# Advanced Calibration Techniques for Astronomical Spectrographs

Paul Bristow[1]
Florian Kerber[1]
Michael R. Rosa[2,3]

[1] ESO
[2] Space Telescope European Coordinating Facility, ESO
[3] Affiliated to the Science Operations and Data Systems Division, Science Department, European Space Agency

**ESO's Calibration and Model Support Group is involved in a variety of activities related to the calibration and physical description of instruments, with the objective of supporting the reduction of science data and facilitating operations. Here we describe the construction, optimisation and application to scientific data reduction of physical instrument models. Such models have been implemented for the HST STIS spectrograph and form an integral part of the data reduction pipelines for CRIRES and X-shooter. These models are supported by validated physical data of the instrumental components and calibration reference data.**

The life cycle of an instrument can be described as follows:

1. Science Requirements
2. Optical Design (Code V/Zemax)
3. Engineering Expertise

---

4. Testing and Commissioning
5. Operation and Data Flow
6. Calibration of Instrument
7. Scientific Data and Archive

Experience shows that it is difficult to ensure that the know-how and expertise that went into designing and building the instrument (steps 1–3) is brought to full use in the instrument calibration and scientific operations (steps 6 and 7).

A case in point is the wavelength calibration, in which well-understood physics is employed to design a spectrograph with an optimal format while during operations the dispersion solution is then derived over and over again in a purely empirical manner by, for example, fitting polynomials to a sparse calibration line spectrum.

One way to ensure that the engineering data propagates from instrument building to operations is to capture all the engineering information in a physical model-based description of the instrument. This model accompanies the instrument throughout its life cycle and is used to drive the science data reduction pipeline. In our concept the model is combined with validated physical data of the instrumental components and calibration reference data.

## Implementation and application of an instrument physical model

Our approach comprises an instrument-specific model kernel and associated software to optimise the model parameters and to apply the model's predictive power to the calibration of science data.

### Model kernel

First of all a streamlined model of the dispersive optics, that enables a rapid evaluation of where any photon entering the instrument arrives on the detector array, is constructed. Though based upon the optical design, it is no substitute for the fully-fledged optical (e.g. Zemax/Code V) models developed by the designers. Clearly this model kernel is specific to each instrument, but the following sub-components and associated parameters are typical:

- Entrance slit and collimator
  - Relative position and orientation of the slit
  - Focal length of collimator
- Pre-disperser (e.g. Prism)
  - Orientation of entrance surface
  - Orientation of exit surface
  - Temperature
  - Refractive index as a function of wavelength and temperature
- Main disperser (e.g. reflection grating)
  - Orientation
  - Grating constant
- Camera and detector array
  - Focal length of focusing optics
  - Orientation of detectors
  - Relative positions of detectors
  - Dimensions of pixel grid

We follow the prescription of Ballester and Rosa (1997) in constructing this model.

Most of the computations involve rotation matrices to represent the change of orientation of the optical ray at the surfaces of the components. For example, the matrix representation of the order *m* transformation performed by an echelle grating with constant $\sigma_E$ at off-blaze angle $\theta$, operates on a 4D vector with components ($\lambda$, x, y, z) representing a ray of wavelength $\lambda$. Here $\theta$ and $\sigma_E$ are amongst the physical model parameters for this instrument.

Hence there is a complete set of parameters that describe the passage of a photon through the spectrograph. These parameters are physical quantities (angles, distances, temperatures, etc.) and describe the actual status of components. They can always be adjusted to match the observed behaviour of the instrument or to predict the effects of tilting/modifying a component. For example, adjusting the camera focal length will change the scale on the detector.

### Optimisation

The model parameter set can be optimised to reflect the performance of the operational instrument with suitable calibration data, in a similar way that a polynomial dispersion solution would be fit. The difference is that the parameters optimised here have physical meaning and represent the actual configuration of the instrument. There are essentially two scenarios in which one needs to perform the optimisation.

Before the instrument is actually built, the only parameters available are those from the instrument design. Inevitably, once the instrument has been built, it will differ from the design predictions, so it is necessary to establish the true values. This may also be the case after a major maintenance intervention, upgrade to the instrument or even an earthquake, resulting in a physical change in the instrument. In this situation a comprehensive and uniform set of robustly identified calibration features from dedicated calibration exposures is required. The core model function is then iteratively called for the identified calibration wavelengths and the results of each iteration are compared with the centroids for these wavelengths as measured in the calibration data. We employ the Taygeta (Carter 2001) implementation of the Simulated Annealing technique to continually adjust, in a statistically sound manner, *all* of the model parameters until the best match between predicted and measured centroids is found. Figure 1 is a schematic representation of this procedure.

