	in (e/ADU	GAINS10	=	0.615742	/	CCD	amplifier	gain	slope	times	65535
GAIN11	=	1.550713	/ (CCD	amplifier	gain factor	in (e/ADU	GAINS11	=	0.638433	/	CCD	amplifier	gain	slope	times	65535
GAIN12	=	1.558488	/ (CCD	amplifier	gain factor	in (e/ADU	GAINS12	=	0.604920	/	CCD	amplifier	gain	slope	times	65535
GAIN13	=	1.550717	/ (CCD	amplifier	gain factor	in (e/ADU	GAINS13	=	0.625721	/	CCD	amplifier	gain	slope	times	65535
GAIN14	=	1.551005	/ (CCD	amplifier	gain factor	in (e/ADU	GAINS14	=	0.656871	/	CCD	amplifier	gain	slope	times	65535
GAIN15	=	1.561832	/ (CCD	amplifier	gain factor	in (e/ADU	GAINS15	=	0.651176	/	CCD	amplifier	gain	slope	times	65535
GAIN16	=	1.588823	/ (CCD	amplifier	gain factor	in (e/ADU	GAINS16	=	0.637058	/	CCD	amplifier	gain	slope	times	65535
RON1	=	2.242	/ (CCD	amplifier	readout noi	se in	n ADU	RON9	=	2.258	/	CCD	amplifier	reado	out noi	ise in	ADU
RON2	=	2.149	/ (CCD	amplifier	readout noi	se in	n ADU	RON10	=	2.233	/	CCD	amplifier	reado	out noi	ise in	ADU
RON3	=	2.032	/ (CCD	amplifier	readout noi	se in	n ADU	RON11	=	1.810	/	CCD	amplifier	reado	out noi	ise in	ADU
RON4	=	2.149	/ (CCD	amplifier	readout noi	se in	n ADU	RON12	=	2.097	/	CCD	amplifier	reado	ut noi	ise in	ADU
RON5	=	2.112	/ (CCD	amplifier	readout noi	se in	n ADU	RON13	=	2.040	/	CCD	amplifier	reado	ut noi	ise in	ADU
RON6	=	1.972	/ (CCD	amplifier	readout noi	se in	n ADU	RON14	=	2.071	/	CCD	amplifier	reado	ut noi	ise in	ADU
RON7	=	2.178	/ (CCD	amplifier	readout noi	se in	n ADU	RON15	=	2.130	/	CCD	amplifier	reado	out noi	ise in	ADU
RON8	=	2.157	/ (CCD	amplifier	readout noi	se in	n ADU	RON16	=	2.116	/	CCD	amplifier	reado	ut noi	ise in	ADU

The resulting image with extension **bss** will only retain modified **IMASEC** list of keywords to define the position of each amplifier, which may be used later for some other applications (e.g. CCD gain calibration).

What is not shown in the dialog window but used in the Image Processing pipeline is the use of a master bias or dark image specific for a given CCD device. The master images are part of the calibration sequence and comprise a Windsor sum of a large number of exposures (e.g. 300) to minimize readout noise. For the master bias image the exposure time is zero and for the dark is an hour. The dark master image is then scaled with the exposure time to the bias subtracting image.







Figure 2: Shown a fragment of the raw ThAr image where overscan areas in CCD columns (horizontal bands) and CCD rows (vertical band) is visible as well as the gap between spectral orders for 200 μ m fiber with five image slices. The image origin (0,0) is on the top left. Shown the location of each image slicer for the left (SX) and right (DX) sides for target (T) and sky (S). The blue arrow shows the direction of échelle orders increase for the blue and red arms.



Figure 3: Shown bias subtracted and trimmed master flat fields images for the blue CD123 (top) and the red CD456 (bottom).





4.3 Wavelength calibration

The wavelength calibration is performed on the image of standard extraction (std) of the ThAr calibration lamp. The wavelength calibration is part of the Image Processing pipeline which processes the image without user interaction. In order to inspect the quality of the fit or for testing or development purposes it can be opened from Tools menu of the Image Browser or by pressing Alt-W.



