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Representations of spectral coordinates in FITS

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Abstract. In Paper I, Greisen & Calabretta (2002) describe a generalized method for specifying the coordinates of FITS data samples. Following that general method, Calabretta & Greisen (2002) describe detailed conventions for defining celestial coordinates as they are projected onto a two-dimensional plane. The present paper extends the discussion to the spectral coordinates of wavelength, frequency, and velocity. World coordinate functions are defined for spectral axes sampled evenly in wavelength, frequency, or velocity, evenly in the logarithm of wavelength or frequency, as projected by ideal dispersing elements, and as specified by a lookup table.

Key words. Methods: data analysis – Techniques: image processing – Techniques: radial velocities – Techniques: spectroscopic – Astronomical data bases: miscellaneous

1. Introduction

The present manuscript is the third in a series of papers intended to establish a clear method by which information about the physical coordinates of FITS data may be transferred along with the binary image, random groups, and table data. In "Paper I" Greisen & Calabretta (2002) describe a revised method for transferring coordinate information in the FITS header and outline some rules governing the values assigned to the new standard header keywords. In "Paper II" Calabretta & Greisen (2002) specify the conventions necessary to define celestial coordinates in a two-dimensional projection of the sky. In this paper, the parameters and conventions needed to specify spectral information including frequency, wavelength, and velocity are defined. In addition to these basic conversions, a world coordinate function is defined to describe ideal optical dispersers of several standard types. In "Paper IV", Calabretta et al. (2002) specify methods to describe the distortions inherent in the image coordinate systems of real astronomical data.

Paper I describes the computation of the world or physical coordinates as a multi-step process. The vector of pixel offsets from the reference point is multiplied by a linear transformation matrix and then scaled to physical units. Mathematically, this is given by

$$x_i = s_i \; q_i = s_i \sum_{j=1}^{N} m_{ij} \; \left(p_j - r_j\right) , \qquad (1)$$

where p_j are pixel coordinates, r_j are pixel coordinates of the reference point given by `CRPIX`j, m_{ij} is a linear transformation matrix given either by `PC`i`_`j or `CD`i`_`j, N is the dimensionality of the WCS representation given by `WCSAXES`, and s_i is a scaling given either by `CDELT`i or by 1.0.

The final step in the computation is the conversion of these linear relative coordinates into the actual physical coordinates. The conventions to be applied to spectral axes, i.e. to frequency, wavelength, and velocity axes, are described in this paper.

2. Coordinate definition

At this stage in the discussion, we consider the spectral world coordinate at the reference point on all other axes. This covers the relatively simple case in which the spectral world coordinate is not dependent on the other world coordinates. Methods to describe deviations from this assumption due to the choice of spectral reference system are discussed in Sect. 7, while instrumental distortions are discussed briefly in Sect. 9 and, in more detail, in Paper IV.

Spectral coordinates are commonly given in units of frequency, wavelength, velocity, and other parameters proportional to these three. The coordinate types discussed here are then frequency, wavelength, and Doppler relativistic velocity denoted by the symbols ν, λ, and v. There are also three conventional "velocities" frequently used in astronomy. These are the so-called "radio" velocity, "optical" velocity, and redshift, denoted here by V, Z, and z. The velocities are defined so that an object that is receding from the observer has a positive ve-

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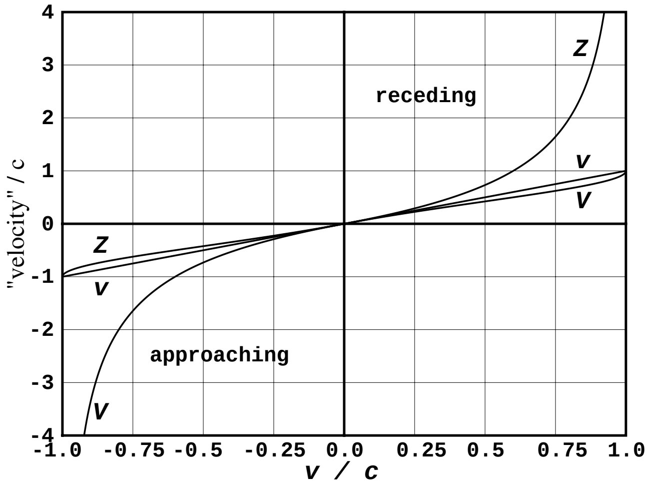


Fig. 1. Conventional velocities as function of physical velocity. The functional forms of Z and V reflect each other through the origin. Large approaching velocities may occur for relativistic jets beamed toward the Earth.

locity. The "velocities" V and Z are plotted with respect to v in Fig. 1.

For the purposes of this section and the next, we consider those spectral axes at a single celestial coordinate that are linearly sampled in wavelength, frequency, or true velocity. The radio and optical "velocities" are directly proportional to frequency and wavelength, respectively, and thus do not constitute additional cases for the type of sampling. Frequency and wavelength axes may also be regularly sampled in their logarithm. Wavelengths are sometimes given "in air" rather than in vacuum, a non-linear distinction that is discussed in Sect. 4. Frequency may also be described in energy (= $h\nu$) units and in Kaysers ("wave number" = $1/\lambda$) units.

As described in Papers I and II, the first four characters of `CTYPE`*ka*[1] specify the coordinate type, the fifth character is `'-'` and the next three characters specify a predefined algorithm for computing the world coordinates from intermediate physical coordinates. When k is the spectral axis, the first four characters shall be one of the codes shown in Table 1. The mathematical symbols we will use for the codes, the non-linear algorithm with which they are associated, and their default units are also listed. The IAU-standard prefixes for scaling the units are described in Paper I and should be used with all coordinate types, except that the dimensionless ones are not scaled.

The non-linear algorithm in use is described by the final 3 characters of `CTYPE`*ka*. The first of the three characters specifies the physical parameter type in which the data are regularly sampled and the third character specifies the physical parameter type in which the coordinate is expressed. This is summarized in Table 2. When the algorithm in use is linear, the last four characters of `CTYPE`*ka* shall be blanks. For logarithmic axes, defined in Sect. 3.2, the last four characters shall be `'-LOG'`. The original FITS paper by Wells, Greisen, & Harten (1981) contained a number of suggestions for the values of `CTYPE`*i*. Those suggestions are to be replaced by the conventions of this manuscript and of Papers I and II.

The relationships between the basic physical quantities ν, λ, and v are shown in Table 3. The relationships between the derived quantities and the basic quantities with which they are associated are shown in Table 4. Derivatives are included in both tables since they will be needed in the coordinate computation.

[1] While Papers I and II use the generic intermediate axis number i, we use here the axis number k as the spectral intermediate axis number. The single-character version code a was introduced in Paper I. It has values blank and `A` through `Z`.

Table 1. Spectral coordinate type codes.

Code	Name	Symbol	Assoc.	Default units
`FREQ`	Frequency	ν	ν	Hz
`ENER`	Energy	E	ν	J
`WAVN`	Wavenumber	σ	ν	m^{-1}
`VRAD`	Radio velocity	V	ν	$\mathrm{m\,s}^{-1}$
`WAVE`	Vacuum wavelength	λ	λ	m
`VOPT`	Optical velocity	Z	λ	$\mathrm{m\,s}^{-1}$
`ZOPT`	Redshift	z	λ	–
`AWAV`	Air wavelength	λ_a	λ_a	m
`VELO`	Relativistic velocity	v	v	$\mathrm{m\,s}^{-1}$
`BETA`	Beta factor (v/c)	β	v	–

Table 2. Non-linear algorithm codes.

Code	Regularly sampled in	Expressed as
`F2W`	Frequency	Wavelength
`F2V`	Frequency	Velocity
`F2A`	Frequency	Air wavelength
`W2F`	Wavelength	Frequency
`W2V`	Wavelength	Velocity
`W2A`	Wavelength	Air wavelength
`V2F`	Velocity	Frequency
`V2W`	Velocity	Wavelength
`V2A`	Velocity	Air wavelength
`A2F`	Air wavelength	Frequency
`A2W`	Air wavelength	Wavelength
`A2V`	Air wavelength	Velocity

3. Basic coordinate computation

This section describes the computation of coordinates with are sampled linearly or logarithmically in a coordinate of similar type and of coordinates which are sampled linearly in a coordinate of different type. The intermediate world coordinate for spectral axis k, given by Eq. (1), will be denoted, for convenience, by

$$w \equiv x_k \,. \tag{2}$$

The final world coordinate will be denoted by S. At the reference point, it has the value S_r, which is denoted by the keyword `CRVAL`*ka*.

3.1. Linear coordinates

Linear coordinates are represented in `CTYPE`*ka* by characters 1-4 containing any code in column one of Table 1 and characters

Table 3. Basic spectral transformation equations.

$\nu = \frac{c}{\lambda}$	(5)	$\frac{d\nu}{d\lambda} = -\frac{c}{\lambda^2}$	(6)
$\nu = \nu_0 \frac{c - v}{\sqrt{c^2 - v^2}}$	(7)	$\frac{d\nu}{dv} = -\frac{c\nu_0}{(c+v)\sqrt{c^2 - v^2}}$	(8)
$\lambda = \frac{c}{\nu}$	(9)	$\frac{d\lambda}{d\nu} = -\frac{c}{\nu^2}$	(10)
$\lambda = \lambda_0 \frac{c + v}{\sqrt{c^2 - v^2}}$	(11)	$\frac{d\lambda}{dv} = \frac{c\lambda_0}{(c-v)\sqrt{c^2 - v^2}}$	(12)
$v = c\frac{\nu_0^2 - \nu^2}{\nu_0^2 + \nu^2}$	(13)	$\frac{dv}{d\nu} = -\frac{4c\nu\nu_0^2}{(\nu^2 + \nu_0^2)^2}$	(14)
$v = c\frac{\lambda^2 - \lambda_0^2}{\lambda^2 + \lambda_0^2}$	(15)	$\frac{dv}{d\lambda} = \frac{4c\lambda\lambda_0^2}{(\lambda^2 + \lambda_0^2)^2}$	(16)

5-8 blank. The world coordinate value for spectral axis k is computed with the above definitions and Eq. (1) as

$$S = S_r + w\,. \quad (3)$$

3.2. Log-linear coordinates

Spectra are sometimes sampled in logarithmic increments of wavelength or frequency. With this type of sampling the source motion, expressed as V, Z, or z, shifts the "pixel" coordinates of spectral features by the same amount over the whole image. This allows relative velocities between spectra to be determined using cross-correlation methods in the pixel arrays.

