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# FOS Post-Operational Archive and STIS Calibration Enhancement

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**Abstract.** The first part of this report summarizes the scientific quality enhancement for FOS/BL data—the Post-Operational Archive project. Part two describes the status and planning for the follow up, a calibration enhancement for the 66,095 data sets obtained with STIS between 1997 and 2001 when it was operated using "Side 1 electronics."

## 1. Introduction

When in 1999 the Memorandum of Understanding (MoU) between NASA and ESA about funding and specific contributions towards the continuation of the multi-agency *HST* project had to be renewed, it became clear that there was little room for hardware contributions from ESA's side. The agencies agreed that the additional ESA contributions will instead concentrate on the "users end," for our purposes here in particular the science data archives and the science data calibration status.

As a result, the "Instrument Physical Modeling Group" was created at the ST-ECF with 3 additional staff from ESA *HST* funds. In October 1999 we could start with the first project, the "Post-Operational Archive for FOS," concluded at year's end in 2001. Since January 2002 we are now fully engaged in the "STIS Calibration Enhancement" (STIS/CE) project. In the following status, results and plans for these two projects, implemented under NASA/ESA MoU, are present with emphasis on the science end user's point of view.

## 2. Scopes and Interfaces

The prime responsibility for *HST* science operations rests with the STScI, including the dissemination and archival of data in a form useful for the science end user. It has always been a key objective for these activities at STScI to ensure a very high standard of calibration on the data. This high quality default calibration was (and still is) to be available not weeks or years after the actual observation took place, but right from the moment the raw data are received on the ground and subjected to the pipeline for the first time.

At the occasion of the first *HST* calibration workshop in the new millennium it should be noted that the staff at STScI, with the support from IDTs and others, has done a very good job on maintaining the high standards for the "instantaneous" calibration, even under the adverse conditions of responsibility for operations, planning and dissemination of products in almost real time. Naturally, this goal could only be reached by investing in an 80/20-like fashion, that is, assuring a good level for almost all data at all times from all frequently used modes, rather than concentrating on a few specific or difficult modes at a

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particular epoch. Also, the operational requirement to make available calibration solutions "momentarily" did not help in understanding long term trends.

The de-commissioning of the first generation of *HST* instruments, in particular the FOS, offered the ideal case to take a break and to view the entire set of data, calibration observations and science exposures as well, as a coherent set. On the firm basis of an existing, usually quite well documented calibration pipeline system the key objectives for POA/FOS project were then initially defined by

1. A comprehensive review of the calibration (documentation, calibration data, suitable science data in comparison to expectations)
2. Analysis of the trends, isolating slowly varying instrumental effects from *HST* environmental ones (long baseline for trending)
3. Selection of the calibration areas with best ratio of scientific value per effort for follow up
4. Implementation of superior solutions into the pipeline
5. Release of re-calibrated data and documentation, user support

Ultimately the recipients of the products should be the scientific users world wide. And, while STScI on behalf of NASA is formally the primary customer, it can also act efficiently as a redistribution center both ways, products and user inquiries. In order to maximize the benefits and to minimize the overhead close collaboration and exchange of information between ST-ECF and STScI were agreed upon as well and set up as required. Reporting is annually to the ST-ECF Users Committee and at the ESA/*ESO* Annual Review of the ST-ECF on this side of the Atlantic. Progress reports are usually also included in the regular meetings of the STScI Users Committee.

## 3. A New Paradigm

From the outset it was clear that our group with a nominal power of 2.5 FTE would never be able to repeat (even partially) the work of many that had covered the calibration of an instrument like FOS as members of the IDT, as participants in the laboratory testing before launch, as instrument scientists and archive specialists at STScI. In order to improve the calibration of the entire set of archived data of the FOS at a scientifically significant level we therefore had to choose a paradigm quite different from the canonical, empirical one.

Our approach then rests on the idea that a large (well above 90 percent) fraction of the calibration relations is very well described by functions that are either directly derived from first principles or well known laws from physics textbooks. The description of dispersion relations through trigonometric functions from physical optics, with meaningful parameters, rather than by fitting of unspecific low order polynomials may serve as an example.

