Frederik De Ceuster

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I am a **Research Scientist** (onderzoekskader; OZK) at the Leuven Gravity Institute, KU Leuven. My research focuses on developing **efficient and quantifiably accurate computational methods** to simulate complex astrophysical processes, such as relativistic hydrodynamics, radiation transport, and chemistry, to allow us to compare our most sophisticated models with our best observations.

EMPLOYMENT

- Research Scientist (onderzoekskader; OZK) 2024 –
  Leuven Gravity Institute, **KU Leuven** (Belgium)

- Postdoctoral Research Fellow 2022 – 2024
  Research Foundation - Flanders (FWO), working
  at the Institute of Astronomy, **KU Leuven** (Belgium)

- Postdoctoral Researcher (KU Leuven Type 2 Postdoctoral Mandate) 2021 – 2022
  Institute of Astronomy, **KU Leuven** (Belgium)

- Training, Web, and Social Media Manager (part-time: 20%) 2017 – 2021
  DiRAC: Distributed Research utilising Advanced Computing (UK)

- Research Assistant Aug. – Oct., 2016
  Solid State Physics Laboratory of Prof. Dr. J.-P. Locquet,
  KU Leuven (Belgium)

INTERNSHIPS

- February 2018, 6-month internship with **Intel** at the University of Edinburgh, *Parallelisation and scaling analysis of the transport solver Magritte*, supervisor: Prof. Dr. Peter Boyle.
- October 2019, 6-month internship with **Intel** (remotely), *Implementation and analysis of hardware acceleration in the transport solver Magritte*, supervisor: Prof. Dr. Peter Boyle.

EDUCATION

- Doctor of Philosophy (PhD; Computational Astrophysics) 2017 – 2021
  University College London, United Kingdom
  Thesis: *Simulating 3D Radiation Transport, a modern approach to discretisation and an exploration of probabilistic methods*
  Supervisors: Prof. Dr. Jeremy Yates, Prof. Dr. Leen Decin,
    Prof. Dr. Peter Boyle, and Prof. Dr. James Hetherington

- Master of Science (MSc; Theoretical Physics) 2014 – 2016
  KU Leuven, Belgium (Magna Cum Laude)
  Thesis: *Holographic explorations of spacetime singularities*
  Supervisors: Dr. Adam Bzowski, and Prof. Dr. Thomas Hertog

- Bachelor of Science (BSc; Major Physics, Minor Mathematics) 2011 – 2014
  KU Leuven, Belgium (Magna Cum Laude)

SELECTED PUBLICATIONS

out of **30 peer-reviewed** of which **8 first-author** publications
(A complete list can be found below and online.)

- F. De Ceuster, et al., *Bayesian Model Reconstruction Based on Spectral Line Observations*, The Astrophysical Journal Supplement Series, Vol. 275, no. 2, Art. nr. 44, 2024, arXiv:2402.18525v2.
- S. Maes, F. De Ceuster, M. Van de Sande, and L. Decin, *MACE: A Machine-learning Approach to Chemistry Emulation*, The Astrophysical Journal, Vol. 969, Nr. 2, Art. no. 79, 2024, arXiv:2405.03274.
- F. De Ceuster, et al., *Radiative Transfer as a Bayesian Linear Regression Problem*, Monthly Notices of the Royal Astronomical Society, Vol. 518, Issue 4, pp. 5536–5551, 2023, arXiv:2211.12547.
- F. De Ceuster, et al., *Magritte, a modern software library for 3D radiative transfer: II adaptive ray-tracing mesh construction and reduction*, Monthly Notices of the Royal Astronomical Society, Vol. 499, Issue 4, pp. 5194 – 5204, 2020, arXiv:2011.14998.

SOFTWARE PROJECTS

(All my projects can be found at github.com/FredDeCeuster)

- **pomme:** an open-source Python library for probabilistic 3D reconstruction of spectral line observations, github.com/Magritte-code/pomme, see also pomme.readthedocs.io.
- **MACE:** a surrogate model for astrochemical kinetics simulations, in collaboration with Silke Maes, github.com/silkemaes/MACE, see also mace-code.readthedocs.io.
- **Magritte**: an open-source software library for simulating 3D radiation transport & synthetic observations, github.com/Magritte-code/Magritte, see also magritte.readthedocs.io.
- **Paracabs**: parallelisation and acceleration abstractions for performance scaling and portability, github.com/Magritte-code/Paracabs.

