Fully automated wavelength calibration method optimizes data accuracy

An intelligent new routine

The recent launch of Princeton Instruments' powerful LightField® 64-bit data acquisition software also heralded the arrival of a brand new, fully automated wavelength calibration method developed to achieve unprecedented accuracy for spectroscopy applications (see Figures 1–4). Currently offered as a LightField package option, patent-pending IntelliCal® technology from Princeton Instruments enables fast, reliable wavelength calibration with minimal user input (see Appendix).

In essence, IntelliCal is a full-spectrum calibration routine that refines a theoretical spectrograph model based on the physical properties of the actual instrument being utilized. This technical note will first provide a review of critical problems inherent to traditional calibration techniques and then present basic IntelliCal theory, comparative data, and key implications of the new method.

Motivation

The development of IntelliCal was fueled by the desire to surmount several shortcomings associated with traditional wavelength calibration methods, especially overreliance on user input for accuracy. By and large, the post-calibration wavelength accuracy is not known by the software programs utilized in these traditional routines, so its determination is left up to the user.

Using a source with multiple known emission lines to illuminate the entrance slit of the spectrograph, it is possible to determine a direct wavelength-to-detector pixel coordinate correlation. There are two common types of wavelength space calibration: (1) a polynomial fit here only two or three emission lines are used and (2) a fit to the Czerny-Turner model.

Some routines utilize a polynomial fit to define the spectral dispersion across the focal plane and thus obtain calibration results at the pixel level. This technique, in which a polynomial is fit to a plurality of known emission lines, is both the more accurate and more tedious of the aforementioned methods. The user must not only determine which emission lines are seen by the detector, but must redo the calibration each time the grating is moved. Furthermore, the accuracy of this approach is partially limited by the number of lines used to generate the fit; typically, only two or three observed spectral emission lines are used.

The most commonly utilized wavelength space calibration is a fit to the Czerny-Turner model. Here, the user is prompted to select a known emission line and the grating is moved so as to position the selected line at two or more locations across the CCD. The grating is then moved to a different line. This process is repeated at least once. Next, the wavelength space residual is defined and minimized with respect to the standard Czerny-Turner model. Accuracy is correlated to *n*, the number of wavelength points used in the refinement.

Figure 1.
IntelliCal source installed on an Acton Series SP2300 spectrograph from Princeton Instruments.