The procedure then is to replace a multitude of isolated empirical corrections (instrumental signatures) available for the various modes, environmental conditions and epochs by a physically correct chain of transformations that are motivated by insight into the engineering and physics of the instrument, its optical setup and its detectors. Early successes in that direction include for example the scattered light model for the FOS, described in the Appendix C (M. Rosa) of the *FOS Instrument Handbook*, (Keyes et at. 1995) and in Rosa (1994).

## 4. Post-Operational Archive for the FOS

The review and subsequent improvement of the calibration of the FOS archival data started in 1999 and was concluded with the final release of the upgraded pipeline software (version 1.2.1), necessary reference data and on-line documentation in November 2001 (see http://www.stecf.org/poa/fos/, and Alexov et al. 2002). The data actually corrected concern all spectrophotometric observations FOS/BL mode. Excluded are FOS/BL spectropolarimetry and FOS/RD all modes (see also the last subsection further down).

### 4.1. Wavelength Calibration—Zero Points

In agreement with STScI we focused in 1999 on known and suspected issues of the wavelength calibration. User reports and the analysis of data obtained annually for the check of the dispersion solutions pointed towards problems with the wavelength calibration in all modes. The findings included inconsistencies of radial velocity measurements between repeated exposures, between different wavelength ranges, between *HST* FOS data and observations from the ground and even within the wavelength range visible in certain high resolution modes.

Even without the user driven suspicion towards the dispersion solutions and zero points it was clear to us that a close review of the wavelength calibration and its stability over the entire FOS lifetime was of high interest. This because the dispersion solution reference data (polynomial parameters) employed by the *calfos* pipeline had remained unchanged since 1992. Indications of large, albeit random-like wavelength zero point shifts from trending analysis while FOS was still operational had always been explained with the so-called "filter-grating-wheel un-repeatability."

We undertook a mass analysis of all internal wavelength calibration lamp observations available, dedicated ones planned by FOS instrument scientists and those taken by GOs in connection with science exposures on targets. In total we had some 1800 such observations spread over the entire lifetime of FOS (1990 to 1996) at our disposal. The raw data were cross-correlated with those that had formed the basis for the dispersion coefficients installed in CDBS.

Soon it became clear that there were rather large uncertainties in the zero points of the wavelength scale. On the blue channel modes there were very well defined almost linear trends with time amounting to an offset of 4 pixels for data taken in late 1996. On the red channel modes the situation was much more complicated, presenting a seemingly random scatter $-2$ to $+6$ pixels throughout the entire lifetime (see Rosa et al. 1998).

In the end the in-famous geomagnetic image motion problem (GIMP) noted in September 1990, and the attempts to correct it on-board after April 1994 were found to be the primary source of the scatter in the wavelength scale zero-points. The long term steady increase in zero point deviation for the FOS/BL data could be identified with the side-effects of the repeated adjustment of the Digicon image focusing parameter YBASE during operational life, and with the general increase of the *HST* aft-shroud temperature. Details can be found in the POA/FOS Technical Reports #1 and #2 (Rosa et al., 2002a, b) available from the above mentioned web site.

Correction for the blue side FOS data was achieved using a model that combined the detector physics (Digicon magneto-electrical focusing) with highly accurate models of the *HST* orbit (from NORAD) and the geomagnetic field (from GSFC). This code segment was implemented into a POA/FOS modification of *calfos* (*poa_calfos*) released in August 2000.

### 4.2. Wavelength Calibration—Dispersion Relations

After correction of the GIMP/YBASE/Temperature related drifts and shifts of the wavelength zero points (really the location of the photocathode image on the diodes), it was possible to analyze the dispersion relations and their variations in shape for the different epochs. Not surprisingly—the FOS was built according to high standards—it was found that the shapes did NOT vary at all. The alleged variation of dispersion solutions had in fact been the zero point shifts masked by the use of unspecific low order polynomials.