Figure 4: A ThAr standard extraction image with extension std for all orders and each slice (here for 130L slicer with nine slices) on the left and the image with extension gss for the Gaussian profile lines fit on the right.

	File Select Ta	ble											
	X B 7 B	Μ Σ 🕥	S						æ	80000			
	order slice	px	ру	wl	res	fwhn	respow	qns	cor A	60000			
	121 4	6894.740	5506.525	5070.7780		4.67		1653	0.9715				
Central wavelength: 611839	121 4	6994.969	5516.282	5071.7534	-3.6250e-01	3.84		329	0.6653	40000			
	121 4	7055.479	5522.045	5072.6288	-2.7385e-04	4.24	141387	915	0.8439	20000			
Development 200420	121 4								0.8613				
Resolving power: 268416	121 4				-4.4769e-01	4.19			0.9976	•			
	121 4	7204.033	5535.784	5074.6465	7.6592e-01	4.00	172067	2517	0.9002				
	121 4	7394.193	5552.526	5075.4659	6.5926e-04	3.62	169191	2624	0.9920				
Num of orders:	121 4					4.47		297	0.8817	<			
	121 4		5578.022	5079.1374		4.52			0.8420				
Num of unuers 00 A	121 4	7716.281	5578.720	5079.1374	1.0326e+00	5.81		838	0.7872	40 0 the	0.0800.00		
Num of waves: 80	121 4	7726.906	5579.538	5079.1374	9.4644e-01	5.14		805	0.8965			200	
	121 4	7781.210	5583.672	5079.1374	5.0723e-01	4.98		705	0.8963	20			8.990 00
EAD: 20 Å	121 4								0.8815	- 67 A22			Contraction and a second s
FAP: 30	121 4								0.8179	o - 1000			
	121 4			5079.1374					0.5282				
Sigma clipping: 1	121 4	8134 116	5608 655	5081 4462	4 41310.04	4 00	161317	14023	0 9981	-20			North States
Sigma cripping: 1	121 4	8283.749	5618.266	5882.6224	3,19420-03	5.52	101517	2058	0.9492				
	122 4	2305.581	4123.736	4985.3725	1.6184e-04	2.46	188212	71178	0.9996	2000			
Tolerance: 10	122 4	2328.389	4128.890	4985.3725	-2.4682e-01	3.56		271	0.9448	2000			
Toterance: 10	122 4	2359.329	4135.859	4985.9486	-5.9933e-04	2.78	167209	2412	0.9704				
	122 4	2369.615	4138.170	4985.9486	-1.1174e-01	2.41			0.9761				
Zoom: 10 A	122 4	2379.320	4140.348	4985.9486	-2.1657e-01	3.62		328	0.9824	50	2 2 . Oak	37.50 12	1 3 2 .
700III. 10 A	122 4		4149.280						0.9232		Sec. 201	1 1 A 1 2	10.000
	122 4				4.5062e-01				0.7953		10.00		
	122 4	2451.330	4156.421	4987.1470	2.1543e-01	3.88	100743	399	0.5309	• - 9	ALC: NO		ALC: LAND