There are only three log-linear coordinates allowed, namely `FREQ-LOG`, `WAVE-LOG` and `AWAV-LOG`. The other combinations one could envision, such as velocity units for a log of wavelength axis or even log of velocity, are not used in astronomy because they are not needed or have little physical meaning. Many of the combinations are also intractable mathematically. The three allowed combinations are evaluated simply by

$$S = 10^{S_r + w}\,. \quad (4)$$

Users of this data form must be careful with units. The units of the reference coordinate and scale keywords given by `CRVAL`*ka*, `CDELT`*ka*, and `CD`*k_ja* are specified by the `CUNIT`*ka* keyword as defined in Paper I. These quantities are in log units such as `'log(Hz)'` for `FREQ-LOG` and `'log(m)'` for `WAVE-LOG`. The prefixes and alternate units described in Paper I may be used, such as `'log(MHz)'` and `'log(Angstrom)'`. However, the units of the final world coordinates produced by Eq. (4) are in linear units, e.g., `Hz` and `m`. Therefore, users should not directly use `CUNIT`*ka* to label or described the units of the world coordinates

3.3. General non-linear coordinates

We now consider the case where an axis is linearly sampled in spectral variable X but is to be expressed in terms of variable S.

Table 4. Extended spectral transformation equations.

$\nu = \nu_0(1 - \frac{V}{c})$	(17)	$\frac{d\nu}{dV} = -\frac{\nu_0}{c}$	(18)
$V = c\frac{\nu_0 - \nu}{\nu_0}$	(19)	$\frac{dV}{d\nu} = -\frac{c}{\nu_0}$	(20)
$\nu = E/h$	(21)	$\frac{d\nu}{dE} = 1/h$	(22)
$E = h\nu$	(23)	$\frac{dE}{d\nu} = h$	(24)
$\nu = c\sigma$	(25)	$\frac{d\nu}{d\sigma} = c$	(26)
$\sigma = \nu/c$	(27)	$\frac{d\sigma}{d\nu} = 1/c$	(28)
$\lambda = \lambda_0(1 + \frac{Z}{c})$	(29)	$\frac{d\lambda}{dZ} = \frac{\lambda_0}{c}$	(30)
$Z = c\frac{\lambda - \lambda_0}{\lambda_0}$	(31)	$\frac{dZ}{d\lambda} = \frac{c}{\lambda_0}$	(32)
$\lambda = \lambda_0(1 + z)$	(33)	$\frac{d\lambda}{dz} = \lambda_0$	(34)
$z = \frac{\lambda - \lambda_0}{\lambda_0}$	(35)	$\frac{dz}{d\lambda} = \frac{1}{\lambda_0}$	(36)
$v = c\beta$	(37)	$\frac{dv}{d\beta} = c$	(38)
$\beta = v/c$	(39)	$\frac{d\beta}{dv} = 1/c$	(40)

Given the large number of spectral variables in Table 1 it is clear that there are very many pairwise combinations; in general, the relationship between any pair may be non-linear. However, each of the spectral variables in Table 1 is linearly related to one or other of ν, λ, λ_a, or v. Thus we may restrict X to one of these four basic variables.

Even with this restriction on X there are still many possible combinations of X and S. In order to reduce the number still further we introduce an intermediate variable, denoted by P, which is the basic variable, ν, λ, λ_a, or v, with which S is associated via a linear relation. This associate variable is listed for each spectral variable in column 4 of Table 1.

Table 3 lists the equations, $X = X(P)$, and their inverses, $P = P(X)$, linking the basic spectral types ν, λ, and v (discussion of λ_a is deferred to Sect. 4). These equations are generally non-linear. Likewise, Table 4 lists the linear relations, $S = S(P)$, and their inverses, $P = P(S)$, linking each spectral variable with its associate. When S is one of the basic types, ν, λ, λ_a, or v, then $P \equiv S$ and $S(P)$ is identity.

Thus the functional relationship between S and X is specified via intermediate variable P as $S(X) = S(P(X))$ with inverse $X(S) = X(P(S))$. Since $S(P)$ is linear, P and X must always differ, otherwise $P(X)$ would be identity with the result that $S(X)$ would be linear, contrary to the assumption of a non-linear axis.

Non-linear spectral coordinate codes are constructed on this basis by combining the spectral coordinate type code for S from Table 1 with the non-linear spectral algorithm code in Table 2. The first letter of the algorithm code defines X as `F`requency, `W`avelength, `A`ir wavelength, or `V`elocity, and the third letter likewise defines P. For example, in `ZOPT-F2W`, X is `F`requency, P is `W`avelength, and the non-linear conversion between the two (`F2W`) is defined in Table 3. The desired spectral coordinate S is redshift (`ZOPT`), and this is related to associate variable P, the `W`avelength, by the linear equation given in Table 4.

It is apparent from the foregoing that it is possible to construct invalid spectral coordinate codes. For example, `ZOPT-F2V` is unrecognized since z is associated with λ, not v. That is not to say that this code could not be interpreted in principle, after all, equations linking z and v could have been included in Table 4; simply that it is not recognized in practice. The associate variable, P, was introduced in the first place to reduce the possible number of combinations and adding new ones like this would defeat that purpose. This is particularly relevant to the software implementation; `ZOPT-F2V` tells software to chain its $\nu - v$ function with a $v - z$ function but, in general, the latter function will not have been defined.

Consider now the computation of spectral coordinate S for an axis that is linearly sampled in X. The statement that an axis is linearly sampled in X simply means that

$$X = X_{\mathrm{r}} + w\,\frac{\mathrm{d}X}{\mathrm{d}w}\,, \tag{41}$$

where $\mathrm{d}X/\mathrm{d}w$ is constant. This constant is determined by imposing the requirement that

$$\left.\frac{\mathrm{d}S}{\mathrm{d}w}\right|_{\mathrm{r}} = 1\,, \tag{42}$$

so that Eq. (3) is satisfied to first order at points near the reference point:

$$S \approx S_{\mathrm{r}} + w\,. \tag{43}$$

Thus

$$\frac{\mathrm{d}X}{\mathrm{d}w} = \left.\frac{\mathrm{d}P}{\mathrm{d}S}\right|_{\mathrm{r}} \Big/ \left.\frac{\mathrm{d}P}{\mathrm{d}X}\right|_{\mathrm{r}}\,. \tag{44}$$

Given that the functions $S = S(P)$ and $P = P(X)$ are known, as are their inverses $X = X(P)$ and $P = P(S)$, then the equation for S as a function of w may be obtained from Eqs. (41) and (44)

$$S(w) = S\left(P\left(X(P(S_{\mathrm{r}})) + w \left.\frac{\mathrm{d}P}{\mathrm{d}S}\right|_{\mathrm{r}} \Big/ \left.\frac{\mathrm{d}P}{\mathrm{d}X}\right|_{\mathrm{r}}\right)\right)\,, \tag{45}$$

where S_{r} is given by `CRVAL`ka.

Equation 45 suggests a three-step algorithm chain:

1. Compute X at w using Eq. (41); $X_{\mathrm{r}} = X(P(S_{\mathrm{r}}))$ and $\mathrm{d}X/\mathrm{d}w$ are constants which need be computed once only, the latter from Eq. (44).
2. Compute P from X using the appropriate equations from Table 3.
3. Compute S from P using the appropriate equations from Table 4.

The inverse computation by which the intermediate coordinate w is computed for a given value of S is effected by traversing the algorithm chain in the reverse direction. The inverse equations required are all listed in Tables 3 and 4. The inverse of Eq. (41) is, trivially,

$$w = (X - X_{\mathrm{r}}) \Big/ \frac{\mathrm{d}X}{\mathrm{d}w}\,. \tag{46}$$

3.3.1. Example non-linear calculation

As an example of a non-linear coordinate computation, consider a `ZOPT-F2W` axis. `F` in the `F2W` code indicates that the axis is linearly sampled in frequency, but it is to be expressed in terms of redshift as indicated by the spectral coordinate type of `ZOPT`. Table 1 indicates that redshift is associated with wavelength, hence the `W` in `F2W` is correct. Of the X, P, and S variables in the preceding section, the axis is linear in frequency so X is ν, the associated variable is wavelength, so P is λ, and the required variable is redshift, so S is z.

Since `CRVAL`ka for the `ZOPT-F2W` axis would be recorded as a redshift, z_{r}, this must first be converted to frequency by applying Eqs.(33),

$$\lambda_{\mathrm{r}} = \lambda_0(1 + z_{\mathrm{r}})$$

and (5),

$$\begin{aligned}\nu_{\mathrm{r}} &= \frac{c}{\lambda_{\mathrm{r}}}\\ &= \frac{c}{\lambda_0(1 + z_{\mathrm{r}})}\,.\end{aligned}$$

This provides X_{r} for Eq. (41). Then $\mathrm{d}\nu/\mathrm{d}w$ (i.e. $\mathrm{d}X/\mathrm{d}w$) is obtained from Eqs. (34) & (10) evaluated at the reference point:

$$\begin{aligned}\frac{\mathrm{d}\nu}{\mathrm{d}w} &= \left.\frac{\mathrm{d}\lambda}{\mathrm{d}z}\right|_{\mathrm{r}} \Big/ \left.\frac{\mathrm{d}\lambda}{\mathrm{d}\nu}\right|_{\mathrm{r}}\\ &= \lambda_0 \Big/ \frac{-c}{\nu_{\mathrm{r}}^2}\\ &= \frac{-c}{\lambda_0(1 + z_{\mathrm{r}})^2}\,.\end{aligned}$$

Redshift may now be computed for any given value of w. The first step is to compute ν (i.e. X) at w using Eq. (41):

$$\nu = \nu_{\mathrm{r}} + w\,\frac{\mathrm{d}\nu}{\mathrm{d}w}\,.$$

In this instance w will be a redshift. Then λ (i.e. P) may be computed from ν using Eq. (9) from Table 3:

$$\lambda = c/\nu\,.$$

The third and final step is to compute z (i.e. S) from λ using Eq. (35) from Table 4:

$$z = \frac{\lambda - \lambda_0}{\lambda_0}\,.$$

It is also possible to combine the three steps into a single equation, although there are many pair-wise combinations of

Table 5. Sample non-linear coordinate combinations.

`FREQ-W2F`	$\nu = \left(\dfrac{\nu_r}{\nu_r - w}\right)\nu_r$	(47)			
`VELO-W2V`	$v = c\,\dfrac{A_\lambda^2 - 1}{A_\lambda^2 + 1}$	(48)	where $A_\lambda \equiv \dfrac{c^2 - v_r^2 + cw}{(c - v_r)\sqrt{c^2 - v_r^2}}$	(49)	
`VRAD-W2F`	$V = \dfrac{V_r(c - V_r) + cw}{c - V_r + w}$	(50)			
`WAVE-F2W`	$\lambda = \left(\dfrac{\lambda_r}{\lambda_r - w}\right)\lambda_r$	(51)			
`VELO-F2V`	$v = c\,\dfrac{A_\nu^2 - 1}{A_\nu^2 + 1}$	(52)	where $A_\nu \equiv \dfrac{c^2 - v_r^2 - cw}{(c + v_r)\sqrt{c^2 - v_r^2}}$	(53)	
`VOPT-F2W`	$Z = \dfrac{Z_r(c + Z_r) + cw}{c + Z_r - w}$	(54)			
`ZOPT-F2W`	$z = \dfrac{z_r(1 + z_r) + w}{1 + z_r - w}$	(55)			
`WAVE-V2W`	$\lambda = \lambda_0\sqrt{\dfrac{1 + B_\lambda}{1 - B_\lambda}}$	(56)	where $B_\lambda \equiv \dfrac{\lambda_r^4 - \lambda_0^4 + 4\lambda_0^2\lambda_r w}{(\lambda_0^2 + \lambda_r^2)^2}$	(57)	
`FREQ-V2F`	$\nu = \nu_0\sqrt{\dfrac{1 - B_\nu}{1 + B_\nu}}$	(58)	where $B_\nu \equiv \dfrac{\nu_0^4 - \nu_r^4 - 4\nu_0^2\nu_r w}{(\nu_0^2 + \nu_r^2)^2}$	(59)	
`VOPT-V2W`	$Z = c\left(\sqrt{\dfrac{1 + D_Z}{1 - D_Z}} - 1\right)$	(60)	where $D_Z \equiv \dfrac{Y_Z^4 - 1 + 4Y_Z w/c}{(1 + Y_Z^2)^2}$	(61)	with $Y_Z \equiv 1 + Z_r/c$ (62)

spectral variables and for some the combined equations may be quite cumbersome. For the sake of illustration, consider the above equations for the `ZOPT-F2W` axis. Eq. (41) becomes

$$\nu = \frac{c}{\lambda_0(1 + z_r)} - \frac{cw}{\lambda_0(1 + z_r)^2}.$$

Substituting this in the equations for λ and z and simplifying we obtain

$$z = \frac{z_r(1 + z_r) + w}{1 + z_r + w}.$$

A representative sample of these direct translation equations is shown in Table 5. They are useful in showing the nature of the coordinate non-linearity.