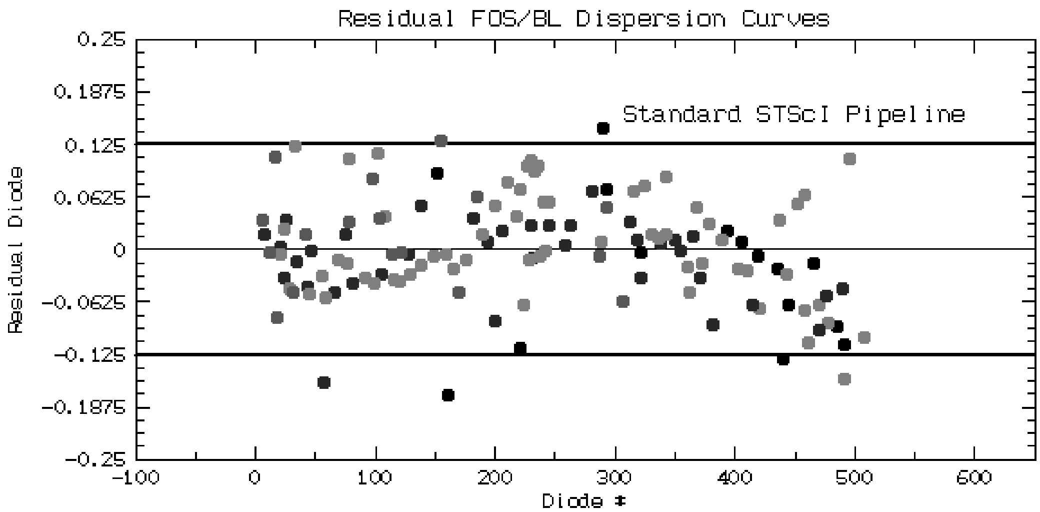


Figure 1. Residuals of the *calfos* dispersion relations (different shades are different high resolution modes). Although most of the data points are within the nominal error limit of a pixel (= 1/4 diode indicated by horizontal bars), there is a clear structure common to all modes—actually the $S$-Distortion not fully matched by the 3rd order polynomials. In addition, several lines of the original line lists are either blends or have bad identifications.

During the review of the dispersion solutions we also found that the scarcity of useful, unblended lines in almost all of the FOS wavelength ranges combined with the use of low order polynomial solutions led to unphysical behavior of those solutions at the wavelength range limits (run-away).

Accordingly, STPOA *poa_calfos* release version 1.1 in May 2001 included an entirely new wavelength calibration module based on a physical optics model of the FOS spectrograph. This model is a derivative of a generic spectrograph model described by Ballester and Rosa (1997), and contains only engineering parameters such as focal lengths, grating constants and configuration angles. The solution implemented for the FOS/BL high resolution modes represents the best set of such parameters for those components that are common between all modes (collimator, overall configuration, camera). It also includes the effects of $S$-Distortion in the Digicon detector. For each of the high resolution modes the internal accuracy of the solutions are a factor 5 to 10 improved over the original polynomial solutions.

## 4.3. Update of Flats and Dark Correction

Subsequently the entire suite of flat fields needed to be redone, because the FOS/BL raw data were now adjusted in zero point location. We used the occasion to investigate areas of improvement for the flat fields, but concluded that any additional improvement was visible only for exposures of exceptional total length and signal to noise ratios. The only set of such exposures in the FOS/BL archive are, however, the standard star observations made for the purpose of deriving flat fields.

A noticeable improvement was possible for the dark correction module of the pipeline. As noted earlier (Rosa 1993), the scaling of darks in the *calfos* pipeline was insufficient at the extremes of geomagnetic latitudes traveled by *HST*. Since the new pipeline *poa_calfos* had already been augmented with a module that predicted HST orbital location and geomagnetic parameters to a much higher accuracy than previously *calfos*, we were able to scale the darks using a physical connection with the energetic particle density through the so-called Shell-parameter $L$. This new dark scaling and correction of an error in the scaling algorithm in

