Executive Summary

This report focuses on the issue of the optimum collimator focal length in the “baseline upgrade.” (Refer to the September 2003 for a comprehensive report on the project.) We present a conservative analysis of the worst-case scenario in which geometric (de)magnification dominates the optical error budget, and degradation of the instrumental resolution must be offset by gains in precision from increased signal-to-noise (S/N). Resolution is carefully defined as the achievable centroid or width precision obtained in a fixed observing time for a given source. The trade-offs between centroid and width precision and S/N are calibrated with realistic data simulations and analysis tools. We conclude that a 800mm focal-length collimator does not degrade the delivered spectral resolution over the current system performance, but does yield substantial gains in throughput for programs that are not resolution-limited. Moreover, the increased magnification with a faster collimator will yield better pixel sampling and improve accuracy of line-width estimation near the limiting instrumental resolution at all S/N.

On the basis of this and the previous (September 2003) report we hereby request SAC approval of the short collimator focal length of 800mm so we may proceed to CDR with this design. We suggest the following motion:

The SAC approves moving forward with the 800mm focal-length collimator design subject to the following proviso:

• there is a demonstration that the model delivered image quality of the upgraded system is as good as or superior to the model delivered image of the current system.
1. Goals

The goal of this report is to evaluate two performance characteristics that lead to limiting changes in the spectral resolution of the Bench Spectrograph in the upgraded design. A complete list of the upgrade changes that may lead to alterations in the achieved spectral resolution are as follows:

1. finer pixel sampling with a new CCD;
2. reduced optical aberrations of the camera and collimator with the off-axis corrector elements;
3. reduced defocus with a flatter CCD;
4. increased S/N with a faster, off-axis collimator; and
5. decreased demagnification of the system due to a shorter focal-length collimator.

All of the above changes work toward improving the achievable spectral resolution except for the last item (5). Whether item (5) will be a limiting factor depends on the width of the fiber and the anamorphic demagnification of the setup, i.e., whether the geometric projection of the monochromatic fiber image is the limiting width, or whether aberrations and sampling contribute significantly to the width of the recorded monochromatic image.

While items (1-3) are difficult to assess in quantitative detail, the last two items are straightforward to estimate. In this report we consider the limiting case where items (4) and (5) are the dominant factors contributing to the achievable spectral resolution in the upgraded system. This is a worse-case scenario since the high-resolution setups (echelle, 850 l/mm, and 1200 l/mm gratings) have considerable anamorphic factors such that the overall demagnification yields geometric fiber images of 37 μm, or 1.5 pixels, for the 200 μm (red) fibers. In the highest-resolution configurations with the echelle, the large anamorphic factors yield demagnifications as high as 6.8, equivalent to 28 μm images, or 1.2 pixels, for 200 μm fibers.

2. Merit Function

To explore the trade-offs between increased S/N and magnification on the achieved spectral resolution, we define spectral resolution to be the achievable precision of a line centroid and line width (FWHM).

3. Simulations

Simulations were made over a wide range of S/N of single line-emission and multiple absorption-line spectra. The spectra span physical conditions suitable for both low-order and echelle configu-
Emission line spectra were generated via `artdata.mkidspec` and `mknoise` with no residual background or continuum structure, and fit using `stsdas.analysis.fitting.ngaussfit` with no prior assumptions about peak, centroid, or width, but with a suitable error model. Line-widths ranging from 1.25 to 20 pixels (FWHM) were used, and centers were chosen spanning the full sub-pixel scale from edge-centered to pixel-centered line profiles.

Absorption-line spectra were generated from adding noise to a high S/N WIYN Bench Spectrograph echelle observation of HD 126053 (G1 V) taken with SparsePak and a standard order-11 setup ($\lambda_c \sim 513\text{nm}$). Hence simulations were limited at the upper S/N end by the observations (S/N $\sim 100$ per pixel in the continuum). The observed template was shifted in velocity, and broadened by Gaussian smoothing functions of 12.5, 25, and 50 km/s ($\sigma$), equivalent to FWHM of 4, 8 and 16 pixels, respectively. Parameter estimation was made via cross-correlation of the shifted, broadened, noise-aberrated spectra against the original template. Consequently, there is no template-mismatch in our simulations.

Examples of simulated spectra are shown in Figure 1.

