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Numerical simulation of spectral equipment

T.A. Fatkhullin, M.V. Yushkin, V.E. Panchuk

Special Astrophysical Observatory, Nizhnij Arkhyz 369167, Zelenchukskiy region, Karachai-Cherkessian Republic, Russian Federation
e-mail: timur@sao.ru

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ABSTRACT

We present the results of numerical simulation of high- and low-resolution spectral equipment, as well as its real-life application. A ray-tracing method is implemented in the C++ programming language by using the nVidia CUDA (Compute Unified Device Architecture) technology. The results of simulation for the ground- (BTA/NES, Big Telescope Alt-azimuth Nasmyth Echelle Spectrograph) and space-based (Spectr-UF) spectrographs are exposed. It is shown that the model two-dimensional echelle and long-slit spectra can be used to estimate the energy efficiency of the proposed optical design, to calculate the characteristics of gradient anti-reflection coatings, as well as to create and refine an automatic processing pipeline for observational data long before the launch of space observatories. By using the NES spectrograph simulation, an analysis of the differences between the "ideal" optical design and its real technical implementation is demonstrated. For example, some manufacturing details of the ruled echelle gratings may cause significant differences as compared to expected characteristics. As a result, we show that the implemented mathematical model is a useful and truly powerful tool for designing astronomical spectral equipment, calculating and justifying its basic characteristics, as well as for planning an astrophysical experiment itself.

Key words: spectrographs, space and ground-based astronomy, computational methods

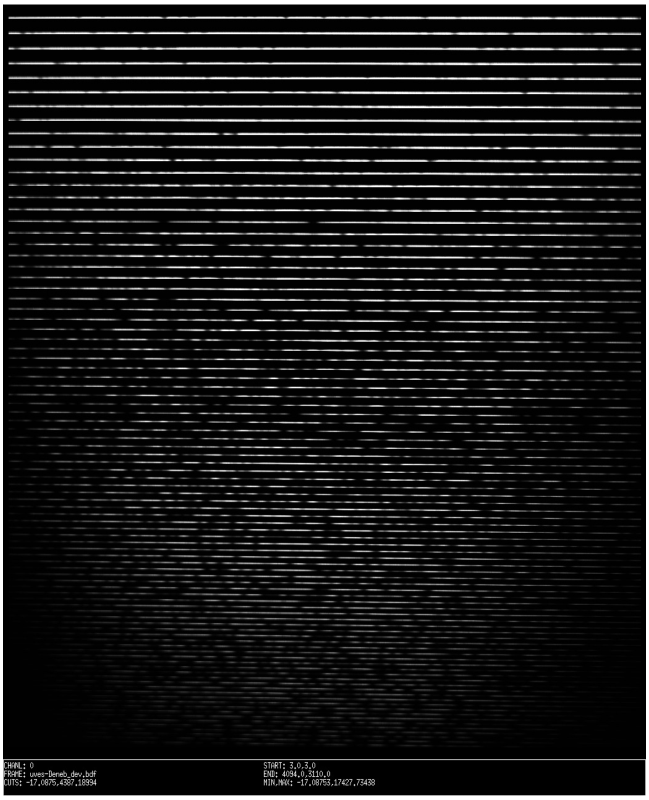
1 Introduction

The current level of computational power, advancement in mathematical methods, and the emergence of various software technologies on their basis (e.g., CUDA[1]) have provided new perspectives on the design, manufacturing, and technical support of observational instruments in astronomy. Various nuances arising during observational tasks, particularly at the limits of instrumental capabilities, also lead to the idea about approaches in modeling instrument behavior or characteristics in advance, prior to experiments, or about applying this modeling, for example, as input parameters for processing and interpretation of the derived measurements (see, e.g., Ballester, Rosa, 1997; Ghavamian et al., 2009). In our view, modern computational capabilities have primarily affected the development of methods for modeling astronomical experiments in space missions. Our involvement in the Spektr-UV project (Boyarchuk et al., 2013), combined with the considerations above, motivated us as developers of spectroscopic instrumentation and, importantly, potential end-users of observational data to elaborate a mathematical model of the instruments under design.