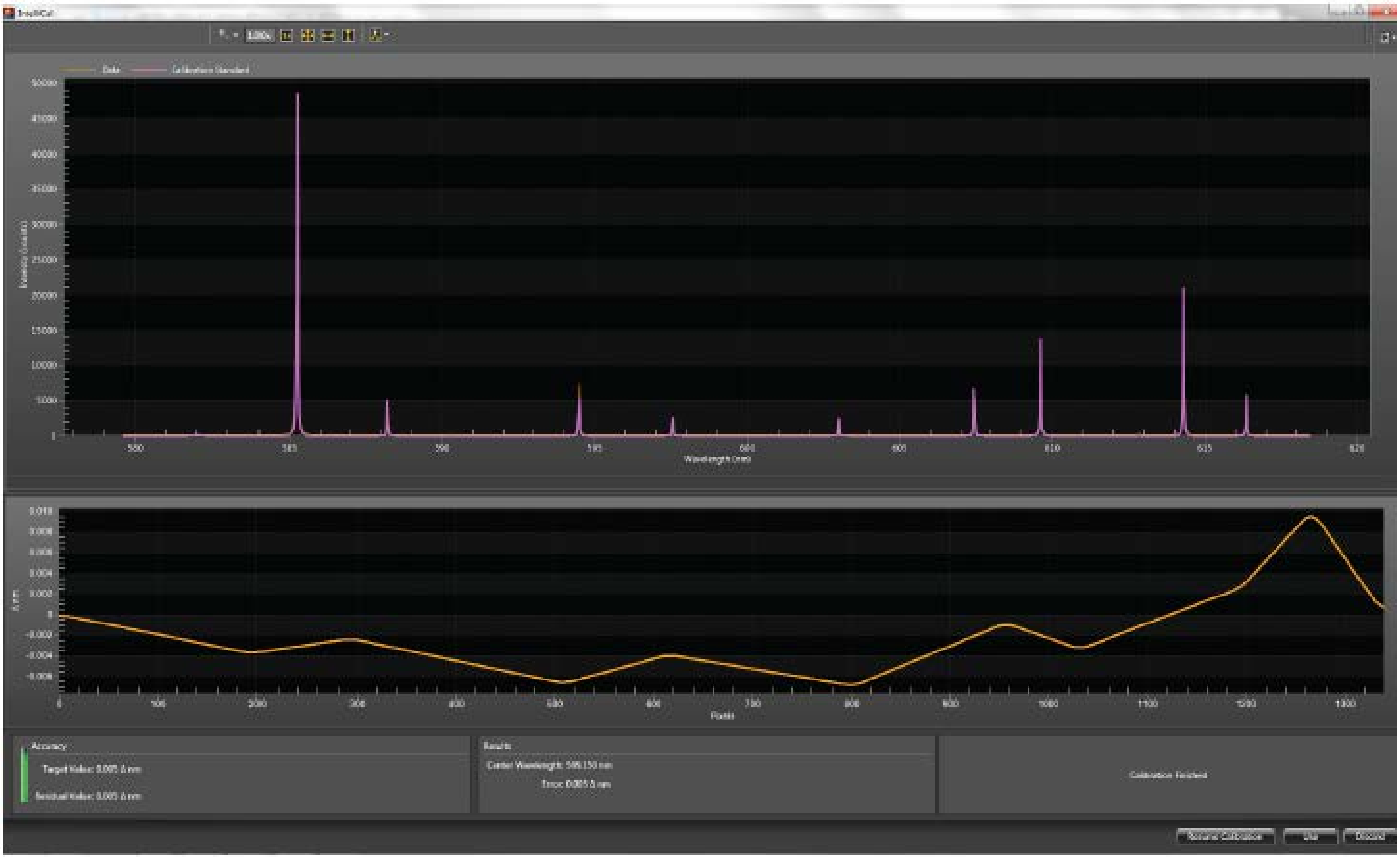

Figure 2.

IntelliCal source installed on an Acton Series SP2300 spectrograph from Princeton Instruments. Acton Series SP2500 spectrograph