In the case of an instrument such as CRIRES which has multiple modes defined by the orientations of optical components (and therefore by parameters in the physical model), we are able to optimise the parameter set for multiple modes simultaneously by assigning a unique value to each of the changing parameters on the basis of all data collected for the corresponding mode. We can then characterise the parameters associated with the moving components that determine the mode.

Most spectrographs have some moving components that allow selection of a given wavelength range. Since there are physical limits to the repeatability and accuracy of these mechanisms, it is useful to be able to fine tune the model to match the performance of the instrument at the time of a given observation. Moreover, even without human intervention, instruments develop malfunctions such as a drift in wavelength zero points that are not well understood initially. Other affects such as thermal or gravitational flexure occur at some level during routine operations and also subtly affect the exact details of the instrument optics. In such cases it is clear that there must be some deviation from the initial parameter calibration that was done with data acquired in the absence of these effects (or in the presence of another alignment of these effects).

For these reasons we have developed the capability to re-optimise specific parameters, using either automatically identified wavelength features in contemporaneous calibration exposures or wavelength standards specified by users (e.g. known sky lines seen in science exposures). These are used in a similar way to that depicted in Figure 1, except that only the known changing parameters, or parameters suspected of causing the spurious drifts, are optimised. Moreover, one can choose to optimise more parameters when more data points are available.

