Wavelength Calibration of the Goddard High Resolution Spectrograph

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Abstract

The Goddard High Resolution Spectrograph (GHRS) is capable of obtaining data with a wavelength accuracy of 1 km/sec in the echelle modes. Both proper observing and data reduction techniques are required to achieve this accuracy.

Shifts of the spectral format at the GHRS diode array can be as large as 300 microns (six diode widths) with time and environmental factors. We have modeled this motion as a function of temperature, time, and the component of the Earth's magnetic field in the direction of dispersion. In the absence of calibration observations of the onboard spectral calibration lamp, this model can be used to reduce the errors from spectral motion in routine processing to approximately one diode width or 3 km/sec in the echelle modes.

I. Method

The following steps are used to compute the calibration coefficients used for routine reduction of GHRS science data. The calibration includes a model for thermal, time, and geomagnetically induced image motion.

1. Compute the dispersion coefficients for each spectral calibration lamp observation. The dispersion relation gives the photocathode sample position as a function of spectral order and wavelength (section i.i).

2. Compute a new cubic dispersion coefficient by fitting residuals in step 1 simultaneously for all observations made with the same grating mode (section i.ii). Repeat step 1 with the new cubic coefficient.

3. Fit of the central wavelength of each observation as a function of carrousel position. The carrousel controls which grating is selected and the grating scan angle (section i.iii).

4. Shift the dispersion relation to a coordinate system where the photocathode sample position is a function of the differences of the spectral order and wavelength from the central spectral order and wavelength (section i.iv).

5. Compute a global dispersion relation for each grating where the dispersion coefficients in step 4 are modeled by least square polynomials of the carrousel position (section i.v).

6. Compute a thermal/temporal motion model (section i.vi).

7. Determine the motion caused by the Earth's magnetic Field (section i.vii).

8. Model changes in linear dispersion as a linear function of temperature (section i.viii).

i.i Compute Dispersion Coefficients for each spectral calibration lamp observation

The GHRS dispersion relation is given by:

\[ s = a_0 + a_1 m \lambda + a_2 m^2 \lambda^2 + a_3 m + a_4 \lambda + a_5 m^2 \lambda + a_6 m \lambda^2 + a_7 m^3 \lambda^3 \]

where,
- \( s \) is the photocathode sample position in 50 micron (one diode) units.
- \( m \) is the spectral order
- \( \lambda \) is the wavelength
- \( a_0, a_1, ..., a_7 \) are the dispersion coefficients.

A single set of dispersion coefficients are computed for multiple spectral orders in the echelle mode when the data are taken without moving the carrousel between observations. In all other cases the dispersion coefficients, \( a_0, a_1, ..., a_7 \) are fit for each individual spectral calibration lamp observation. A typical GHRS spectral calibration lamp observation is shown in Figure 1.

**a)** Determine the photocathode sample positions of the spectral lines in the lamp observation with known wavelengths.

**b)** Compute \( a_0, a_1, a_2, \) and \( a_4 \) by least-squares fit. There are typically too few lines in a single observation to accurately fit the cubic term, \( a_7 \). The \( a_7 \) coefficient is user supplied (its computation is described in a later section). \( a_3, a_5, \) and \( a_6 \) are fixed at 0. \( a_5 \) and \( a_6 \) are not used for the GHRS but have been included in the relation for compatibility with the International Ultraviolet Explorer dispersion definition. \( a_3 \) is used only for the incidence angle correction from the spectral calibration lamp aperture to the science apertures. \( a_4 \) is set to 0 for the first order gratings and single order echelle observations.