Slice: 4 🔂 All: 🖌 Fit: 🖌	122 4	24/1.489	4168.877	4987.1470	-5.91898-04	2.48	188742	4366	0.9935	688	18.12	an an an an	40.46
	122 4	2589 883	4169.383	4987.5582	6.3219e-04	2.43	192556	3377	0.9947		Sec. 18, 14, 19		1.10110.000
	122 4								0.8500		1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 -	S	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
Order: 121 All: V	122 4	2555.339	4179.378	4987.5582	-4.8684e-01	4.16		60	0.8123	كتصا			
	122 4	2562.653	4180.981	4987.5582	-5.6518e-01	1.86		220	0.7495	2000			
	122 4	2571.204	4182.853	4987.5582	-6.5674e-01	2.34		181	0.6760			<u> </u>	
rms, mA: 0.42 nfree: 4326	122 4		4189.314	4989.3086	7.9157e-01	3.28		183	0.6134	l I I I I I I I I I I I I I I I I I I I			
	122 4	2674.982	4205.406	4989.3086	-3.1259e-04	2.50	189052	28009	0.9991	6			
rms ms: 25 err ms: 2	122 4								0.6472				
11115, 1115. 25 CH, 1115. 2	122 4					9.42			0.7447	°			1. 21. 23
	122 4		4243 896		-4.76010-03				0.0253	4		2 96. Same 9	
	122 4		4246.198	4991.2038					0.9377	1.1			B. B. A.M.
💌 Single 🕥 Multiple	122 4								0.6195	3 E 10 E			A CONTRACTOR OF
	122 4	2912.040	4255.778	4992.1257	3.2714e-01	3.29		143	0.5984	2	a second second		•
	122 4	2943.099	4262.260	4992.1257	-1.6554e-04	2.58	185485	2971	0.9971	• •			
Draiact: papei wava	122 4	2956.863	4265.124	4992.1257	-1.4506e-01	2.30			0.9969	2000			
Project. pepsi.wave	122 4	2966.882	4267.205			3.58		401	0.5637				
	122 4				4.8405e-01	3.28			0.8070				
	122 4	3070.916	4288.647	4993.7488	2.94146-01	4.68	199105	340	0.8367				
Open Locate Seek	122 4	3099.050	4294.394	4993.7400	-3.72098-04	2.00	100105	2212	0.9992				
open cocate ocek	122 4	3133.468	4301.392	4994.1058	-2.3172e-05	2.50	193054	5114	0.9991				
	122 4	3177.650	4310.327	4994.1058	-4.6095e-01	4.50		449	0.8732	2e+05	And a state of the		
Power Focus Wower	122 4	3209.414	4316.716	4995.2981	4.1039e-01	2.34			0.8693				
rocus waves	122 4	3228.640	4320.570	4995.2981	2.1038e-01			329	0.8676			A LAND	
	122 4	3249.003	4324.640	4995.2981	-1.2759e-03	2.83		840	0.9782		N 89 1 1 1 1	1 8 9 9 9	1.5 4 1
	122 4	3297.333	4334.253	4995.2981	-5.0285e-01	2.28		369	0.9268	1e+05		-	
Stop Erase Close									v		4900	5000	\$200
	Record: 1264	3 Ma	rked: 0	Included: (Erase	d: 16742	Tot	al: 21194					