One thing to notice about the equations of Table 5 is that the meaning of w differs for each. For example, Eq. (54) may not be obtained from Eq. (55) simply by multiplying both sides by c: in Eq. (55) w is a redshift (`ZOPT`), whereas in Eq. (54) it is an optical velocity (`VOPT`).

3.3.2. Coordinate parameters

Aside from `CRVAL`*ka*, the coordinate computations of Sect. 3.3 require one extra parameter when evaluating the `F2V`, `V2F`, `W2V`, `V2W`, `A2V`, and `V2A` non-linear algorithms, namely the rest frequency or wavelength of the spectral-feature of interest. These are fundamental physical parameters so, rather than use the `PV`*i_ma* parameters defined in Paper I which would tend to disguise them, the special floating-valued keywords

`RESTFRQ`*a* (floating-valued),

and

`RESTWAV`*a* (floating-valued),

are hereby reserved for the purpose. Their units are `'Hz'` and `'m'` respectively, fixed to save having additional keywords to define them. `RESTWAV`*a* is for wavelengths in vacuum only. One or other of these keywords must be included for the above-mentioned algorithm codes, usually `RESTFRQ`*a* would be given for `F2V` and `V2F`, and `RESTWAV`*a* for the others. FITS writers should always write one or other of these when it is meaningful to do so, even for algorithm codes such as `F2W` or `W2A` which do not require them.

Keyword `RESTFREQ` has been used in previous FITS files and should be recognized as equivalent to `RESTFRQ`.

4. Air wavelengths

The wavelengths so far discussed are measured in vacuum. However, dispersion coordinates for UV, optical, and IR spectra at $\lambda > 200$ nm are commonly given as wavelengths in air. The relative difference between the two varies between 0.028% and 0.032% across this range. To identify wavelengths measured in dry air at standard temperature and pressure rather than in vacuo, we introduce the coordinate type `AWAV` for which the reference value and increment must be expressed accordingly.

The two measures of wavelength are related by

$$\lambda = n(\lambda_a)\lambda_a, \tag{63}$$

where λ is the wavelength in vacuum, λ_a is the wavelength in air, and $n(\lambda_a)$ is the index of refraction of dry air at standard temperature and pressure. This varies non-linearly with wavelength, the standard relation given by Cox (2000) is

$$n(\lambda_a) = 1 + 6432.8 \times 10^{-8} + \frac{2949810}{146 \times 10^8 - \sigma_a^2} + \frac{25540}{41 \times 10^8 - \sigma_a^2}, \tag{64}$$

where $\sigma_a = 1/\lambda_a$ is the wave number in cm^{-1}. This formula suffices for conversions from air to vacuum when no more than eight-figure accuracy is required (Peck & Reeder, 1972). The derivative, which may be required in Eq. (44), is

$$\frac{\mathrm{d}\lambda}{\mathrm{d}\lambda_a} = n - 2\sigma_a^2 \left(\frac{2949810}{(146 \times 10^8 - \sigma_a^2)^2} + \frac{25540}{(41 \times 10^8 - \sigma_a^2)^2} \right). \tag{65}$$

While the inversion of Eq. (64) is algebraically intractable, the vacuum wavelength may be used to evaluate Eq. (64) since it differs so little from the air wavelength. The resulting error in the index of refraction amounts to $1 : 10^9$, and this is less than than the accuracy of the empirical formula. Thus,

$$\lambda_a = \lambda / n(\lambda). \tag{66}$$

As usual, an axis that is linearly sampled and expressed in air wavelengths is described with a `CTYPE`*ka* of `'AWAV    '` and evaluated with Eq. (3).

Algorithm codes for the non-linear conversions are `A2F`, `A2W`, `A2V`, and their complements, `F2A`, `W2A`, and `V2A` as listed in Table 2. Use of the three-step procedure described in Sect. 3.3 would require λ_a as a function of each of the other spectral variables, together with their inverses and derivatives. Thus it is much simpler to handle air wavelengths as a separate, extra step in the algorithm chain. For example, to compute world coordinates for `VRAD-A2V`, the value of `CRVAL`*ka* would first have to be converted from radio velocity to air wavelengths via Eqs. (17), (9), and (66), and $\mathrm{d}\lambda_a/\mathrm{d}w$ for Eq. (44) would be obtained from Eqs. (18), (10), and (65). Then, the value of λ_a computed for w via Eq. (41) would be transformed to vacuum wavelengths via Eq. (63), and then to radio velocity via Eqs. (5) and (19).

5. Dispersed spectra

One common form of spectral data is produced by imaging the light from a *disperser*. The wavelengths of the light at some position in the image are related to the position and wavelength of the light in the field of view illuminating the disperser; the relation is defined by the physics of the disperser. In general the light received at a pixel in the detector is a superposition of different wavelengths from different points in the field of view. However, if the field of view is limited spatially, usually by aperture masks and fiber optics, each pixel receives light from only a small range of wavelengths. It is then possible to define a world coordinate function relating pixel position and effective wavelength. This is the basis of many astronomical spectrographs.

In the following section we use the physical relation applicable to the dispersers commonly used in astronomical spectrographs to define a world coordinate function for computing spectral coordinates. The relation applies to the simple, though common, case of single dispersers. More complex spectrographs with multiple dispersers, such as those using multiple passes through prisms, is not described by the methods of this section. Alternatives to using this ideal world coordinate function, based on the physics of dispersers, are the table lookup described in section 6 and empirical function fits provided by the the distortion function mechanism described in Paper IV.

We require that the dispersion occurs along just one direction on the detector and that the intermediate coordinates are computed so that only one world coordinate axis corresponds to wavelength. Paper IV describes how distortions and effects of the aperture shape can be removed to satisfy this requirement. The distortion correction is also used to remove aberrations causing departures from the ideal physical behavior of the dispersers assumed here.

The dispersers we consider are *gratings*, *prisms*, and *grisms*, which are a combination of a prism with a grating within or on the surface of the prism. Gratings may be reflecting or transmissive and may be fabricated with surface relief rulings, holographic surface relief patterns, and holographic volume phase patterns. In the discussion we use the terms *grooves*, *lines* and *ruling* to refer to the periodic diffraction structures that produce the interference. By combining the two physical equations for interference and refraction a single world coordinate function covers all these cases with appropriate choice of parameters.

5.1. The grism coordinate function

This section defines a world coordinate function using the basic laws of refraction and interference. It is beyond the scope of this discussion to give the full background for the laws and concepts underlying dispersive spectroscopy. Of the many texts on the subject, a standard reference is *Astronomical Optics* by Schroeder (1999).

Spectroscopic dispersers are based on interference and refraction effects which are naturally described in terms of wavelength. Moreover, they are most often used in the regime where wavelength is commonly the spectral coordinate. For these reasons the grism function is defined in terms of wavelength. The function assumes that the all the dispersion occurs at one place. This is why combinations of dispersers, other than a single grism, are not described by this function. This assumption means that for prisms and grisms the function is rigorously correct only when the light enters perpendicular to the face of the prism and the grating is at the exit face. However, even when these conditions are not exactly met the function may still be a good approximation with slight adjustments of the parameters.

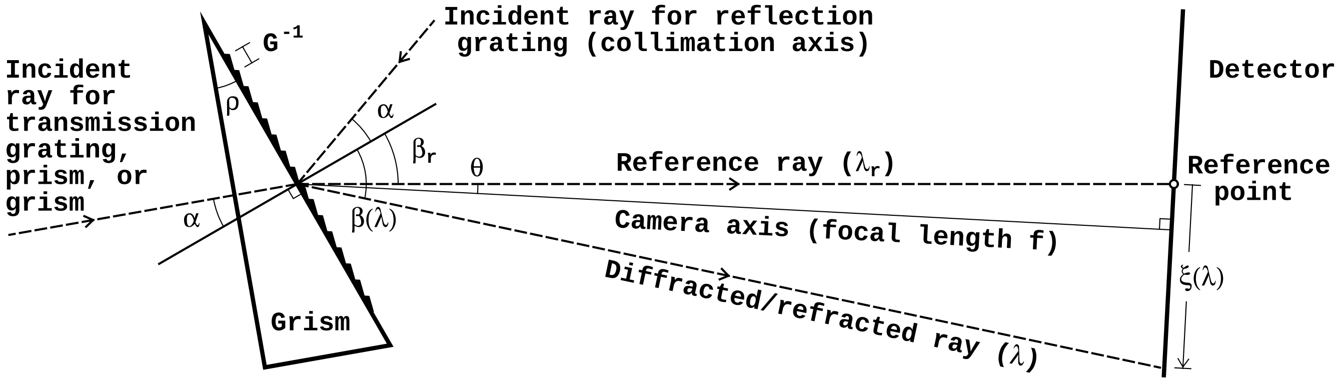


Fig. 2. Geometry of gratings, prisms, and grisms. This simplified representation omits the collimation and focusing optics. Dashed lines mark ray paths in the plane of the figure – the "dispersion plane". The normal to the grating/exit prism face and the normal to the detector plane are each projected onto the dispersion plane, and angles α, β, and θ are measured with respect to these projected normals. Usually the incident ray for a prism or grism is perpendicular to the entry face so that α is equal to the prism angle, ρ. Angle β is wavelength-dependent, and consequently so is the offset ξ in the dispersion direction on the detector. The intermediate spectral world coordinate, w, is proportional to ξ. Reference wavelength λ_r follows the reference ray defined by β_r and illuminates the reference point at $w = \xi = 0$. The normal to the detector plane is shown tilted by angle θ from the reference ray though typically this angle is zero. The grating spacing G^{-1} is indicated.