### 4. Results

From inspection of Figures 2-5 we find both centroid and width (FWHM) precision scales with line-width at a given S/N, and is a simple, inverse function of S/N. For direct-fitting of single emission lines:

$$ \sigma_c / \text{FWHM} = 0.6 \left( \frac{S}{N} \right)^{-1}, $$

and

$$ \sigma_{\text{FWHM}} / \text{FWHM} = 1.5 \left( \frac{S}{N} \right)^{-1}, $$

where $\sigma_c$ is the standard deviation about the mean centroid determination, and $\sigma_{\text{FWHM}}$ is the standard deviation about the mean width determination – both determined at a given S/N. For cross-correlation of absorption line spectra:

$$ \sigma_c / \text{FWHM} = 0.6 \left( \frac{S}{N} \right)^{-1}, $$

and

$$ \sigma_{\text{FWHM}} / \text{FWHM} = 0.80 \left( \frac{S}{N} \right)^{-1}. $$

The inverse dependence of centroid precision on S/N agrees with the literature (Griffin & Gunn 1974, Campbell & Walker 1979, and Merline 1984). Particularly informative is equation (1) of Campbell & Walker (1979). Our results here extend this relation to the line-width, demonstrate the relation holds with realistic absorption and emission-line spectra germane to the Bench Spectrograph, and calibrate the relations for these spectra.
Hence at fixed collimator focal length (demagnification), we may write:

\[
R \equiv \frac{\lambda}{\Delta \lambda} \propto \begin{cases} 
\sqrt{\epsilon} & \text{photon limited} \\
\epsilon & \text{detector limited}
\end{cases},
\]

where \( \epsilon \) is the mean system efficiency (or throughput). Considering the changing geometric factors with collimator focal length, \( R \) becomes:

\[
R \propto \epsilon^a \times \text{collimator f.l.},
\]

where \( a = 0.5, 1 \) for photon- and detector-limited cases, respectively. Therefore the merit function, \( f_R \) becomes

\[
 f_R = \left( \frac{\epsilon}{\epsilon_{on,1023}} \right)^a \frac{\text{collimator f.l.}}{1023 \text{ mm}},
\]

where \( \epsilon_{on,1023} \) is the efficiency of the current Bench Spectrograph with an on-axis collimator with a focal-length of 1023 mm.

The above merit function, plotted in Figure 6, shows that for the most conservative case with high-resolution setups in the photon-limited regime, the merit function is above, or equal to, the current system for collimator focal-lengths of 800 mm or greater. On the other hand, a collimator focal-length which is as short as possible improves the throughput for applications which are not resolution-limited (bottom panel). **Conclusion:** The optimal collimator focal length is 800 mm since this maximizes throughput while maintaining the merit-function at a high level for detector-limited applications (top panel).

5. Discussion

5.1. Limitations of the current analysis

There remains anecdotal evidence that increased S/N cannot be traded for instrumental resolution, contrary to the results of these simulations. Why this disparity? One possibility is the limitations of field-flattening of the data – an effect not included in these simulations. Field-flattening errors will, to first order, add in quadrature with the detector and photon noise, effectively producing a pedestal S/N. It would therefore be worthwhile to determine the amplitude of field-flattening errors and to consider data-taking schemes minimizing these effects. Shorter, more numerous exposures interleaved with flat-field exposures should help even with the current system. Better pixel sampling and charge shuffling are two considerations to improve field-flattening errors in an upgraded system. The former is accomplished with a faster collimator; both are accomplished with a new CCD camera with smaller pixels and an appropriate control and read-out electronics.
5.2. Pixelization Issues: Resolution Gains from Increased Magnification

We find no dependence of our results to sub-pixel positioning of the simulated emission-line spectra. But not surprisingly, for FWHM < 2.5 pixels it is no longer possible to retrieve accurate line-widths from the \texttt{ ngaussfit} fitting algorithm at any S/N (see Figure 3). Despite this pixelization limit, the trend of precision with S/N obeys the same scaling relation as the larger line-width simulations.