Figure 5: Shown the dialog window (left), the line identification table (middle), and the resulting plots of the wavelength solution (right).

4.3.1 The dialog window

 \Box Central wavelength in Å is the wavelength in the first échelle order in the image center. The value is used as the initial approximation for the wavelength solution and is specific for each spectrograph.





- □ **Resolving power** is used as the initial approximation of the linear dispersion for each order as one half of its inverse value (hence for two CCD pixels). The value is the same for different fibers with various resolving powers and for different CCD binning modes, but specific for each spectrograph
- \Box Num of orders allows to change the central échelle order number within a range e.g. ± 1 of the number given. This may assume that the central order number for the image center is not exact as it can fall exactly between two orders.
- □ Num of waves specifies the swing range in wavelength around the central wavelength. One step is 10 CCD pixels.
- \Box FAP stands for the False Alarm Probability and used for the 3D polynomial fits to reject insignificant polynomial coefficients. Low FAP retains less significant terms and high FAP retains the most significant terms. The integer FAP parameter here is $-\log 10$ of the probability value.
- \Box Sigma clipping defines the separation level between statistical and systematical noises in the resistant statistic in order to mask out outlayers of the fit.
- \Box Tolerance defines the final accepted quality of the fit as the error of the fit in m/s in the image center divided by half of the median FWHM of all line widths, e.g. for an image with two pixels line width FWHM, the tolerance is 10 m/s. This definition makes it invariant for different fibers with various resolving powers (and line widths FWHM) and for different CCD binning modes
- \Box Zoom is the width as the multiple of the line FWHM to display the original line and its Gaussian fit in the window (upper left) when browsing the line identification table.
- \Box Slice displays the resulting fit only for a given slice.
- \Box Order displays the resulting fit only for a given order.
- $\checkmark\,$ All displays the resulting fit for all slices or orders
- \checkmark Fit displays polynomial fit curves to the plot panels of the resulting fit (which may be too dense in some cases).
- ★ The four status boxes show the merit parameters of the fit: rms in mÅ, rms in m/s, number of free parameters, and the error of the fit in the image center in m/s.
- \odot Single or Multiple is to make the wavelength solution for a single image of a number of selected images.
- **Project** opens the file selector window to select another project file. All parameters of this application can be saved into a specific project file and retrieved any time later.
- **Open** opens another image from the Image Browser.
- Locate starts to detect all spectral lines in the image for every slice of each order and make a Gaussian fit to them.
- Seek starts to seek the wavelength solution by swinging around the central wavelength and central order. It starts with a fit of the robust polynomial to the trial wavelength table to select good lines for a slice in all orders, then it proceeds with the resistant 2D polynomial fit to all slices and orders in five stages. The successful fits is saved into a binary file with extension was and the merits of the fit are stored in the FITS header of the file (as in Sec.4.3.4).
- Power creates separate 1D FITS spectra for each slice in all orders of the 3D robust polynomial fit to the resolving power estimate for all spectral lines used in the wavelength solution. These are used for the spectral synthesis to define the instrumental profile FWHM at a given wavelength and for the quality control.





- Focus makes the best focus position for a given slice selected from the series of focusing sequence images for the quality control and is not using or requires the wavelength solution to be made. This auxiliary function makes a 3D robust polynomial fit to FWHM of all lines in the line identification table versus their position in CCD rows, order number, and the focus position of the optical camera. The minimum of the fit for a given CCD row and order number along the focus is the best focus value. The resulting 1D FITS file is saved with extension focus for all orders and 50 equally spaced CCD rows.
- Waves makes wavelength calibrated image (in wavelength scale, wlc) from the ThAr calibration image and slices merged image (mrg).
- **Stop** interrupts processing.
- **Erase** removes all items in the line identification table and erases the polynomial fit.
- Close closes the dialog window.

4.3.2 The line identification table

The table is stored as the FITS binary table with extension wat with its columns described as follows. The lines which are used in the wavelength solution are of the normal state in the Table Browser (i.e. in blue color) and the lines which are rejected to the fit are in erased state (i.e. in light gray color).

order - order number of the line.

slice - slice number of the line.

- px the Gaussian centroid of the line fit in CCD rows.
- py position of the line center in CCD columns from the tracing polynomial fit.

wl - wavelength of the line after wavelength solution.

 ${\tt res}$ - residual of the wavelength fit for a given line in Å which is scaled to the wavelength of the central order.

fwhm - line width in pixels.

respow - resolving power for the line given its FWHM, wavelength, and the dispersion after the fit.

amp - intensity of the line.

cor - correlation coefficient of the line defined by the Gaussian profile fit.

4.3.3 The wavelength solution plots

- 1. The top plot shows the Gaussian profile fit to the line selected in the line identification FITS Table Browser. The width of the plot in CCD rows is controlled by the Zoom multiplier to the line FWHM.
- 2. The wavelength solution fit is the difference in radial velocity (km/s) of the dispersion polynomial of a given order and of the central order of the image. It has a characteristic obtuse trapezoid shape whose orientation depends on the blue or red arm. The horizontal axis is CCD rows.
- 3. The residuals of the fit in radial velocity (m/s) with the error of the fit polynomial overplotted at 3σ level. The horizontal axis is CCD rows.
- 4. FWHM plot in pixels versus CCD rows for all lines used in the fit
- 5. The resolving power estimates for each line used in the fit overplotted with the 3D robust polynomial fit versus wavelength scale.





4.3.4 The wavelength solution merit parameters

The wavelength solution (WAS) merit parameters are saved into the FITS header of the ThAr image and also automatically added as columns of the Browser Table.