LEADERSHIP

- **Group leader** of the **Computational Research Division** in Prof. Decin's group at the Institute of Astronomy, KU Leuven. Supervision of 5 PhD students (1 at University of Leicester), defining and coordinating the computational research path, and stimulating collaborations.
- **PI** of the **Scientific Programming in The Age of AI** research initiative, in collaboration with DiRAC (in the UK) and Vlaams Supercomputer Centrum (VSC; in Flanders). Chairing discussions between the academic DiRAC advisory group, VSC, and our industrial partners (Nvidia, Google, AWS, Intel, OpenAI, Microsoft/GitHub, and Graphcore) to help align our research and training with the latest developments in relevant domains of AI.
- **Organiser/Chair** of the **ENSOR** meetings: monthly meetings that started during the covid pandemic bringing together physicists, chemists, engineers, and mathematicians from University College London, KU Leuven, University of Oxford, and other institutes, to discuss transferable methods, and foster new collaborations. This led e.g. to the PhD project of Silke Maes, a collaboration between KU Leuven, UCL, University of Leeds, and Leiden University.
- **co-I** of the **DiRAC HPC project** - RAC 12 call: **dp147**: *Simulations and Models of the ALMA ATOMIUM Project Data*, 25.76 million cpu hours + 318 TB storage (Data Intensive Cambridge), 10.56 million cpu hours + 751 TB storage (Data Intensive Leicester). Allocation doubled in the RAC 13.5 call; hence total of 72.64 million cpu hours, 2138 TB storage, awarded after peer-review.
- **co-I** of the **ALMA Large Program** (ID 2018.1.00659.L), **ATOMIUM**: *ALMA Tracing the Origins of Molecules in dUst-forming oxygen-rich M-type stars*, 113.2 hr, awarded after peer-review.

TEACHING

- **Lecturer** for *Physics I: Mechanics*, BSc Physics & Mathematics at KU Leuven, Fall terms 2021, 2022, 2023, 2024, substituting for Prof. Dr. Leen Decin.

- **Teaching assistant** for *Physics I: Mechanics*, BSc Physics & Mathematics at KU Leuven, Fall terms 2016, 2018, 2019, 2020.

- **Teaching assistant** for *Physics II: Electromagnetism*, BSc Physics & Mathematics at KU Leuven, Spring terms 2015, 2016.

SUPERVISION

including **6 PhD** and **9 MSc** students

PhD

- Tom Colemont (**Mathematical Engineering**, **KU Leuven**), topic: *Probabilistic Numerics to compress and accelerate General Relativistic Hydrodynamics*, 2024-2028.
- Owen Vermeulen (**Astronomy & Astrophysics**; **FWO**, **KU Leuven**), topic: *3D modelling of CO spectral lines in AGB outflows*, 2024-2028.
- Shiqi Su (**Computational Astrophysics**, **University of Leicester**), topic: *Artificial neural networks for emulating radiative transfer simulations*, 2021-2025.
- Thomas Ceulemans (**Astronomy & Astrophysics**; **FWO**, **KU Leuven**), topic: *Computational aspects of radiative transfer*, 2021-2025.
- Silke Maes (**Astronomy & Astrophysics**, **KU Leuven**), topic: *Tracing the wind dynamics and chemistry in evolved stars*, 2020-2024.
- Jolien Malfait (**Astronomy & Astrophysics**, **KU Leuven**), topic: *Shaping of AGB outflows by wind-companion interactions*, 2020-2024.

MSc   (*This research culminated in a PhD project.)

