











Astronomical échelle spectroscopy data analysis with `muler`

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Summary

Modern astronomical échelle spectrographs produce information-rich 2D echellograms that undergo standard reduction procedures to produce extracted 1D spectra. The final post-processing steps of these 1D spectra are often left to the end-user scientists, since the order of operations and algorithm choice may depend on the scientific application. Implementing these post-processing steps from scratch acts as a barrier to entry to newcomers, taxes scientific innovation, and erodes scientific reproducibility. Here we assemble and streamline a collection of spectroscopic data analysis methods into a single easy-to-use Application Programming Interface (API), `muler`. The `specutils`-based fluent interface enables method chaining that yields compact 1-line code for many applications, a dramatic reduction in complexity compared to existing industry practices. When applicable, some algorithms are customized to the pipeline data products of three near-infrared spectrographs: HPF, Keck NIRSPEC, and IGRINS. The framework could be extended to other spectrographs in the future. The tutorials in `muler` may also serve as a central onboarding point for new entrants to the practice of near-infrared échelle spectroscopy data. The open-source permissively licensed Python 3 implementation lowers the barrier to entry and accelerates the investigation of astronomical spectra.

Statement of need

In its most elemental form, an astronomical spectrum consists of a list of wavelength coordinates and their flux values. Additional metadata for uncertainties, date, time, sky pointing coordinates, and instrumental configuration are common. The Astropy-affiliated `specutils` package serves as a unifying container for virtually any astronomical spectrum, by providing a way to represent, load, manipulate, and analyze these data and metadata. It is therefore possible for each new practitioner to load a pipeline-produced output spectrum with, numpy arrays, pandas dataframes, or `specutils` objects and write standard post-processing operations from scratch. This bespoke approach requires expert knowledge, is time-consuming, and may be error prone. Ideally, we would have an easy-to-use post-processing tool that takes in the raw 1D pipeline output filename and produces a refined spectrum ready for scientific analysis. The `muler` framework fills this role.

Each spectrograph and pipeline has peculiarities, and so `muler` provides domain-specific layers for individual spectrographs. The `muler` framework therefore enables user code to be compact and easily transferable among projects.

The Python spectroscopy ecosystem has dozens or hundreds of packages. Here we compare `muler` to a few recent examples to show how it fits into that ecosystem. The `wobble` ([Bedell](#)

[et al., 2019](#)) framework performs advanced modeling on groups of dozens of échelle spectra of the same celestial object, assuming they have already been normalized, continuum-flattened, sky subtracted, etc. So in this case, `muler` serves as the layer that takes in the pipeline output, processes each spectrum identically, and then feeds these refined spectra into `wobble`. Similarly, the `starfish` framework ([Czekala et al., 2015](#)) expects spectra to reside in an HDF5 format with telluric lines either corrected or masked. `muler` can satisfy these requirements. You can therefore view `muler` as taking care of these necessary pre-processing steps to get from the pipeline products to the inputs of virtually any other Python spectroscopy analysis package.

Some packages such as `igrins_rv` ([Tang et al., 2021](#)) conduct pre-processing steps as a matter of course in their analyses. These packages could hypothetically be refactored to make `muler` a dependency, with the boilerplate steps taken over by `muler`. This refactoring step would simplify the code, possibly making it more maintainable in the long term. In other cases, popular methods in `muler` may move upstream into `specutils`.

`muler` depends on `astropy` ([Astropy Collaboration et al., 2018, 2013](#)), `numpy` ([Harris et al., 2020](#)), `specutils`, `scipy` ([Virtanen et al., 2020](#)), and others.

Architecture and design considerations

The design of `muler` shares three key inspirations from `lightcurve` ([Lightcurve Collaboration et al., 2018](#)), which provides a well-liked open-source fluent interface to NASA Kepler/K2/TESS data. First, pipeline products have reliable and predictable formats that make them a *de facto* standard. You can then make an API that relies on that standard for accessing attributes and metadata, and build methods that combine the data, metadata, and optionally user inputs to conduct essentially all routine operations.

The second key idea is that the output of an operation is usually self-similar: a `lightcurve` operation usually takes in a `lightcurve` and outputs a `lightcurve`. Here a `muler` operation takes in a `Spectrum1D`-like object and returns a `Spectrum1D`-like. This key idea makes method chaining both possible and desirable.

Finally, `lightcurve` objects inherit key behaviors from the `Astropy TimeSeries` module, reducing the duplication of code relevant to time series data. Here in `muler` we gain similar extensibility through an object-oriented design with `specutils`, abstracting away many routine spectroscopy tasks, and keeping the `muler` code lean.