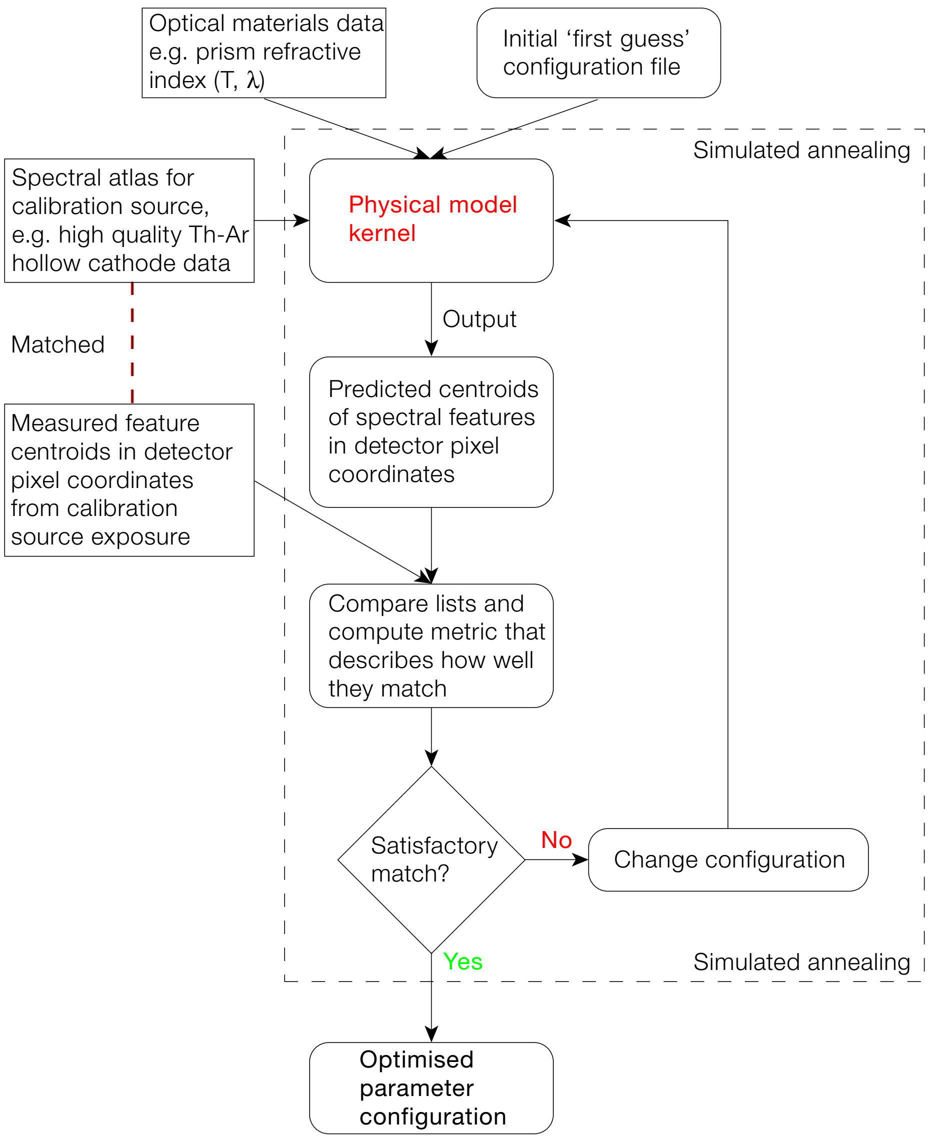



**Figure 1:** Schematic representation of the optimisation process for instrument physical models.

We have recently achieved the full automation of this process for CRIRES. The procedure is illustrated by Figure 2. First the model is used to trace the locus on the detector of a given entrance slit position. A 1D spectrum is then extracted from a Th-Ar hollow cathode lamp (HCL) full slit exposure along this locus and bright features are identified. Using the baseline physical model parameter configuration, we predict the positions of wavelength features along this locus (red crosses in Figure 2). A crucial point here is that we only consider wavelength features that we know will be well isolated (see "Optimising Calibration Systems" below) in order to avoid the possibility of false matches. The significant offset between the red crosses and the corresponding features identified in the data (magenta circles) is due to a shift in spectral format that has occurred in CRIRES between the acquisition of the calibration data used to determine the baseline model parameter configuration and the epoch of this data. Hence known wavelengths are reliably matched to measured positions in the new data and the model parameters can be re-optimised to match the actual performance of CRIRES. As well as recovering the predictive power of the physical model for calibration applications, this process also gives us some insight into which parameters need to be modified in order to match the changing spectral format. In this case we found that the grating and associated focusing optics were the parameters responsible.

## Calibration

The principal purpose of the physical modelling approach is to provide accurate wavelength calibration for spectroscopic science data. Once the physical model parameter set is optimised to match the instrument reality and, where necessary, fine tuned to match the actual operating conditions, it is trivial to recover the wavelength corresponding to each pixel in the 2D detector array or each bin in extracted 1D spectra. For CRIRES and X-shooter this is incorporated in the standard data reduction software (DRS) pipeline.

The application to the Space Telescope Imaging Spectrograph (STIS) provided encouraging verification of the validity of wavelength calibration using this technique. Many spectral features occur in adjacent spectral orders in cross-dispersed echelle spectrograms. An accurate dispersion solution should assign identical wavelengths to these features regardless of which spectral order they are measured from. Figure 3 is a histogram of the wavelength offset between wavelengths assigned to line positions on adjacent orders. The blue histogram is that found for the standard STIS data reduction software, *calstis*. Note that STIS is arguably one of the best empirically calibrated modern astronomical spectrographs. The red histogram is what we obtain with the physical model approach. The goodness of the latter dispersion solution is even more impressive if one recalls that it is a global solution across the entire 2D dispersion map, while the 2D polynomials of the canonical *calstis* pipeline are matched locally (per order).

The physical model can also be used to drive the extraction of 1D spectra from 2D data since it will predict the locus on the detector array of wavelengths entering at a given entrance slit position. A further possibility, which has not yet been fully exploited, is to use a physical model to fully map flux in the 2D detector pixel array plane back to the slit position/wavelength plane.

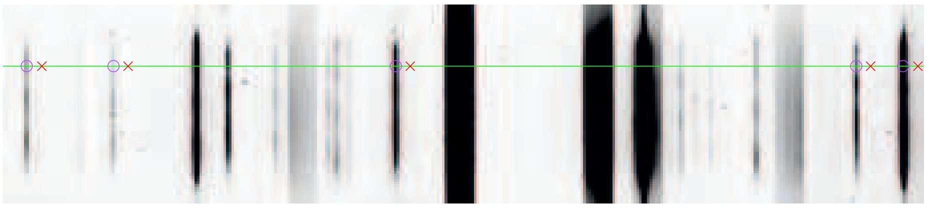


Figure 2: A CRIRES full slit Th-Ar Hollow Cathode Lamp exposure used to discover the change in spectral format. The green line is the locus of a chosen entrance slit position on the detector array. Red crosses mark the predicted positions of isolated spectral features according to the baseline model parameter configuration. Purple circles mark the actual position of these features after a shift in spectral format.

