Dries Van De Putte

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Technical Skills

- Software development in a research context – Approximately 6 years of experience in developing software for my research goals. This technical skills overview mentions several codes: PAHFIT, the BEAST, SKIRT, and RADAGAST. Please refer to the experience, education, and projects sections for more information about these project and my development work.
- Python – Daily use for the reduction and analysis of astronomical data. Notable and frequently used packages are numpy, scipy, matplotlib, astropy and affiliated packages (specutils, photutils), and the jwst pipeline package. Development experience by contributing to BEAST and PAHFIT.
- git and GitHub – Daily use for code specific to my scientific projects. All collaborative software projects I contributed to used GitHub.
- Software practices – Experience with writing issues and pull requests, and best practices such as continuous integration and test driven development. The BEAST and PAHFIT have automated building and testing routines based on GitHub actions, Tox, and pytest, as set up by the astropy package template, and I added new regression tests for new features or bug fixes I worked on.
- Documentation and user support – Recent experience by responding to GitHub issues of PAHFIT, and writing a demonstration notebook for this tool. Experience editing the documentation that is build for those projects, by the Sphinx system. Experience with the Doxygen automated documentation system for C++ code; it is used by SKIRT, and I used the same system for RADAGAST, and where all functions are thoroughly documented.
- Project management – Working on multiple science projects simultaneously throughout my PhD program and postdoctoral appointment, and managing my collaborations with multiple teams. Short-term projects include writing observing proposals for HST and JWST, and adding features to the scientific codes of my collaborators.
- C++ proficiency – Author of the RADAGAST C++ code, and have deep knowledge of the SKIRT C++ code by implementing a parallelization scheme and coupling it to RADAGAST (see experience and projects). Experience with the GCC and CLang compilers, and writing CMakeLists.txt files for the CMake build system, as well as writing and edit regular make files. Basic knowledge of C concepts.
- HPC and parallel programming – Experience using the multi-node High Performance Computers of the Flemish Supercomputer Center, and their job queue system. The SKIRT C++ code uses a hybrid parallelization combining multi-processing and multi-threading, and I implemented several inter-process communication steps with MPI (Message Passing Interface). Experience using Valgrind to profile the code and find bottlenecks. Use of command line tools such as GNU parallel, and the Python multiprocessing module to speed up research tasks that are straightforward to parallelize. Attended introduction to OpenMP training at Ghent University. Attended introduction to Docker training at STScI.
- Numerical methods – Experience with using solvers (from scipy, GSL, or Eigen): numerical integration, root-finding, ordinary differential equations, linear systems of equations (via RADAGAST). Monte Carlo radiation transport, 3D grids (Octree, Cartesian, Voronoi), postprocessing output of other astrophysical simulations (via SKIRT). Bayesian methods, forward modeling, model fitting (via BEAST and PAHFIT). Statistical methods to estimate uncertainty and covariance such as Monte Carlo estimation, bootstrapping, error propagation.
- Data experience – Daily use of FITS files produced by various observatories, and transforming the data within them, including images, spectral data cubes, and binary tables. Working with the JWST pipeline for NIRSpec and MIRI IFU data. Working with astropy Table or pandas DataFrame, and reading and writing CSV and HDF5. Experience writing custom file reading routines in C++ and Python, to read atomic data or simulation output in non-standard formats.
- Astrophysical knowledge – Astrophysical research experience with the following specializations: Radiative transfer, interstellar gas and dust, photodissociation regions observations and modeling (photochemistry processes, heating and cooling processes, chemical networks, molecular excitation and energy level populations), molecular hydrogen, fitting spectra and photometric observations, JWST data reduction.

Experience and Education

2021-today **Postdoctoral Research Fellow** Space Telescope Science Institute, Baltimore, MD

- Member of the PDRs4All (JWST ERS-1288) data reduction team, with a focus on NIRSpec IFU and MIRI IFU spectroscopy. Maintained the PDRs4All data reduction Python package, containing workarounds to resolve issues with early versions of the JWST pipeline. The delivery of improved data products we created, to the other team members, was crucial for the work on the first four PDRs4All papers (Berné et al. 2023, Habart et al. 2023, Peeters et al. 2023, Chown et al. 2023). Currently leading the fifth PDRs4All paper: an overview and initial analysis of the mid-IR emission lines in the Orion Bar.
- Contributed to the open-source Python code PAHFIT, a tool for spectral decomposition of the typical features in near-IR and mid-IR spectra. Contributions include the redesign of the main user-facing API, and the development and presentation (see presentations: JWebbinar 23) of a Jupyter notebook to demonstrate and communicate the new features to the community. Developed PAHFITcube, a separate package with utilities to apply PAHFIT to data cubes from JWST (see projects for details).
- Member of the Horsehead and NGC 7023 collaboration (JWST GTO-1192), where I led the reduction of the NIRSpec and MIRI IFU data. Currently leading a paper concerning the decomposition and spatial mapping of spectral features based on these IFU spectra.
- Dust extinction projects: Published Van De Putte et al. (2023) concerning the connection beween H_2 and UV dust extinction. Wrote dust extinction observation proposals for Hubble Space Telescope and James Webb Space Telescope concerning, and contributed to observing proposals of collaborators as a co-investigator.