WASRMS - rms in m/s

WASERR - fit error in m/s for the image center

WASTOL - tolerance for two pixels in m/s

WASFREE - degrees of freedom

WASTIME - processing elapsed time in sec

WASREP - median resolving power of all lines

WASREQ - resolving power quartile

WASFWHM - median FWHM of spectral lines in pixels

WASFWHQ - FWHM quartile in pixels

CENTRODE - central échelle order number

 ${\tt WASCENT}$ - image center wavelength for the first order at which the wavelength solution was committed

WASREPO - resolving power for two pixels at which the wavelength solution was committed

The last two parameters are also propagated along the dependency tree up to the original raw image, so that in case the image has to be re-processed next time it will have a better initial guess parameters.

If the two parameters WASCENT and WASREPO are not present in the FITS header, the application uses the default parameters from the project file displayed in the dialog window.

In the case the central order number **CENTRODE** has been changed in the wavelength solution, its new value updates the order definition polynomial fit file (**trace**) and saved into the FITS header of the associated tracing flat image and propagated up along the dependency tree.





4.4 Math on images

Image	Polar	CCD		
			Im	age & Constant
۲	Add		C) Subtract
C) Divide		С) Multiply
Co	nst: 0			Make
				Image & Image
C) Add		0) Subtract
۲	Averag	e	0) Divide
C) Multiply		0) RelDiff
C) Variano	e	C) Windsor
C) Inner			
۲	Process	all:	0	In pairs:
0	In time:		0	In sort:
Ex	tension:	avr		Make
			V	/ariance & Mask
	timate SN	IR	O Est	timate variance
O Se	et variance	•	O De	lete variance
O Re	eset mask		O De	lete mask
() A(dd noise		O As	sert noise
0 0	uantile flu:	×		
Vari	ance: 1		< >	Make

- Image & Constant
 - ◎ Add, Subtract, Divide, Multiply selects the function to use.
 - \Box Constant value.
 - Make starts operation on a single or selected images. Division and multiplication also changes the variances of the images. The resulting image is saved with the same name.
- Image & Image
 - $\odot\,$ Add makes a sum of selected images according to the processing mode.
 - Subtract subtracts all selected images in pairs or one image (tagged as Included) from all selected (tagged as Marked).
 - \odot Average makes a weighted average according to the processing mode.
 - ⊙ Divide divides all selected images in pairs or all selected images (tagged as Marked) by one image (tagged as Included).
 - \odot Multiply makes a product of all selected images in pairs or all selected images. .
 - \odot RelDiff makes a relative difference of all selected images in pairs.
- Variance makes the variability image of all selected images.
- \odot Windsor makes the Windsor (trimmed) sum of all selected images (by ignoring the five lowest and five highest values in each pixel).
- Inner makes the inner region of all selected images by selecting the innermost part of these images for testing purposes.
- Process all allows to process all selected images tagged as Marked (with Ins). The common image tagged as Included (with Alt-Ins) is used in the Subtract mode as the image to be subtracted and in the Divide mode as the denominator image.
- \odot In pairs allows to process all selected images tagged as Marked (with Ins) in pairs.
- ◎ In time allows to process all selected images tagged as Marked (with Ins) which are exposured on the same date.
- ◎ In sort allows to process all selected images tagged as Marked (with Ins) according to the sorting criteria, e.g. if sorted by fiber and cross-disperser it will process all images separately with the same combination of the fiber and cross-disperser. It opens the table sort window to make the sorting combination.
- \Box Extension for the resulting image.
- Make starts selected sequence.
- Variance & Mask
 - Estimate SNR processes all selected images and estimates 75% quantile of the signal/noise for all pixels given their intensity and variance. Has sense only for extracted images.
 - \odot Estimate variance processes all selected images and estimates their variances according to Photon statistics with the use of GAIN FITS keyword (CCD gain factor e/ADU) and RON as the readout noise in ADUs.
 - \odot Set variance to a constant value given in the edit window.
 - Delete variance removes image section with the variance matrix.
 - Reset mask changes the image mask values to its normal state.





