

# ONEDSPEC/IMRED Package Revisions Summary: IRAF Version 2.10

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May 1992

## 1. Introduction

The IRAF NOAO spectroscopy software, except for the **longslit** package, has undergone major revisions. The revisions to the aperture extraction package, **apextract**, are described in a separate document. This paper addresses the revisions in the **onedspec** package and the spectroscopic image reduction packages in the **imred** package. In addition to the revisions summary given here there is a new help topic covering general aspects of the new **onedspec** package such as image formats, coordinate systems, and units. This help topic is referenced under the name "onedspec.package".

There are a large number of revisions both minor and major. To avoid obscuring the basic themes and the major revisions in a wealth of minor detail, this document is organized into sections of increasing detail. The most important aspects of the revisions are described in a major highlight section followed by a minor highlight section. Then a reorganization chart for the **onedspec** package is presented showing where various tasks have been moved, which have been deleted, and which are new. Finally, a summary of the revisions to each task is presented.

I hope that the many new capabilities, particularly as presented in the highlight section, will outweigh any disruption in accomodating to so many changes.

## 2. Major Highlights

The major highlights of the revisions to the NOAO spectroscopy software are listed and then discussed below.

- Non-linear dispersion calibration
- Integration of dispersion coordinates with the core system
- Sinc interpolation
- Plotting in user selected units including velocity
- Integration of long slit spectra and 1D formats
- New **imred** packages featuring streamlined reductions

Possibly the most significant revision is the generalization allowing non-linear dispersion calibration. What this means is that spectra do not need to be interpolated to a uniform sampling in wavelength or logarithmic wavelength. The dispersion functions determined from calibration arc lines by **identify**, **reidentify**, **ecidentify**, or **ecreidentify** can be simply assigned to the spectra and used throughout the package. It is also possible to assign a dispersion table or vector giving the wavelengths at some or all of the pixels. Note, however, that it is still perfectly acceptable to resample spectra to a uniform linear or log-linear dispersion as was done previously.

For data which does not require geometric corrections, combining, or separate sky subtraction the observed sampling need never be changed from the original detector sampling, thus avoiding any concerns over interpolation errors. In other cases it is possible to just interpolate one spectrum, say a sky spectrum, to the dispersion of another spectrum, say an object spectrum, before operating on the two spectra. There are several new tasks that perform interpolations to a common dispersion, not necessarily linear, when operating on more than one spectrum. In particular, the new

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<sup>††</sup>Operated by the Association of Universities for Research in Astronomy, Inc. under cooperative agreement with the National Science Foundation.

task **sarith** and the older task **splot** now do arithmetic on spectra in wavelength space. Thus, one no longer need be concerned about having all spectra interpolated to the same sampling before doing arithmetic operations as was the case previously.

The trade-off in using non-linear dispersion functions is a more complex image header structure. This will make it difficult to import to non-IRAF software or to pre-V2.10 IRAF systems. However, one may resample to a linear coordinate system in those cases before transferring the spectra as FITS images having standard linear coordinate keywords.

On the subject of interpolation, another important addition is the implementation of sinc interpolation. This is generally considered the best interpolation method for spectra, however, it must be used with care as described below. Sinc interpolation approximates applying a phase shift to the fourier transform of the spectrum. Thus, repeated interpolations do not accumulate errors (or nearly so) and, in particular, a forward and reverse interpolation will recover the original spectrum much more closely than other interpolation methods. However, for undersampled (where the fourier transform is no longer completely represented), strong features, such as cosmic rays or narrow emission or absorption lines, the ringing can be much more severe than the polynomial interpolations. The ringing is especially a concern because it extends a long way from the feature causing the ringing; 30 pixels with the truncated algorithm that has been added. Note that it is not the truncation of the interpolation function which is at fault but the under-sampling of the narrow features!

Because of the problems seen with sinc interpolation it should be used with care. Specifically, if there are no under-sampled, narrow features it is a good choice but when there are such features the contamination of the spectrum by ringing is more severe, corrupting more of the spectrum, than with other interpolation types.

