

# 3D Line Radiative Transfer & Synthetic Observations with Magritte

Frederik De Ceuster<sup>12¶</sup>, Thomas Ceulemans<sup>2</sup>, Atulit Srivastava<sup>2</sup>, Ward Homan<sup>3</sup>, Jan Bolte<sup>2</sup>, Jeremy Yates<sup>1</sup>, Leen Decin<sup>24</sup>, Peter Boyle<sup>56</sup>, and James Hetherington<sup>7</sup>

1 Department of Physics and Astronomy, University College London, London, UK 2 Institute of Astronomy, KU Leuven, Leuven, Belgium 3 Institut d'Astronomie et d'Astrophysique, Université Libre de Bruxelles, Brussels, Belgium 4 School of Chemistry, University of Leeds, Leeds, UK 5 School of Physics and Astronomy, The University of Edinburgh, Edinburgh, UK 6 Brookhaven National Laboratory, NY, USA 7 Department of Computer Science, University College London, London, UK ¶ Corresponding author

**DOI:** 10.21105/joss.03905

#### **Software**

- Review 🗗
- Repository 🗗
- Archive ♂

Editor: Juanjo Bazán ♂ Reviewers:

@gonsie

Ocfgrote

**Submitted:** 27 October 2021 **Published:** 01 March 2022

#### License

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

## **Summary**

Electromagnetic radiation is a key component in many astrophysical simulations. Not only does it dictate what we can or cannot observe, it can provide radiation pressure, efficient heating and cooling mechanisms, and opens up a range of new chemical pathways due to photo-reactions. Magritte is a software library that can be used as a general-purpose radiative transfer solver, but was particularly designed for line radiative transfer in complex 3D morphologies, such as, for instance, encountered in the stellar winds around evolved stars (see Decin, 2020). It is mainly written in C++ and can either be used as a Python package or as a C++ library. To compute the radiation field, a deterministic ray-tracer and a formal solver are employed, i.e., rays are traced through the model and the radiative transfer equation is solved along those rays (De Ceuster et al., 2019). This is in contrast to most radiative transfer solvers which employ (probabilistic) Monte Carlo techniques (Noebauer & Sim, 2019). By virtue of minimal assumptions about the underlying geometric structure of a model, Magritte can handle structured and unstructured input meshes, as well as smoothed-particle hydrodynamics (SPH) data. Furthermore, tools are provided to optimise different input meshes for radiative transfer (De Ceuster et al., 2020).

#### Statement of need

Recent high-resolution observations exposed the intricate and intrinsically 3D morphologies of stellar winds around evolved stars (Decin et al., 2020). The sheer amount of complexity that is observed, makes it difficult to interpret the observations and necessitates the use of 3D hydrodynamics, chemistry and radiative transfer models to study their origin and evolution (El Mellah et al., 2020; Maes et al., 2021; Malfait et al., 2021). Their intricate morphokinematics, moreover, makes their appearance in (synthetic) observations far from evident (see e.g. the intricate structures in Figure 1). Therefore, to study these and other complex morpho-kinematical objects, it is essential to understand how their models would appear in observations. This can be achieved, by creating synthetic observations with Magritte. Examples and analytic as well as cross-code benchmarks can be found in the documentation and in (De Ceuster et al., 2019, 2020).



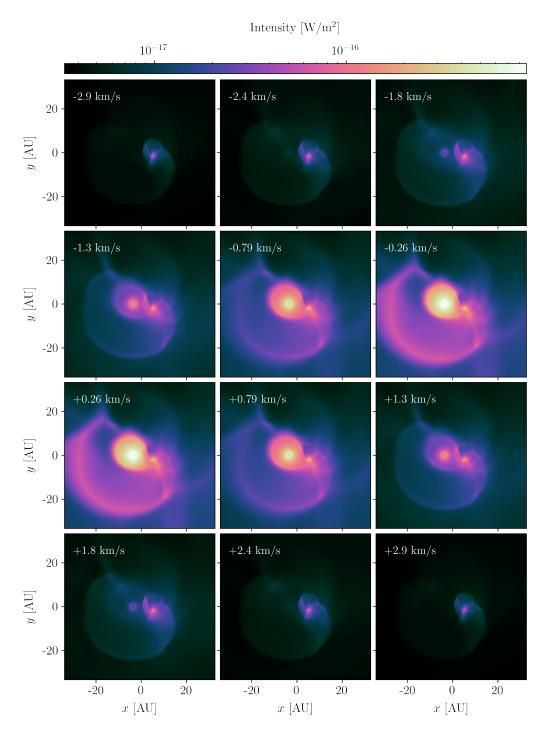


Figure 1: Example of a synthetic observation of the  $CO(v=0,\ J=1-0)$  transition, created with Magritte for a hydrodynamics model of an asymptotic giant branch (AGB) star, as it is perturbed by a companion (this is model v10E50 in Malfait et al., 2021).