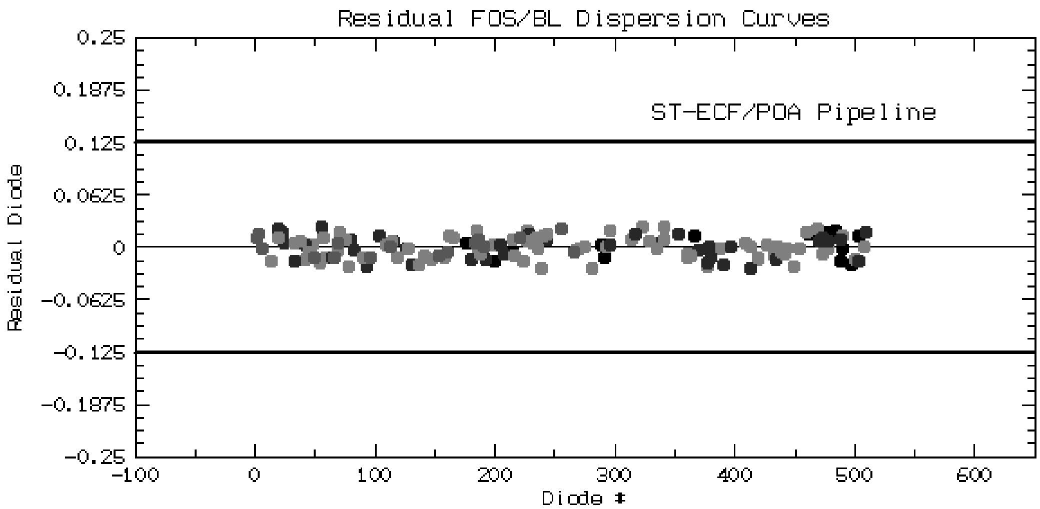


Figure 2. Residuals from the FOS Dispersion model, same total number of lines used. Improvement by a factor of 5 to 10 is mostly due to the generic inclusion of the $S$-Distortion and the ability to select against blends or misidentifications without significant change of the shape of the solution.

the pipeline itself were implemented into the final release of STPOA in late 2001 (Bristow et al. 2002b).

Additional dependencies of the dark rate on solar cycle or day-night differences could be seen in the data, but the large spread of actual dark measurements at any given geomagnetic location and epoch did not warrant any further modeling. In any event, the residual uncertainty in dark scaling is only relevant for the faintest of all targets. However, for such observations the only trustworthy dark measurements could have been obtained only by simulating a near-simultaneous sky or dark observation through use of a 50/50 cycle rapid beam switching in the Digicon—actually never performed.

### 4.4. And What about FOS/RD Data...

The entire suite of successful improvements made for the FOS/BL data archive rests on the ability to correct the GIMP/YBASE/temperature induced zero point shifts of the raw data in the first place. In the case of the blue side FOS Digicon the magnetic shielding was near spec, so that the GIMP (and its, albeit wrong, on-board compensation) were small compared to the other two sources of error.

However, the magnetic shielding of the red side detector was so poor (factor 8 less than on the blue side), that the GIM and the subsequent on-board compensation are significant nominally 4 pixel max each. The seemingly stochastic variation of the zero-points on the red side from −2 to +6 pixel exceeded this range about twice (see Rosa et al. 1998). The suspicion, that the on-board GIM compensation was sometimes out of phase is—very probably—the answer. Probably, because our deep investigation into the convoluted sequence of scheduling software, telemetry up, execution of the on-board GIM segment and telemetry down did lead nowhere. Actually it led into a US Government storage facility near Bowie, MD, where some 10,000 reels of 16 inch magtape from VAX resided—to be destroyed within a month's time (that was in June 2000). More details on this sad outcome can be found in Bristow et al. (2002c).