5.1.1. The grism equation

The basic physical relationship between the wavelength, λ, the angle of incidence of the light, α, and the diffracted/refracted angle, β (not to be confused with the velocity ratio of Table 1), is given by a combination of the grating interference equation and Snell's law of refraction:

$$\frac{Gm\lambda}{\cos\epsilon} = n(\lambda)\sin\alpha + \sin\beta\,, \tag{67}$$

where G is the grating ruling density, m is the interference order, and $n(\lambda)$ is the wavelength-dependent index of refraction of the prism material. For a pure prism the order m is zero and for a reflection or transmission grating $n(\lambda)$ is the unit function. The plane containing α and β is the *dispersion plane*, illustrated in Fig. 2, and the angles are measured relative to the projection in the dispersion plane of the normal to the grating or exit prism face. Usually the normal does lie in the dispersion plane, but small values of ϵ, the angle between the normal and the dispersion plane, are sometimes used for instrumental design reasons.

By convention, the angles of incidence and diffraction/refraction are measured *from* the normal *to* the beam and α is always measured positive in the anticlockwise direction. The sign changes on either side of the normal and this determines the sign of β. Thus, for the reflection grating in Fig. 2, $\alpha > 0$ and $\beta < 0$, and vice versa for a transmission grating, prism, or grism.

Reflection grating geometry is sometimes defined by the angle ϕ measured from the camera axis to the collimator axis and the tilt t of the bisector relative to the grating normal. If ϕ and t obey the same sign convention as α, then $\alpha = \phi/2 + t$.

In spectrographs with prisms or grisms the requirement that the incident light be normal to the prism entry face means that α is equal to the prism angle (ρ in Fig. 2). Even for oblique entry, identifying α with the prism angle is often a good initial approximation.

The requirement that the diffraction and refraction occur at one point means that α is fixed and independent of wavelength. The variation of β with wavelength then defines the relation between wavelength and position ξ on the detector. The reference wavelength λ_r is the wavelength at the reference point corresponding to the zero point of ξ and the intermediate spectral world coordinate w.

The prism's dispersive power derives from the variation of its index of refraction with wavelength. While this variation depends on the material and is generally non-linear, it is sufficient to approximate it by a first-order Taylor expansion about the reference wavelength, λ_r:

$$n(\lambda) \approx n_r + n'_r(\lambda - \lambda_r)\,, \tag{68}$$

where we have written n_r as a shorthand for $n(\lambda_r)$, and likewise n'_r for $\mathrm{d}n/\mathrm{d}\lambda|_r$. Combining Eqs. (67) and (68) yields the grism equation

$$\lambda = \frac{(n_r - n'_r\lambda_r)\sin\alpha + \sin\beta}{Gm/\cos\epsilon - n'_r\sin\alpha}\,, \tag{69}$$

where the denominator must not be zero, though Gm, n'_r, and α may be zero in different types of spectrographs.

In order to define a world coordinate function we need λ as a function of the intermediate world coordinate, w, which is proportional to ξ. Since Eq. (69) gives λ as a function of β it remains to determine the relationship between β and ξ. First note that Eq. (69) evaluated at $\lambda = \lambda_r$ provides

$$\beta_r = \sin^{-1}\left(Gm\lambda_r/\cos\epsilon - n_r\sin\alpha\right)\,, \tag{70}$$

the exit angle of the reference ray for which $w = \xi = 0$, as in Fig. 2.

Figure 2 shows an angle θ which is measured from the reference ray to the camera axis using the same sign convention as β, i.e. if β is clockwise-positive as for a grism then so is θ. Normally θ would be zero, but it is included here to provide a small correction. Depending on the sign convention for β, simple geometry for a flat detector gives

$$\beta = \beta_r + \theta + \tan^{-1}(\pm\xi/f - \tan\theta)\,, \tag{71}$$

where f is the effective focal length of the camera. The plus sign is taken when the sign convention for β is such that ξ increases as β increases, and the minus sign otherwise. Section 5.1.3 discusses the resolution of this potential sign ambiguity.

5.1.2. GRI coordinate axes

In keeping with the preceding sections we wish to define general grating, prism, and grism world coordinate representations such as WAVE-GRI, FREQ-GRI, etc.

Bearing in mind that the grism equation, Eq. (69), is expressed in terms of wavelength, then given a FREQ-GRI axis, for example, it would be straightforward to convert the reference frequency, ν_r, given by CRVALk, from frequency to wavelength via $\lambda = c/\nu$. However, it would not be valid to convert the intermediate spectral world coordinate, w, from frequency to wavelength like this because it is not a true frequency. While it may be a close approximation near the reference point it deviates at points away from it.

Thus, interpretation of an axis such as FREQ-GRI necessarily involves a procedure similar to that of Sect. 3.3, and to apply that methodology we need a parameter, the *grism parameter*, Γ, that is a known function of the spectral variables and for which the axis is linearly sampled; this will substitute for X in Eq. (41). Since ξ is proportional to w

$$\xi = \kappa w\,, \tag{72}$$

where κ is a constant. Combining this with Eq. (71) we have

$$\tan(\beta - \beta_r - \theta) = -\tan\theta \pm w\kappa/f\,. \tag{73}$$

Thus the grism parameter may be identified as

$$\Gamma = \tan(\beta - \beta_r - \theta)\,, \tag{74}$$

and this satisfies Eq. (41) at the reference point:

$$\Gamma_r = -\tan\theta. \tag{75}$$

The grism parameter has a simple geometrical interpretation in Fig. 2; it is the offset on the detector from the point of intersection of the camera axis measured in units of the effective focal length, f.

Following Sect. 3.3 (with X replaced by Γ), we have

$$\Gamma = \Gamma_r + w\frac{\mathrm{d}\Gamma}{\mathrm{d}w} \tag{76}$$

where $d\Gamma/dw$ is constant:

$$\frac{\mathrm{d}\Gamma}{\mathrm{d}w} = \left.\frac{\mathrm{d}\Gamma}{\mathrm{d}P}\right|_r \left.\frac{\mathrm{d}P}{\mathrm{d}S}\right|_r \left.\frac{\mathrm{d}S}{\mathrm{d}w}\right|_r\,. \tag{77}$$

As before, S is the spectral variable in which the axis, and hence w, is expressed, and P is the basic variable, ν, λ, λ_a, or v, with which S is most closely associated. Recognized spectral variables and their associates are listed in Table 1. When S is one of the basic types, ν, λ, λ_a, or v, as is often the case, then $P \equiv S$ whence $\mathrm{d}P/\mathrm{d}S|_r = 1$.

As previously, we require that CDELTi or CDi_j be set so that

$$\left.\frac{\mathrm{d}S}{\mathrm{d}w}\right|_r = 1 \tag{78}$$

(exactly how this is done is addressed in Sect. 5.1.3). Since we only have Γ directly in terms of β we may use

$$\left.\frac{\mathrm{d}\Gamma}{\mathrm{d}P}\right|_r = \left.\frac{\mathrm{d}\Gamma}{\mathrm{d}\lambda}\right|_r \left.\frac{\mathrm{d}\lambda}{\mathrm{d}P}\right|_r\,, \tag{79}$$

where $\mathrm{d}\Gamma/\mathrm{d}\lambda|_r$ itself may be deduced from the derivatives of Eqs. (74) & (69):

$$\begin{aligned}\left.\frac{\mathrm{d}\Gamma}{\mathrm{d}\lambda}\right|_r &= \left.\frac{\mathrm{d}\Gamma}{\mathrm{d}\beta}\right|_r \Big/ \left.\frac{\mathrm{d}\lambda}{\mathrm{d}\beta}\right|_r \\ &= \frac{Gm/\cos\epsilon - n'_r\sin\alpha}{\cos\beta_r\cos^2\theta}\,.\end{aligned} \tag{80}$$

Combining Eqs. (77) to (80) we have

$$\frac{\mathrm{d}\Gamma}{\mathrm{d}w} = \frac{Gm/\cos\epsilon - n'_r\sin\alpha}{\cos\beta_r\cos^2\theta} \left.\frac{\mathrm{d}\lambda}{\mathrm{d}P}\right|_r \left.\frac{\mathrm{d}P}{\mathrm{d}S}\right|_r\,, \tag{81}$$

where $\mathrm{d}\lambda/\mathrm{d}P|_r$ and $\mathrm{d}P/\mathrm{d}S|_r$ come from Tables 3 & 4 respectively. In the common case where S, and hence P, is wavelength then $\mathrm{d}\lambda/\mathrm{d}P|_r$ and $\mathrm{d}P/\mathrm{d}S|_r$ are both unity.

The foregoing provides everything needed to compute Γ from w, and this forms the first step of a five-step algorithm chain for computing S from w:

1. Compute Γ at w using Eq. (76). Γ_r and $\mathrm{d}\Gamma/\mathrm{d}w$ are constants which need be computed once only; Γ_r from Eq. (75) and $\mathrm{d}\Gamma/\mathrm{d}w$ from Eq. (81) using the appropriate equations from Tables 3 & 4.
2. Compute β from Γ using the inverse of Eq. 74:
$$\beta = \tan^{-1}(\Gamma) + \beta_r + \theta\,. \tag{82}$$
3. Compute the wavelength λ from β via Eq. (69).
4. Compute P from λ using the appropriate equation from Table 3.
5. Compute S from P using the appropriate equation from Table 4.

If S, and hence P, is wavelength then the last two steps are no-ops.

As usual, the inverse computation is effected by traversing the algorithm chain in the reverse direction. The inverse equations required for the backward steps have already been given except that for Eq. (69):

$$\begin{aligned}\beta = {} & \sin^{-1}(\lambda(Gm/\cos\epsilon - n'_r\sin\alpha) - \\ & (n_r - n'_r\lambda_r)\sin\alpha)\,,\end{aligned} \tag{83}$$

and also the inverse of Eq. (76) which is trivial.

Grism parameters required for these calculations are provided by the PVi_ma keywords defined in Table 6, with β_r given by Eq. (70), and λ_r computed from the coordinate reference value, CRVALk, by the appropriate equations from Tables 3 & 4. Default values for missing parameters are also defined in the table. Generally only the first three parameters will appear for gratings and the first five for grisms.

Table 6. Grism parameters, their default values, and units.

Keyword	Default	Units
PVk_0a = G	0	m^{-1}
PVk_1a = m	0	
PVk_2a = α	0	degrees
PVk_3a = n_r	1	
PVk_4a = n'_r	0	m^{-1}
PVk_5a = ϵ	0	degrees
PVk_6a = θ	0	degrees

5.1.3. Determination of the grism scale

A question raised above was how CDELTi or CDi_j may be set by a WCS composer so that $\mathrm{d}S/\mathrm{d}w|_\mathrm{r} = 1$.