The dispersion coordinates are now interfaced through the IRAF WCS (world coordinate system) interface. This is important to users for two reasons. First, operations performed on spectral images by IRAF core system tasks and the IRAF image I/O system will have access to the dispersion coordinates and will properly modify them as necessary. The most common such operation is applying an image section to a spectrum either during an image copy or as input to another task. In this case the relation between the pixels in the image section and their wavelengths is preserved. For example one may **splot** a section of a large spectrum and get the correct wavelengths. The second reason is to allow use of proper dispersion coordinates in such IRAF tasks as **listpixels**, **implot**, and **graph**.

The new package supports a variety of spectral image formats. The older formats are understood when reading them. In particular the one dimensional "onedspec" and the two dimensional "multispec" format will still be acceptable as input. Note that the image naming syntax for the "onedspec" format using record number extensions is a separate issue and is still provided but only in the **imred.iids** and **imred.irs** packages. Any new spectra created are either a one dimensional format using relatively simple keywords and a two or three dimensional format which treats each line of the image as a separate spectrum and uses a more complex world coordinate system and keywords. For the sake of discussion the two formats are still called "onedspec" and "multispec" though they are not equivalent to the earlier formats.

In addition, the one dimensional spectral tasks may also now operate on two dimensional images directly. This is done by using the DISPAXIS keyword in the image header or a package dispaxis parameter if the keyword is missing to define the dispersion axis. In addition there is a summing parameter in the packages to allow summing a number of lines or columns. If the spectra are wavelength calibrated long slit spectra, the product of the **longslit.transform** task, the wavelength information will also be properly handled. Thus, one may use **splot** or **specplot** for plotting such data without having to extract them to another format. If one wants to extract one dimensional spectra by summing columns or lines, as opposed to using the more complex **apextract** package, then one can simply use **scopy** (this effectively replaces **proto.toonedspec**).

The tasks **splot** and **specplot** allow use of and changes between various dispersion units. Spectra may be plotted in units all the way from Hertz to Mev. The units may also be inverted to plot in wavenumbers, such as inverse centimeters, and the decimal log may be applied, to plot something like log wavelength or log frequency. One special "unit" which is available is a velocity computed about a specified wavelength/frequency. The multiple unit capability was one of the last major changes made before the V2.10 release so the complete generalization to arbitrary units has not been completed. Dispersion calibration and image world coordinate system generally must still be done in Angstroms, particularly if flux calibration is to be done. The generalization to other units throughout the package is planned for a later release.

The last of the changes categorized as a major highlight is the addition of a number of special packages for generic or specific types of instruments and data in the **imred** package. Most of these package include a highly streamlined reduction task that combines all of the reduction operations into a single task. For example, the **spectred.doslit** task can extract object, standard star, and arc spectra from long slit images, apply a consistent dispersion function based on only a single interactively performed dispersion solution, compute a sensitivity function and end up with flux calibrated spectra. Another example, is **hydra.dohydra** for extracting, flatfielding, dispersion calibrating, and sky

subtracting spectra from the NOAO Hydra multifiber spectrograph. There are user's guides for each of these new reduction tasks.

### 3. Minor Highlights

There are some further highlights which are also quite important but which are secondary to the previous highlights. These are listed and discussed below.

- Greater use of package parameters
- An observatory database
- A more flexible **identify/reidentify**
- Only one **dispcor**
- Spatial interpolation of dispersion solutions
- Deblending of arbitrary number of gaussian components
- Manipulating spectral formats
- Improved fitting of the continuum and related features
- Various new tasks

There is an even greater use of package parameters than in the previous release. Package parameters are those which are common to many of the the tasks in the package and which one usually wants to change in one place. The new package parameters are the default observatory for the data if the observatory is not identified in the image header (discussed further below), the interpolation type used when spectra need to be resampled either for dispersion calibration or when operating on pairs of spectra with different wavelength calibration, and the default dispersion axis and summing parameters for long slit and general 2D images (as discussed in the last section). You will find these parameters not only in the **onedspec** package but in all the spectroscopic packages in the **imred** package.

A number of spectroscopic tasks require information about the location of the observation. Typically this is the observatory latitude for computing air masses if not defined in the header. Radial velocity tasks, and possible future tasks, may require additional information such as longitude and altitude. The difficulty is that if such parameters are specified in parameter files the default may well be inappropriate and even if the users set them once, they may forget to update them in later reductions of data from a different observatory. In other words this approach is prone to error.

