CALIBRATION AND DATA REDUCTION SYSTEM REQUIREMENTS AND PRELIMINARY DESIGN

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1 INTRODUCTION

1.1 Purpose

This document presents the design requirements and design concept for the calibration and data reduction systems. The calibration system provides iSHELL with wavelength and flat field calibration. It consists of arc lamps and a gas cell for wavelength calibration, continuum lamps for flat fielding, and illumination optics. The data reduction system is the software to manipulate raw spectral images to the point where spectra can be extracted, to remove the instrument signature, to merge spectral orders into continuous spectra, and to remove telluric contamination.

2 CALIBRATION SYSTEM DESIGN REQUIREMENTS

2.1 Fundamental requirements

iSHELL acquires cross-dispersed (echelle) spectra at resolving powers up to R=70,000 (4.3 km/s) and with anywhere between ~ 5-40 orders per setting depending on wavelength and slit length. The grating blaze shape and overall instrument throughput variations are removed by observing a standard star of known spectral shape (e.g. A0V star), while detector pixel-to-pixel variations are removed by observing a uniformly illuminated field (a flat-field) projected onto the detector array (e.g. Cushing et al. 2004 PASP 116, 362; Vacca et al. 2003 PASP 115, 387). Flat fielding should achieve S/N>1000 across 1.1-5.4 µm. This requires a summed signal of >10^6 photo-electrons. In addition the flat field must illuminate the full length of the longest slit (25″) equivalent to a diameter >14 mm. A low-order change in flux of about 1% (typical of integrating spheres) across this field should be adequate to meet the S/N requirement.

A good wavelength solution requires at several arc lines per order, since angular dispersion varies with angle of diffraction, for a good (non-linear) fit and the centroiding of individual lines to about one tenth of the narrowest slit (one tenth of three pixels or about 0.4 km/s). This accuracy of centroiding requires peak line detections with S/N>10. At wavelengths where the arc line density is low (λ>2.5 µm), telluric features can be used. See, for example, the echelle plots in the H band and L band illustrated in Figure 1. Since

\[
\frac{m\lambda}{n} = \text{constant}
\]

where \(m\) is the order, \(\lambda\) is the wavelength, and \(n\) is the refractive index of the immersed grating medium (Silicon for iSHELL), an option is to collapse the orders into one ‘super order’. This is done successfully with SpeX to increase the effective number of calibration lines. The complication for iSHELL is that \(n\) is now a function of wavelength and needs to be carefully calibrated. Optical distortion across the array also needs to be mapped out.
Figure 1. Symbols indicate the position of Argon (green square) and Thorium (purple diamond) lines from a Th-Ar arc lamp lines. The free spectral range of each spectral order is plotted. A box indicates the H2RG array. Example echelle formats: H band (left) and L band (right).

Planet detection through radial velocity measurements requires much higher velocity precision. Experiments with CSHELL by Plavchan and Anglada indicate that long-term precisions of ~ 10m/s can be obtained by using iSHELL in conjunction with a $^{13}$CH$_4$ gas cell working in the $K$ band (high density of methane absorption features). The gas cell (see Figure 2) is placed immediately in front of the cryostat entrance window. Use of heavy methane shifts lines by ~0.010 $\mu$m relative to telluric methane to avoid contamination. The pressure of the gas (4 psi) is optimized to match the width of stellar lines.

Figure 2. The methane gas cell used in CSHELL. The cell is 150 mm long and 50 mm diameter.
2.2 Practical requirements

The calibration system must fit in the space surrounding the cryostat entrance window, ~0.5m x 0.5m (wide) x 0.3m (high).

Total integration times to obtain flat and arcs per mode should be no longer than a few minutes. Given the limitations on space (and therefore lamp size and brightness) this will possibly require the use of flux concentrators to increase the solid angle of flux intercepted from the lamps.

It is important to duplicate the telescope illumination on the array with the calibration system. Therefore the illumination optics are designed to accurately match the input beam from the telescope (f/38.3). The illumination optics also need to be achromatic across the range of use (1.1-5.4 µm).

The calibration optics must be shielded from stray light although, since the lamps are bright, the light path does need to be absolutely light tight.

The calibration system should be made as simple reasonable, minimizing the number of mechanisms (e.g. use an integrating sphere to feed multiple lamps rather than moving lamps into position over an entrance aperture).

Since a uniform patch of illumination is projected onto the slits (>14 mm diameter) stability and reproducibility of the illuminating optics are not significant design drivers (~0.5 mm at the slits).

For long-term radial velocity stability the gas cell needs to be stable to about 1 K. Since seasonal variations on the MIM are about ± 5 K temperature control of the gas cell will be required.