## Simulation tools

Such an instrument model can also be used to simulate spectroscopic data. In addition to the geometric capabilities of the physical model, basic photometric simulation is also implemented. Blaze efficiency can be computed directly from the model parameter set, whilst other throughput issues such as quantum efficiency, dichroic transmission, etc. are incorporated through reference data for the materials used.

In order to produce a simulated 2D exposure of a given spectrum, the model kernel is then called iteratively for photons in the given spectral energy distribution with a realistic distribution on the entrance slit. If so required, one can generate a stochastical and probabilistic observational result model. The pixel that would be illuminated on the detector array is recorded, and a 2D array describing where the flux arrives on the detector is built up. Before the instrument is even built we are able to provide simulated 2D data (flat fields, arc lamp exposures or astronomical objects) that can be used in the development of the data reduction software or can be used as an aid when aligning the instrument in the laboratory (e.g. Vernet et al. 2007).

Figure 4a shows a section of a Th-Ar hollow cathode lamp X-shooter VIS exposure made using a nine-pinhole mask, while 4b shows the equivalent section from a model based simulation. Figure 5 shows a 2D simulation of an observation of the Orion nebula on the UVB and VIS detectors of X-shooter.

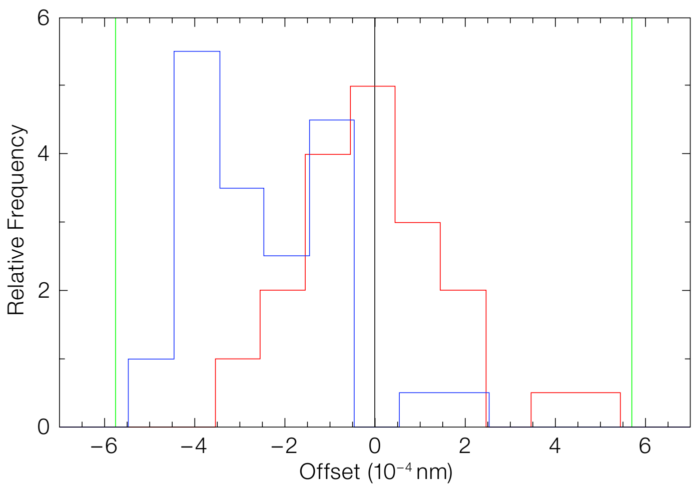
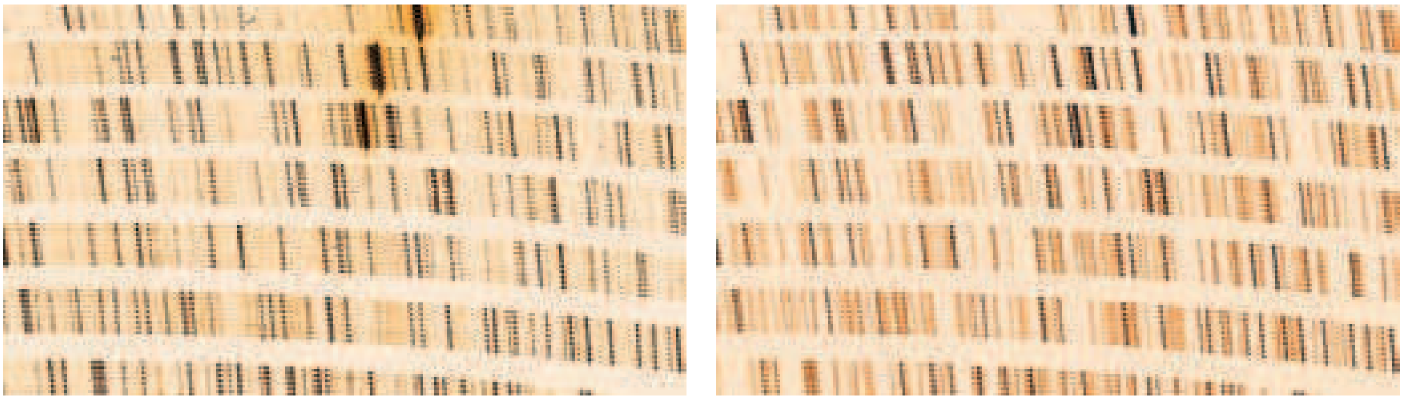



Figure 3: Histograms of the discrepancy in the wavelength assigned to features appearing in adjacent orders in STIS E140H exposures by the standard STIS DRS (blue) or the physical model derived dispersion solution (red). The green bars indicate the size of one STIS pixel.