**c)** Apply an incidence angle correction from the spectral calibration lamp aperture to the small science aperture (SSA). This correction is given by:

\[
\begin{align*}
    a_i &= a_i (1.0 - p_0) \quad \text{for } i = 1,7 \\
    a_0 &= a_0 - p_1 \\
    a_3 &= a_3 - p_2
\end{align*}
\]

where \( p_0, p_1, p_2 \) vary with carrousel position, \( R \), by the following relations:

\[
\begin{align*}
    p_0 &= c_2 + c_3 R \\
    p_1 &= c_0 + c_1 R + c_4 R^2 \\
    p_2 &= c_5
\end{align*}
\]
c₀, c₁, c₂, c₃, c₄, and c₅ are coefficients that were computed by least squares fit to pre-launch offset measurements between the SSA and the spectral calibration lamp apertures.

i.ii Computation of the Cubic Term in the dispersion relation.

The cubic term, a₇, of the dispersion relation can not be reliably fit from a single observation. To obtain the value of the cubic coefficient it is necessary to combine the results from multiple observations for the grating mode taken at multiple carrousel positions. This is done by computing the dispersion relations for all of the observations with the cubic term, a₇, set to 0.0. The residuals (observed spectral line positions minus the spectral line positions computed from the fitted dispersion relation) are combined from all observations. The combined residuals are fit as a least-squares polynomial of the difference m(λ−λ_c). λ_c is the wavelength at the center of the diode array. Figure 2 shows the results for grating mode G160M. The cubic term of the polynomial can now be used as the a₇ dispersion coefficient. The other coefficients are then recomputed for each observation with the new a₇ coefficient.
i.iii  Fit the central wavelength as a function of carrousel position:

The central wavelength of an observation can be modeled as a function of carrousel position by the following relation which can be derived from the grating equation:

\[ \lambda_c = \frac{(A \cdot \sin(C-R))/10430.378}{m_c} \]

where:

- \( \lambda_c \) is the central wavelength for spectral order \( m_c \),
- \( m_c \) is the central order (1 for first order gratings, 42 for echelle A, and 25 for echelle B),
- \( A \) and \( C \) are coefficients fit for each grating mode,
- 10430.378 is used to convert from carrousel positions to radians.

A and C (tabulated in Table 1) are computed from the dispersion coefficients by:

- **a)** adjust \( a_0 \) term by subtracting previous thermal/time/geomagnetic model (if available).
- **b)** for each dispersion relation compute the wavelength, \( \lambda_{c_x} \), at the x-center of photocathode (sample position = 280.0) for central spectral order, \( m_c \) (1 for first order gratings, 42 for echelle A, 25 for echelle B).
c) Combining all observations for each grating mode, compute the coefficients $A$ and $C$ by using a non-linear least squares fit. Do not use observations in the echelle mode when only a single order was used to generate the dispersion coefficients.

i.iv Shift each dispersion relation to new coordinate system:

The dispersion coefficients, as defined in section i.i, are not useful for analysis of image motion. Small changes in the computed values of higher order coefficients cause large variations of the lower order coefficients. These large variations also make interpolation between calibrated carrousel positions invalid except for linear interpolation. Linear interpolation between carrousel positions has been shown to be inadequate. These problems can be avoided by changing the coordinate system of the dispersion coefficients so that the sample position is a function of the difference of the wavelength from a predicted central wavelength (the wavelength at the center of the photocathode). This new relation can be specified by:

$$s = f_0 + f_1 U + f_2 U^2 + f_3 U^3 + f_4 V + f_5 X$$

where:

- $U = m\lambda - m_c\lambda_c$
- $V = \lambda - \lambda_c$
- $X = m - m_c$
- $\lambda_c = (A*\sin(C-R)/10430.378)/m_c$
- $A$ and $C$ are coefficients fit in section i.iii.
- $m_c = 1$ for first order gratings, 24 for Ech-A, 25 for Ech-B
- $R$ is the carrousel position.