- \odot Delete mask removes image section with the mask matrix.
- Add noise adds normal noise to each pixel intensity with the variance specified in the edit window.
- ◎ Assert noise replaces each pixel intensity with a mean value averaged in a window with its size specified in the edit window. This is useful for signal/noise estimation of flat field images. Saves the resulting image with extension snr.
- \odot Quantile flux makes a random selection of image pixels and takes the difference between 5% quantiles of the intensities (i.e. 5% smallest and 5% largest). Writes the result into FITS keyword FLUX.

Image	Polar	CCD		
			Polarim	etric reduction 1
Тур	e: Stoke	≥s IQUV	0	Start
	Sub			O Rat
🗌 Ma	ike I±V	🗌 Ma	ake I±Z	🔲 In pairs
			Polarim	etric reduction 2
Ту	pe: Circ	ular 🗘		Stack Start
		🗌 Reta	rder axis	
				Radial velocity
Rad	dvel 1:	OBSVEL		
Rad	dvel 2:	RADVEL		
Exte	nsion:	hwl		Remove
				Unpack spectra
Orders	• •		Stretch	: 0
Rectify	• 0		Rows: (O Unpack
Extens	ion: re	с		

- Polarimetric reduction 1
 - **Type** specifies the expected type of Stokes vector derived.
 - $\odot~{\tt Sub}$ derives Stokes parameters with the difference method
 - $\odot\,$ Rat derives Stokes parameters with the ratio method
 - ✓ Make $I \pm V$ produces additional images where I + V and I V are calculated.
 - ✓ Make $I \pm Z$ produces additional images where I + Z and I Z are calculated, where Z is the null profile.
 - $\checkmark\,$ In pairs processes images in pairs for the two polarization angles.
 - Start processes selected images to derive Stokes *IQUV* parameters and creates separate images for each Stokes parameter with extensions i, q, u, v, and z.
- Polarimetric reduction 2
 - **Type** specifies the expected type of Stokes vector derived.
 - \checkmark Retarder axis specifies the type of the fit.
 - Stack processes selected images to combine them versus polarization optics angle.
 - Start makes a global linear least-squares fit of the polarization modulation function versus angle of the retarder to the data. In case the Retarder axis is included, it performs a non-linear least-squares fit with the retarder axis versus wavelength as a free parameter.





4.5 Image Processing

This menu command opens Image Processing window to start the pipeline manually for e.g. development and testing. The pipeline can be restarted from any point of the Image Processing up to the end. It can take all available images to process or a number of selected images, as well as specific slices (fibers) or cross-dispersers (CD) can be selected.