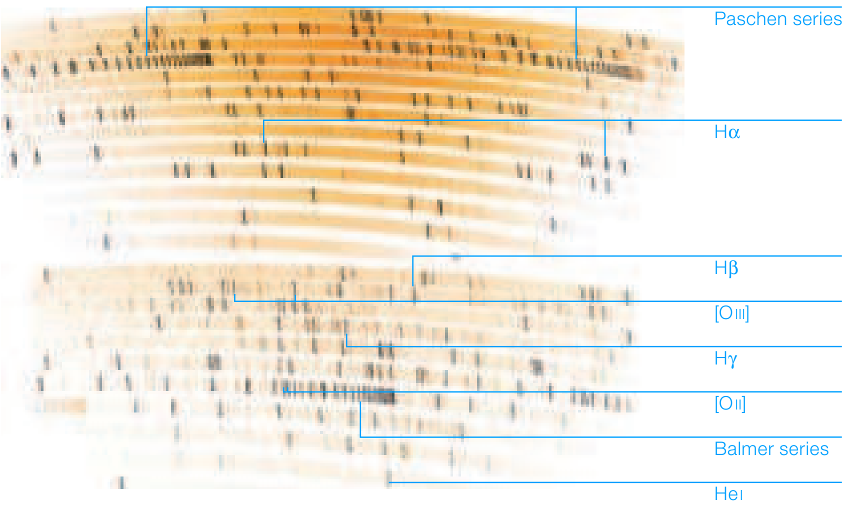



Figure 4 (above): Left: Section of an X-shooter VIS 180 s exposure of a Th-Ar HCL through a nine-pinhole mask obtained in the laboratory. Right: Physical model based simulation of the above left image.

Figure 5 (left): Simulated 2D echellogram exposures with the X-shooter UVB arm (below) and VIS arm (above) of the Orion nebula. Some familiar emission lines are indicated.

## Calibration Reference Data and Model Support

The Calibration and Modelling Support Group performs several activities that are aimed at obtaining data that will ensure optimum calibration of the science instruments at ESO.

### Properties of physical materials

A realistic description of an instrument requires data describing the physical properties of critical components. For example, in CRIRES a ZnSe prism is used as a pre-disperser making it essential to quantitatively know the properties of ZnSe at CRIRES' cryogenic operating temperature. Since no such data were available in the literature, new laboratory measurements, taken at NASA's CHARMS facility (Kerber et al. 2006), were included in the model. The validity of the model in this respect was verified by comparing it with data taken during a temperature ramp during testing.

### Wavelength standards

Like any other approach to wavelength calibration, the use of instrument physical models requires high quality reference data traceable to laboratory standards, such as the wavelength standards emitted by calibration lamps. For CRIRES, ESO, in collaboration with the the Space Telescope European Co-ordinating Facility (ST-ECF) and the US National Institute of Standards and Technology (NIST), embarked on a project to establish Th-Ar wavelength standards in the 950–5 000 nm operating range of CRIRES. Through dedicated laboratory measurements at NIST, a catalogue of about 2 400 lines between 750 and 4 800 nm with highly accurate wavelengths (accuracy 0.001 $cm^{-1}$ for strong lines) was obtained. This now forms the backbone of wavelength calibration for CRIRES up to 2 500 nm (Kerber et al. 2008). For longer wavelengths, gas cells ($N_2O$ and OCS) are being established as calibration sources by using NIST reference data and laboratory measurements with ESO's Fourier Transform Spectrometer to characterise the gas cells as a function of fill gas pressure and temperature.