- Raphael Annys (**Mathematical Engineering**, **KU Leuven**), topic: *GPU-accelerated solvers for General Relativistic Hydrodynamics*, 2024-2025.
- Kriti Sharma (**Astronomy & Astrophysics**, **KU Leuven**), topic: *3D reconstruction of the environment of the AGB star R Aquilae*, 2024-2025.
- Ke Peng (**Mathematics**, **KU Leuven**) topic: Forward and *inverse Non-LTE line radiative transfer modelling leveraging PyTorch*, 2023-2024.
- *Owen Vermeulen (**Astronomy & Astrophysics**, **KU Leuven**) topic: *3D modelling of CO spectral lines in AGB outflows*, 2023-2024. (Won Paul Smeyers Prize for best thesis in Astrophysics 2024.)
- Arnout Coenegrachts (**Astronomy & Astrophysics**, **KU Leuven**) topic: *Modelling the 3D distribution of NaCl around the AGB star IK Tauri*, 2021-2022.
- *Mats Esseldeurs (**Astronomy & Astrophysics**, **KU Leuven**) topic: *Implementing a ray-tracing 3D radiative transfer solver in the smoothed-particle hydrodynamics code PHANTOM*, 2021-2022. (Won Paul Smeyers Prize for best thesis in Astrophysics 2022.)
- *Atulit Srivastava (**Astronomy & Astrophysics**, **KU Leuven**) topic: *Machine Learning solutions to accelerate Radiative Transfer computations*, 2020-2021.
- *Thomas Ceulemans (**Mathematics**, **KU Leuven**), topic: *Multigrid solutions for Radiative Transfer*, 2020-2021.
- *Shiqi Su (**Applied Mathematics**, **University College London**), topic: *Artificial neural networks for uncertainty quantification*, 2020-2021.

Other

- Astha (**Research project**, **MSc Physics**, **KU Leuven**) topic: *Probabilistic numerics for solving linear partial differential equations*, spring semester 2022.
- Anirudh Sharma (**Research Project**, **MSc Physics, KU Leuven**) topic: *Operator-adapted wavelets for optimal function approximation*, spring semester 2022.
- Annika Lauwerys (**High school final project**, **ZAVO Zaventem**), topic: *Astronomical image deprojection using the Doppler shifts of spectral lines*, 2021-2022.
- Jelle Vandersnickt (**BSc Honours project**, **KU Leuven**) topic: Analysis of a 1D self-consistent AGB star model, summer 2021.

GRANTS

Personal

- **Research Foundation - Flanders (FWO)**, a 3-year **Junior Postdoctoral Research Fellowship** at KU Leuven (FWO: 1253223N; 2022-2025).
- **KU Leuven**, Belgium, a 1-year **Postdoctoral Mandate Type 2** (PDMT2/21/066; 2021-2022) for excellent researchers to bridge the gap with the end of their PhD and follow-up funding.
- **Intel**, United Kingdom, 6 months **paid internship**, in addition to the internship that was already included in my iCASE PhD project (see below).
- **Engineering & Physical Sciences Research Council (EPSRC)**, United Kingdom, industrial Cooperative Awards in Science & Technology (iCASE), a 4-year **PhD project** at University College London, Project Reference: 1878976, including a 6 months internship at Intel.

As supervisor

- **Research Foundation - Flanders (FWO)**, a 4-year **PhD Fellowship** for Owen Vermeulen at KU Leuven (FWO: 1173025N; 2024-2028).
- **Research Foundation - Flanders (FWO)**, a 4-year **PhD Fellowship** for Thomas Ceulemans at KU Leuven (FWO: 1166722N; 2021-2025).
- **PhD Fellowship** for Shiqi Su at the University of Leicester, 2021-2025.

Other

- **Project funding** for the **Scientific Programming in The Age of AI** initiative, DiRAC (Science and Technologies Facilities Council; STFC, UK).
- **HPC time** (as co-I): **DiRAC RAC 12 call: dp147**: 25.76 million cpu hours + 318 TB storage (Data Intensive Cambridge), 10.56 million cpu hours + 751 TB storage (Data Intensive Leicester). Allocation doubled in the RAC 13.5 call; hence total of 72.64 million cpu hours, 2138 TB storage, awarded after peer-review.
- **Telescope time** (as co-I): **ALMA Large Program** (ID 2018.1.00659.L), ATOMIUM, 113.2 hr, awarded after peer-review.

TALKS
including **7 invited** and **4 contributed** talks

Invited

- ProbNum24: Probabilistic Numerics Workshop, London, UK (July 15, 2024): *Probabilistic Numerics for Astrophysical simulation*.
- Webinar for BASE-II: Blueprinting AI for Science at Exascale (June 5, 2024; online): *"Lossy acceleration" of astrophysical simulations with surrogate models*.
- Probabilistic Numerics School, University of Southampton, UK (April 10, 2024): *Probabilistic Numerics for quantifiably accurate approximations in astrophysics*.