2.3 Summary of calibration system high-level design requirements

1. Arc line wavelength reference > 6 lines per order (TBC), ±0.4 km/s
2. Otherwise use telluric features
3. Precision RV ~ 10 m/s with gas cell
4. Flat field S/N > 1000, uniformity ~ 1% across field of largest slit (25")
5. Integration times less than a few minutes (use lamp concentrators if necessary)
6. Fit in 0.5m x 0.5m (wide) x 0.3m (high) space immediately in front of the cryostat window
7. Illumination optics should mimic the beam from telescope (f/38.3) and be achromatic across the range 1.1-5.4 µm
8. Shield calibration optics from stray light
9. Minimize moving parts
10. Optical stability and reproducibility < 0.5 mm at slits
11. Temperature control of gas cell ± 0.5 K
3 CALIBRATION SYSTEM CONCEPT

In concept iSHELL’s calibration system is similar to that used in SpeX (see Figure 3). The uniform flux distribution across the exit aperture of an integrating sphere is reimaged onto the telescope focal plane (TFP) inside the cryostat at a magnification sufficient to cover the longest slit. The function of the integrating sphere is to integrate and scramble the spatial structure in the flux from lamps placed at the three entrance apertures into a uniform (flat) distribution at the exit port. This is done by an arrangement of baffles inside the sphere that force rays entering the sphere to undergo multiple reflections before exiting. A highly reflective non-specular and spectrally flat coating is applied to the surface of the sphere (Infragold from Labsphere) to enhance uniformity and throughput.

Figure 3. The calibration system used in SpeX. Mirrors feed light from the exit port of an integrating sphere through the entrance window and into the cryostat. Flat field lamps and arc lamps are positioned at the three entrance ports of the integrating sphere. The only mechanism is the in/out mirror that moves into the f/38 beam from the telescope (shown in the calibration position) to project light from the calibration lamps into SpeX.

In the optical layout for iSHELL (see Figure 4) a 600 mm focal length spherical mirror re-images a magnified virtual image of the integrating sphere exit port (10 mm diameter) onto the TFP at one to one magnification (30 mm diameter – sufficient to cover the longest slit). An achromatic lens (a LiF/BaF$_2$ doublet) is placed at the image of the entrance pupil (the secondary mirror) in the spherical mirror (643 mm behind the mirror). The exit port of the integrating sphere is then placed 186 mm behind the lens.
((1200-643)/3) to form a three-times magnified virtual image of the exit port (30 mm) at 1200 mm from the spherical mirror (i.e. at a distance of two focal lengths). The aperture of the lens is adjusted to match the required input beam speed (about 15 mm gives f/38.3). The re-imaged pupil is imaged onto the internal spectrograph pupil by fine-tuning the distance between the lens and spherical mirror. (In this way both the TFP and internal pupil are evenly illuminated.)

Figure 4. Optical layout of calibration system. Side view (top), plan view (bottom). For scale the integrating sphere is 50 mm diameter and the gas cell 150 mm long.

The integration times needed to meet the S/N requirements are calculated from simple considerations of lamp brightness, lamp illumination geometry ($A\Omega$), and integrating sphere throughput (see Mathcad document). The brightness of the flat field lamps is determined by the filament size and temperature. The temperature is set by the need for the flux to pear in the near infrared (1.15 µm for a standard QTH lamp
at 3200 K and 3.34 µm for a standard IR lamp at 1100 K). Therefore lamp brightness effectively scales with lamp size (filament area). Working at resolving powers of up to R=2000 SpeX requires only relatively small lamps to limit flat field integrations to about one minute. The lamps were positioned about 20 mm in front of the 10 mm diameter input ports (see Figures 3 and 5).

![Figure 5. SpeX integrating sphere showing QTH lamps (top), IR lamps middle), argon arc lamp (bottom), positioned in front of their respective input ports.](image)

Since iSHELL works at resolving of up to R=70,000 about 35 times more flux is needed to achieve the similarly short integration times. Given the space limitations this cannot be achieved by increasing the brightness (size) of the lamps. The best solution is to intercept more photons from the lamps by using optical concentrators (1-2 orders of magnitude more is relatively simple to do). This will also require more space but not significantly.

Since spectral lines from the Argon arc lamp are unresolved even at R=70,000, flux is not an issue. More of a concern is the number of lines. We need at least three lines per order to provide a good wavelength solution. A simple Argon arc lamp does not provide sufficient lines. A Thorium-Argon arc lamp of the type used in CRIRES seems like the best solution for iSHELL (see Figure 6). However, the lamp is larger than the simple Argon arc. Even then there are fewer lines at longer wavelengths (> 3 µm) and so telluric features will to be used where necessary. A better solution is to use the ‘super order’ discussed in Section 2.1.