In principle the code we produced for FOS/BL can be used to analyze some 1000 wavelength calibration data from FOS/RD and to investigate whether a suitable and meaningful scaling of the parameters might explain the zero point shifts in a homogeneous and

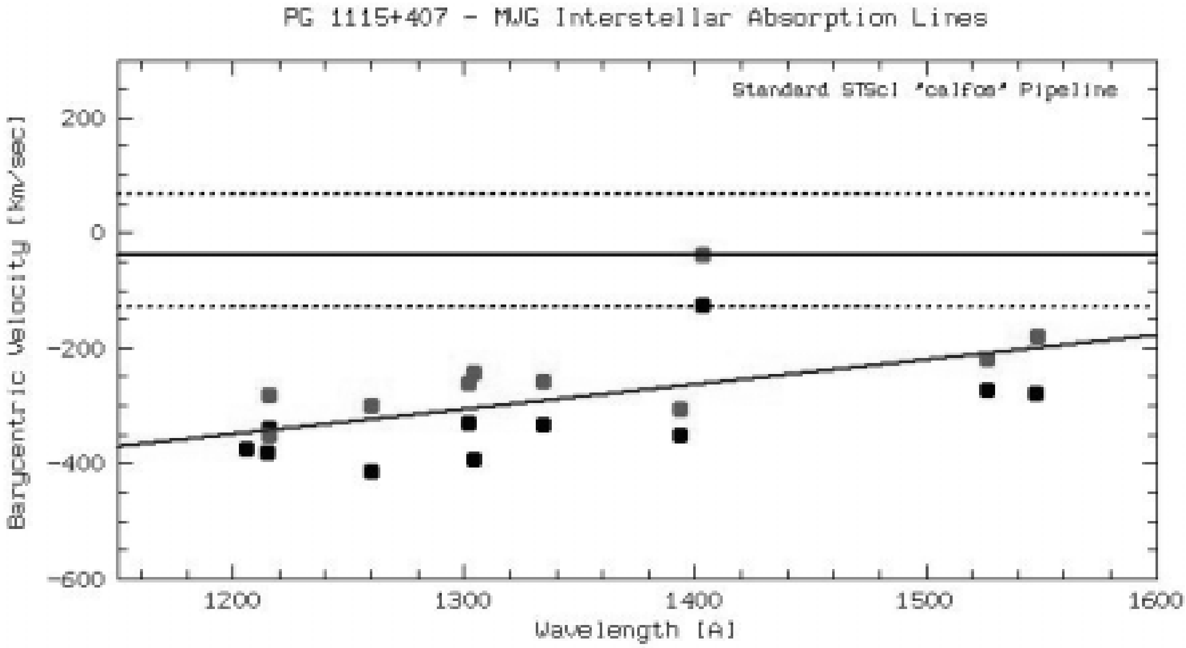


Figure 3. MWG halo absorption line velocities measured in data from two successive orbits as calibrated in the original FOS archive. Note the unphysical slope (wavelength dependency), and offset relative to the values expected from 21 cm line data bracketed by the dashed horizontal lines.

comprehensive manner. Our peers and the internal review of plans between STECF and STScI however felt that we should now concentrate on the 66,095 data sets from STIS side 1 instead (see below)—and this is why there will likely never come a POA-like improvement to the FOS/RD part of the archive.

### 4.5. Science Verification of POA/FOS

Finally, the improved calibration of the FOS/BL data was verified on science data in two ways. The consistency of the wavelength calibration across several adjacent wavelength ranges was shown using the emission lines of several LMC planetary nebulae (Kerber et al. 2002).

The full impact of the POA/FOS correction of zero-points and dispersion solutions can be judged from a "before and after" comparison shown in Figures 3 and 4. Galactic halo absorption lines seen against the background of quasar continua have been measured in data sets calibrated with both, the standard *calfos* and with the new *poa_calfos* pipelines respectively. Shown are data from two successive orbits denoted by symbols of different grey-scale. The horizontal lines indicate the range of radial velocities expected from the line of sight velocity distribution in the $H_2$ column. The old calibration resulted in a velocity distribution that was (a) not commensurate with the 21 cm data, (b) displaying an unphysical correlation with wavelength, and (c) not even consistent from one orbit to the next. Surprisingly, a reasonably strong absorption line at 140 nm, if identified as a prevalent feature seen in many lines of sight through the halo, seems to be the only one matching up with expectation.