The new sets of dispersion coefficients $f_0$, $f_1$, $f_2$, $f_3$, $f_4$, and $f_5$ can computed from the previous coefficients by:

- $f_0 = a_0 + a_1 K + a_2 K^2 + a_3 K^3 + a_4 \lambda_c + a_5 m_c$
- $f_1 = a_1 + 2a_2 K + 3a_3 K^2$
- $f_2 = a_2 + 3a_4 K$
- $f_3 = a_4$
- $f_4 = a_4$
- $f_5 = a_3$

where:

$$K = m_c^*\lambda_c$$

We now have a set of $f_i$ coefficients for each observation which vary smoothly with carrousel position.
Table 1: GHRS Wavelength Calibration Coefficients

<table>
<thead>
<tr>
<th></th>
<th>G160M</th>
<th>G200M</th>
<th>G270M</th>
<th>ECH-B</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>4020.518</td>
<td>4615.5419</td>
<td>5539.2643</td>
<td>63192.867</td>
</tr>
<tr>
<td>C</td>
<td>54807.949</td>
<td>30600.929</td>
<td>14887.347</td>
<td>50575.473</td>
</tr>
<tr>
<td>m_c</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>25</td>
</tr>
<tr>
<td>F_{00}</td>
<td>-415.91319</td>
<td>76.751444</td>
<td>226.64578</td>
<td>688.63565</td>
</tr>
<tr>
<td>F_{01}</td>
<td>2.75097431e-02</td>
<td>1.59030662e-02</td>
<td>1.12093029e-02</td>
<td>-2.08831168e-02</td>
</tr>
<tr>
<td>F_{02}</td>
<td>-2.71933142e-07</td>
<td>-3.10844897e-07</td>
<td>-5.86011762e-07</td>
<td>2.66752644e-07</td>
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<tr>
<td>F_{10}</td>
<td>231.28828</td>
<td>75.862971</td>
<td>21.996576</td>
<td>95.848666</td>
</tr>
<tr>
<td>F_{11}</td>
<td>-8.08765830e-03</td>
<td>-4.38208344e-03</td>
<td>-1.82872974e-03</td>
<td>-4.52938433e-03</td>
</tr>
<tr>
<td>F_{12}</td>
<td>7.50778582e-08</td>
<td>7.49774546e-08</td>
<td>6.92031147e-08</td>
<td>5.42651856e-08</td>
</tr>
<tr>
<td>F_{20}</td>
<td>-0.42947955</td>
<td>-8.78849405e-02</td>
<td>6.51991907e-03</td>
<td>9.25916323e-03</td>
</tr>
<tr>
<td>F_{21}</td>
<td>1.73033639e-05</td>
<td>6.94837105e-06</td>
<td>-9.28531869e-07</td>
<td>-4.01144167e-07</td>
</tr>
<tr>
<td>F_{22}</td>
<td>-1.73384021e-10</td>
<td>-1.34734267e-10</td>
<td>4.12024736e-11</td>
<td>4.27596025e-12</td>
</tr>
<tr>
<td>F_{30}</td>
<td>-7.29502865e-05</td>
<td>-4.72720577e-05</td>
<td>-3.00016807e-05</td>
<td>-6.05639617e-08</td>
</tr>
<tr>
<td>F_{31}</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>F_{32}</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
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<tr>
<td>F_{40}</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
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<td>F_{41}</td>
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<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
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<td>F_{42}</td>
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<td>0.0</td>
<td>0.0</td>
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<td>F_{50}</td>
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<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
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<td>F_{51}</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>F_{52}</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>T_{1REF}</td>
<td>11.190587 (zdett1^a)</td>
<td>-1.8843722 (zfict^b)</td>
<td>19.027338 (zcst^c)</td>
<td>17.604019 (zcst)</td>
</tr>
<tr>
<td>D_1</td>
<td>0.17227277</td>
<td>-0.37546803</td>
<td>-0.70566530</td>
<td>-0.40634180</td>
</tr>
<tr>
<td>T_{2REF}</td>
<td>19.289868 (zcst)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>D_2</td>
<td>-0.48700304</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>J D_0</td>
<td>48111.5</td>
<td>48109.7</td>
<td>48109.8</td>
<td>48111.0</td>
</tr>
<tr>
<td>D_3</td>
<td>-1.42976053e-03</td>
<td>-1.09159957e-03</td>
<td>-1.51320847e-03</td>
<td>-5.44631437e-04</td>
</tr>
<tr>
<td>T_{REF}</td>
<td>33.370072 (zpabt2^d)</td>
<td>31.751161 (zpabt2)</td>
<td>32.713316 (zpabt2)</td>
<td>29.752718 (zpabt2)</td>
</tr>
<tr>
<td>E_1</td>
<td>4.61042115e-04</td>
<td>4.41550158e-04</td>
<td>3.36457557e-04</td>
<td>6.09907132e-05</td>
</tr>
</tbody>
</table>

