Probabilistic Numerics
in Astronomy & Astrophysics

Frederik De Ceuster (FWO Fellow, Institute of Astronomy, KU Leuven)
(Research Scientist, Gravity Institute, KU Leuven)

in collaboration with

Thomas Ceulemans, **Silke Maes**, **Marie Van de Sande**, Jon Cockayne, Leen Decin, Jeremy Yates,
Taïssa Danilovich, Mats Esseldeurs, Jolien Malfait, Shiqi Su, Mark Wilkinson, Tjonnie G.F. Li, …

Context

Context — A&A: from stellar winds to supernovae

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Stellar evolution: **what?** **why?** **how?**

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Stellar evolution: **what?** why? how?

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  They are born and die

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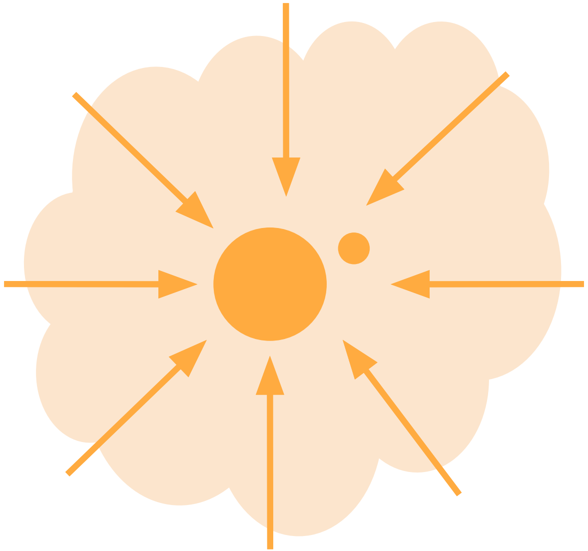

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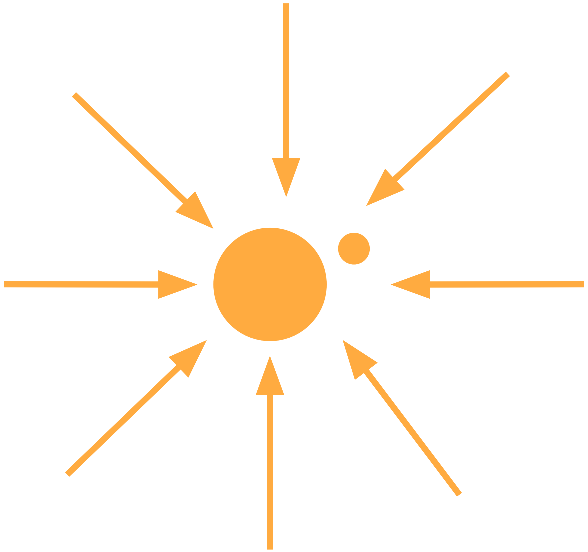

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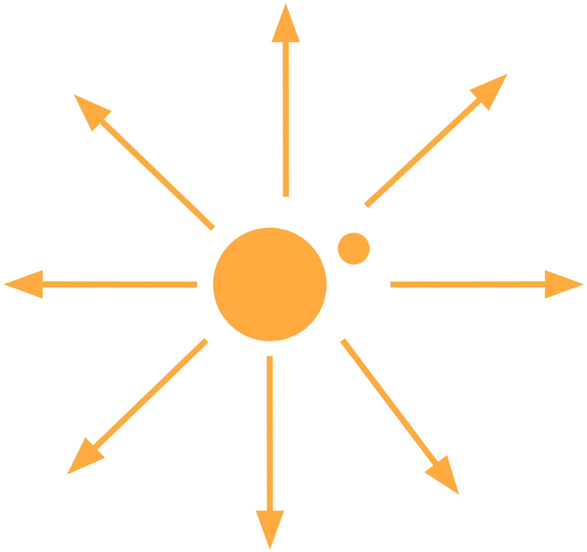
- Dying stars lose mass

  in outwards-directed **stellar winds**



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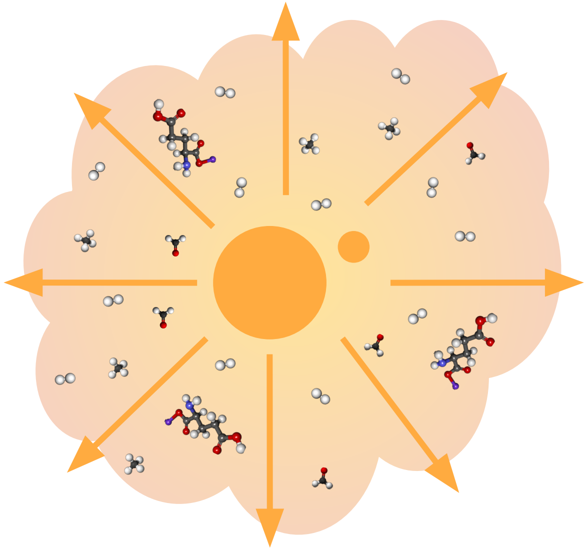