- DataSig seminar, University of Oxford, UK (March 21, 2024; remotely): *Data-driven surrogate modelling for astrophysical simulations: from stellar winds to supernovae*.
- RT24: Radiative Transfer in Astrophysics: Codes and Algorithms, Heidelberg, Germany (March 13, 2024): *A differentiable Radiative Transfer model for Probabilistic 3D reconstruction and Uncertainty Quantification*.
- Vlaams Supercomputer Centrum (VSC) users day (November 24, 2023; Brussels): *Scientific Programming in the Age of AI*, together with Geert Jan Bex and Frédéric Wautelet.
- IAU Symposium 366: The Origin of Outflows in Evolved Stars (November 1, 2021; online); **invited training session**: *3D Radiative Transfer & Synthetic Observations with Magritte*.

Contributed
- ATOMIUM 2023 fall meeting, Leuven, (November 25, 2023): *Probabilistic 3D Reconstruction of Spectral Line Observations with p3droslo*.
- European Astronomical Society (EAS) Annual Meeting 2023, Krakow (Poland), (July 13, 2023): *Probabilistic 3D reconstruction of the circumstellar environments of evolved stars*.
- ATOMIUM 2023 winter meeting, Meudon (France), (March 8, 2023): *Probabilistic 3D reconstruction of spectral line images*.
- DELVE: The death-throes of evolved stars, a virtual encounter (April 12, 2021; online): *Beyond the Treachery of Images: 3D Radiative Transfer with Magritte*.

Seminars
- Department of Physics and Astronomy, Ghent University (March 24, 2022): *Approximate Radiative Transfer*.
- Institute of Astronomy, KU Leuven (February 26, 2021; online), together with Silke Maes and Jolien Malfait: *Hydro/radiative modelling of AGB wind-companion interactions*.
- Institute of Astronomy, KU Leuven (October 10, 2019): *Magritte, a modern software library for 3D radiative transfer*.

OUTREACH

- AI-accelerated science, online video tutorial of MACE: Machine-accelerated Chemistry Emulation, for the DiRAC online learning platform, to be published in February 2025.
- Public lecture at Urania (amateur astronomy group) in Hove: *"Numerical Simulation: the 3rd pillar of modern science"*, October 8, 2024.
- Interview with Kennismakers (online outreach platform of the Research Foundation – Flanders, FWO): kennismakers.be/mijn-job-als-sterrenkundige.
- *"Eigen kweek"* outreach talks about my research for the student organisation at Lerkeveld (Filosofisch en Theologisch College, Heverlee), 2017, 2023.
- *"Life as a PhD student in Astronomy"* outreach talk for first year students in physics and mathematics at KU Leuven, February 17, 2016.
- Whenever possible, I have been helping out at the various outreach activities of the Institute of Astronomy and the Leuven Gravity Institute, KU Leuven.

REFERENCES

- **Prof. Dr. Tjonnie G.F. Li**
  Leuven Gravity Institute, KU Leuven
  Email: tjonnie.li@kuleuven.be

- **Prof. Dr. Leen Decin** (Postdoc supervisor)
  Institute for Astronomy, KU Leuven
  Email: leen.decin@kuleuven.be

- **Prof. Dr. Jeremy Yates** (PhD supervisor)
  Department of Computer Science & UCL Centre for Space Exo-chemistry Data,
  University College London
  Email: j.a.yates@ucl.ac.uk

- **Dr. Clare Jenner** (supervisor at DiRAC)
  Deputy director at DiRAC, Project Scientist at University College London
  DiRAC, University College London
  Email: c.jener@ucl.ac.uk

PUBLICATIONS

30 peer-reviewed of which **8 first-author** publications
(This list can also be found online.)

- F. De Ceuster, et al., *Bayesian model reconstruction based on spectral line observations with pomme*, Journal of Open Source Software, Vol. 9, nr. 104, pp. 7321, 2024.

- F. De Ceuster, et al., *Bayesian Model Reconstruction Based on Spectral Line Observations*, The Astrophysical Journal Supplement Series, Vol. 275, no. 2, Art. nr. 44, 2024, arXiv:2402.18525v2.