from Princeton Instruments with 1200 gr/mm grating and neon-argon USB lamp — after

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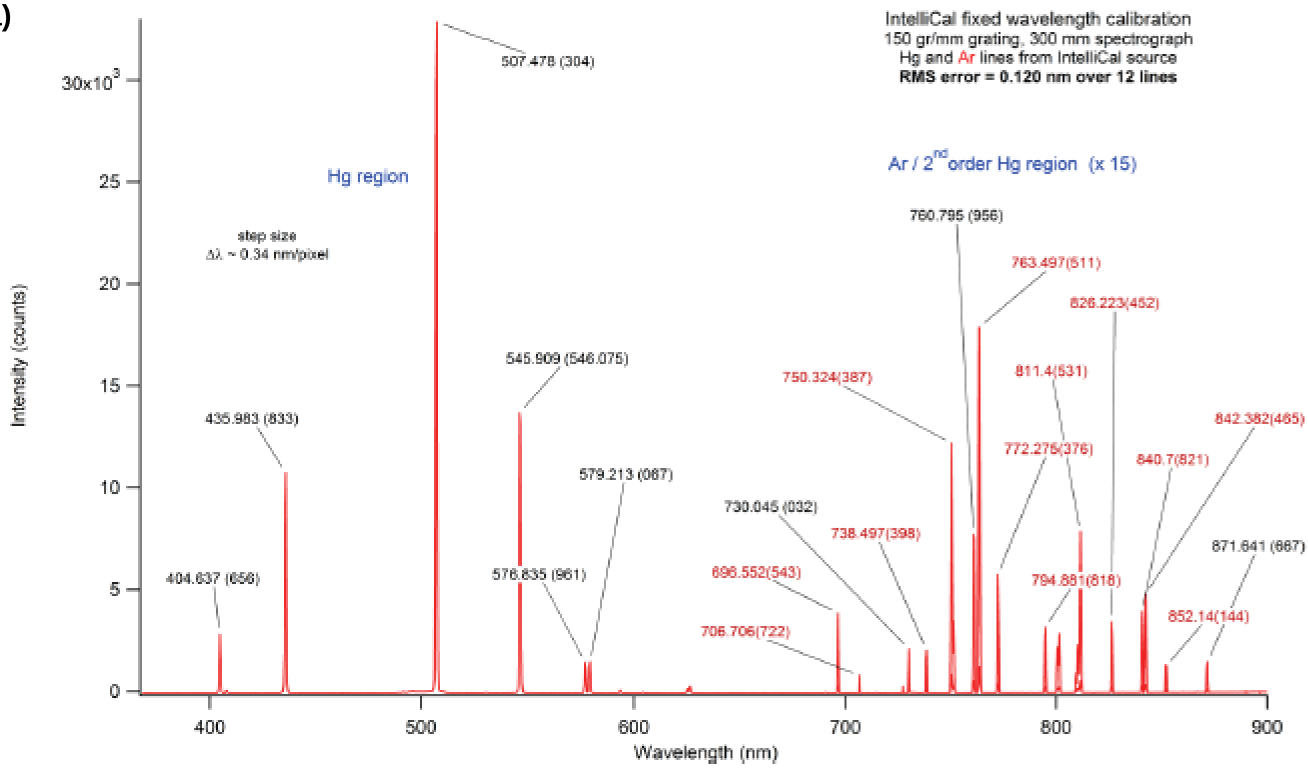
(a)