In the conservative limit where geometric factors dominate the monochromatic line-width, the proposed $\sim$20\% increase in magnification with a shorter focal-length collimator will change the sampling of the geometric projection of the monochromatic fiber image from $\sim$1.6 pixels to $\sim$1.9 pixels. Hence the faster collimator will yield more adequate sampling for the limiting ($\sim$2.5 pixel) resolution. The prospect of a new CCD with 1.5-2 times smaller pixels (12-15$\mu$m instead of 24$\mu$m) will enable adequate sampling for even smaller fibers or the highest-resolution echelle configurations.

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REFERENCES


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HD 126053 (G1 V) at 0.128 A/pix, broadened by 25 km/s Gaussian (8 pix FWHM)

Gaussian emission-line, 1A FWHM (5 pix), centered at 6563 A

S/N = 3 per pixel

S/N = 10 per pixel

S/N = 30 per pixel

Fig. 1.— Examples of emission and absorption-line spectra discussed in the text. The emission-line spectra (right panels) have S/N within the line FWHM of 3, 10 an 30. The absorption-line spectrum (left panels) have the same S/N values but defined in terms of S/N per pixel.
Fig. 2.— Centroid precision (top and middle panels) and accuracy (bottom panel) as a function of S/N for single, Gaussian line-emission simulated in the background- or detector-noise-limited regime (300 realizations per S/N point). Solid lines are weighted according to line-widths (FWHM, as marked) between 1.25 and 20 pixels. S/N is defined within the line FWHM. Line-fitting uses no prior assumptions about peak, centroid, or width, but with a suitable error model. For S/N < 10, line detection completeness falls rapidly below 100%, the precision asymptotes to about 25% of the spectral range, and the accuracy rapidly degrades. (Error bars in the bottom panel are the standard error in 300 measurements of the mean deviation, $\Delta_c$, from the model centroid.) Above S/N = 10 there is a direct inverse dependence of precision on S/N, with a value normalized to units of line-width (middle panel). This relation holds for line-widths of 1.25 pixels (FWHM) or greater.
Fig. 3.— Width (FWHM) precision (top and middle panels) and accuracy (bottom panel) as a function of S/N for single, Gaussian line-emission in the background- or detector-noise-limited regime. Other features as in previous figure. Low-S/N precision and accuracy tends to the width of a characteristic noise feature (~ 1 pixel). Note again the inverse relation between width precision and S/N for S/N > 10. For line-widths below 2.5 pixels the scaling relation with FWHM breaks down because the lines are insufficiently resolved.
Fig. 4.— Centroid precision (top and middle panels) and accuracy (bottom panel) as a function of S/N for multiple, absorption-line spectra and Gaussian line-broadening in the photon-limited regime (50 realizations per S/N point). Solid lines are weighted according to line-widths (FWHM) of 4, 8 and 16 pixels. S/N is defined per pixel – NB: this is different than in Figures 2 and 3. Parameter estimation is done via cross-correlation with a suitable error model. At all S/N there is a direct inverse dependence of precision on S/N, with a value normalized to units of line-width (middle panel). The relation is identical to the emission-line case (Figure 2).
Fig. 5.— Width (FWHM) precision (top and middle panels) and accuracy (bottom panel) as a function of S/N for multiple, absorption-line spectra and Gaussian line-broadening in the photon-limited regime. Other features as in previous figure. characteristic noise feature (~1 pixel). Note again the inverse relation between width precision and S/N, but in this case the normalization is nearly half that for the single, Gaussian line-width vs S/N relation.
Fig. 6.— Spectral resolution gain (the merit function $f_R$, top and middle panels) and throughput gain (bottom panel), averaged along the spectrograph slit for the WIYN Bench Spectrograph and an off-axis collimator as a function of collimator focal-length. The current collimator focal-length is 1023mm. Top panels are the spectral resolution gain merit function, $f_R$, of equation (3) (see text) for the photon- and detector-limited regimes. The bottom panel is the mean vignetting for the off-axis collimator normalized by the mean vignetting for the current, on-axis collimator, as taken from the September 2003 Bench Upgrade Report. Results are shown for a variety of spectrograph setups (labeled). The echelle order 11, 850 order 2, and 316 order 1 setups are close to on-order. The echelle order 8 and 9 are at the blue and red half-order points respectively (both are roughly at order 8.5). Note that in the worse case scenario for high-resolution spectrograph setups, there is no loss in the spectral resolving power, $f_R$, for collimator focal-lengths above 800 mm.