- J. Malfait, L. Siess, M. Esseldeurs, F. De Ceuster, S.H.J. Wallström, A. de Koter, L. Decin, *Impact of HI cooling and study of accretion disks in asymptotic giant branch wind-companion smoothed particle hydrodynamic simulations*, Astronomy & Astrophysics, Vol. 691, Art. no. A84, 2024, arXiv:2408.13158.

- J. Malfait, et al., *SPH modelling of AGB wind morphology in hierarchical triple systems and a comparison to observation of R Aql*, Astronomy & Astrophysics, Vol. 691, Art. no. A57, 2024, arXiv:2408.16565.

- T. Ceulemans, F. De Ceuster, L. Decin, and J. Yates, Magritte, a modern software library for spectral line radiative transfer, Astronomy & Computing, Vol. 49, Art. nr. 100889, 2024, arXiv:2411.03040.

- M. Van de Sande, C. Walsh, T. Danilovich, F. De Ceuster, and T. Ceulemans, *Modelling predicts a molecule-rich disc around the AGB star L2 Puppis*, Monthly Notices of the Royal Astronomical Society, vol. 532, no. 1, pp. 734–754, 2024, arXiv:2406.12768.

- S. Maes, F. De Ceuster, M. Van de Sande, and L. Decin, *MACE: A Machine-learning Approach to Chemistry Emulation*, The Astrophysical Journal, Vol. 969, Nr. 2, Art. no. 79, 2024, arXiv:2405.03274.

- T. Danilovich, et al., *Chemical tracers of a highly eccentric AGB-main-sequence star binary*, Nature Astronomy, Vol. 8, pp. 308–327, 2024, arXiv:2407.16979.

- S. H. J. Wallström, et al., ATOMIUM: *Molecular inventory of 17 oxygen-rich evolved stars observed with ALMA*, Astronomy & Astrophysics, Vol. 681, Art. nr. A50, 2024, arXiv:2312.03467

- K. Matsumoto, P. Camps, M. Baes, F. De Ceuster, K. Wada, T. Nakagawa, K. Nagamine, *Self-consistent dust and non-LTE line radiative transfer with SKIRT,* Astronomy & Astrophysics, Vol. 678, nr. A175, 2023, arXiv:2309:02628.

- A. Coenegrachts, T. Danilovich, F. De Ceuster, L. Decin, *The unusual 3D distribution of NaCl around the asymptotic giant branch star IK Tau,* Astronomy & Astrophysics, Vol. 678, nr. A85, 2023, arXiv:2302.06221.

- S. Maes, M. Van de Sande, T. Danilovich, F. De Ceuster, L. Decin, *Sensitivity study of chemistry in AGB outflows using chemical kinetics,* Monthly Notices of the Royal Astronomical Society, Vol. 522, Issue 3, pp. 4654–4673, 2023, arXiv:2304.05924.

- M. Esseldeurs, L. Siess, F. De Ceuster, W. Homan, J. Malfait, S. Maes, T. Konings, T. Ceulemans, L. Decin, *3D simulations of AGB stellar winds. II. Ray-tracer implementation and impact of radiation on the outflow morphology,* Astronomy & Astrophysics, Vol. 674, nr. A122, 2023, arXiv:2304.09876.

- Montargès, M., et al., *The VLT/SPHERE view of the ATOMIUM cool evolved star sample. I. Overview: Sample characterization through polarization analysis,* Astronomy & Astrophysics, Vol.671, nr. A96, arXiv:2301.02081.

- F. De Ceuster, T. Ceulemans, J. Cockayne, L. Decin, J. Yates, *Radiative Transfer as a Bayesian Linear Regression problem,* Monthly Notices of the Royal Astronomical Society, Vol. 518, Issue 4, pp. 5536–5551, 2023, arXiv:2211.12547.

- J. Malfait, S. Maes, W. Homan, J. Bolte, L. Siess, F. De Ceuster, L. Decin, *3D hydrodynamical survey of the impact of a companion on the morphology and dynamics of AGB outflows,* Proceedings of the International Astronomical Union, Vol. 16, Symposium S366, 2022, arXiv:2207.14032.