Supported spectrographs

We currently support custom operations for three spectrographs: the Immersion Grating Infrared Spectrograph, IGRINS ([Mace et al., 2018](#); [Park et al., 2014](#)) reduced with the `plp` ([Lee et al., 2017](#)); the Habitable Zone Planet Finder Spectrograph, HPF ([Mahadevan et al., 2012, 2014, 2018](#)) with either the `Goldilocks` or `Penn State` pipelines; and the Keck Near-Infrared Spectrograph, NIRSPEC ([McLean et al., 1998, 2000](#)) with the `MSDRP` pipeline.

In principle, `muler` could be extended with devoted classes for other échelle spectrographs, so long as the pipeline outputs deliver standardized files with common metadata, such as date, time, celestial coordinates, etc.

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References

- Astropy Collaboration, Price-Whelan, A. M., Sipőcz, B. M., Günther, H. M., Lim, P. L., Crawford, S. M., Conseil, S., Shupe, D. L., Craig, M. W., Dencheva, N., Ginsburg, A., VanderPlas, J. T., Bradley, L. D., Pérez-Suárez, D., de Val-Borro, M., Aldcroft, T. L., Cruz, K. L., Robitaille, T. P., Tollerud, E. J., ... Astropy Contributors. (2018). The Astropy Project: Building an Open-science Project and Status of the v2.0 Core Package. *156*, 123. <https://doi.org/10.3847/1538-3881/aabc4f>
- Astropy Collaboration, Robitaille, T. P., Tollerud, E. J., Greenfield, P., Droettboom, M., Bray, E., Aldcroft, T., Davis, M., Ginsburg, A., Price-Whelan, A. M., Kerzendorf, W. E., Conley, A., Crighton, N., Barbary, K., Muna, D., Ferguson, H., Grollier, F., Parikh, M. M., Nair, P. H., ... Streicher, O. (2013). Astropy: A community Python package for astronomy. *558*, A33. <https://doi.org/10.1051/0004-6361/201322068>
- Bedell, M., Hogg, D. W., Foreman-Mackey, D., Montet, B. T., & Luger, R. (2019). WOBBLE: A Data-driven Analysis Technique for Time-series Stellar Spectra. *158*(4), 164. <https://doi.org/10.3847/1538-3881/ab40a7>
- Czekala, I., Andrews, S. M., Mandel, K. S., Hogg, D. W., & Green, G. M. (2015). Constructing a Flexible Likelihood Function for Spectroscopic Inference. *812*, 128. <https://doi.org/10.1088/0004-637X/812/2/128>
- Harris, C. R., Millman, K. J., Walt, S. J. van der, Gommers, R., Virtanen, P., Cournapeau, D., Wieser, E., Taylor, J., Berg, S., Smith, N. J., Kern, R., Picus, M., Hoyer, S., Kerkwijk, M. H. van, Brett, M., Haldane, A., R'io, J. F. del, Wiebe, M., Peterson, P., ... Oliphant, T. E. (2020). Array programming with NumPy. *Nature*, *585*(7825), 357–362. <https://doi.org/10.1038/s41586-020-2649-2>
- Lee, J.-J., Gullikson, K., & Kaplan, K. (2017). *Igrins/plp 2.2.0*. Zenodo. <https://doi.org/10.5281/zenodo.845059>
- Lightkurve Collaboration, Cardoso, J. V. d. M., Hedges, C., Gully-Santiago, M., Saunders, N., Cody, A. M., Barclay, T., Hall, O., Sagar, S., Turtelboom, E., Zhang, J., Tzanidakis, A., Mighell, K., Coughlin, J., Bell, K., Berta-Thompson, Z., Williams, P., Dotson, J., & Barentsen, G. (2018). *Lightkurve: Kepler and TESS time series analysis in Python*. Astrophysics Source Code Library.
- Mace, G., Sokal, K., Lee, J.-J., Oh, H., Park, C., Lee, H., Good, J., MacQueen, P., Oh, J. S., Kaplan, K., Kidder, B., Chun, M.-Y., Yuk, I.-S., Jeong, U., Pak, S., Kim, K.-M., Nah, J., Lee, S., Yu, Y.-S., ... Jaffe, D. T. (2018). IGRINS at the Discovery Channel Telescope and Gemini South. In C. J. Evans, L. Simard, & H. Takami (Eds.), *Ground-based and airborne instrumentation for astronomy VII* (Vol. 10702, p. 107020Q). <https://doi.org/10.1117/12.2312345>
- Mahadevan, S., Anderson, T., Balderrama, E., Bender, C. F., Bevins, E., Blakeslee, S., Cole, A., Conran, D., Diddams, S., Dykhouse, A., Darling, J., Fredrick, C., Halverson, S., Hearty, F., Jennings, J., Kaplan, K., Kanodia, S., Levi, E., Lubar, E., ... Wright, J. (2018). The habitable-zone planet finder: engineering and commissioning on the Hobby Eberly telescope (Conference Presentation). In C. J. Evans, L. Simard, & H. Takami (Eds.), *Ground-based and airborne instrumentation for astronomy VII* (Vol. 10702). International Society for Optics; Photonics; SPIE. <https://doi.org/10.1117/12.2313835>
- Mahadevan, S., Ramsey, L. W., Terrien, R., Halverson, S., Roy, A., Hearty, F., Levi, E., Stefansson, G. K., Robertson, P., Bender, C., Schwab, C., & Nelson, M. (2014). The