a. zdett1 - detector 1 temperature  
b. zfict - Fixture interface C temperature  
c. zcst - Carrousel stator temperature  
d. zpabt2 - Detector 2 preamp assembly box temperature
i.v Compute a Global dispersion relation for each grating mode.

The dispersion coefficients $f_0, f_1, ..., f_5$ defined in section i.iv can be used to construct a dispersion model for arbitrary carrousel positions. A least squares polynomial can be fit to each coefficient $f_i$ as a function of carrousel position, $R$.

$$f_i = F_{i0} + F_{i1}R + F_{i2}R^2$$

$F_{i0}$, $F_{i1}$, and $F_{i2}$ give the least squares polynomial coefficients for dispersion coefficient $f_i$. Because of an ambiguity between the $f_0$ and $f_4$ terms in echelle modes when only an observation of a single order was used to compute the dispersion relation, only multiple order echelle dispersion relations should be used in the preceding polynomial fit.

The order of the polynomial varies for each $f_i$. We presently use a second order (quadratic) polynomial for $f_0$, $f_1$, $f_2$, and $f_4$ and a zeroth order (average value) for $f_3$ and $f_5$. Table 1 shows the computed values for $F_{i0}$, $F_{i1}$, and $F_{i2}$.

i.vi Computation of new spectral motion model

At this point any adjustment for a previous motion model subtracted from $a_0$ in section i.iii should be added to the $f_0$ values. We are ready to compute an improved motion model. Compute the fitted dispersion coefficients for each observation by using the polynomial from section i.v:

$$f_{i_{-fit}} = F_{i0} + F_{i1}R + F_{i2}R^2.$$  

For echelle mode observations of a single order where $a_4$ and $f_4$ could not be computed, set $f_4$ equal to $f_{4_{-fit}}$ and adjust the $f_0$ term accordingly:

$$f_4 = f_{4_{-fit}},$$

$$\lambda = A \sin((C-R)/10430.378)/m,$$

$$f_0 = f_0 - f_{4_{-fit}}(\lambda - \lambda_c),$$

where $m$ is the spectral order observed and $\lambda_c$ is the central wavelength for order $m_c$ computed in section i.iii. The differences of the $f_i$ values with the fitted values can be used to generate a motion model by:

a) For each observation compute the residual, $\Delta f_0$, of $f_0$ from the value computed using the fit in section i.v.

$$\Delta f_0 = f_0 - f_{0_{-fit}}.$$  

b) If already calibrated, subtract the contribution to $\Delta f_0$ due to geomagnetically induced motion. The geomagnetically induced motion will be computed in section i.vii by combining the results of all grating modes for the same detector:

$$\Delta f_0 = \Delta f_0 - G^*B_x.$$
where: $B_x$ is the x-component of the Earth's magnetic field for the midpoint of the observation
$G$ is the geomagnetic image motion coefficient (diodes/Gauss)

c) Perform a least squares fit to the equation to determine $D_0$, $D_1$, $D_2$, and $D_3$

$$\Delta f_0 = D_0 + D_1 (T_1 - T_{1REF}) + D_2 (T_2 - T_{2REF}) + D_3 (J \, D - J \, D_0)$$

where: $T_1$ is the temperature reading from the selected thermistor,
$T_2$ is an optional second temperature from a second thermistor,
$T_{1REF}$ is the average $T_1$ for all observations,
$T_{2REF}$ is the average $T_2$ for all observations,
$J \, D$ is the Julian Date - 2400000,
$J \, D_0$ is the minimum $J \, D$ for all observations.