To address this concern observatory parameters are now obtained from an observatory database keyed by an observatory identifier. If the image data contains an observatory keyword, **OBSERVAT**, the tasks will look up the required parameters from the observatory database. Thus, if the images contain the observatory identifier, as does data from the NOAO observatories, they will always be correctly reduced regardless of the setting of any parameters. Of course one has to deal with data from observatories which may not include the observatory identifier and may not have an entry in the observatory database. There are provisions for sites and individual users to define local database files and to set the default observatory parameters. This is all discussed in the help for the **observatory** task.

The dispersion function fitting tasks **identify** and **reidentify** have been improved in a number of important ways. These tasks now treat the input images as units. So for long slit and multispectrum images one can move about the image with a few keystrokes, transfer solutions, and so on. When transferring solutions between a multispectrum reference image and another multispectrum image with the same apertures using **reidentify**, the features and dispersion solutions are transferred aperture by aperture. This avoids problems encountered by having to trace successively between apertures and having the apertures be in the same order.

On the subject of tracing in **reidentify**, in some cases it is desirable to use the same reference spectrum with all other sampled lines or columns in a long slit spectrum or apertures in a multispectrum image rather than propagating solutions across the image. The latter method is necessary if there is a continuous and progress shift in the features. But if this is not the situation then the loss of features when tracing can be a problem. In this case the alternative of reidentifying against the same starting reference is now possible and there will not be the problem of an increasing loss of features. On the other hand, the problem of lost features, whether tracing or not, can also be addressed using another new feature of **reidentify**, the ability to add features from a line list. For both tracing and nontracing reidentifications, another useful new feature is automatic iterative rejection of poorly fitting lines in determining a new dispersion function noninteractively.

The nontracing reidentifications, the automatic addition of new lines, and the iterative rejection of poorly fitting lines in determining a new dispersion function are all responses to make the reidentification process work better without intervention. However, as a last resort there is also a new interactive feature of **reidentify**. By monitoring the log output of the reidentification process one can have a query be made after the automatic reidentification and function

fitting to allow selectively entering the interactive feature identification and dispersion function fitting based on the logged output. Thus if a fit has a particularly large RMS or a large number of features are not found one can choose to intervene in the reidentification process.

Dispersion calibration is now done exclusively by the task **dispcor** regardless of the spectrum format or dispersion solution type; i.e. solutions from **identify** or **ecidentify**. In addition to allowing assignment of non-linear dispersion functions, as described earlier, **dispcor** has other new features. One is that, in addition to interpolating dispersion solutions between two calibration images (usually weighted by time), it is now possible to interpolate zero point shifts spatially when multiple spectra taken simultaneously include arc spectra. This is mostly intended for the new generation of multifiber spectrographs which include some fibers assigned to an arc lamp source. However, it can be used for the classic photographic case of calibration spectra on the same plate.

The limitation to four lines on the number of gaussian components which can be deblended by the deblending option in **splot** has been removed. A new feature is that line positions may be input from a line list as well as the original cursor marking or terminal input. In addition an option to simultaneously determine a linear background has been added. As a spinoff of the deblending option a new, noninteractive task, called FITPROFS, has been added. This task takes a list of initial line positions and sigmas and simultaneously fits gaussians with a linear background. One can constrain various combination of parameters and output various parameters of the fitting. While it can be used to fit an entire spectrum it becomes prohibitively slow beyond a number like 30. A banded matrix approach is required in that case.

As mentioned earlier there is a new task called **scopy** for manipulating spectra. It allows changing between various formats such as producing the separate, simple keyword structure, one dimensional images from multispec format images, combining multiple one dimensional spectra into the more compact multispec format, and extracting line or column averaged one dimensional spectra from two dimensional images. It can also be used to select any subset of apertures from a multispec format, merge multiple multispec format spectra, and extract regions of spectra by wavelength.

The **continuum** task has been revised to allow independent continuum fits for each aperture, order, line, or column in images containing multiple spectra. Instead of being based on the **images.fit1d** task it is based on the new task **sfit**. **Sfit** allows fitting the **icfit** functions to spectra and outputting the results in several ways such as the ratio (continuum normalization), difference (continuum subtraction), and the actual function fit. In addition it allows outputting the input data with points found to be deviant by the iterative rejection algorithm of **icfit** replaced by the fitted value. This is similar to **images.lineclean**. In all cases, this may be done independently and interactively or noninteractively when there are multiple spectra in an image.