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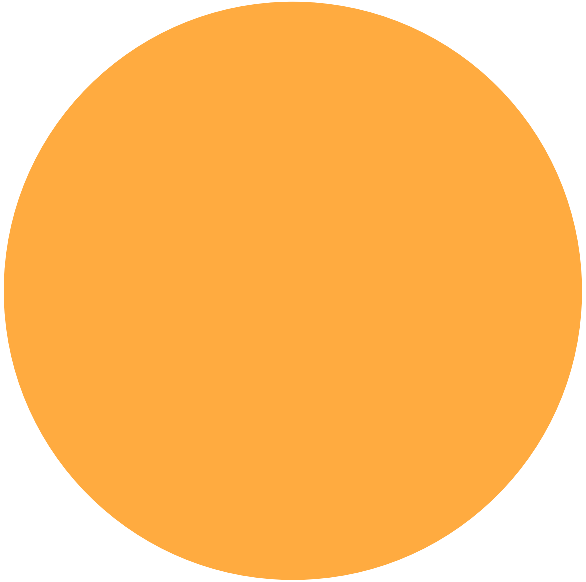

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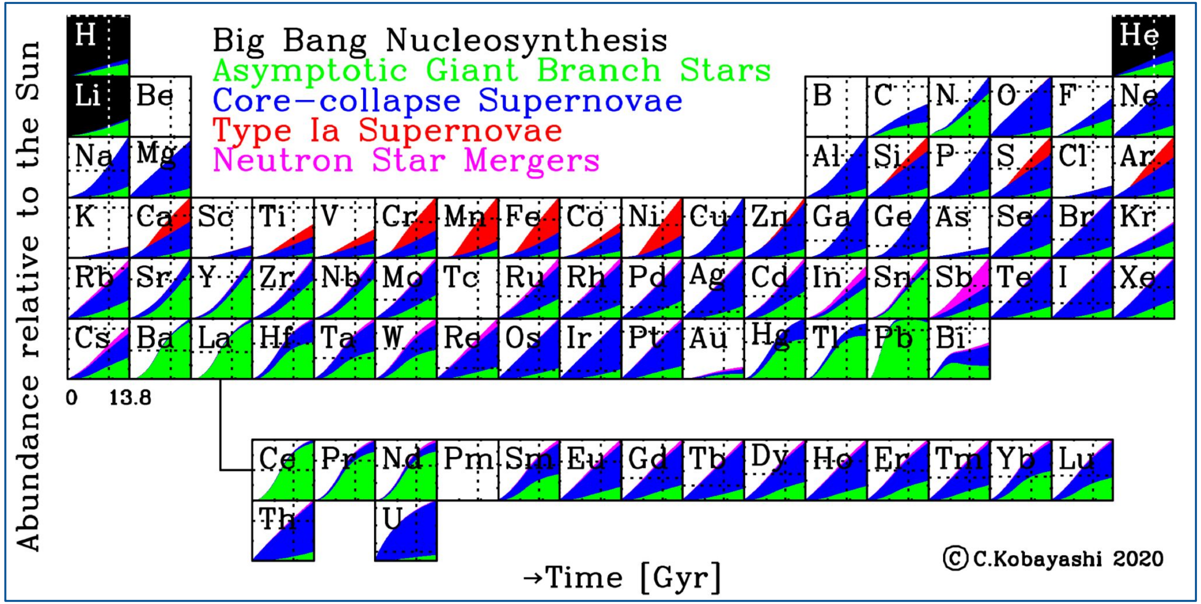
- Chemical history