Repeat for each thermistor or pair of thermistors. Select thermistors which give the best fit.

d) Adjust $F_{00}$ computed in step V to correspond to temperature $T_{1REF}$, $T_{2REF}$ and day $J \, D_0$. $F_{00} = F_{00} + D_0$.

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**Figure 3: G270M spectral motion versus carousel stator temperature.** The diamonds are the motion for each individual observation and the solid line is the model.
Figure 3 shows a sample plot of spectral motion versus temperature for grating G270M. G270M was the only grating mode which showed a significant improvement in the fit when a two temperature thermal model was used. We set $D_2$ to 0.0 for all other grating modes. Figure 4 shows the spectral motion for G270M as a function of time. It appears that a linear model of motion with respect to time will not be sufficient in the future. The rate of change with time appears to be decreasing. The thermal and time motion coefficients computed by this model are tabulated in Table 1.

Figure 4: G270M spectral motion versus time. The diamonds are the motion for each individual observation and the solid line is the model.

i.vii Computation of sensitivity to the Earth's Magnetic Field.

To determine the spectral motion resulting from changes in the Earth's magnetic field vector as the HST orbits the Earth, subtract contributions to $\Delta f_0$ caused by thermal and time motion as modeled in the previous section. This gives any remaining residual from the global dispersion coefficient model that is not predicted by our thermal and time motion model. Since the magnetically induced motion is a detector problem, we can combine the results for all grating modes for the same detector. We then compute the least-squares linear fit to the residuals as a function of the component of the Earth's magnetic field in the dispersion ($x$) direction of the detector. The slope of the least-squares line gives the spectral motion in diodes/Gauss. Figure 5 shows the results for detector 2. Each + mark is the average of the residuals for 25 individual observations.
i.viii Changes in the linear dispersion with temperature.

In addition to motion of the spectrum with temperature, results show that the linear dispersion, term, $f_1$, also changes with temperature. To model these changes:

**a)** For each dispersion relation compute the residual, $\Delta f_1$, of $f_1$ from the value fit by the coefficients derived in section i.v.

$$\Delta f_1 = f_1 - f_1_{\text{fit}}$$

**b)** Perform a least squares fit to the following equation to determine $E_0$ and $E_1$ (tabulated in Table 1).

$$\Delta f_1 = E_0 + E_1(T - T_{\text{REF}})$$

where:

- $T$ is the temperature reading from the selected thermistor, and
- $T_{\text{REF}}$ is the average $T$ for all observations.

Repeat for each thermistor and select the results for the thermistor which gives the best fit.
c) Adjust $F_{10}$ computed in section i.v to correspond to temperature $T_{REF}$:

$$F_{10} = F_{10} + E_0.$$ 

Figure 6 shows the changes in the linear dispersion for grating G160M as a function of the thermistor with the best correlation.

II. Sources of GHRS Wavelength Calibration Errors.

The major sources of errors in the assignment of wavelengths to GHRS science observations are shown in Table 2. When the object is observed in the Large Science Aperture (LSA) the major source of errors are inaccuracies in the centering of the target in the aperture by the onboard flight software and the lack of an accurate incidence angle correction for the LSA. These errors are estimated to be as large as 1.5 diodes.

Wavelengths accurate to 1.0 diodes can obtained for observations with the target in the SSA using the spectral motion model described in this report. A WAVECAL/SPYBAL observation taken near the time of a science observation can be used to correct the data for inadequacies in the thermal/time motion model. Errors in carrousel repeatability and the short term thermal motion between the WAVECAL/
SPYBAL and the science apertures will then be the dominant errors. The most precise wavelengths can be obtained by taking a WAVECAL observation at the same carrousel position as the science observation.