¿From Eqs. (1) & (2)

$$w = s_k q_k \tag{84}$$

so

$$\begin{aligned} s_k &= \frac{\mathrm{d}w}{\mathrm{d}q_k} \\ &= \left.\frac{\mathrm{d}w}{\mathrm{d}S}\right|_\mathrm{r} \left.\frac{\mathrm{d}S}{\mathrm{d}P}\right|_\mathrm{r} \left.\frac{\mathrm{d}P}{\mathrm{d}\lambda}\right|_\mathrm{r} \left.\frac{\mathrm{d}\lambda}{\mathrm{d}q_k}\right|_\mathrm{r} . \end{aligned} \tag{85}$$

Now, $\mathrm{d}w/\mathrm{d}S|_\mathrm{r} = 1$ by design, $\mathrm{d}S/\mathrm{d}P|_\mathrm{r}$ and $\mathrm{d}P/\mathrm{d}\lambda|_\mathrm{r}$ come from Tables 4 & 3 respectively, and $\mathrm{d}\lambda/\mathrm{d}q_k|_\mathrm{r}$ is the wavelength dispersion (e.g. in nm/pixel) measured at the reference point and this is an instrumental parameter. Thus we have everything needed to compute s_k. When S is wavelength, then all but the last factor in Eq. (85) is unity, and $s_k = \mathrm{d}\lambda/\mathrm{d}q_k|_\mathrm{r}$.

It is the correct choice of sign for $\mathrm{d}\lambda/\mathrm{d}q_k|_\mathrm{r}$ that resolves the sign ambiguity in Eq. (73).

5.1.4. GRA: grisms in air

Thus far we have ignored the distinction between vacuum and air wavelengths in the discussion of grism world coordinates. In fact, the λ variable that appears in the grism equation may be either, and in general $n(\lambda)$ in Eq. (67) is the index of refraction of the prism material with respect to the surrounding medium, either air or vacuum.

If the dispersion takes place in vacuum, as it does, for example, in a spectrograph on a spacecraft, then the grism equation is correct for vacuum wavelengths; if in air, it is correct for air wavelengths and λ in Sects. 5.1.1, 5.1.2, and 5.1.3 should be replaced everywhere by λ_a. Then as discussed in Sect. 4, the computation of quantities such as $\mathrm{d}\lambda_\mathrm{a}/\mathrm{d}P|_\mathrm{r}$ in Eq. 81 is best handled by using the vacuum wavelength, λ, as an intermediary, effectively introducing an extra step into the algorithm chain.

In order to distinguish between grisms operated in air and in vacuum we hereby reserve the use of GRI exclusively for vacuum operation and introduce GRA for operation in dry air at standard temperature and pressure.

Note that for real spectrographs operated in air at an observatory, the actual wavelength system that GRA describes is for air at the local conditions. The coordinate value and increment at the reference point are normally adjusted to the values at standard conditions during calibration. If the accuracy of the wavelength measurement requires it, any further correction between wavelength at local conditions and wavelength at standard conditions may be accomplished via the methods of Paper IV.

5.2. AWAV-GRA examples

This section illustrates application of the GRA world coordinate function with three real-world examples of spectral images from Kitt Peak National Observatory (KPNO) spectrographs. Each spectrum is of an arc calibration lamp which produces emission lines of known wavelength. The position of each line in the image along the spectral world coordinate axis is measured by centroiding on the spectral line profile and identified with the known rest wavelength to create a list of pixel positions and wavelengths.

Each example figure shows plots of the positions and wavelengths for a particular spectrograph. The pixel positions are plotted along the bottom axis. Rather than plot the wavelengths directly, where it would be difficult to see the shape of the curve, the difference or correction between the known (air) wavelengths and the simple linear world coordinate function 'AWAV   ' ($\lambda = S_\mathrm{r} + w$) are shown. The corrections are plotted along the left axes. In these examples the wavelength units are consistently Ångstroms.

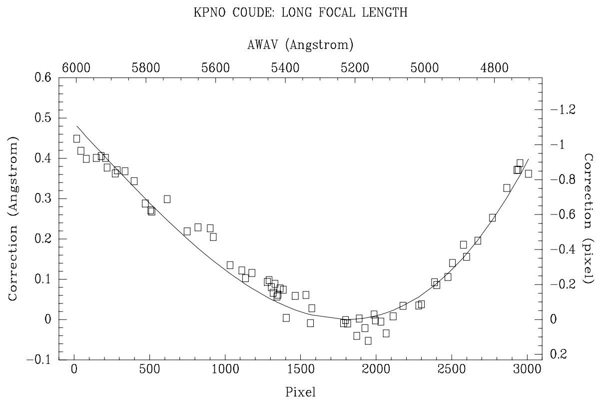
The top axis gives the simple 'AWAV   ' linear coordinates, which in this case is just a linear scaling of the pixel axis. The right axis divides the wavelength correction by CDELT1, the linear dispersion at the reference pixel. This represents the shift, in pixels, of the wavelengths on the detector relative to where they would occur in a spectrograph with a linear dispersion relation.

The departure of the data points from zero indicate the magnitude of the world coordinate errors that would occur by using the simple linear AWAV world coordinate function. The solid line in the figures are the difference between the wavelengths produced by the AWAV-GRA grating coordinate function and the linear AWAV coordinate function evaluated at the pixel positions in the image.

The usefulness of the ideal grating coordinate function is that the curves go through the measured data points with an appropriate choice of parameters. The parameters are essentially those known for the spectrograph and disperser with small adjustments to some of the parameters to produce the best fit to the calibration data. In these examples the dispersion function represented by the grating world coordinate relation is as good as typically provided by empirical polynomial functions. Higher order effects due to aberrations are corrected by the distortion correction methods defined in Paper IV.

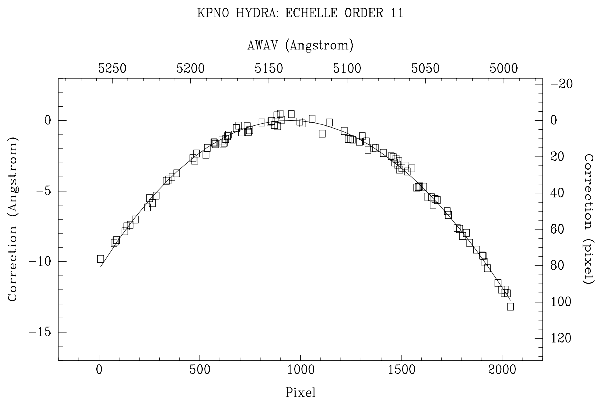
Each figure shows the arc line measurements, the coordinate function curve, and the relevant world coordinate keywords used to produce the curve. Not all of the WCS keywords are shown and the keywords are reformatted by removing leading whitespace in the value field to fit the allowed space.

The first example shows the behavior of a long focal length spectrograph with a reflection grating used at a low angle of incidence. Because of the long focal length the deviation from




```
CTYPE1  = 'AWAV-GRA' / Grating dispersion function
CUNIT1  = 'Angstrom' / Dispersion units
CRPIX1  =     1801.7 / [pixel] Reference pixel
CRVAL1  =     5225.2 / [Angstrom] Reference value
CDELT1  =    -0.4334 / [Angstrom/pixel] Dispersion
PV1_0   =     3.16E5 / [m^(-1)] Grating density
PV1_1   =          1 / Diffraction order
PV1_2   =       13.9 / [deg] Incident angle
```

Fig. 3. KPNO Coudé Feed spectrograph with a long focal length and a 3K CCD.

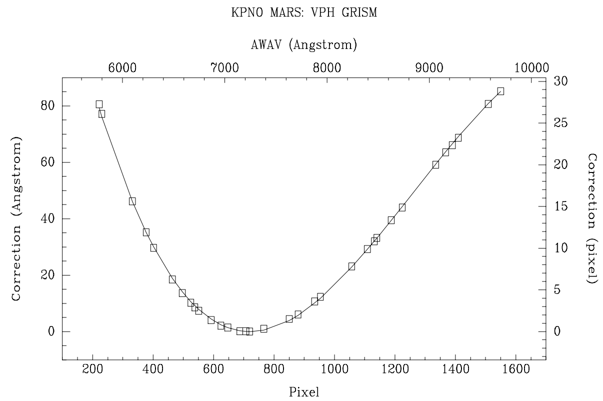



```
CTYPE1  = 'AWAV-GRA' / Grating dispersion function
CUNIT1  = 'Angstrom' / Dispersion units
CRPIX1  =      944.8 / [pixel] Reference pixel
CRVAL1  =     5136.8 / [Angstrom] Reference value
CDELT1  =    -0.1287 / [Angstrom/pixel] Dispersion
PV1_0   =     3.16E5 / [m^(-1)] Grating density
PV1_1   =         11 / Diffraction order
PV1_2   =       64.8 / [deg] Incident angle
```

Fig. 4. KPNO Hydra Fiber Bench Spectrograph using an echelle grating in 11^{th} order with a 2K CCD.

linearity is relatively small though still clearly significant. The grating has a density of 316 lines per mm and is used in first order to produce a spectrum centered near 5000 A with a dispersion of 0.43 Å/pixel.

The next example uses a 316 lines/mm echelle reflection grating, a grating designed for use at large angles from the grating normal, operated in a higher order. It is used to produce a spectrum centered near 5000 A with a dispersion of 0.13 Å/pixel. The departure from linearity is in the opposite sense from the other examples because the echelle grating is used with the diffracted angle at a greater angle than the incidence angle. The higher order results is a fairly large departure from a linear WCS.




```
CTYPE1  = 'AWAV-GRA' / Grating dispersion function
CUNIT1  = 'Angstrom' / Dispersion units
CRPIX1  =      719.8 / [pixel] Reference pixel
CRVAL1  =     7245.2 / [Angstrom] Reference value
CDELT1  =      2.956 / [Angstrom/pixel] Dispersion
PV1_0   =     4.50E5 / [m^(-1)] Grating density
PV1_1   =          1 / Diffraction order
PV1_2   =       27.0 / [deg] Incident angle
PV1_3   =      1.765 / Reference refraction
PV1_4   =   -1.077E6 / [m^(-1)] Refraction deriv
```

Fig. 5. KPNO MARS spectrograph with a 450 lines/mm volume phase holographic grism and a 2K CCD.

The last example illustrates use of a grism. However this is not the more common grism with a ruled grating on the output face and the input face oriented normal to the incident beam. Instead, the grating is sandwiched in the middle of the prism. The prism is oriented with the beam entering and leaving the prism at equal angles to the faces resulting in a straight through configuration as with a standard grism.

Another unusual feature of this grism is that it uses a volume phase holographic (VPH) grating. While the intensity response is different from a surface relief grating (ruled or holographic) the dispersion behavior is the same.

The full optical equation is complex even in this symmetric configuration. But as shown in the figure using the `GRA` function, a very good description of the coordinates can be obtained.

The prism has a 27 degree angle with an index of refraction of 1.764 near the reference wavelength. The grating has an equivalent interference pattern of 450 lines/mm. Using these values and adjusting the slope of the index of refraction produces Fig. 5.

6. Coordinates by table lookup

There are numerous instances in which a physical coordinate is well defined at each pixel along an image axis but the relationship of the coordinate values between pixels is essentially arbitrary. A simple example of this would be a 3-dimensional image consisting of a sequence of 2-dimensional images of an astronomical object recorded at an arbitrary sequence of times determined in part by weather and time assignment committees. As another example, the calibration of some spectrographs, such as when a diode array detector is used, is represented best by a list of frequencies or wavelengths for each pixel on the spectral axis rather than some functional form.