- Habitable-zone Planet Finder: A status update on the development of a stabilized fiber-fed near-infrared spectrograph for the Hobby-Eberly telescope. In S. K. Ramsay, I. S. McLean, & H. Takami (Eds.), *Ground-based and airborne instrumentation for astronomy v* (Vol. 9147, p. 91471G). <https://doi.org/10.1117/12.2056417>
- Mahadevan, S., Ramsey, L., Bender, C., Terrien, R., Wright, J. T., Halverson, S., Hearty, F., Nelson, M., Burton, A., Redman, S., Osterman, S., Diddams, S., Kasting, J., Endl, M., & Deshpande, R. (2012). The habitable-zone planet finder: a stabilized fiber-fed NIR spectrograph for the Hobby-Eberly Telescope. In I. S. McLean, S. K. Ramsay, & H. Takami (Eds.), *Ground-based and airborne instrumentation for astronomy IV* (Vol. 8446, p. 84461S). <https://doi.org/10.1117/12.926102>
- McLean, I. S., Becklin, E. E., Bendiksen, O., Brims, G., Canfield, J., Figer, D. F., Graham, J. R., Hare, J., Lacayanga, F., Larkin, J. E., Larson, S. B., Levenson, N., Magnone, N., Teplitz, H., & Wong, W. (1998). Design and development of NIRSPEC: a near-infrared echelle spectrograph for the Keck II telescope. In A. M. Fowler (Ed.), *Infrared astronomical instrumentation* (Vol. 3354, pp. 566–578). <https://doi.org/10.1117/12.317283>
- McLean, I. S., Graham, J. R., Becklin, E. E., Figer, D. F., Larkin, J. E., Levenson, N. A., & Teplitz, H. I. (2000). Performance and results with the NIRSPEC echelle spectrograph on the Keck II telescope. In M. Iye & A. F. Moorwood (Eds.), *Optical and IR telescope instrumentation and detectors* (Vol. 4008, pp. 1048–1055). <https://doi.org/10.1117/12.395422>
- Park, C., Jaffe, D. T., Yuk, I.-S., Chun, M.-Y., Pak, S., Kim, K.-M., Pavel, M., Lee, H., Oh, H., Jeong, U., Sim, C. K., Lee, H.-I., Nguyen Le, H. A., Strubhar, J., Gully-Santiago, M., Oh, J. S., Cha, S.-M., Moon, B., Park, K., ... Park, B.-G. (2014). Design and early performance of IGRINS (Immersion Grating Infrared Spectrometer). *Society of Photo-Optical Instrumentation Engineers (SPIE) Conference Series, 9147*, 1. <https://doi.org/10.1117/12.2056431>
- Tang, S.-Y., Stahl, A., Johns-Krull, C., Prato, L., & Llama, J. (2021). IGRINS RV: A Python Package for Precision Radial Velocities with Near-Infrared Spectra. *The Journal of Open Source Software, 6*(62), 3095. <https://doi.org/10.21105/joss.03095>
- Virtanen, P., Gommers, R., Oliphant, T. E., Haberland, M., Reddy, T., Cournapeau, D., Burovski, E., Peterson, P., Weckesser, W., Bright, J., van der Walt, S. J., Brett, M., Wilson, J., Millman, K. J., Mayorov, N., Nelson, A. R. J., Jones, E., Kern, R., Larson, E., ... SciPy 1.0 Contributors. (2020). SciPy 1.0: fundamental algorithms for scientific computing in Python. *Nature Methods, 17*, 261–272. <https://doi.org/10.1038/s41592-019-0686-2>