(b)

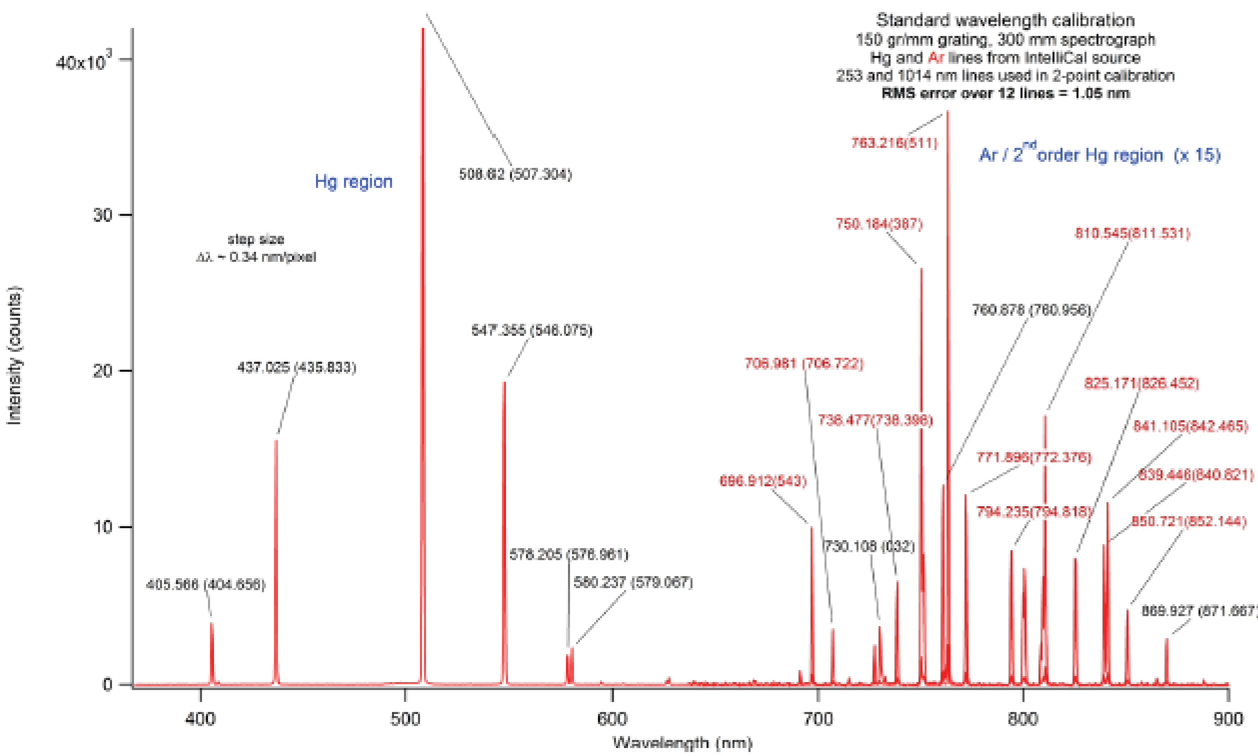
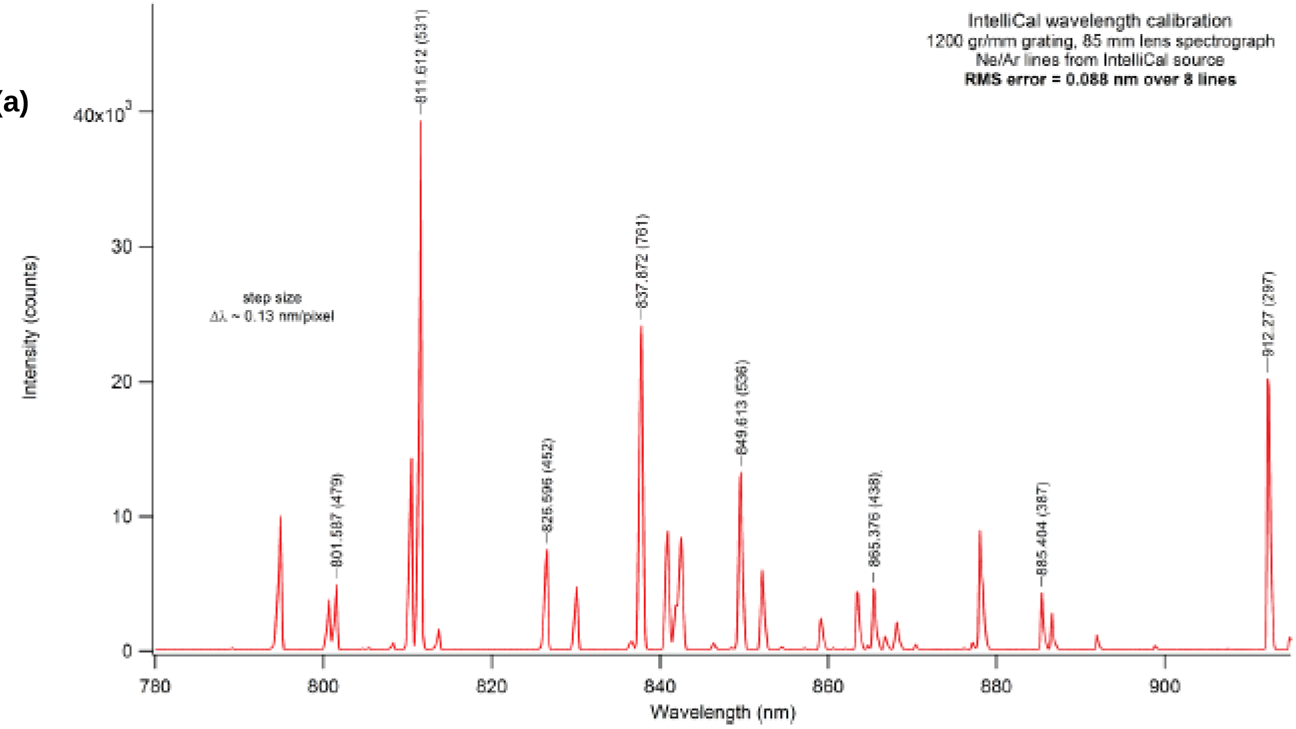