- Bias subtraction: it uses bias overscan to remove bias offset and trim the image according to the TRIMSEC keyword in the FITS header. Then it uses available master bias or dark CCD image to remove any structure in the bias level. The ADU values in the image are transformed to photoelectrons according to the GAIN factor for each amplifier given in the FITS header and the photon noise is estimated taking into account the slope of the gain factor with ADUs. All these parameters are introduced to the FITS header by the Archon CCD readout software (which is part of the PEPSI control program). Creates image with extension bss.
- Master flat image correction remove CCD pixel-to-pixel noise with the use of a master flat field image which comprises a sum of 300 exposures of the de-focused flat field. The master flat image is not normalized to the blaze function, hence, the processed image will have essentially blaze function removed after division. All science and calibration images are divided by the master flat. Creates image with extension mfc.
- Scattered light subtraction removes any residual flux between spectral orders by using a 2D spline fit with resistant statistics to avoid spectral orders from the fit. Creates image with extension sls.
- Order definition uses special calibration tracing flat field spectra made for each slice separately to define traces for each order and every slice with a 3D polynomial fit. It uses the FITS keyword CENTRODE to define the échelle order number in the image center for each CD and the direction of its increase. This parameter is introduced by the PEPSI control program. Creates polynomial fit files with extension trace.
- Standard extraction of orders applies to the wavelength calibration images with ThAr lamp or Fabry-Perot etalon (FPE). It takes the nearest in time order definition file and uses it for integration of the flux for every order and all slices in each CCD row. It results in the image with the flux integrated for each slice and all orders. Creates image with extension std.
- Wavelength calibration makes the wavelength solution of the extracted ThAr image: first it locates all emission spectral lines and searching for the best fit with the given approximate wavelength in the first order in the image center and the expected resolving power for two pixels (to define the dispersion). Creates several files associated with the wavelength solution having extension was and wat, and the image of the Gaussian fit to the ThAr lines with extension gss.
- Optimal extraction of orders integrates the flux of the science exposure image and its cosmic spikes elimination by constructing spatial profile for each order and every slice. Once it is smoother with a spline it is linearly fitted to the raw data for each CCD row. It results in the image with the flux integrated for each slice and all orders. Creates images with extension opt and spp.
- Wavelength calibration applies the wavelength solution of the associated ThAr image to the optimally extracted image by adding wavelength grid for every slice in all order for each CCD row. It proceeds with merging slices in wavelength scale of the central slice into one spectrum for each spectral order. Creates image with extension wlc and mrg.
- Master flat spectrum correction make the division of the master flat field spectrum which reduced the same way as the science échelle image. This removes any optical fringes and other features common to both images. Creates image with extension ffc.
- Continuum normalization make a low degree 2D polynomial fit to the continuum level of the normalized image by using a resistant statistics to avoid spectral lines from the fit. It proceeds with the constrained least-squares solution to fit the overlapping in wavelength parts of adjacent spectral orders to each other. Creates image with extension con.





- Rectification of spectra creates an 1D spectrum out of the normalized image by averaging overlapping parts of the spectral order with their weights as the inverse variance in each pixel. The wavelength scale is preserved for each spectral order. Creates spectrum with extension rec.
- Continue proceeds with the image processing interrupted as some point. The pipeline starts to resolve all dependencies, i.e. checking that the intermediate files for a given science image exist in every step of image processing. In case the file does not exist, it proceeds at that point for a given science image.



Figure 6: The Image Processing dialog window which stars the reduction pipeline (left). A typical Image Processing printout on a terminal shows the steps involved and the time spent (right).

- ◎ All instructs the pipeline that all science images in the current working directory are to be processed depending on the selection of the check-boxes for the slicers (fibers) and cross-dispersers.
- Selected instructs the pipeline that only selected science images are to be processed (with extension fits).
- \checkmark 100 200 300 200P 100L 130L all or some image slicers can be selected.
- $\checkmark\,$ CD1 CD2 CD3 CD4 CD5 CD6 all or some cross-dispersers can be selected
- **Process** starts image processing from a given step and selection criteria.





- **Prepare** starts processing only calibration images in the working directory and can be used prior to the processing of the science images.
- **Stop** interrupts image processing at any step. To resume the process use **Continue** radio-box in the reduction steps.
- Close closes the image processing window.

4.5.1 Image dependency tree

The Image Processing pipeline creates a number of intermediate files which are used at different stages of the processing. They define the dependencies of the processing flow which means that if the file with a certain extension is absent, the pipeline with continue processing the image at that step.

- fits the original raw image.
- **bss** bias subtracted image.
- mfc image after master flat field image correction.
- **sls** scattered light subtracted image.
- trace an internal binary file with the order definition fit.
- std standard extraction image.
- was an internal binary file with the wavelength solution fit.
- wat an internal FITS binary table where the wavelength solution lines and their positions are stored.
- gss image where the Gaussian fit profiles are stored for wavelength calibration.
- opt optimally extracted image.
- ${\tt spp}$ spatial profile image for optimal extraction.
- wlc wavelength calibrated image.
- mrg image with the slices merged into one order.
- ffc image after master flat field spectrum correction.
- con normalized image after 2D continuum fit.
- rec the resulting 1D spectrum after orders rectification.
- pol2dc, pol2dr, pol2drc polynomial fit images produced at various stages of image processing.

An internal binary file means that it will not appear in the FITS Image Browser. All other regular images will be added to the Browser Table and can be displayed and inspected in the Browser Imager.