- S. Maes, L. Siess,, W. Homan, J. Malfait, F. De Ceuster, T. Ceulemans, D. Donné, M. Esseldeurs, L. Decin, *Route towards complete 3D hydro-chemical simulations of companion-perturbed AGB outflows,* Proceedings of the International Astronomical Union, Vol. 16, Symposium S366, 2022, arXiv:2206:12278.

- C. A. Gottlieb, L. Decin, A. M. S. Richards, F. De Ceuster, et al., *ATOMIUM: ALMA tracing the origins of molecules in dust forming oxygen-rich M-typestars. Motivations, sample, calibration, and initial results,* Astronomy & Astrophysics, Vol. 660, nr. A94, 2022, arXiv:2112.04399.

- F. De Ceuster, et al., *3D Line Radiative Transfer & Synthetic Observations with Magritte,* Journal of Open Source Software, Vol. 7, nr. 71, pp. 3905, 2022.

- S. Maes, W. Homan, J. Malfait, L. Siess, J. Bolte, F. De Ceuster, L. Decin, *SPH modelling of companion-perturbed AGB outflows including a new morphology classifications scheme,* Astronomy & Astrophysics, Vol. 653, nr. A25, 2021, arXiv:210.00505.

- J. Malfait, W. Homan, S. Maes, J. Bolte, L. Siess, F. De Ceuster, L. Decin, *SPH modelling of wind-companion interactions in eccentric AGB binary systems,* Astronomy & Astrophysics, Vol. 652, nr. A51, 2021, arXiv:210.01074.

- W. Homan, et al., *ATOMIUM: The astounding complexity of the near circumstellar environment of the M-type AGB star R Hydrae. I. Morpho-kinematical interpretation of CO and SiO emission,* Astronomy & Astrophysics, Vol. 651, nr. A82, 2021, arXiv:2104.0729.

- F. De Ceuster, J. Bolte, W. Homan, S. Maes, J. Malfait, L. Decin, J. Yates, P. Boyle, J. Hetherington, *Magritte: 3D radiative transfer library*, Astrophysics Source Code Library, ascl:2012.025, 2020.

- F. De Ceuster, et al., *Magritte, a modern software library for 3D radiative transfer: II adaptive ray-tracing mesh construction and reduction*, Monthly Notices of the Royal Astronomical Society, Vol. 499, Issue 4, pp. 5194-5204, 2020, arXiv:2011.14998.

- W. Homan et al., *ATOMIUM: A high-resolution view on the highly asymmetric wind of the AGB star π^1Gruis. I. First detection of a new companion and its effect on the inner wind*, Astronomy & Astrophysics, Vol 644, nr. A61, 2020, arXiv:2010.05509.

- L. Decin, et al., *(Sub)stellar companions shape the winds of evolved stars*, Science, Vol. 369, Issue 6510, pp. 1497-1500, 2020, arXiv:2009.11694.

- F. De Ceuster, et al., *Magritte, a modern software library for 3D radiative transfer: I Non-LTE atomic and molecular line modelling*, Monthly Notices of the Royal Astronomical Society, Vol. 492, Issue 2, pp. 1812-1826, 2020, arXiv:1912.08445.

- F. De Ceuster, J. Yates, P. Boyle, L. Decin, J. Hetherington, MAGRITTE: a new multidimensional accelerated general-purpose radiative transfer code, Why Galaxies Care About AGB Stars: A Continuing Challenge through Cosmic Time, Proceedings of the International Astronomical Union, Vol. 343, pp. 381-382.

- T. Danilovich, A. M. S. Richards, A. I. Karakas, M. Van de Sande, L. Decin, F. De Ceuster, *An ALMA view on CS and SiS around oxygen-rich AGB stars*, Monthly Notices of the Royal Astronomical Society, Vol. 484 Issue 1, pp. 494-509, 2019, arXiv:1901.00070.

- M. Van de Sande, J. O. Sundqvist, T. J. Millar, D. Keller, W. Homan, A. de Koter, L. Decin, F. De Ceuster, *Determining the effects of clumping and porosity on the chemistry in a non-uniform AGB outflow,* Astronomy & Astrophysics, Vol. 616, nr. A106, 2018, arXiv:1803.0176.