Figure 3. *Calibration error for an Acton Series SP2300 spectrograph from Princeton Instruments utilizing* ***(a)*** *IntelliCal and* ***(b)*** *standard routines. The relatively high RMS calibration error is due to the low dispersion of the grating used; much greater accuracies can be obtained with high-groove-density gratings.*

(a)



(b)

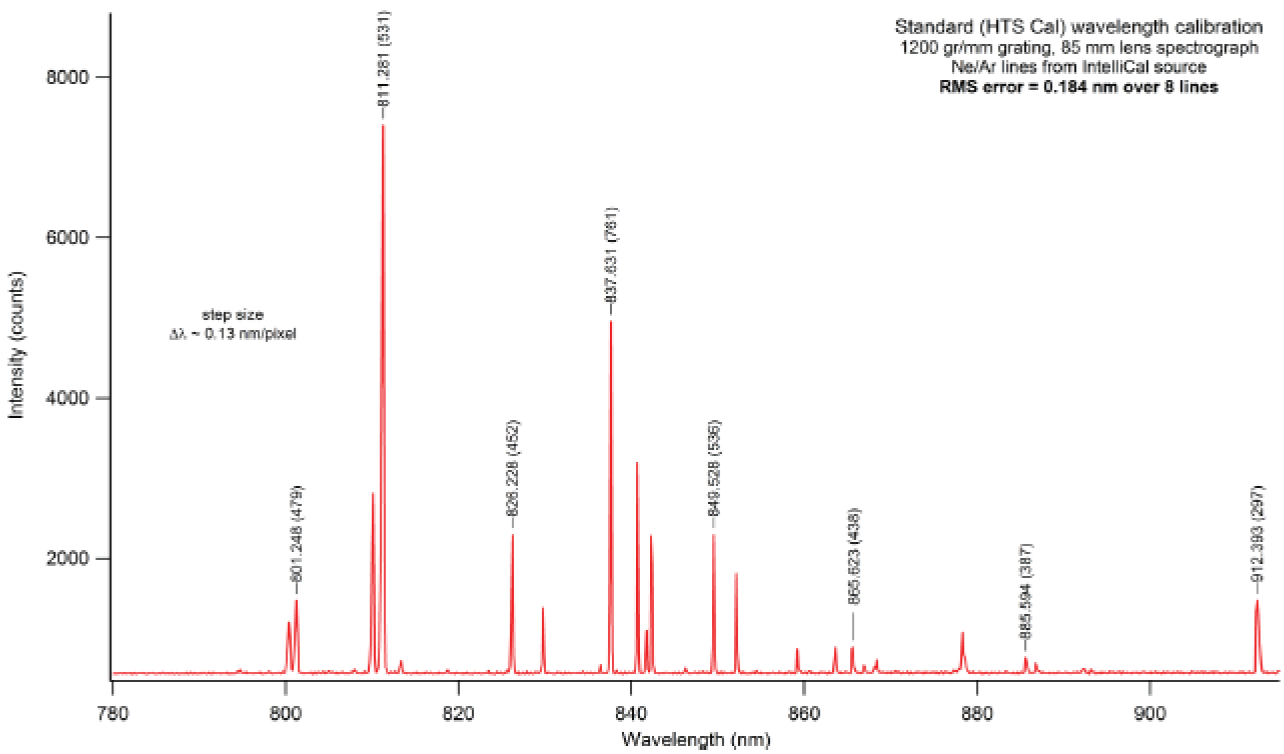


Figure 4. *Calibration error for an Acton Series LS785 spectrograph from Princeton Instruments utilizing (a) IntelliCal and (b) standard routines.*

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Basic theory

IntelliCal is a fully automated calibration routine in which a non-linear least squares refinement algorithm is derived that minimizes the intensity space residual with respect to a theoretical model of the spectrograph. IntelliCal simulates the entire observed spectrum; the number of observables is always equal to the number of horizontal pixels in the CCD array. No significant user input is required.

The ultimate aim of IntelliCal is to minimize the residual difference between observed and calculated emission line spectral intensities. This goal is realized in three major steps.

1. Define an intensity function for a calculated spectrum.

$$I\left(\lambda'\left(x; f\gamma\delta\right)\right) = I_o + \sum_{i=1}^{n} I_{rel_i} e^{-\left(\lambda'(x)-\lambda_i\right)^2/2\sigma^2}$$

2. Define the residual that will be minimized.

$$r_i(x,\phi) = I_{obs\,i} - I_{Calc_i}\left(\lambda'\left(x; f\gamma\delta\right)\right)$$

3. Define how the light is dispersed by the spectrograph.

Czerny-Turner:

$$\lambda'\left(x; f\gamma\delta\right) = \left(\frac{d}{m}\right)\left\{\sin\left(\psi - \frac{\gamma}{2}\right) + \sin\left(\psi + \frac{\gamma}{2} + \xi(x)\right)\right\}$$

Where:

$$\psi_i = \sin^{-1}\left(\frac{m\lambda_{c_i}}{2d\cos\left(\frac{\gamma}{2}\right)}\right) \quad \xi = \tan^{-1}\left(\frac{nx\cos\delta}{f + nx\sin\delta}\right)$$

Definitions

d = groove spacing	f = focal length
m = diffracting order	δ = detector angle
n = pixel number	s = spectral FWHM
x = pixel width	λ' = dispersed wavelength
γ = inclusion angle	ψ = grating angle

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Comparative data

Figures 5, 6, and 7 show the comparative calibration accuracy of IntelliCal versus traditional techniques. The comparisons are made in terms of wavelength error as a function of calibration line wavelength.

Figure 5.

Wavelength error as a function of calibration line wavelength shows comparative calibration accuracy of IntelliCal versus Czerny-Turner model (500 mm focal length).