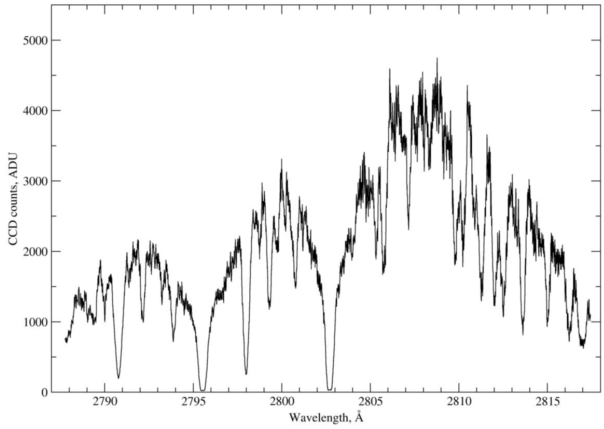
2 Mathematical model

In our work on the creation of spectroscopic instrumentation for the Spektr-UV space observatory, the primary requirement was to justify the selected optical design, particularly the calculation of the total energy efficiency of the spectrographs under development. Here, we imply efficiency across the entire operational spectral range, including the efficiency of the supposed diffraction gratings. For more complex designs, such as in the NES spectrograph, it becomes crucial to account for internal losses due to vignetting of the working beam. For ground-based instruments, losses at the entrance slit are also significant, as unlike space experiments, the turbulent stellar disk is typically much larger than the slit width. Collaboration with the engineering team on elaborating control methods for manufacturing the instrument, its alignment procedures, and the application of gradient anti-reflective coatings on CCD detectors required precise knowledge on the positions of spectral echelle orders on the detector plane. Based on the above, we can formulate specifications for our model. The input parameters of the model are the optical designs of telescopes and spectrographs, transmission or reflection coefficients of optical elements, diffraction grating parameters, quantum efficiency of CCD detectors, and the spectral energy distribution of the radiation source (e.g., a star). For ground-based instruments, an additional input parameter is the size of the turbulent stellar disk. Then, it is required that in the implemented model, the outputs include the geometric position of spectral orders on the detector, their curvature and the tilt of spectral lines in them, the total quantum efficiency of the telescope–spectrograph–detector system, and a simulated image of the CCD frame derived

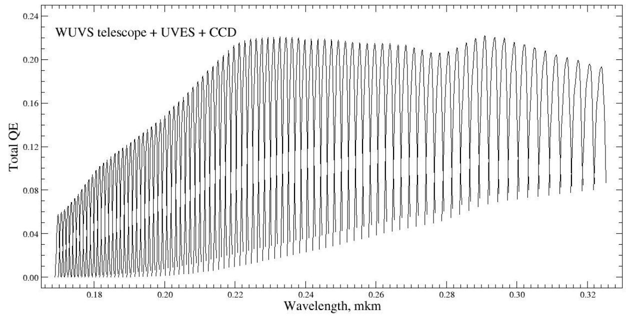
[1] https://developer.nvidia.com/cuda-zone