We will use FITS-standard binary table (`XTENSION = 'BINTABLE'`) extensions to hold the list of coordinates. The list of coordinate values is a vector in a single cell of a column of the table. A second vector list of the same dimension may appear in a second column in the same row of the same table to be used in addressing the list of coordinates in the first vector. We will call these the "coordinate vector" and "indexing vector," respectively. The indexing vector would be useful in attaching, for example, a distance measure within an instrument to the wavelength observed at that position. The two lists could then be sampled at small intervals over that portion of the range in which the instrument is seriously non-linear and sampled more coarsely over regions in which it is better behaved. If the indexing vector is absent, it is taken to have values $1, 2, 3, \ldots, N$, where N is the number of values in the coordinate vector.

6.1. *xxxx*-TAB *non-linear algorithm*

To support representations for separable, one-dimensional axes of primary images and image extensions, we define a table-lookup form for the value of CTYPE*ia* as *xxxx*-TAB, where *xxxx* are four letters representing the type of coordinate, e.g. TIME or FREQ. Note that *xxxx* is a real coordinate such as RA, not an intermediate coordinate needing deprojection, such as RA---TAN. To determine the coordinate value on such an axis, one first determines an index for addressing the appropriate vector location in the table by evaluating

$$v_i = x_i + \mathtt{CRVAL}\,ia\,, \tag{86}$$

where x_i is computed following the prescriptions of Eq. (1). v_i is an index into the vector of values. One finds the location in the indexing vector corresponding to index value v_i and takes the corresponding value from the coordinate vector as the coordinate value of type *xxxx*. If an exact match to v_i is not found in the indexing vector, then one must interpolate linearly between the coordinate values of the two indexing vector locations most closely corresponding to v_i. Note that, when the indexing vector is absent, its default converts the v_i into a direct index (vector subscript) for the coordinate vector.

The specified coordinate table is found in the same FITS file as the data which reference it.

The parameters required by -TAB are the table extension name (EXTNAME), the table version number (EXTVER), the table level number (EXTLEVEL), the column name for the coordinate vector (TTYPE*n*), and the column name for the indexing vector (TTYPE*m*). The keywords used for this purpose are PS*i*_0, PV*i*_1, PV*i*_2, PS*i*_1, and PS*i*_2, respectively. For images, PS*i*_0 has no default; for tables a missing or blank PS*i*_0 is taken to be the current table (see below). PV*i*_1 and PV*i*_2 both have a default value of 1. PS*i*_1 never has a default; it must be present and be assigned a value actually occurring in table PS*i*_0. If PS*i*_2 is missing or has a value of all blanks, the indexing vector is taken to be a list of integers from 1 to N and v_i becomes a direct index into the column specified by PV*i*_1. If PV*i*_2 is present and assigned a value, then that value must actually occur in table PS*i*_0.

If a FITS file contains multiple XTENSION HDUs with the specified EXTNAME, EXTLEVEL, and EXTVER, then the result of the WCS table lookup is undefined. If a FITS BINTABLE contains no, or multiple, columns with the specified TTYPE*n*, then the result of the WCS table lookup is undefined.

No units conversions are to be performed. CUNIT*i* must be the same as TUNIT*c* of the binary table, where *c* is the column number corresponding to PS*i*_1.

The lookup-table representation is not needed for binary table extensions containing pixel lists; there are better ways to manage this issue within such tables. However, binary table extensions containing vector columns may need a lookup function for coordinate values. Seemingly the most convenient form of lookup would be one in which the lookup vector(s) are also vector cells in the same row as the data vector. However, a separate coordinate table would be more economical if it were able to apply to a number of the data vectors. The -TAB keywords for such tables are *i*CTYP*n*, *i*PS*n*_0, *i*PV*n*_1, *i*PV*n*_2, *i*PS*n*_1, and *i*PS*n*_2, where *n* is the column number of the vector of data and *i* is the intermediate world coordinate axis number. If *i*PS*n*_0 is missing or blank, the present binary table is taken to be the coordinate lookup table. In that case, the coordinate lookup vector(s) are taken to be single-cell vectors in the same row as the data vector and keywords *i*PV*n*_1 and *i*PV*n*_1 are ignored.

There are several suggestions we can make for using this facility. The first is that, if one chooses EXTNAME to begin with the four letters WCS-, then generic programs will recognize the table as part of the WCS portion of the data and will be less likely to separate the table from the rest of the WCS. The second is that the data in the vectors should be sorted in ascending order of the indexing vector's values. Otherwise, the application programs may be forced to do the sort themselves. In general, this representation will result in tables with only one row, since no provision is made to direct the algorithm to a row greater than one. As a result, the usual table sort programs will not break the algorithm.

6.2. *Possible* *xxxx*-TB2 *non-linear algorithm*

The -TAB algorithm above covers separable, one-dimensional axes only. It could be extended, with another algorithm code such as -TB2, to two non-separable axes ($x_1 = f(q_1, q_2)$ and $x_2 = g(q_1, q_2)$) by having three vector lists in three columns: one for x_1, one for x_2, and one for q_1, which would be optional. A fourth column, required in order to defend against sorting and with single-value cells, would then be used to lookup q_2 to select the row to be considered for the particular pixel. Since we believe that there may be much better representations for this problem, including dispensing with an image in the primary HDU entirely, we do not propose -TB2 at this time.

```
CTYPE1  = 'WAVE-TAB'  / Coordinate type
CUNIT1  = 'Angstrom'  / Coordinate units
PS1_0   = 'WCS-TAB '  / Coord table extension name
PS1_1   = 'WAVELENTH' / Coord table column name
```

Fig. 6. WCS keywords in the spectral image for FOS and GHRS example.

```
1CTYP4  = 'WAVE-TAB'   / Coordinate type
1CUNI4  = 'Angstrom'   / Coordinate units
1PS4_1  = 'WAVELENGTH' / Coords for gross spectrum

1CTYP5  = 'WAVE-TAB'   / Coordinate type
1CUNI5  = 'Angstrom'   / Coordinate units
1PS5_1  = 'WAVELENGTH' / Coords background spectrum
```

Fig. 7. WCS keywords in the STIS table for two of the spectral columns.

6.3. `-TAB` examples: HST data

Since there has been no generally agreed upon FITS format for spectral data with explicit wavelengths assigned to each pixel, data providers have had to define their own formats. Two such cases, which can now be represented by the `-TAB` algorithm, were defined for Hubble Space Telescope data. The two cases illustrate the evolution from simple images to the more powerful constructs provided by FITS extensions and binary tables. The purpose of discussing these formats is not to explain the HST formats, but to illustrate a couple of types of data which can be represented by the `-TAB` algorithm. Therefore, some details of these formats are ignored.

The early HST spectrographs, FOS and GHRS, adopted a format based only on simple FITS images. The basic concept is that the spectral flux values are given in one image and the vacuum wavelengths, in Angstroms, are given as the pixel values in another image. The two are associated by filenames. The filenames have the same basename, but different filename extensions for an exposure. To represent these spectra with a FITS WCS based on the `-TAB` method, while continuing to use an image representation for the spectral fluxes, one replaces the separate wavelength image with a table extension.

Figure 6 shows the minimum WCS keywords required in the primary image header. The `PS1_0` keyword value defines the coordinate table to be in a binary table extension with name `'WCS-TAB'`. The coordinate table extension consists of one column, named `'WAVELENGTH'`, and one row. The vector values and length correspond to the original image format.

Other WCS keywords defined in paper I would also be included as needed. The intermediate coordinate transformation must produce indexing values equal to the pixel coordinate in the image. Since the defaults for these keywords are defined in Paper I to produce pixel coordinates, it is not strictly necessary to include these keywords.

The second generation HST spectrograph, STIS, adopted a binary table format very close to one of those defined for the `-TAB` algorithm. In the STIS one-dimensional extracted echelle format each exposure is stored in a separate binary table. The extracted data from an exposure consist of a number of echelle orders each of which is stored in a separate row. The wavelengths and various associated "spectra" are vector elements in different columns. An associated spectrum is a vector of a single type data quantity such as fluxes, errors, or data quality flags.

To convert this format to the `-TAB` representation only requires adding the `1CTYP`n and `1PS`n`_1` keywords to specify the coordinate type and coordinate column name for each spectral column n. There are six types of spectral quantities for each order: gross, background, net, flux, error, and data quality flag. So there must be six pairs of keywords. Since the same wavelength column applies to each of the spectra, the keyword values are repeated six times, but with different column numbers in the keywords. Figure 7 shows the WCS keywords for two of the spectral columns.

As noted for the FOS and GHRS format, additional WCS keywords are included as needed and the intermediate coordinate transformation values may be absent since this defines an indexing by pixel coordinate. In the STIS data, the units of the wavelength vector are vacuum Angstroms so the `1CUNI`n keyword would be required.

6.4. `-TAB` example: radio interferometry

Radio interferometry data are now best represented in binary tables with each row representing the visibility at one time on one antenna pair with a vector of data representing the complex values for all polarizations and frequencies observed. These telescopes often allow the user to observe N_i regularly-sampled spectral channels starting from M "randomly" chosen "IF" frequencies. Furthermore, this spectral data pattern may be used with one receiver and, a few minutes later, with other receivers at very different frequencies. Because of the "randomness" of the IF frequencies and the choice of receivers, the frequencies present in the data may only be described by a table. Because that description is very repetitive, we choose to put it in a table separate from the visibility table.

Considering, for the moment, only one receiver, we could construct a single column table of all $\sum_{i=1}^{M} N_i$ frequencies observed for that receiver. However, by using the second lookup column, we can take advantage of the regular sampling of the N_i spectral channels. If we set i`CRVL`k, i`CDLT`k, and i`CRPX`k to one, then Table 7 may represent the actual frequencies, where ν_i is the frequency of channel 1 in IF i and δ_i is the increment in frequency between the regularly sampled channels of IF i. A second receiver could be added to the table by adding one or two more vector columns – two would be needed if the number of channels in each IF (N_i) was not the same. This is illustrated in the table using Υ_i as the frequency of channel 1 in IF i or receiver 2 and Δ_i as the increment in frequency between the regularly sampled channels of IF i for that receiver and taking the number of channels in each IF to be constant.

7. Coordinate reference frames

Frequencies, wavelengths, and velocities are always referred to some selected standard of rest (reference frame), and while they are measured, of necessity, in the observer's rest frame,

Table 7. Sample coordinate table. Each displayed column is actually a one-cell vector of the table.

iPSn_2	iPSn_1	2nd iPSn_1	...
1	ν_1	Υ_1	...
N_1	$\nu_1 + (N_1 - 1)\delta_1$	$\Upsilon_1 + (N_1 - 1)\Delta_1$	...
$N_1 + 1$	ν_2	Υ_2	...
$N_1 + N_2$	$\nu_2 + (N_2 - 1)\delta_2$	$\Upsilon_2 + (N_2 - 1)\Delta_2$	...
$N_1 + N_2 + 1$	ν_3	Υ_3	...
$N_1 + N_2 + N_3$	$\nu_3 + (N_3 - 1)\delta_3$	$\Upsilon_3 + (N_3 - 1)\Delta_3$	...
...	...	...	...
$\sum_1^{M-1} N_i + 1$	ν_M	Υ_M	...
$\sum_1^M N_i$	$\nu_M + (N_M - 1)\delta_M$	$\Upsilon_M + (N_M - 1)\Delta_M$	...