Focal length	500 mm
Aperture ratio	f/6.5
Linear dispersion	1.52 nm/mm
CCD resolution	0.09 nm

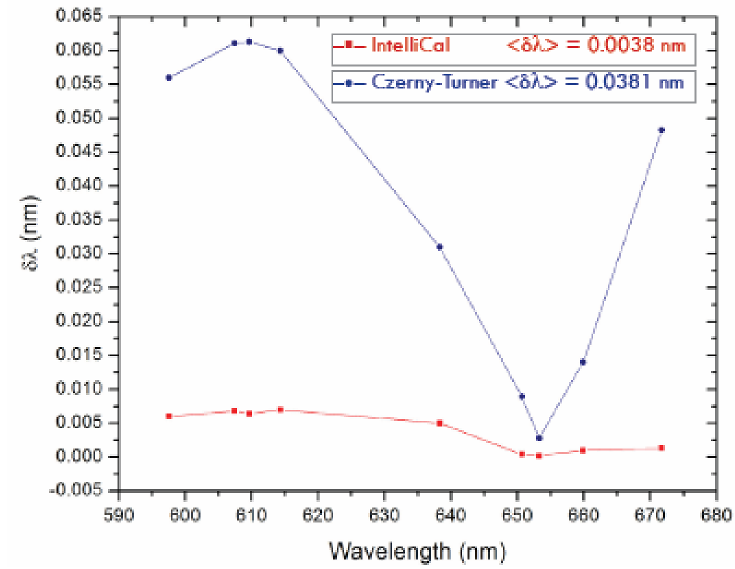

Figure 6.

Wavelength error as a function of calibration line wavelength shows comparative calibration accuracy of IntelliCal versus Czerny-Turner model (300 mm focal length).

Focal length	300 mm
Aperture ratio	f/3.9
Linear dispersion	2.38 nm/mm
CCD resolution	0.14 nm

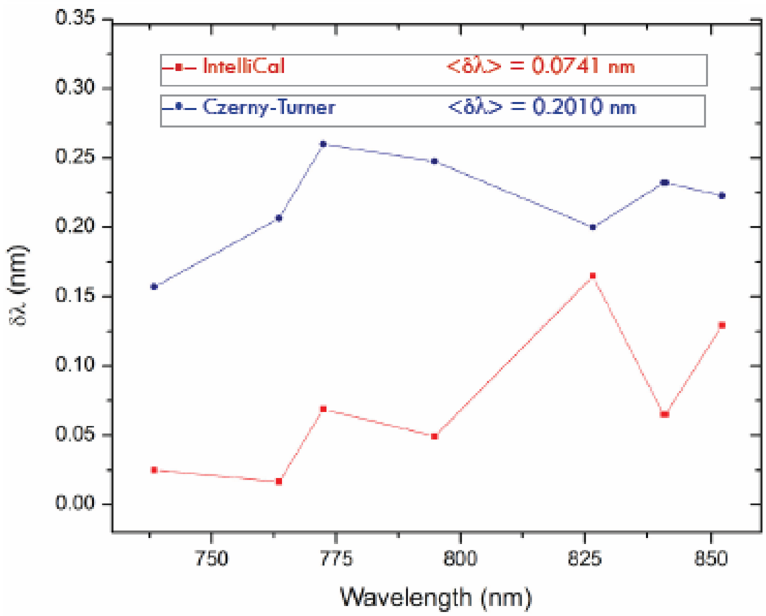

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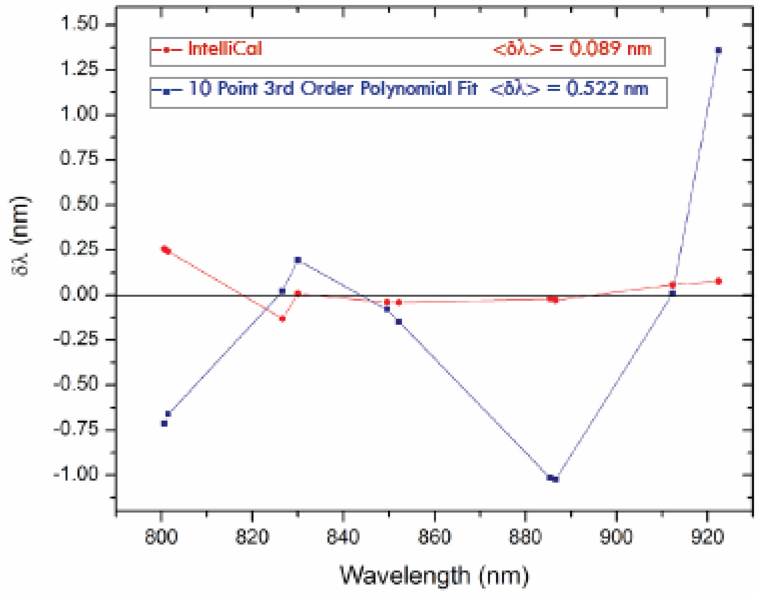
Figure 7.