The measurements of the same data sets, now from the POA/FOS archive, dramatically demonstrate the science potential for archival research with the improved FOS data. The measurements are now in agreement with expectation, from one orbit to the next as well, and independent from wavelength. In addition, the "mystery" line can now clearly identified

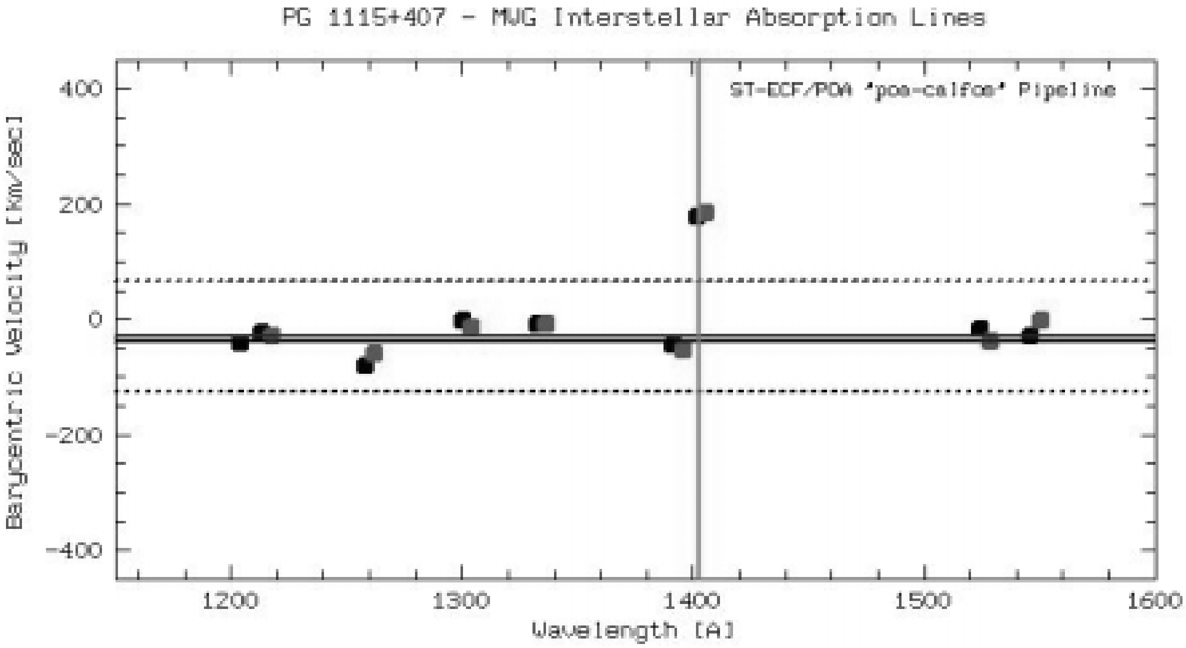


Figure 4. Same raw data as Figure 3, now calibrated with the POA/FOS pipeline. The feature at 140 nm is definitely not a MWG halo absorption, but $Ly_\alpha$ from the quasar host galaxy at the redshift indicated by the vertical line.

with $Ly_\alpha$ absorption in the quasar host galaxy at the expected redshift (indicated by the vertical line in Figure 4).

### 4.6. User Support

Upon delivery and release of STPOA v1.2.1 (August 2001), the STECF assumed full responsibility for the FOS user support world wide. Users entering the STScI *HST* help pages are transparently routed through to http://www.stecf.org/poa/fos/, and mail links are set to our POA help desk at *ecf-poa@eso.org*.

## 5. STIS Calibration Enhancement—STIS/CE

Since January 2002 we are engaged in a follow-up project that will bring to the STIS data all the insight gained with implementing the new paradigm for FOS. Since STIS is not a post-operational instrument yet, extra care has to be taken to not interfere with the operational pipeline and calibration data base. Hence, the STIS Calibration Enhancement (STIS/CE) project has as its objective the archive of STIS data obtained between the commissioning after Servicing Mission 3 (March 1997) and the switching of electronics to Side 2 (July 2001). This STIS Side 1 archive comprises 66,095 data sets.

Between January and March 2002 we collected and digested a very near complete pile of relevant STIS documentation from STScI, from the IDT archives at GSFC and from the manufacturer (Ball Aerospace). In April we discussed the resulting 4-year-plan with the STScI and presented it to both the STECF and the STScI Users Committees. The plan is a phased approach to the key areas of STIS calibration for which a significant improvement of science data can be expected from our paradigm of reducing calibration to understanding an instrument and list environment in physical terms.