### **Future work**

Currently, Magritte is mainly being used for post-processing hydrodynamics simulations by creating synthetic observations, such that the models can be compared with real observations. However, Magritte is still under active development. In future work, we aim to explicitly



include continuum radiation and improve on the computational speed to clear the path for on-the-fly radiative transfer in hydrodynamics models. Furthermore, aside from being a practical research tool, we also aim for Magritte to be the starting point for further research in computational radiative transfer. Current active research topics include: efficient parallelisation and acceleration strategies on modern high-performance computing systems, acceleration of convergence in the non-linear coupling between the radiation field and the medium, and uncertainty quantification in radiative transfer through probabilistic numerical methods (e.g., De Ceuster, 2021).

## Acknowledgements

FDC is supported by the EPSRC iCASE studentship programme, Intel Corporation and Cray Inc. FDC, JB, and LD acknowledge support from the ERC consolidator grant 646758 AEROSOL. TC is a PhD fellow of the Research Foundation – Flanders (FWO). WH acknowledges support from the Fonds de la Recherche Scientifique (FNRS) through grant 40000307.

#### References

- De Ceuster, F. (2021). Simulating 3D Radiation Transport [PhD]. University College London.
- De Ceuster, F., Bolte, J., Homan, W., Maes, S., Malfait, J., Decin, L., Yates, J., Boyle, P., & Hetherington, J. (2020). Magritte, a modern software library for 3D radiative transfer: II. Adaptive ray-tracing, mesh construction, and reduction. *Monthly Notices of the Royal Astronomical Society*, 499(4), 5194–5204. https://doi.org/10.1093/mnras/staa3199
- De Ceuster, F., Homan, W., Yates, J., Decin, L., Boyle, P., & Hetherington, J. (2019). Magritte, a modern software library for 3D radiative transfer: I. Non-LTE atomic and molecular line modelling. *Monthly Notices of the Royal Astronomical Society*, 492(2), 1812–1826. https://doi.org/10.1093/mnras/stz3557
- Decin, L. (2020). Evolution and Mass Loss of Cool Ageing Stars: a Daedalean Story. *arXiv e-Prints*, arXiv:2011.13472. https://doi.org/10.1146/annurev-astro-090120-033712
- Decin, L., Montargès, M., Richards, A. M. S., Gottlieb, C. A., Homan, W., McDonald, I., El Mellah, I., Danilovich, T., Wallström, S. H. J., Zijlstra, A., Baudry, A., Bolte, J., Cannon, E., De Beck, E., De Ceuster, F., de Koter, A., De Ridder, J., Etoka, S., Gobrecht, D., ... Yates, J. (2020). (Sub)stellar companions shape the winds of evolved stars. *Science*, 369(6510), 1497–1500. https://doi.org/10.1126/science.abb1229
- El Mellah, I., Bolte, J., Decin, L., Homan, W., & Keppens, R. (2020). Wind morphology around cool evolved stars in binaries: The case of slowly accelerating oxygen-rich outflows. *Astronomy and Astrophysics*, *637*, A91. https://doi.org/10.1051/0004-6361/202037492
- Maes, S., Homan, W., Malfait, J., Siess, L., Bolte, J., De Ceuster, F., & Decin, L. (2021). SPH modelling of companion-perturbed AGB outflows including a new morphology classification scheme. *Astronomy & Astrophysics*, *653*, A25. https://doi.org/10.1051/0004-6361/202140823
- Malfait, J., Homan, W., Maes, S., Bolte, J., Siess, L., De Ceuster, F., & Decin, L. (2021). SPH modelling of wind-companion interactions in eccentric AGB binary systems. *Astronomy & Astrophysics*, 652, A51. https://doi.org/10.1051/0004-6361/202141161
- Noebauer, U. M., & Sim, S. A. (2019). Monte Carlo radiative transfer. *Living Reviews in Computational Astrophysics*, 5(1), 1. https://doi.org/10.1007/s41115-019-0004-9