Wavelength error as a function of calibration line wavelength shows comparative calibration accuracy of IntelliCal versus polynomial fit (lens spectrograph).

Focal length	85 mm
Aperture ratio	f/2
Linear dispersion	6.68 nm/mm
CCD resolution	0.20 nm



Key implications

First and foremost, as the name implies, IntelliCal provides truly intelligent calibration. Unlike traditional methods, the software is now aware of the instrument it is calibrating. Furthermore, the fully autonomous IntelliCal routine eliminates user error.

Of course, the name of the game is accuracy. By treating every pixel in the detector as an observable element, IntelliCal delivers tremendous gain in wavelength accuracy via highly over-determined refinement. In fact, spectra calibrated using IntelliCal can demonstrate up to a full order-of-magnitude improvement in wavelength accuracy versus traditional calibration routines.

Every observable emission line is used and spectral dispersion is refined at every pixel in the CCD array. The observed spectrum is simulated to the pixel level; even doublets in a spectrum are accurately modeled and used in the calibration. Each calculated spectrum displays the wavelength accuracy, quantitatively, at every pixel (see Figure 8, below). In addition, the refinement is insensitive to line intensity.

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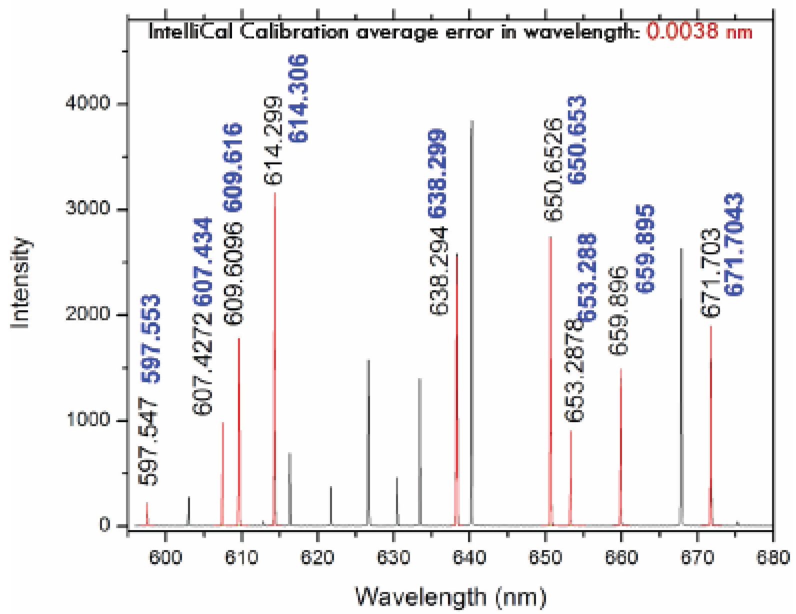
Figure 8.

IntelliCal has been designed to instill pixel-by-pixel confidence in data collected after calibration.



Post-refinement capabilities are impressive as well. These include simulating how any emission spectrum will appear at the detector for an arbitrary grating position, seamless combination with a pattern recognition algorithm, and searching all possible grating angles so as to fully determine the state of the instrument.

The most recent version of IntelliCal also provides intensity calibration, further improving the accuracy of recorded spectra.

Appendix

IntelliCal provides highly accurate wavelength calibration quickly and simply:

1. Install the IntelliCal source on the spectrograph.
   (Alternatively, use the source to illuminate a fiber or place it at the sample position.)
2. Plug the source into the spectrograph's USB port.
3. Collect a background.
4. Click "calibrate".
5. Either accept, or repeat to refine further.

It's that easy!

For additional information about IntelliCal technology, please contact Princeton Instruments.

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