### 5.1. Preparations

Phase 1 (2002) foresaw the consolidation of a documentary archive, additional hardware installation to mass process the 66,095 data sets repeatedly, and to archive raw and processed data in an on-line storage for analysis. By mid-2002 we had installed a 5 TB raid array on a SUN Fire 280R machine with two 900 MHz CPUs, supported by the over-night processing power of additional 4 SUN Blade 150 Workstations. By late 2002 we have now in place the complete raw data archive of all STIS Side 1 data processed by STIS OTFR Opus v 1.4.2. This will serve as the reference against which improvements are verified (to be updated as necessary).

### 5.2. Geometry

As was the case with FOS, paramount to this approach is a firm basis of the instrumental geometry for all epochs of data taking, both for imaging and for spectral long slit or echelle data. The pipeline ultimately will contain a module that comprises geometric distortion, 2D spectrometric imaging and wavelength assignment in a coherent fashion. Phase 2 (2002–2003) calls for the implementation of the 2D spectrograph model (Ballester & Rosa, 1997), which has been working successfully already for the UVES Echelle spectrograph on the *ESO* VLT. Testing of the analysis part of the code has been very successful by June 2002 already for both, the FUV and the NUV echelle modes. As an example for the E140H FUV mode we predict the location wavelength calibration lines to better than 0.3 pixel (chi-square for 400 lines) from first principles across the entire frame (2 by 2 K).

In support of this Phase 2 (geometry and wavelengths) several calibration lamps (vintage STIS flight spares and newly produced) have been observed with the UV vacuum spectrograph at NIST to obtain highly accurate laboratory list of the Pt, Cr and Ne spectra as observed in orbit. This is necessary because the laboratory list currently in use by the default STIS pipeline are not based on any observation of a STIS vintage lamp and, in particular do not have a single entry for the abundant lines of Cr.

Also in support of the geometry phase we have begun to build up a physical CCD readout model that will be able to correct the raw data for the effects of CTE deficiencies. It is a well known fact that the loss and redistribution of charge during readout is not only a nuisance for photometric applications, but also leads to geometric distortion of the data in an illumination/scene dependent manner. The CCD readout model will serve also during Phase 4 (flux calibration).

### 5.3. Trending and Orbital Environment

Phase 3 (mid-2003 to mid-2004) will make use of the STIS internal geometry corrected data to assess the impact of orbital environments (MSM repeatability, aft-shroud temperature variations, breathing of the telescope, etc.). The analysis of the data will also have an impact on the predictability of dark frames, hot pixels and other items related to photometry.

### 5.4. Flux Calibration

After conclusion of Phase 3 the data processed by the STIS/CE Side 1 pipeline will be ready to establish a new system for flux calibration. Improvements of the geometric stability and predictability will be used to address again the optimal extraction of spectral data, this time aided by the predictions from the 2D echelle or long slit model—particularly beneficial for faint targets or deep absorption troughs. Phase 4 then will include the review of flux calibration items (e.g., flats, darks, extraction, inverse sensitivity, throughput and vignetting).

### 5.5. And what about STIS Side 2...

Between the STIS project at STScI and the STIS/CE project we have a close collaboration and information exchange, supported and regulated by several agreed upon documents. In order to protect the operational STIS pipeline at STScI from the experimental versions of our STIS/CE pipeline there will not be a direct port of modules and builds into *calstis*.

However, the collaboration stipulates to exchange all insight gained into STIS calibration and functioning at the earliest possible date. For example it will certainly be possible to upgrade the operational *calstis* to the improved geometry and wavelength calibration once these modules have been tested extensively for STIS/CE of Side 1 data, if the STScI STIS project opts to do so. In any case it will be necessary to evaluate the situation—i.e. the evolutionary stage of both pipelines, STIS Side 1 *ce_calstis* and STIS Side 2 *calstis*—at around 2004 and to discuss possibilities for mergers for the benefit of all STIS users.

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