Table 8. Recognized values for `SPECSYS`*a* and `SSYSOBS`*a*.

Value	Definition	Magnitude	Reference
`TOPOCENT`	Topocentric	0.0 km/s	
`GEOCENTR`	Geocentric	0.5	
`BARYCENT`	Barycentric	30	Stumpf (1980)
`HELIOCEN`	Heliocentric	30	Stumpf (1980)
`LSRK`	Local standard of rest (kinematic)	20	Delhaye (1965)
`LSRD`	Local standard of rest (dynamic)	16.6	Delhaye (1965)
`GALACTOC`	Galactocentric	220	Kerr & Lynden-Bell (1986)
`LOCALGRP`	Local group	300	de Vaucouleurs (1976)
`SOURCE`	Source rest frame	any	

they may also be corrected to some other frame. The velocity correction is computed from the vector dot product of the direction vector and the (constant) relative velocity vector of the two reference frames.[2] In addition, the corrections from topocentric, the frame in which the observations are usually made, to geocentric and then to barycentric or heliocentric are dependent on the dot product with time-variable velocity vectors. As a consequence, the "velocity" with respect to the reference frame depends on direction. Differential effects over a field of view may be important in some high precision applications; for example, they may amount to 5 km/s for the local group correction over a field of one degree. In another example, observations of Galactic CO over two-degree fields separated by two degrees failed to align by two spectral channels (Mangum et al. 2000).

If a frequency, wavelength or velocity associated with an image plane has been corrected to some other frame by transforming the `CRVAL`*ka* et al. values, then differential errors may arise at points away from the reference point. For example, it is normal in radioastronomy to observe a field while holding constant the velocity of the reference point with respect to the local standard of rest.

Nonetheless, each image plane shares a constant topocentric frequency (or velocity). The velocity (*and* frequency and wavelength) with respect to the local standard of rest is then a function of celestial coordinate within the image. In order to denote this, we introduce two character-valued keywords. The first, `SPECSYS`*a*, describes the reference frame in use for the spectral-axis coordinate(s). The second, `SSYSOBS`*a*, describes the spectral reference frame that is constant over the range of the non-spectral world coordinates and has default value `SPECSYS`*a*. The recognized values are given in Table 8. In this table, the magnitude column gives the approximate magnitude of the velocity vector that defines the particular reference frame. The radio-astronomy example described above has `SPECSYS = 'LSRK'` and `SSYSOBS = 'TOPOCENT'` indicating that the spectral axis is expressed as a kinematic Local Standard of Rest velocity, but that each right ascension by declination image plane is at a constant topocentric spectral coordinate.

Many spectrometers suffer from a significant variation in their spectral coordinate as a function of celestial coordinate. Such variations are the primary subject of Paper IV, while the concepts of this manuscript refer to images produced by, or corrected to, an ideal spectrometer. In general we can hope that the frame corrections will get folded into the instrumental ones and that the image produced after the Paper IV corrections will have identical `SSYSOBS` and `SPECSYS`. This is not required, but certainly simplifies matters.

It is not appropriate for this manuscript to define the parameters of the recognized rest frames. The parameters needed to compute geocentric frequencies/velocities from topocentric are the sidereal time and the observatory location.[3] The observing date is needed to convert from geocentric to barycentric coordinates. The new keyword `MJD-AVG` is reserved to give a repre-

[2] The actual mathematics used should be done with proper relativistic formulæ; see Gibbs & Tao (1997) or Rindler (1982).

[3] The keywords in Tables 9 and 10 apply to terrestrial observers only. Observations from spacecraft require additional description of their motions – either a position and velocity or an ephemeris. The required keywords and/or tables for this are beyond the scope of this paper.

sentative time for the whole observation, suitable for calculating proper motion, apparent place, local apparent sidereal time, velocity with respect to the center of the Earth and barycenter, etc. In the absence of this keyword, DATE-OBS may be used to determine the representative time, although DATE-OBS refers to the beginning of an observation and hence is not entirely suitable. For high-precision applications, a time system to apply to MJD-AVG must be defined in the manner proposed by Bunclark & Rots (1997).

Astronomers have traditionally quoted telescope positions using terrestrial longitude, latitude, and height, but, for computation of topocentric velocity, these values are immediately converted into a geocentric Cartesian triple. A precise conversion from longitude, latitude, and height, however, requires knowledge of the geodetic datum in which they are expressed. There are about 1000 geodetic datums in use. These are described by the United States Department of Defense (2000) in a printed document also available over the Internet. Some of the datums deviate from geocentricity by over a kilometer.

Rather than burden FITS with these details of geodetic tradition, three new keywords OBSGEO-X, OBSGEO-Y, and OBSGEO-Z are reserved to define a representative location for the observation in a standard terrestrial reference frame. The location values should be right-handed, geocentric, Cartesian coordinates valid at the epoch of MJD-AVG. Position errors of several kilometers should have negligible impact on the computation of the diurnal velocity correction, so for this purpose geodetic accuracy is not a requirement. However, it should be possible to provide coordinates with an accuracy of 1m or better based on a recent satellite-based geodetic reference frame and we recommend that FITS writers do so.[4]

More general geodetic information is available from http://www.nima.mil/GandG/pb.html and a solution based on the outputs of almost any hand-held GPS unit is found at
http://www.ngs.noaa.gov/TOOLS/XYZ/xyz.html.
These references, together with information about the origin of the traditional telescope position, should allow the determination of the keyword values defined in this manuscript.

The frame of rest defined with respect to the source (SOURCE) is useful for comparing internal velocities in objects at different redshifts. This allows the FITS writer to apply all the proper relativistic corrections, leaving a low-velocity, non-relativistic coordinate. For this frame of rest, it is necessary to define the velocity with respect to the observer at which the velocity is zero with respect to the source. This may be given in km/s via the keyword VSOURCE*a* or in unitless optical velocity via the keyword ZSOURCE*a*. It may be helpful for the FITS writer to provide information on the relative velocity between the observer and the selected standard of rest in the direction of the celestial reference coordinate. The keyword VELOSYS*a* is hereby reserved for this purpose. Units will be km/s. CUNIT*ka* is not used since the WCS version *a* may not be expressed in velocity units. The new floating-valued keywords hereby reserved are listed in Table 9.

Table 9. Velocity reference parameters.

SPECSYS*a*	Spectral reference frame (from Table 8)
SSYSOBS*a*	Spectral reference frame fixed during observation (from Table 8)
OBSGEO-X	Observation X (m)
OBSGEO-Y	Observation Y (m)
OBSGEO-Z	Observation Z (m)
MJD-AVG	Average date of observation (Julian days−2400000.5)
VSOURCE*a*	Physical velocity of source for SOUR cases (km/s)
ZSOURCE*a*	Optical "velocity" of source for SOUR cases (unitless)
VELOSYS*a*	Velocity wrt standard of rest (km/s)
RESTFRQ*a*	Line rest frequency (Hz)
RESTWAV*a*	Line rest wavelength in vacuum (m)

An alternative to leaving the computation of correct relative velocities to the FITS reader is provided in Paper IV. By declaring that the two reference frames are the same (e.g. SPECSYS = SSYSOBS) and then providing a velocity distortion correction using the methods described in Paper IV, the FITS writer may save the FITS reader from having to understand this, normally forgotten, correction.

8. Alternate FITS image representations: pixel list and vector column elements[5]

The use of coordinate keywords to describe a multi–dimensional vector in a single element of a FITS binary table (Cotton et al. 1995), and a tabulated list of pixel coordinates in a FITS ASCII (Harten et al. 1988) or binary table was discussed in sections of Papers I and II. In this section, we extend those discussions to the keywords specific to spectral coordinates. This convention is considered an integral part of the full world coordinates convention.

8.1. Keyword naming convention

Table 10 lists the corresponding set of coordinate system keywords for use with each type of FITS image representation. The allowed values for these keywords are identical for all three types of images as defined in the main body of this paper. The following notes apply to the naming conventions used in Table 10:

- *a* are 1-character coordinate version codes and may be blank (primary) or any single uppercase character from A through Z.
- *n* is an integer table column number without any leading zeros (1–999).

[4] It is beyond the scope of this paper to define particular terrestrial reference frames or tectonic models, but most post-1980 reference frames, including GPS, agree to about 0.1 m.

[5] Suggested by contributions from William Pence, Arnold Rots, and Lorella Angelini of the NASA Goddard Space Flight Center, Greenbelt, MD 20771.

Table 10. Alternate coordinate keywords.

Keyword Description	Primary Array	BINTABLE Vector	Pixel List
Reference Frame	SPECSYS*a*	SPEC*na*	SPEC*na*
Constant Frame	SSYSOBS*a*	SOBS*na*	SOBS*na*
Observation X .	OBSGEO-X	OBSGX*n*	OBSGX*n*
Observation Y	OBSGEO-Y	OBSGY*n*	OBSGY*n*
Observation Z	OBSGEO-Z	OBSGZ*n*	OBSGZ*n*
Date of obs (avg)	MJD-AVG	MJDAV*n*	MJDAV*n*
Source velocity	VSOURCE*a*	VSOU*na*	VSOU*na*
Source velocity	ZSOURCE*a*	ZSOU*na*	ZSOU*na*
Relative velocity	VELOSYS*a*	VSYS*na*	VSYS*na*
Rest frequency	RESTFRQ*a*	RFRQ*na*	RFRQ*na*
Rest wavelength	RESTWAV*a*	RWAV*na*	RWAV*na*

When using the BINTABLE vector image format, if the table only contains a single image column or if there are multiple image columns but they all have the same value for any of the keywords in Table 10 then the simpler form of the keyword name, as used for primary arrays, may be used. For example, if all the images in the table have the same location, then one may use one set of OBSGEO-X, OBSGEO-Y, and OBSGEO-Y keywords rather than multiple OBSGX*n*, OBSGY*n*, and OBSGZ*n* keywords. The other keywords, however, must always be specified using the more complex keyword name with the column number suffix and the axis number prefix.

In principle, more than one pixel list image can be stored in a single FITS table by defining more than one pair of i and j pixel coordinate columns. Under the convention defined here, however, all the images must share the same values for the keywords in Table 10.

9. Spectral coordinate variation with other coordinates

There are instruments having spectral coordinates which are a function of other coordinates in the resulting image, e.g. celestial position. For example, optical astronomers use imaging Michelson interferometers and scanning Fabry-Perot instruments to produce three-dimensional images with two celestial and one spectroscopic coordinate. Because the path length through such instruments increases off the optical axis of the telescope, the observed wavelength is a function of celestial coordinate in each plane of the image cube. In general, this is a subject reserved for Paper IV since such instruments almost always have lesser distortions which need to be parameterized and corrected along with the path length correction.