A number of useful new tasks have already been mentioned: **fitprofs**, **sarith**, **scombine**, **scopy**, and **sfit**. There are two more new tasks of interest. The task **dopcor** applies doppler shifts to spectra. It applies the shift purely to the dispersion coordinates by adding a redshift factor which is applied by the coordinate system interface. This eliminates reinterpolation and preserves both the shift applied and the original observed dispersion function (either linear or nonlinear). The task can also modify the pixel values for various relativistic and geometric factors. This task is primarily useful for shifting spectra at high redshifts to the local rest frame. The second new task is called **deredden**. It applies corrections for interstellar reddening given some measure of the extinction along the line of sight.

#### 4. ONEDSPEC Package Task Reorganization

The **onedspec** package dates back to the earliest versions of IRAF. Some of its heritage is tied to the reduction of IRS and IIDS spectra. One of the revisions made for this release has been to reorganize the various tasks and packages. A few tasks have been obsoleted by new tasks or the functionality of the new dispersion coordinate system, a number of new tasks have been added, and a number of IRS and IIDS specific tasks have been moved to the **imred** packages for those instruments. While these packages are organized for those particular instruments they may also be used by data having similar characteristics of beam switching, coincidence corrections, and the requirement of sequential numeric extensions.

The table below provides the road map to the reorganization showing tasks which have disappeared, been moved, been replaced, or are new.

V2.9	V2.10	ALTERNATIVE	V2.9	V2.10	ALTERNATIVE
addsets		irs/iids	process		irs/iids
batchred		irs/iids	rebin		scopy/dispcor
bplot	bplot		refspectra	refspectra	
bswitch		irs/iids	reidentify	reidentify	
calibrate	calibrate		sapertures		
coincor		iids	sarith		
combine		scombine	scombine		
continuum	continuum		scopy		
	deredden		sensfunc	sensfunc	
dispcor	dispcor		setdisp		hedit
	dopcor		sextract	scopy	
	fitprofs		sfit		
flatdiv		irs/iids	sflip		scopy/imcopy [-*,*]
flatfit		irs/iids	shedit		hedit
identify	identify		sinterp	sinterp	
lcalib	lcalib		slist	slist	
mkspec	mkspec		specplot	specplot	
names	names		splot	splot	
	ndprep		standard	standard	
observatory		noao	subsets		irs/iids
powercor		iids	sums		irs/iids

## 5. IMRED Packages

Many of the **onedspec** tasks from the previous release have been moved to the **iids** and **irs** packages, as indicated above, since they were applicable only to these and similar instruments.

A number of new specialized spectroscopic instrument reduction packages have been added to the **imred** package. Many of these have been in use in somewhat earlier forms in the IRAF external package called **newimred**. In addition the other spectroscopic package have been updated based on the revisions to the **onedspec** and **apextract** packages. Below is a table showing the changes between the two version and describing the purpose of the spectroscopic packages. Note that while many of these package are named for and specialized for various NOAO instruments these packages may be applied fairly straightforwardly to similar instruments from other observatories. In addition the same tools for multifiber and slit spectra are collected in a generic package called **specred**.

V2.9	V2.10	SPECTROSCOPY PACKAGE
	argus	Fiber: CTIO Argus Reductions
specphot	ctioslit	Slit: CTIO Slit Instruments
echelle	echelle	Fiber Slit: Generic Echelle
	hydra	Fiber: KPNO Hydra (and Nessie) Reductions
iids	iids	Scanner: KPNO IIDS Reductions
irs	irs	Scanner: KPNO IRS Reductions
coude	kpnocoude	Fiber/Slit: KPNO Coude (High Res.) Reductions
	kpnoslit	Slit: KPNO Slit Instruments
msred	specred	Fiber/Slit: Generic fiber and slit reductions
observatory	-> noao	
setairmass		

An important feature of most of the spectroscopic packages are specialized routines for combining and streamlining the different reduction operations for a particular instrument or type of instrument. These tasks are:

argus.doargus	ctioslit.doslit	echelle.doeclit
echelle.dofoe	hydra.dohydra	iids.batchred
irs.batchred	kpnocoude.do3fiber	kpnocoude.doslit
kpnoslit.doslit	specred.dofibers	specred.doslit

## 6. ONEDSPEC Task Revisions in V2.10

### ADDSETS

Moved to the **iids/irs** packages.