### Table 2: Sources of GHRS Wavelength Errors

<table>
<thead>
<tr>
<th>Source of Error</th>
<th>Max Error (diodes)</th>
<th>Correction</th>
</tr>
</thead>
<tbody>
<tr>
<td>1) Computation of dispersion coefficients</td>
<td>0.1</td>
<td>None</td>
</tr>
<tr>
<td>2) Incidence angle offset between spectral lamp aperture and SSA</td>
<td>0.1</td>
<td>None</td>
</tr>
<tr>
<td>3) Errors in thermal/time model</td>
<td>1.0</td>
<td>Use WAVECAL or WAVECAL/SPYBAL</td>
</tr>
<tr>
<td>4) Short term thermal motion</td>
<td>0.4 diodes/hour</td>
<td>Take multiple WAVECALs</td>
</tr>
<tr>
<td>5) Carrousel repeatability</td>
<td>0.5 (0.17 typical)</td>
<td>Take WAVECAL at same wavelength as science obs.</td>
</tr>
<tr>
<td>6) Onboard Doppler compensation</td>
<td>increases with time since Doppler zero typical=0.15</td>
<td>Use short obs. times (e.g. 5 minutes). Correct errors with ground software.</td>
</tr>
<tr>
<td>a) round off in orbital period causing phase shift</td>
<td></td>
<td></td>
</tr>
<tr>
<td>b) round off in Doppler magnitude to nearest 1/8 diode</td>
<td>0.06</td>
<td></td>
</tr>
<tr>
<td>c) round off of correction to nearest 1/8 diode</td>
<td>0.06</td>
<td></td>
</tr>
<tr>
<td>7) Geomagnetic image motion</td>
<td>0.25</td>
<td>short obs. time. Correct with ground software</td>
</tr>
<tr>
<td>8) Errors in centering target in SSA</td>
<td>0.21</td>
<td>Use the new SSA return to brightest point</td>
</tr>
<tr>
<td>9) Observing in LSA. (centering errors, lack of accurate incidence angle offset calibration)</td>
<td>1.5</td>
<td>Use the SSA</td>
</tr>
</tbody>
</table>

### III. Obtaining the Ultimate Wavelength Precision with the GHRS

Observing in the SSA is the only special observing consideration required to obtain wavelengths accurate to within one diode. If better wavelengths are desired, the following observing guidelines can be followed.

1) Observe in the small science aperture.

2) Use an SSA return to brightest point target acquisition. This decreases the errors caused by mis-centering of the target in the aperture.

3) Limit individual exposures to 5 minutes. This limits the loss of resolution and allows corrections for geomagnetically induced image motion and errors in the onboard Doppler compensation processor.
4) Take a WAVECAL at each wavelength observed. If total time at a single wavelength exceeds 15 minutes, take a WAVECAL both before and after the science observation. This limits the errors resulting from short term thermal motion.

5) For long exposures, take a wavecal every 30 to 60 minutes. Do not allow a WAVECAL/SPYBAL to be performed without a WAVECAL before and after it. The WAVECAL/SPYBAL moves the carrousel.

The following accuracy is achievable by following these guidelines:

<table>
<thead>
<tr>
<th>Source of Error</th>
<th>Error (diodes)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Accuracy of the dispersion relation</td>
<td>0.1</td>
</tr>
<tr>
<td>Spectral cal lamp to SSA offset error</td>
<td>0.1</td>
</tr>
<tr>
<td>Centering error in the SSA</td>
<td>0.125</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td><strong>0.325 diodes = 1 km/sec</strong></td>
</tr>
<tr>
<td>Errors added in quadrature</td>
<td>0.19 diodes = 0.6 km/sec</td>
</tr>
</tbody>
</table>