2016 - 2020 **PhD of Science in Astronomy** Ghent University, Ghent, Belgium
Space Telescope Science Institute, Baltimore, MD

- Wrote a research plan and obtained a four year fellowship from BOF (*bijzonder onderzoeksfonds*), the "exceptional research fund" provided by Ghent University.
- Developed RADAGAST, a new astrophysical C++ code that calculates the local properties of interstellar gas, under the effect of a given local radiation field and dust grain properties. RADAGAST was coupled to SKIRT, a C++ code for radiative transfer through dust in arbitrary 3D geometries. PhD thesis: "Self-consistent modeling of radiation, dust, and gas in the interstellar medium". Supervision: Maarten Baes, Karl Gordon, Julia Roman-Duval.
- Visited the Johns Hopkins University and STScI (Apr 2017 - Apr 2018), to collaborate with the ISM*@ST group. In the context of Van De Putte et al. (2020), modified and applied the Bayesian Stellar and Extinction Tool (BEAST). This is an open-source Python code which combines stellar atmosphere model grids and dust extinction curves to forward model stellar photometry data from the UV to the NIR. Added several tools to the main BEAST code branch, including support for stellar distance fitting, and a method to curb its memory usage when calculating the posterior. Regression tests for these tools were also added.
- Teaching assistant for "Statistics and data processing" for two semesters (Fall 2018, 2019). Supervised the exercise sessions, and set up three Python programming challenges which introduced the students to essential packages such as *numpy* and *scipy*, and numerical statistical tasks such as error propagation and bootstrapping.

2011 - 2016 **BS and MS in Physics and Astronomy** Ghent University, Ghent, Belgium

- Implemented distributed-data multi-processing in the SKIRT C++ code, to enable the distribution of memory usage across compute nodes. This enabled users to run radiative transfer models that exceed the memory capacity of a single node. Added efficient inter-process communications to the existing C++ code base using the industry-standard Message Passing Interface (MPI). These communications facilitated switches in the memory distribution scheme, and to gathered the results for the final output. Co-authored Verstocken et al. (2017), by including a description of this method. *Master's thesis:* "Data parallelization with MPI in a 3D Monte Carlo dust radiative transfer code". *Supervision:* Maarten Baes.
- *Internship at the Royal Observatory of Belgium:* Developed a new pipeline step for the HERMES spectrograph of the Mercator Telescope. This step, written in Python, removes a bias introduced by the spectrum of the flat-field calibration lamps.
- *Notable elective course:* "Software Development I" in C and C++.

Projects

PAHFIT `https://github.com/PAHFIT/pahfit`
An open-source Python package, for the spectral decomposition of near-IR and mid-IR spectra, especially important for its application to JWST spectroscopy. Together with the author of the original IDL version, I am a main contributor and point of contact for users. I have frequently answered user questions and contributed to developer discussions on the GitHub issues page.

PAHFITcube `https://github.com/drvdputt/PAHFITcube`
The application of PAHFIT to the many spectra contained in IFU data cubes is relatively new, and necessary for my own research. Therefore, I created my own Python package with wrappers around PAHFIT that bookkeep the input spectra and fit results for spectral data cubes. Notable quality of life features include multiprocessing, the option to resume a series of fits that was interrupted, and writing a collection of fit results to a multi-extension FITS file.

RADAGAST `https://github.com/drvdputt/RADAGAST`
Astrophysical simulation code written from scratch in C++. Calculates the local properties of interstellar gas, under the effect of a given local radiation field and dust grain properties. Numerical techniques used include: 1D root-finding to determine the temperature based on the heating-cooling equation; Systems of ordinary differential equations to solve evolve the chemical network; Linear systems of equations to determine the energy level populations of H and H_2; Numerical integration of the radiation field over a given cross sections. The above calculations are based on atomic data, coming from various of sources, and therefore various file formats had to be read in.

SKIRT `https://skirt.ugent.be`
The above RADAGAST code was coupled to SKIRT, a C++ code for radiative transfer through dust in arbitrary 3D geometries. By integrating RADAGAST into SKIRT, I gained experience in interfacing multiple codes, working with the CMake build system, and compile or build issues that can appear in such configurations. The SKIRT/RADAGAST integration is demonstrated in my personal fork `https://github.com/drvdputt/SKIRT9/`.