One particularly difficult case should be mentioned here. Objective prism instruments produce data in which the image of each object in the field has been spread out into a spectrum. Thus the output image is the convolution of the sky with both a spatial point-spread-function and a spectral dispersive point-spread function, both in the two dimensions of the output image. The methods used to specify coordinates described in the present manuscript and in Papers I and II are unable to handle such complex data.[6] Analysis of objective prism images can produce tables of spectra which are easily described by the present methods.

10. Example

10.1. Basic spectral-line header

Let us consider an example. The partial FITS header in Table 11 was produced for data from the Very Large Array, updated to the present conventions. We have left out numerous other header parameters including axes 1, 2, and 4 of the alternate WCS keywords and updated things to the standards of Papers I, II, and III. We will derive additional header keywords which could also have been written. These will be shown in Table 12, again leaving out axes 1, 2, and 4 of the alternate WCS versions.

The spectral-line cube is regularly sampled in frequency and the primary description is of a linear frequency axis (from the CTYPE3 keyword value 'FREQ   '). The observation was at 1.378 GHz, 42 MHz from the rest frequency of neutral hydrogen (1.420 GHz). It is shown as if it had been observed at a constant topocentric frequency. For the moment, let us assume that the observations were made over a short interval and that this is then correct.

The first alternate (O for optical[7]) axis description for the spectral axis reveals that the user requested an optical-convention velocity of 9120 km/s. An optical velocity of 9120 km/s produces a frequency of 1.37847122 GHz using Eqs. (9) and (19). Since this is 120 kHz greater than the actual frequency used, we can deduce that the VLA on-line system applied a correction for the motion of the observatory in order to make the observation be at the requested optical velocity with respect to the kinematic Local Standard of Rest. The amount of this correction may be determined from Eq. (13). The change from a topocentric frequency of 1.37835117405 GHz to a BARYCENT frequency of 1.37847122 GHz corresponds to 26.11 km/s. Thus the correction for the observatory's motion wrt the center of the Earth and the Earth's motion wrt the center of the Solar System added up to 26.11 km/s in the direction of the reference pixel. As illustrated in Table 12, this velocity shift can be represented in the FITS header with the new keyword VELOSYS.

The BARYCENT frequency may be used as another alternate axis description. Note that the frequency increment as well as the reference frequency are adjusted with Eqs. (8) and (7). The velocity increment in axis description O is computed by Eqs. (32) and (10) using the frequency increment appropriate to an BARYCENT reference frame (i.e. as given in axis description F for frequency). The frequency description may be in-

[6] Rather than ignore the world coordinates entirely, writers of such images should consider providing the celestial coordinates that would be correct for the image if it had been taken at a single representative wavelength. That wavelength would be specified in a third WCS axis. Alternate axis descriptions could then be used to specify the same information for other wavelengths.

[7] We use the alternate axis description letter codes in a mnemonic fashion as allowed by Paper I.

verted into a wavelength description simply using Eq. 9, as in axis description `W` (for wavelength).

The frequency description wrt to the `BARYCENT` may also simply be expressed as a radio velocity (also regularly sampled) using Eq. (19). This is shown as axis description version `R` (for radio). A true velocity description (version `V` for velocity) requires the use of Eq. (13) for the reference value and Eq. (14) for the increment.

10.2. Real-world complications

We may now relax the assumption made above. The actual observation required several hours and the frequency used was changed with time so that the `BARYCENT` frequency or velocity – at the reference celestial coordinate – would remain constant. Therefore, the primary spectral axis description, which is given to aid in interferometric analysis, is not correct and should be replaced by the second alternate (`F`) axis description.

A radio interferometer acquires data from all directions within its field of view, not just the direction for which the `BARYCENT` frequency was held constant. The differential error in so doing is greatest when the velocity vector is orthogonal to the direction to the source and least when it is parallel or anti-parallel. Thus the differential correction is greatest when the correction is zero, and least when the correction is greatest.

For diurnal rotation the worst case differential error occurs for a telescope at the equator observing a source on the local meridian. For an angular offset, α, from the tracking center the maximum differential error is $v \sin(\alpha)$ which amounts to 8.7 m/s for $\alpha = 1$ deg. The worst case change in the differential error over the course of 12 hours occurs for a field at the north or south point on the horizon; it is $2v \sin(\alpha)$ or 17.5 m/s for $\alpha = 1$ deg. If data from different days (months really) are combined, then the 30 km/s orbital velocity scales up the worst-case error to 1.0 km/s for $\alpha = 1$ deg. Note that, in the present example, the barycentric correction is nearly the maximum value and so the differential correction is nearly its minimum value.

This example brings out a fundamental limitation to coordinate accuracy for some instruments caused by the motion of the earth. If the instrument requires a significant integration time, then the correction of the observing frequency in the reference direction to some standard at rest wrt the universe will diverge from that correction for other directions within the field of view. For some instruments, it may be possible to correct the data at each time to a consistent WCS and then to perform the time averaging required to obtain a useful sensitivity. For example, a single-dish radio telescope observes a single direction at a time, allowing each observed spectrum to be shifted and scaled before it is added in to the output, three-dimensional image. However, other instruments observe multiple directions at each time and must combine multiple times before imaging. Radio astronomy aperture synthesis telescopes fall in this category since multiple times are required in order to sample the Fourier space adequately to do imaging and deconvolution. In fact, it is common to combine data taken months apart in different telescope array configurations. These data are affected not only by the rotation of the earth but also by its mo-

Table 11. Example image header.

```
SIMPLE  =                    T /
BITPIX  =                  -32 /
NAXIS   =                    4 /
NAXIS1  =                 1024 /
NAXIS2  =                 1024 /
NAXIS3  =                   63 /
NAXIS4  =                    1 /
EXTEND  =                    T /Tables may follow
BLOCKED =                    T /Blocked ok
OBJECT  = '3C353   '           /
TELESCOP= 'VLA     '           /
DATE-OBS= '1998-09-29'         /Start obs
BUNIT   = 'JY/BEAM '           /
EQUINOX =       2.000000000E+03 /
DATAMAX =       5.080558062E-01 /
DATAMIN =      -1.179690361E-01 /
WCSAXES =                    4 /
WCSNAME = 'TopoFreq'           /
CTYPE1  = 'RA---SIN'           /
CRVAL1  =     2.60108333333E+02 /
CDELT1  =      -2.777777845E-04 /
PC1_1   =       1.000000000E+00 /
CRPIX1  =       5.120000000E+02 /
CUNIT1  = 'deg'
CTYPE2  = 'DEC--SIN'           /
CRVAL2  =    -9.75000000000E-01 /
CDELT2  =       2.777777845E-04 /
PC2_2   =       1.000000000E+00 /
CRPIX2  =       5.130000000E+02 /
CUNIT2  = 'deg'
CTYPE3  = 'FREQ    '           /
CRVAL3  =     1.37835117405E+09 /
CDELT3  =       9.765625000E+04 /
PC3_3   =       1.000000000E+00 /
CRPIX3  =       32.00000000E+00 /
CUNIT3  = 'Hz'
SPECSYS = 'TOPOCENT'
CTYPE4  = 'STOKES  '           /
CRVAL4  =     1.00000000000E+00 /
CDELT4  =       1.000000000E+00 /
PC4_4   =       1.000000000E+00 /
CUNIT4  = ' '
OBSGEO-X=      -1.601185365E+06
OBSGEO-Y=      -5.041977547E+06
OBSGEO-Z=       3.554875870E+06
MJD-AVG =           51085.99722

WCSAXESO=                    4 /
WCSNAMEO= 'OpticalV'           /
RESTFRQO=     1.42040575200E+09 / [Hz]
CTYPE3O = 'VOPT-F2V'           /
CRVAL3O =         9.120000E+06   /
CDELT3O =        -2.188774E+04   /
PC3_3O  =       1.000000000E+00 /
CRPIX3O =         32.00000E+00   /
CUNIT3O = 'm/s'
SPECSYSO= 'BARYCENT'
SSYSOBSO= 'TOPOCENT'
```

Table 12. Additional keywords for example header.

```
VELOSYSO=                  26.111 / [km/s]
WCSAXESF=                       4 /
WCSNAMEF= 'BaryFreq'              /
CTYPE3F = 'FREQ    '              /
CRVAL3F =     1.37847122E+09      /
CDELT3F =       9.766475E+04      /
CRPIX3F =       32.00000E+00      /
CUNIT3F = 'Hz'
SPECSYSF= 'BARYCENT'
SSYSOBSF= 'TOPOCENT'
VELOSYSF=                  26.111 / [km/s]
WCSAXESW=                       4 /
WCSNAMEW= 'Waveleng'              /
CTYPE3W = 'WAVE-F2W'              /
CRVAL3W =     0.21106117E+00      /
CDELT3W =      -1.495369E-05      /
CRPIX3W =       32.00000E+00      /
CUNIT3W = 'm'
SPECSYSW= 'BARYCENT
SSYSOBSW= 'TOPOCENT'
VELOSYSW=                  26.111 / [km/s]
RESTFRQR=     1.42040575200E+09 / [Hz]
WCSAXESR=                       4 /
WCSNAMER= 'RadioVel'              /
CTYPE3R = 'VRAD    '              /
CRVAL3R =        8.8507514E+06    /
CDELT3R =       -2.0613236E+04    /
CRPIX3R =        32.00000E+00     /
CUNIT3R = 'm/s'
SPECSYSR= 'BARYCENT'
SSYSOBSR= 'TOPOCENT'
WCSAXESV=                       4 /
WCSNAMEV= 'Velocity'              /
RESTFRQV=     1.42040575200E+09 / [Hz]
CTYPE3V = 'VELO-F2V'              /
CRVAL3V =        8.9813433E+06    /
CDELT3V =       -2.1728665E+04    /
CRPIX3V =        32.00000E+00     /
CUNIT3V = 'm/s'
SPECSYSV= 'BARYCENT'
SSYSOBSV= 'TOPOCENT'
```

tion around the Sun. While current observations are often of small angular fields or modest spectral resolution, instruments now under development will be capable of significantly greater sensitivity over wider spectral and spatial fields of view and hence will need to consider the effects discussed here. Note that this problem cannot be solved by declaring the `SSYSOBS` to be `'BARYCENT'` since at any moment in time the frequency is constant in celestial coordinates in a topocentric sense.

11. Summary

The present paper has presented a consistent set of keyword values to describe spectral information in FITS data files. The, by now, standard header keywords of Papers I and II are given similar meanings when applied to such axes. The wavelength, frequency, true velocity and three conventional "velocities" may be expressed as functions of pixel along an axis regularly sampled in wavelength, frequency, or physical velocity. Common, although idealized, spectral dispersers are also described by a defined world coordinate function. A table lookup function for separable (one-dimensional) axes is also described. The new keywords are summarized in Table 9. They include two new keywords `SPECSYS`*a* and `SSYSOBS`*a* used to specify the standards of rest in use, seven other keywords used to enable conversion between standards of rest, and two keywords used to define the spectral line with respect to which velocities are measured. Extensions to these keywords for use with tabular data are also defined.

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