(a) Simulated CCD image

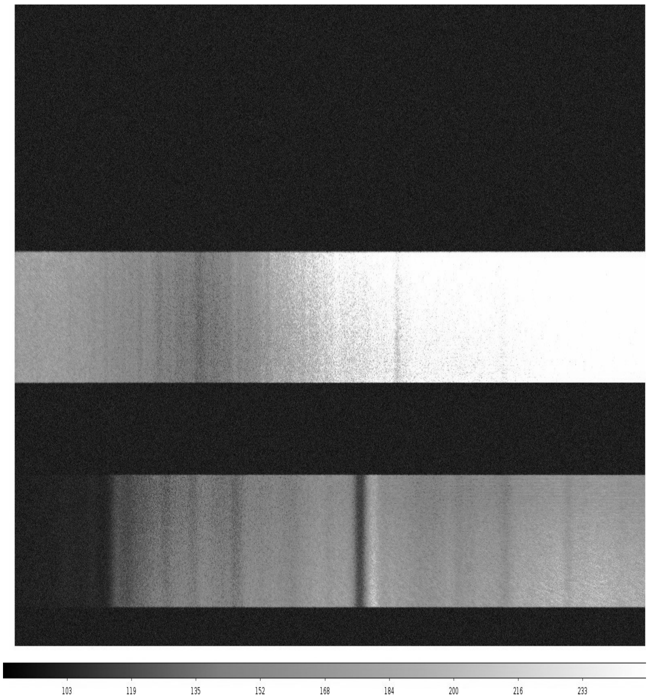


(b) Photometric cross-section of one spectral order

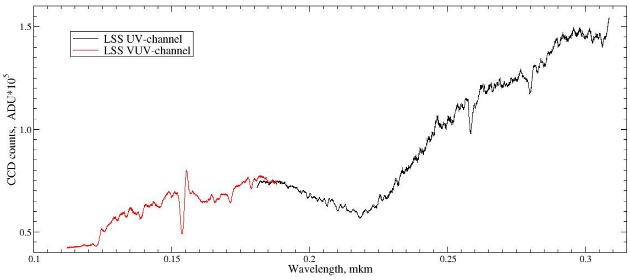


(c) Total quantum efficiency of the telescope–spectrograph–detector system

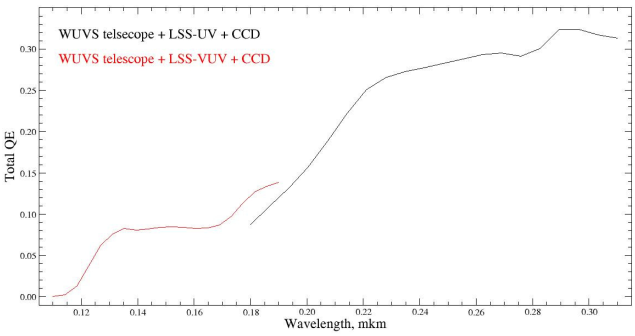
Fig. 1. Results of simulation for the Spektr-UV/UVES spectrograph. The CCD format is 4096×3112 elements, 4.5×10^9 rays for tracing, and the input model spectrum of an A2-type star ($T_{\rm eff}$ = 9200 K). The wavelength range is 169–325 nm.