JWST Data reduction scripts `https://github.com/drvdputt/jwst-pdr-reduction`
Some of the data reduction tools and tweaks developed for the PDRs4All and GTO-1192 JWST programs were made public, as they serve as a useful starting point for researchers wishing to re-reduce their JWST NIRSpec or MIRI IFU data.

Presentations and Conferences

2023/11/14 – Baltimore, MD	*Improving JWST Data Products Workshop:* Poster "Tools and corrections for imaging and IFU spectra of the Orion Bar"
2023/10/29 – Florence, Italy	*Illuminating the Dusty Universe: A Tribute to the Work of Bruce Draine:* Contributed talk "Spatially resolved maps of the IR emission bands in photodissociation regions"
2023/09/26 – Gothenburg, Sweden	*Origin and Fate of Dust in Our Universe:* Contributed talk "Far-UV extinction and H_2; Decomposing and mapping IR bands near the HI-H_2 transition"
2022/12/16 – Remote	*JWebbinar 23: PDRs4ALL Community Telecons in Support of JWST Cycle 2 Proposals; Webinar 3: Tools To Quantify the Spectral Information:* Live PAHFIT demo
2022/11/30 – Ghent, Belgium	*SKIRT Days 2022:* Contributed talk about the implementation of the RADAGAST gas model and its use in SKIRT
2022/07/11 – Paris-Saclay, France	*Interstellar Institute #5 - With Two Eyes:* Discuss PDRs4All and PAHFIT
2022/06/12 – Pasadena, CA	*240th Meeting of the American Astronomical Society:* Poster about the far-UV extinction rise to H_2 relationship

2022/03/15 – Baltimore, MD	*STScI Discovery Seminar Series:* "Far-UV Dust Extinction and Molecular Hydrogen in the diffuse Milky Way Interstellar Medium"
2019/06/24 – Lyon, France	*EWASS2019, Cosmic dust (r)evolution:* Poster about IC 63 project
2018/11/05 – Leiden, Netherlands	*Hendrik van de Hulst Centennial Symposium: The Interstellar Medium of Galaxies: Status and Future Perspectives:* Poster about IC 63 project
2018/06/11 – Copenhagen, Denmark	*CPHDUST2018: Cosmic Dust: origin, applications & implications:* Poster about IC 63 project
2016/10/28 – Florence, Italy	*DustPedia meeting:* Contributed talk about the parallelization of SKIRT
2016/10/04 – Ghent, Belgium	*CHARM meeting:* Contributed talk about the parallelization of SKIRT

Publications

1. Pasquini, S., Peeters, E., Schefter, B., et al. 2023, arXiv e-prints, arXiv:2311.01163 – *PDRs4All VI: Probing the Photochemical Evolution of PAHs in the Orion Bar Using Machine Learning Techniques*
2. Van De Putte et al. (*in prep.*) – *PDRs4All V: Mid-IR emission line inventory of the Orion Bar*
3. Chown, R., Sidhu, A., Peeters, E., et al. 2023, arXiv e-prints, arXiv:2308.16733 – *PDRs4All IV. An embarrassment of riches: Aromatic infrared bands in the Orion Bar*
4. Peeters, E., Habart, E., Berne, O., et al. 2023, arXiv e-prints, arXiv:2310.08720 – *PDRs4All III: JWST's NIR spectroscopic view of the Orion Bar*
5. Habart, E., Peeters, E., Berné, O., et al. 2023, arXiv e-prints, arXiv:2308.16732 – *PDRs4All II: JWST's NIR and MIR imaging view of the Orion Nebula*
6. Berné, O., Martin-Drumel, M.-A., Schroetter, I., et al. 2023, Nature, 621, 56 – *Formation of the methyl cation by photochemistry in a protoplanetary disk*
7. Van De Putte, D., Cartledge, S. I. B., Gordon, K. D., Clayton, G. C., & Roman-Duval, J. 2023, ApJ, 944, 33 – *Far-ultraviolet Dust Extinction and Molecular Hydrogen in the Diffuse Milky Way Interstellar Medium*
8. Berné, O., Habart, É., Peeters, E., et al. 2022, PASP, 134, 054301 – *PDRs4All: A JWST Early Release Science Program on Radiative Feedback from Massive Stars*
9. Van De Putte, D., Gordon, K. D., Roman-Duval, J., et al. 2020, ApJ, 888, 22 – *Evidence of Dust Grain Evolution from Extinction Mapping in the IC 63 Photodissociation Region*
10. Verstocken, S., Van De Putte, D., Camps, P., & Baes, M. 2017, Astronomy and Computing, 20, 16 – *SKIRT: Hybrid parallelization of radiative transfer simulations*
11. Baes, M., Camps, P., & Van De Putte, D. 2017, MNRAS, 468, 927 – *Analytical expressions and numerical evaluation of the luminosity distance in a flat cosmology*