### BATCHRED

Moved to the **iids/irs** packages.

### BPLOT

The APERTURES and BAND parameters been added to select apertures from multiple spectra and long slit images, and bands from 3D images. Since the task is a script calling **splot**, the many revisions to that task also apply. The version in the **iids/irs** packages selects spectra using the record number extension syntax.

### BSWITCH

Moved to the **iids/irs** packages.

### CALIBRATE

This task was revised to operate on nonlinear dispersion corrected spectra and 3D images (the **apextract** "extras"). The aperture selection parameter was eliminated (since the header structure does not allow mixing calibrated and uncalibrated spectra) and the latitude parameter was replaced by the observatory parameter. The observatory mechanism insures that if the observatory latitude is needed for computing an airmass and the observatory is specified in the image header the correct calibration will be applied. The record format syntax is available in the **iids/irs** packages. The output spectra are coerced to have real pixel datatype.

### COINCOR

Moved to the **iids** package.

### COMBINE

Replaced by **scombine**.

### CONTINUUM

This task was changed from a script based on **images.fit1d** to a script based on **sfit**. This provides for individual independent continuum fitting in multiple spectra images and for additional flexibility and record keeping. The parameters have been largely changed.

### DEREDDEN

This task is new.

### DISPCOR

This is a new version with many differences. It replaces the previous three tasks **dispcor**, **edispcor** and **msdispcor**. It applies both one dimensional and echelle dispersion functions. The new parameter **LINEARIZE** selects whether to interpolate the spectra to a uniform linear dispersion (the only option available previously) or to assign a nonlinear dispersion function to the image without any interpolation. The interpolation function parameter has been eliminated and the package parameter **INTERP** is used to select the interpolation function. The new interpolation type "sinc" may be used but care should be exercised. The new task supports applying a secondary zero point shift spectrum to a master dispersion function and a spatial interpolation of the shifts when calibration spectra are taken at the same time on a different region of the same 2D image. The optional wavelength table may now also be an image to match dispersion parameters. The APERTURES and REBIN parameters have been eliminated. If an input spectrum has been previously dispersion corrected it will be resampled as desired. Verbose and log file parameters have been added to log the dispersion operations as desired. The record format syntax is available in the **iids/irs** packages.

### DOPCOR

This task is new.

### FITPROFS

This task is new.

### FLATDIV

Moved to the **iids/irs** packages.

#### FLATFIT

Moved to the **iids/irs** packages.

#### IDENTIFY

The principle revision is to allow multiple aperture images and long slit spectra to be treated as a unit. New keystrokes allow jumping or scrolling within multiple spectra in a single image. For aperture spectra the database entries are referenced by image name and aperture number and not with image sections. Thus, **identify** solutions are not tied to specific image lines in this case. There is a new autowrite parameter which may be set to eliminate the save to database query upon exiting. The new colon command "add" may be used to add features based on some other spectrum or arc type and then apply the fit to the combined set of features.

#### LCALIB

This task has a more compact listing for the "stars" option and allows paging a list of stars when the star name query is not recognized.

#### MKSPEC

This task is unchanged.

#### NAMES

This task is unchanged.

#### NDPREP

This task was moved from the **proto** package. It was originally written at CTIO for CTIO data. It's functionality is largely unchanged though it has been updated for changes in the **onedspec** package.

#### OBSERVATORY

New version of this task moved to **noao** root package.

#### POWERCOR

Moved to the **iids** package.

#### PROCESS

Moved to the **iids/irs** package.

#### REBIN

This task has been eliminated. Use **scopy** or **dispcor**.

#### REFSPECTRA

A group parameter was added to allow restricting assignments by observing period; for example by night. The record format option was removed and the record format syntax is available in the **iids/irs** packages.

#### REIDENTIFY

This task is a new version with many new features. The new features include an interactive options for reviewing identifications, iterative rejection of features during fitting, automatic addition of new features from a line list, and the choice of tracing or using a single master reference when reidentifying features in other vectors of a reference spectrum. Reidentifications from a reference image to another image is done by matching apertures rather than tracing. New apertures not present in the reference image may be added.