With these developments wavelength calibration in the near-IR will become very similar to the UV-visible region, and it is possible to support high accuracy absolute wavelength calibration without having to rely on atmospheric features. In an earlier very similar effort, a multitude of additional lines were measured in the spectrum of Pt/Cr-Ne lamps as used onboard STIS (Sansonetti et al. 2004). The STIS Calibration Enhancement effort using a physical model in combination with these data was recognised by a NASA Group achievement award in 2006 (see The Messenger 126, page 54). For future E-ELT instruments the group has already started a project to study various elements spectroscopically in order to identify the best near-IR calibration sources as a function of spectral resolution. Similarily, improved spectro-photometric standard stars for the near-IR are being established for use with X-shooter (Vernet et al. 2008) and future IR spectrographs.

## Optimising calibration systems

The combination of laboratory measurements with a physical instrument model is a very powerful tool for assessing the predicted performance of an instrument or its calibration subsystem. For the selection of the best-suited wavelength calibration sources for the near-IR arm of X-shooter, we did an in-depth analysis (Kerber et al. 2007). As a result we have been able to identify a combination of the noble gases Ne, Ar and Kr as the best three-lamp combination. Our analysis provides a quantitative order-by-order prediction about the number of lines available from a given source, their relative intensities – including the effect of the blaze function – and an estimate of the line blending between sources.

We have recently extended this concept to develop a technique to customise calibration source line catalogues according to the instrument, mode and operating conditions. By creating a 2D simulation with a given set of physical model parameters, and extracting a 1D spectrum from the simulation, one obtains a realistic flux distribution for the spectral features to which, if desired, a noise level appropriate to the exposure time of calibration observations can be added. This spectrum will include potential blending from neighbouring features and, for some spectrographs, order overlap, an effect that would normally be difficult to evaluate. By measuring centroids in the simulated data and comparing to the known centroids we can determine which features will potentially be blended or poorly resolved and thus not useful for automated wavelength calibration. In the event of a major change in spectral format (intervention, earthquake, etc.), this procedure enables us to identify calibration features that will always be isolated within a window of a size that reflects the uncertainty, hence reducing the chance of false matches.

## Summary and outlook

We have developed streamlined physical models for a variety of astronomical spectrographs that are characterised by a model kernel with an associated set of parameters; each parameter has a clear physical meaning. In addition we have implemented the tools necessary to optimise the parameter sets to match the actual configuration of the real instruments using dedicated calibration observations.

Once optimised, the physical model drives the wavelength calibration inside the data reduction pipeline. This is already an option for CRIRES and is being realised for X-shooter. We have also produced a suite of software to simulate 1D and 2D spectroscopic data using such models. These simulations aid the initial alignment of the instrument in the laboratory, the development of the DRS and, potentially, the planning of observations.

Calibration reference data traceable to laboratory standards provide the ground truth needed for quantitative calibration. A combination of the modelling techniques and calibration reference data can be used to optimise instrument performance throughout all phases of the life cycle of an instrument: design, manufacture, testing and operations.

Key to success and to achieving the best science product is an integrated approach that combines the development of physical instrument models, application of and feedback from these models during instrument integration, testing, commissioning and science verification and their integration in the data reduction software.

Second-generation VLT instruments and E-ELT instruments clearly stand to benefit from this approach.

### Acknowledgements

We would like to thank our CRIRES and X-shooter project colleagues for their support and co-operation and Gillian Nave and Craig Sansonetti at NIST for fruitful collaboration. Special thanks also to Yves Jung for his sterling effort (and patience) interfacing the physical model code with the CRIRES DRS.

### References

Ballester P. and Rosa M. R. 1997, A&A Supp. 563, 126
Carter E. 2001, *http://www.taygeta.com/annealing/simanneal.html*
Kerber F. et al. 2006, SPIE 6269, 42
Kerber F., Saitta F. and Bristow P. 2007, The Messenger 129, 21
Kerber F. et al. 2008, ApJ Supp., submitted
Sansonetti C. J. et al. 2004, ApJS 153, 555
Vernet J. et al. 2007, The Messenger 130, 5
Vernet J. et al. 2008, in "2007 ESO Instrument Calibration Workshop, Proceedings of the ESO Workshop held in Garching, Germany, 23–26 January 2007", eds. A. Kaufer and F. Kerber, Springer

Photo: H. H. Heyer, ESO

VISTA's 67-Mpixel near-infrared camera (black and silver) is shown in the Instrument Preparation Room at VISTA on its blue handling carrier. An autoguider test source is fitted across the camera window. Primary Mirror polishing is close to completion and first light is expected later this year. See *http://www.vista.ac.uk/* for more details.