(a) Simulated CCD image

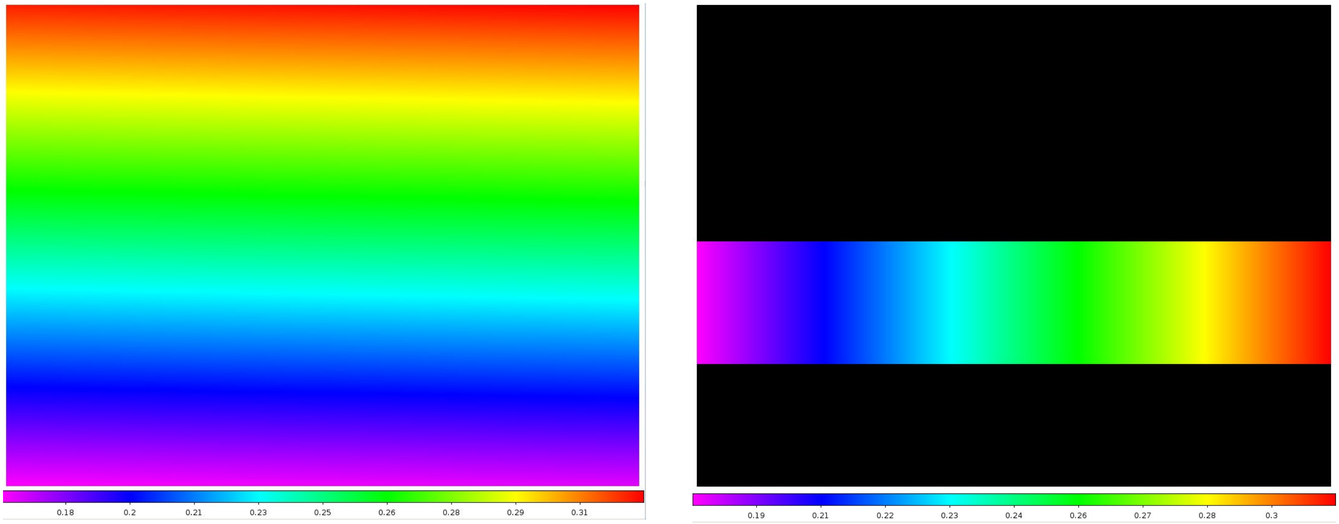


(b) Photometric cross-section of spectral orders



(c) Total quantum efficiency of the telescope–spectrograph–detector system

Fig. 2. Results of simulation for the Spektr-UV/LSS spectrograph. The CCD format is 4096×3112 elements, 10^9 rays for tracing, and the input model spectrum of an A2-type star ($T_{\rm eff}$ = 9200 K). The wavelength range is 110–310 nm.



(a) For the UVES spectrograph

(b) For the LSS spectrograph

Fig. 3. Analytical dependence $\lambda = f(x, y)$ inferred from simulation for applying HfO_2 anti-reflective coating.

during observation. Detailed mathematical derivations and algorithmic features of our model are presented in Yushkin et al. (2016). Note that we applied a ray-tracing method and a scalar theory of the diffraction grating, implementing the model in C++ using CUDA libraries. CUDA technologies allowed us to apply algorithms of the so-called massive parallel computing, significantly reducing computation time by over an order of magnitude compared to classical sequential implementations.

3 Spectrographs of the Spektr-UV space observatory

Within the Spektr-UV project, we contributed to the development of high-resolution spectrographs UVES (Ultraviolet Echelle Spectrograph), VUVES (Vacuum Ultraviolet Echelle Spectrograph), and the moderate-resolution LSS (Long-Slit Spectrograph). The concept, optical designs, and detailed parameters are described in Sachkov et al. (2016). The UVES and VUVES designs differ only in parameters of diffraction gratings, so we focus on UVES here.

Figures 1 and 2 present the results of simulation for UVES and LSS, respectively. As mentioned earlier, gradient HfO_2 anti-reflective coatings were applied to CCDs to enhance quantum efficiency. To calculate the dependence $\lambda = f(x, y)$ (in fact coating thickness) as a function of coordinates on the detector plane, the results of our simulation were used, namely the precise position of orders. Figure 3 shows these dependences for CCD detectors of UVES and LSS spectrographs (for LSS, coating was applied only to the long-wavelength channel). We note the fact that the simulated images of 2D echelle spectra with simulated noise characteristics of CCD detectors can be used to develop data processing systems before the launch of space missions.

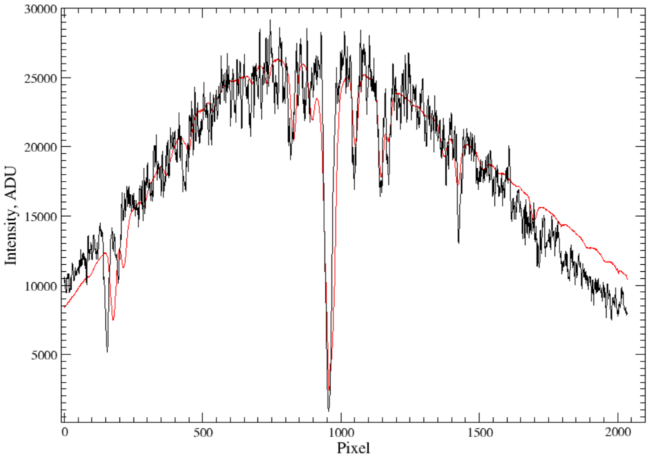
4 NES spectrograph of the BTA telescope

NES is a high-resolution echelle spectrograph mounted on the BTA telescope (SAO RAS). The optical design, detailed description, and the current state of the instrument are presented, for example, in Panchuk et al. (2017). We selected NES as an example of a rather complex and, most importantly, actually used spectroscopic instrument. This allowed us to test our simulation, determine the limits of its applicability, and consider possible directions for further development of the elaborated mathematical method. Figure 4 presents the results of simulation and comparison with actual observations. Let us discuss this comparison in more detail. First of all, we note that the initial attempt (not shown in Fig. 4) revealed that the model produces a "steeper" energy distribution in orders. Investigation of this discrepancy led us to the conclusion that the main reason lies in the difference of the diffraction grating groove shape from an ideal triangular shape.

