




# Bayesian model reconstruction based on spectral line observations with pomme

Frederik De Ceuster <sup>1</sup>, Thomas Ceulemans <sup>1</sup>, Leen Decin <sup>1</sup>, Taissa Danilovich <sup>2,3,1</sup>, and Jeremy Yates <sup>4</sup>

<sup>1</sup> Institute of Astronomy, Department of Physics & Astronomy, KU Leuven, Celestijnenlaan 200D, 3001 Leuven, Belgium <sup>2</sup> School of Physics & Astronomy, Monash University, Clayton, Victoria, Australia <sup>3</sup> ARC Centre of Excellence for All Sky Astrophysics in 3 Dimensions (ASTRO 3D), Clayton, Victoria, Australia <sup>4</sup> Department of Computer Science, University College London, WC1E 6EA, London, United Kingdom

DOI: [10.21105/joss.07321](https://doi.org/10.21105/joss.07321)

## Software

- [Review](#) 
- [Repository](#) 
- [Archive](#) 

Editor: [Josh Borrow](#)  

## Reviewers:

- [@karllark](#)
- [@s-goldman](#)

Submitted: 14 August 2024

Published: 10 December 2024

## License

Authors of papers retain copyright and release the work under a Creative Commons Attribution 4.0 International License ([CC BY 4.0](#)).

## In partnership with



This article and software are linked with research article DOI [10.3847/1538-4365/ad89a2](https://doi.org/10.3847/1538-4365/ad89a2), published in the *Astrophysical Journal Supplement Series*.

## Summary

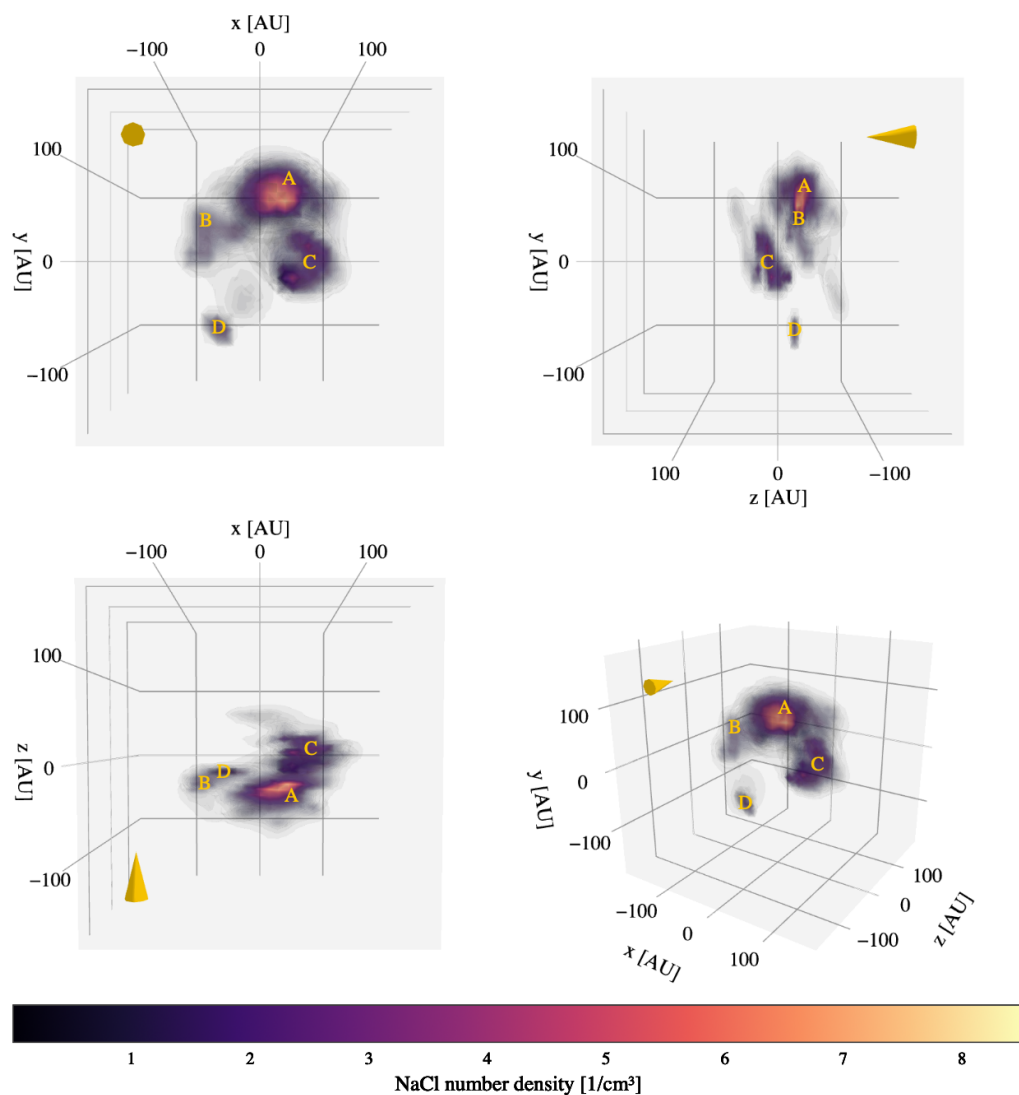
A typical problem in astronomy is that, for most of our observations, we are restricted to the plane of the sky. As a result, these observations are always mere projections containing only partial information about the observed object. Luckily, some frequency bands of the electromagnetic spectrum are optically thin, such that we receive radiation from the entire medium along the line of sight. This means that, at least in principle, from the observed radiation, we can extract information about the physical and chemical conditions along the entire line of sight. This is especially the case for spectral line radiation caused by transitions between the quantized energy levels of atoms and molecules. Rotational transition lines are particularly interesting, since they are excited in many astrophysical environments and can easily be resolved individually. Using spectral line observations, we can infer information about physical and chemical parameters, such as abundance of certain molecules, velocity, and temperature distributions. To facilitate this, we built a Python package, called *pomme*, that helps users reconstruct 1D spherically symmetric or generic 3D models, based on astronomical spectral line observations. A detailed description and validation of the methods can be found in De Ceuster et al. (2024).

