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Representations of Spectral Coordinates in FITS

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Abstract. In Paper I, Greisen & Calabretta (2003) describe a generalized method for specifying the coordinates of FITS data samples. Following that general method, Calabretta & Greisen (2003) in Paper II 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. Papers I and II have been accepted into the FITS standard by the North American, Japanese and European FITS Committees; we expect the present work to be accepted as well. The full text of the proposed standards can be found at http://www.aoc.nrao.edu/~egreisen.

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1. Introduction

Greisen & Calabretta (2003, "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

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

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 ideal spectral axes are described in "Paper III" (Greisen et al. 2003) and summarized here. A later work (Calabretta, et al. 2003, "Paper IV") will address the corrections needed to convert real astronomical data into the ideal axes assumed in the celestial coordinates (Calabretta & Greisen 2003, "Paper II") and present manuscripts.

2. Basic Coordinates

The basic "spectral" coordinates are frequency, wavelength, and Doppler relativistic velocity. There are several other coordinates which are proportional to one of these, including wavenumber, energy, and "radio" and "optical" conventional velocities. Let us consider the case in which an axis is linearly sampled in spectral variable X, but is to be expressed in terms of variable S. We may restrict X to the basic types since all others are linearly proportional to one of them. Let us also introduce an intermediate variable P which is the basic variable associated with S. The relationship between X and S is then $S(X) = S(P(X))$ with inverse $X(S) = X(P(S))$. The statement that an axis is linearly sampled in X simply means that

$$X = X_{\rm r} + w \frac{{\rm dX}}{{\rm dw}} \tag{2}$$

where w is the intermediate value x_i for the spectral axis and dX/dw is a constant. Since, to first order and very near the reference point, the axis is linear in S, i.e., $S \approx S_{\rm r} + w$, we may determine the derivative by

$$\frac{{\rm dX}}{{\rm dw}} = \left.\frac{{\rm dP}}{{\rm dS}}\right|_{\rm r} \Big/ \left.\frac{{\rm dP}}{{\rm dX}}\right|_{\rm r} \;\; . \tag{3}$$

A three-step algorithm chain is then indicated:

1. Compute once $X_{\rm r} = X(P(S_{\rm r}))$ and dX/dw using Equation (3) and then compute X at w using Equation (2).
2. Compute P from X using the set of non-linear relationships between the basic spectral coordinates..
3. Compute S from P using the set of linear relationships between the basic and secondary spectral coordinates.

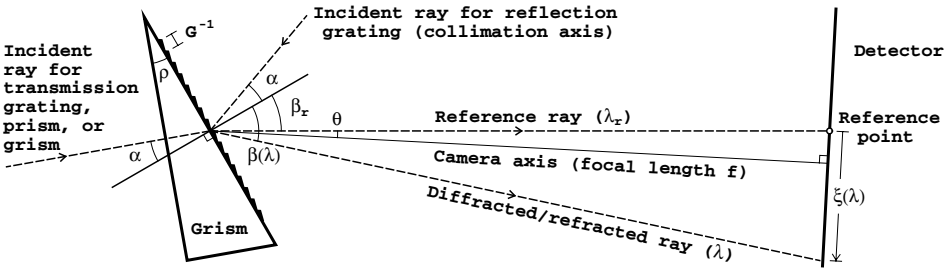

Figure 1. Geometry of gratings, prisms, and grisms. This simplified representation omits the collimation and focusing optics. Dashed lines mark ray paths in the plane of the figure – the "dispersion plane". The normal to the grating/exit prism face and the normal to the detector plane are each projected 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 $\lambda_{\rm r}$ follows the reference ray defined by $\beta_{\rm r}$ 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.

Dispersion coordinates for UV, optical, and IR spectra at $\lambda > 200$ nm are commonly given as wavelengths in air rather than in vacuum. The relationship between these is given by $\lambda = n(\lambda_a)\lambda_a$ and causes a relative difference of around 0.03%. The conversion between wavelengths in air and wavelengths in vacuum adds another step in the chain described above.

Paper III presents a full set of codes to be used in keyword `CTYPE`*ia* for spectral coordinate types and for the non-linear algorithms involved, including air wavelengths. Keywords `RESTFRQ`*a* and `RESTWAV`*a* are reserved to give the line rest frequency (in Hz) or wavelength (in m) needed for the conversion between frequency/wavelength and velocity.

3. Dispersed Spectra: `-GRI` Non-linear Algorithm

One common form of spectral data is produced by imaging the light from a disperser, such as a prism, grating, or grism, as illustrated in Figure 1. Paper III presents the full mathematics by which the wavelength λ and the spacing at the detector $\xi(\lambda)$ may be related. The basic grism equation is given by

$$\lambda = \frac{(n_{\rm r} - n'_{\rm r}\lambda_{\rm r})\sin\alpha + \sin\beta}{Gm/cos\epsilon - n'_{\rm r}\sin\alpha}\,. \tag{4}$$

Despite numerous approximations made in the development of the mathematics, it is found that suitable parameters provide good fits to a variety of spectrometers in use at the KPNO.

4. Coordinates by Table Lookup: `-TAB` Algorithm

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 cannot be described by a simple functional form. Observations of the same object made at an arbitrary set of frequencies or times are the simplest examples. In addition, the calibration of some spectrographs is represented best by a list of wavelengths for each pixel on the spectral axis.

Fully separable, one-dimensional axes of this type may be represented by an algorithm, `-TAB`, defined in Paper III. A FITS binary table containing only one row is used. The coordinates are given by a vector of values in a single cell, optionally accompanied by a second indexing vector in a second cell within the row. The parameters required by `-TAB` are the table extension name, the table version number, the table level number, the column name for the coordinate vector, and the column name for the optional indexing vector. The character-valued generic keyword `PS`i_j is introduced to provide the three character-valued parameters of this algorithm. The coordinate value is found by first evaluating Equation (1) and adding the reference value. The result is used as a value to be looked up in the vector of values found in the indexing vector cell. The corresponding position in the vector of values in the coordinate vector cell then provides the actual coordinate. If the indexing vector is omitted, the value found with Equation (1) is used as a direct index for the coordinate vector.

The `-TAB` algorithm described above is then generalized to cases in which the coordinates on N axes are dependent on each other, but the indexing vectors are independent. In this case, the values of the coordinates are contained in one column of the (one-row) table as an array of dimensions $(N, K_1, K_2, \ldots, K_N)$, where K_i is the number of indexing values on axis i. The indexing vector for axis i, if present, will occupy a separate column and will contain K_i values in a one-dimensional array. An additional parameter is required for each of the N coordinates to give the axis number i within the coordinate array.

5. Summary

Paper I has defined a general framework to describe world coordinates in the FITS format; Paper II has extended that framework to describe ideal celestial coordinate representations. Paper III, summarized here, extends the discussion to ideal spectral coordinates and introduces a general table lookup algorithm. All three papers are well on their way to becoming part of the IAU FITS Standard.

References

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