#### SAPERTURES

This task is new.

#### SARITH

This task is new.

#### SCOMBINE

This task is new.

#### SCOPY

This task is new.

#### SENSFUNC

The latitude parameter has been replaced by the observatory parameter. The 'i' flux calibrated graph type now shows flux in linear scaling while the new graph type 'l' shows flux in log scaling. A new colon command allows fixing the flux limits for the flux calibrated graphs.

#### SETDISP

This task has been eliminated. Use **hedit** or the package DISPAXIS parameter.

#### SEXTRACT

Replaced by **scopy**.

#### SFIT

This task is new.

#### SFLIP

This task has been eliminated. Use image sections.

#### SHEDIT

This task has been eliminated. Use **hedit** if needed.

#### SINTERP

This task is unchanged.

#### SLIST

This task was revised to be relevant for the current spectral image formats. The old version is still available in the **iids/irs** package.

#### SPECPLOT

New parameters were added to select apertures and bands, plot additional dimensions (for example the additional output from the extras option in **apextract**), suppress the system ID banner, suppress the Y axis scale, output a logfile, and specify the plotting units. The PTYPE parameter now allows negative numbers to select histogram style lines. Interactively, the plotting units may be changed and the 'v' key allows setting a velocity scale zero point with the cursor. The new version supports the new spectral WCS features including nonlinear dispersion functions.

#### SPLOT

This is a new version with a significant number of changes. In addition to the task changes the other general changes to the spectroscopy packages also apply. In particular, long slit spectra and spectra with nonlinear dispersion functions may be used with this task. The image header or package dispaxis and nsum parameters allow automatically extracting spectra from 2D image. The task parameters have been modified primarily to obtain the desired initial graph without needing to do it interactively. In particular, the new band parameter selects the band in 3D images, the units parameter selects the dispersion units, and the new histogram, nosysid, and xydraw options select histogram line type, whether to include a system ID banner, and allow editing a spectrum using different endpoint criteria.

Because nearly every key is used there has been some shuffling, consolidating, or elimination of keys. One needs to check the run time '?' help or the help to determine the key changes.

Deblending may now use any number of components and simultaneous fitting of a linear background. A new simplified version of gaussian fitting for a single line has been added in the 'k' key. The old 'k', 'h', and 'v' equivalent width commands are all part of the single 'h' command using a second key to select a specific option. The gaussian line model from these modes may now be subtracted from the spectrum in the same way as the gaussian fitting. The one-sided options, in particular, are interesting in this regard as a new capability.

The arithmetic functions between two spectra are now done in wavelength with resampling to a common dispersion done automatically. The 't' key now provides for the full power of the ICFIT package to be used on a spectrum for continuum normalization, subtraction, or line and cosmic ray removal. The 'x' editing key may now use the nearest pixel values rather than only the y cursor position to replace regions by straight line segments. The mode is selected by the task option parameter "xydraw".

Control over the graph window (plotting limits) is better integrated so that redrawing, zooming, shifting, and the **gtools** window commands all work well together. The new 'c' key resets the window to the full spectrum allowing the 'r' redraw key to redraw the current window to clean up overplots from the gaussian fits or spectrum editing.

The dispersion units may now be selected and changed to be from hertz to Mev and the log or inverse (for wave numbers) of units taken. As part of the units package the 'v' key or colon commands may be used to plot in velocity relative to some origin. The \$ key now easily toggles between the dispersion units (whatever they may be) and pixels coordinates.

Selection of spectra has become more complex with multiaperture and long slit spectra. New keys allow selecting apertures, lines, columns, and bands as well as quickly scrolling through the lines in multiaperture spectra. Overplotting is also more general and consistent with other tasks by using the 'o' key to toggle the next plot to be overplotted. Overplots, including those of the gaussian line models, are now done in a different line type.

There are new colon commands to change the dispersion axis and summing parameters for 2D image, to toggle logging, and also to put comments into the log file.

#### STANDARD

Giving an unrecognized standard star name will page a list of standard stars available in the calibration directory and then repeat the query.



SUBSETS

Moved to the **iids/irs** packages.

SUMS

Moved to the **iids/irs** packages.