## Statement of need

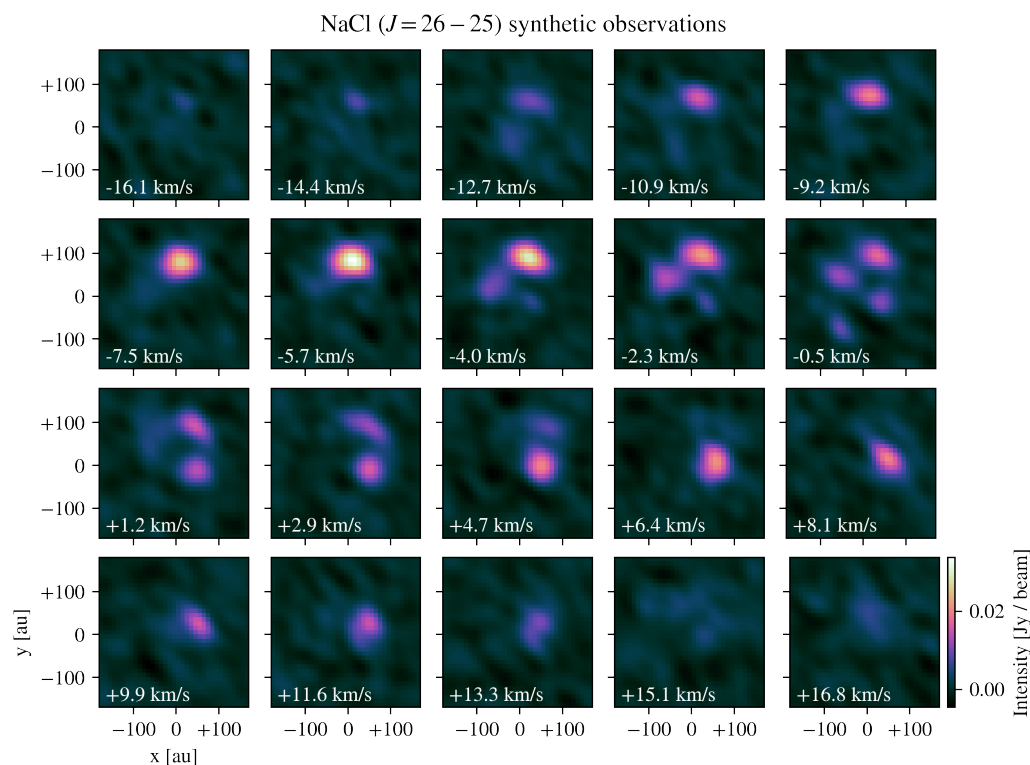
Spectral line observations are indispensable in astronomy. As a result, many line radiation transport solvers exist to solve the (forward) problem of determining what spectral line observations of a certain model would look like (De Ceuster et al., 2022; Matsumoto et al., 2023). However, far fewer tools exist to efficiently solve the more pressing inverse problem of determining what model could correspond to certain observations, commonly referred to as fitting our models to observations. Although one can use existing forward solvers to iteratively solve the inverse problem, the resulting process is often slow, cumbersome, and leaves much room for improvement (Coenegrachts et al., 2023; Danilovich et al., 2024). Therefore, in *pomme*, we have implemented a line radiative transfer solver (the forward problem) in the PyTorch framework (Paszke et al., 2019) to leverage the autograd functionality (Paszke et al., 2017) to efficiently fit our models to the observations (the inverse problem) in a streamlined way (De Ceuster et al., 2024).