![Figure 6. Th-Ar lamp, dimensions in mm.](image)
4 DATA REDUCTION SYSTEM DESIGN REQUIREMENTS

4.1 Fundamental requirements

- Extract spectra from raw cross-dispersed spectral images
- Wavelength calibrate extracted spectra
- Remove instrument signature (preserve spectral shape)
- Merge individual orders into continuous spectra
- Remove telluric contamination

To do this requires that the instrument acquires a variety of calibration data: arc line images, flat field images, dark current and bias frames, bad pixel maps, and data to correct for non-linearity. In addition, telluric contamination can in principle be removed by observing a standard star (e.g. Vacca et al. 2003 PASP 115, 387) or by using an atmospheric model such as ATRAN and as is done with CRIRES.

4.2 Practical requirements

The data reduction system will use a modified version of Spextool – the data reduction system written in IDL for SpeX by Mike Cushing and Bill Vacca. Spextool already contains much of the functionality needed for iSHELL. Spextool has been successfully modified for use in a number of spectrographs including CORMASS and TripleSpec (at Palomar and Apache Point Observatory).

One of the main differences between SpeX and iSHELL is that SpeX has five fixed format spectral modes whereas in iSHELL spectral orders can be moved up and down the array (by tilting the cross-dispersing grating) to place a user-selected wavelength at the center of the array. This requires that the software find the position of the orders rather than use a look-up table. Compared to SpeX the re-imaged slits in iSHELL are tilted by about 2-3 degrees because of the pseudo-Littrow grating illumination. This requires that spectra be resampled to correctly fit spectral lines along the length of the slit. Also, iSHELL has 11-37 orders across the array depending on wavelength and slit length compared to six in SpeX. Therefore automatic order finding and tracing routines are desirable.

The use of A0V stars as telluric standards is practical with SpeX since the wide simultaneous wavelength coverage permits telluric free hydrogen lines to be observed and fitted by a model of Vega. The adjusted Vega model is then used to divide-out the instrument signature and telluric features from spectra. This approach is not so easily implemented with iSHELL since the simultaneously observed wavelength range is not necessarily wide enough to include telluric free hydrogen lines that can fit and used to adjust the Vega model. An alternative is to use ATRAN to model and remove telluric features from spectra. However, this conveys no information about the instrument signature and the spectral continuum shape cannot be preserved.
5 DATA REDUCTION SYSTEM CONCEPT

iSHELL produces cross-dispersed spectral images similar to those produced by SpeX but at higher resolving power and with more orders. The required functionality of the data reduction package required for iSHELL is therefore similar to that built for SpeX - ‘Spextool’ (Cushing et al. 2004 PASP 116, 362). A flowchart of the reduction steps is shown in Figure 7. The procedure requires the following data frames:

- Target spectrum
- Telluric standard spectrum
- Arc lamp spectrum and/or sky telluric spectrum for wavelength calibration
- Flat field frames
- Dark and bias frames
- Bad pixel image
- Linearity data

Figure 7. A flowchart showing the steps in the reduction process for SpeX (Cushing et al. 2004, PASP 116:362-376). A modified version will be used in iSHELL.
An option not included in this procedure is to use a telluric model (e.g. ATRAN) to remove telluric features from target spectra. Some observing programs (e.g. radial velocity and Mars methane observations) require special reduction procedures which are not part of the standard package.

Spextool is run from an interactive GUI the front panel of which is shown in Figure 8. iSHELL will employ a similar GUI.

![Figure 8. The front panel of the Spextool GUI. Other windows are used for calibration, extraction aperture location and tracing, setting the size of extraction apertures, combining spectra, telluric correction, merging orders, and cleaning spectra.](image)

One of the biggest differences between SpeX and iSHELL is that in iSHELL the user needs to be able to set the desired central wavelength of an observation at the vertical (i.e. row) center of the array otherwise surrounding features may fall off the array and require a second set of observations (e.g. setting the
central wavelength to 2.38 µm so that most of the CO bandhead is covered in the K3 mode, see OCCD Figure 11). This means that a simple lookup table cannot be used as first guesses for the order location (red asterisks in Figure 9). For iSHELL a potential solution is to use the measured tilt of the cross-dispersing grating provided by a calibrated Kaman sensor.

Figure 9. SpeX 2.2-4.2 µm flat field image (3200 K QTH lamp combined with 1100 K IR source). Figure shows the detection of the edges of the orders in the flat-field image. The red asterisks represent initial guesses for the centers of each order. The green crosses mark the positions where the order edge is located, and the red lines are the robust polynomial fits through these positions. The blue crosses designate positions that have been excluded from the fits. In iSHELL the orders will be located using a calibrated Kaman sensor providing the tilt of the different cross-dispersing gratings.