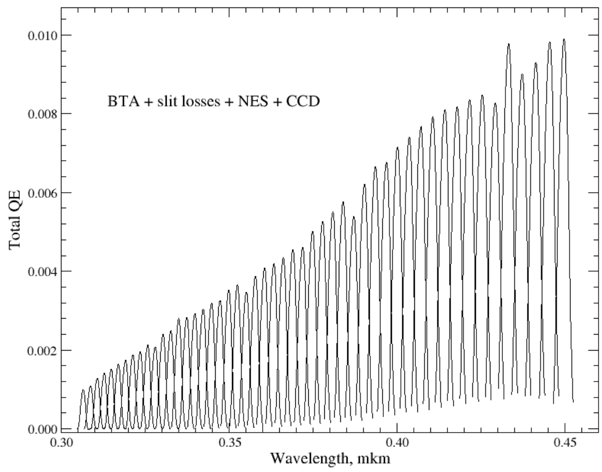
It is known that to reduce the load on the cutting tool when manufacturing gratings with low groove density, cutting is implemented not in a full profile (see Fig. 5a). Additionally, there is an effect of the groove vertex "rounding" during cutting due to incomplete filling of the master grating profile replica with composite material (see Fig. 5b). We simulated these effects by sequentially and iteratively reducing the working surface width of the echelle grating grooves in calculations. As can be seen from Fig. 4, this approach allowed us to achieve satisfactory agreement between simulation and observations. We interpret the residual discrepancy (see Fig. 4c) as deviations of the CCD detector chip axis from its input window axis, differences in the actual positioning angles of the echelle grating, and possible reducing of the blaze angle compared to the calculated values. Reducing the blaze angle is a known fact in manufacturing gratings due to elastic deformations of aluminum during the cutting tool passage. In our view, further calculations with introducing such deviations into the model parameters will allow one to achieve even better agreement between the actual data and

(a) Echelle spectrum image obtained with the NES spectrograph

(b) Simulated echelle spectrum image



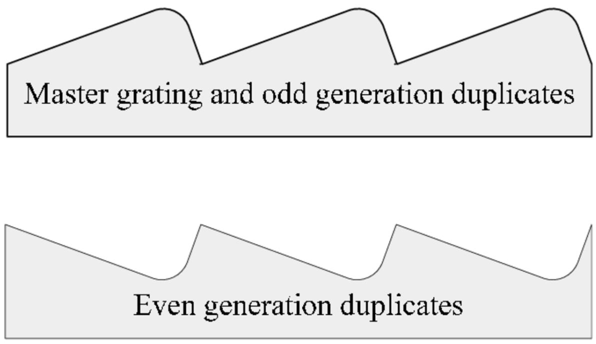
(c) Comparison of photometric cross-sections for one order: simulated cross-section is indicated by the red line and the observed one by the black line. The effective groove width is 60% of nominal (see discussion in the text)



(d) Total quantum efficiency including losses at the spectrograph entrance slit

Fig. 4. Echelle spectrum of α Cyg obtained with the NES spectrograph in the 300–450 nm wavelength range and the results of simulation. The CCD format is 2048×2048 elements, the turbulent disk size for the model $\mathrm{FWHM}_{\mathrm{gauss}} = 1.5$ arcsec, 10^9 rays for tracing, the input model spectrum of an A2-type star ($T_{\mathrm{eff}} = 9200$ K).

(a) A groove of the incomplete profile of the diffraction grating



(b) Rounding of the master grating groove edge (top) and its replica (bottom)

Fig. 5. Defects of the diffraction grating groove profile.

our results; however, this obviously requires significant computational time.

5 Conclusions

We have presented the results of elaboration and application of a method for mathematical simulation of spectrographs in the Spektr-UV space project and the ground-based BTA telescope. Based on the instruments of the Spektr-UV observatory, we demonstrated the possibility of using the results of such calculations when developing instruments, while for BTA/NES, in scientific and technical support of an operational instrument. Such simulation seems to be a useful and powerful tool for designing, justifying optical designs and characteristics, and supporting astronomical spectroscopic instrumentation.

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