## Example

Figure 1 shows an application of pomme, where it was used to reconstruct the abundance distribution of NaCl (table salt) around the evolved star IK Tauri. The reconstruction is based on observations of the NaCl ( $J = 26 - 25$ ) rotational line, taken with the Atacama Large Millimeter/submillimeter Array (ALMA), shown in Figure 2. The original analysis was done by Coenegrachts et al. (2023), and we improved their methods using pomme as described in De Ceuster et al. (2024).



**Figure 1:** Reconstruction of the NaCl abundance distribution around the evolved star IK Tauri, created with pomme. An interactive version of the figure is available in the [documentation](#).



**Figure 2:** NaCl ( $J = 26 - 25$ ) rotational line observations, taken with the Atacama Large Millimeter/sub-millimeter Array (ALMA), which is used as input in pomme to create a reconstruction.

## Acknowledgements

FDC is a Postdoctoral Research Fellow of the Research Foundation - Flanders (FWO), grant number 1253223N, and was previously supported for this research by a KU Leuven Postdoctoral Mandate (PDM), grant number PDMT2/21/066. TC is a PhD Fellow of the Research Foundation - Flanders (FWO), grant number 1166722N. LD acknowledges support from KU Leuven C1 MAESTRO grant C16/17/007, KU Leuven C1 BRAVE grant C16/23/009, KU Leuven Methusalem grant METH24/012, and FWO Research grant G099720N. TD is supported in part by the Australian Research Council through a Discovery Early Career Researcher Award, number DE230100183, and by the Australian Research Council Centre of Excellence for All Sky Astrophysics in 3 Dimensions (ASTRO 3D), through project number CE170100013.

## References

- Coenegrachts, A., Danilovich, T., De Ceuster, F., & Decin, L. (2023). The unusual 3D distribution of NaCl around the asymptotic giant branch star IK Tau. *Astronomy & Astrophysics*, 678, A85. <https://doi.org/10.1051/0004-6361/202346116>
- Danilovich, T., Malfait, J., Van de Sande, M., Montargès, M., Kervella, P., De Ceuster, F., Coenegrachts, A., Millar, T. J., Richards, A. M. S., Decin, L., Gottlieb, C. A., Pinte, C., De Beck, E., Price, D. J., Wong, K. T., Bolte, J., Menten, K. M., Baudry, A., de Koter, A., ... Zijlstra, A. (2024). Chemical tracers of a highly eccentric AGB-main-sequence star binary. *Nature Astronomy*, 8, 308–327. <https://doi.org/10.1038/s41550-023-02154-y>
- De Ceuster, F., Ceulemans, T., Decin, L., Danilovich, T., & Yates, J. (2024). Bayesian model reconstruction based on spectral line observations. *The Astrophysical Journal Supplement*

*Series*, 275(2), 44. <https://doi.org/10.3847/1538-4365/ad89a2>

- De Ceuster, F., Ceulemans, T., Srivastava, A., Homan, W., Bolte, J., Yates, J., Decin, L., Boyle, P., & Hetherington, J. (2022). 3D line radiative transfer & synthetic observations with Magritte. *The Journal of Open Source Software*, 7(71), 3905. <https://doi.org/10.21105/joss.03905>
- Matsumoto, K., Camps, P., Baes, M., De Ceuster, F., Wada, K., Nakagawa, T., & Nagamine, K. (2023). Self-consistent dust and non-LTE line radiative transfer with SKIRT. *Astronomy & Astrophysics*, 678, A175. <https://doi.org/10.1051/0004-6361/202347376>
- Paszke, A., Gross, S., Chintala, S., Chanan, G., Yang, E., DeVito, Z., Lin, Z., Desmaison, A., Antiga, L., & Lerer, A. (2017). Automatic differentiation in PyTorch. *NIPS 2017 Autodiff Workshop*. <https://openreview.net/forum?id=BJJsrnfCZ>
- Paszke, A., Gross, S., Massa, F., Lerer, A., Bradbury, J., Chanan, G., Killeen, T., Lin, Z., Gimelshein, N., Antiga, L., Desmaison, A., Kopf, A., Yang, E., DeVito, Z., Raison, M., Tejani, A., Chilamkurthy, S., Steiner, B., Fang, L., ... Chintala, S. (2019). PyTorch: An imperative style, high-performance deep learning library. *Advances in Neural Information Processing Systems 32 (NeurIPS 2019)*, 32. <https://doi.org/10.48550/arXiv.1912.01703>