Context — A&A: from stellar winds to supernovae

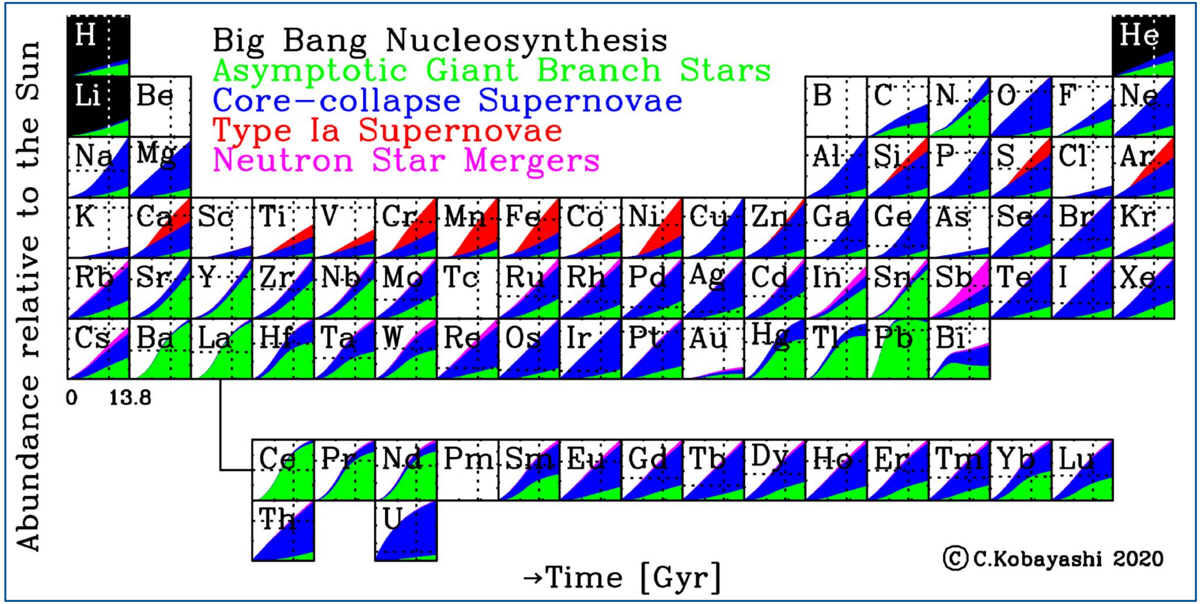
Stellar evolution: what? **why?** how?

- Chemical history
- Chemical future

  building blocks for

  next-gen stars,

  planets, …, life?



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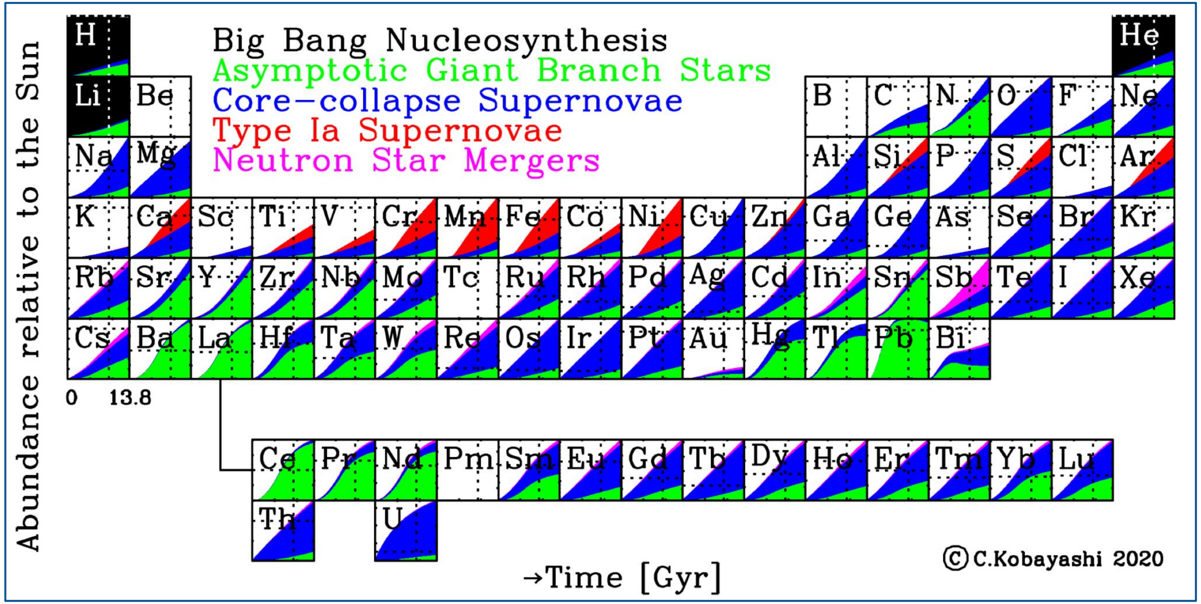

- **(Playground of problems for beautiful <u>math</u>, <u>data science</u>, and <u>engineering</u>!)**

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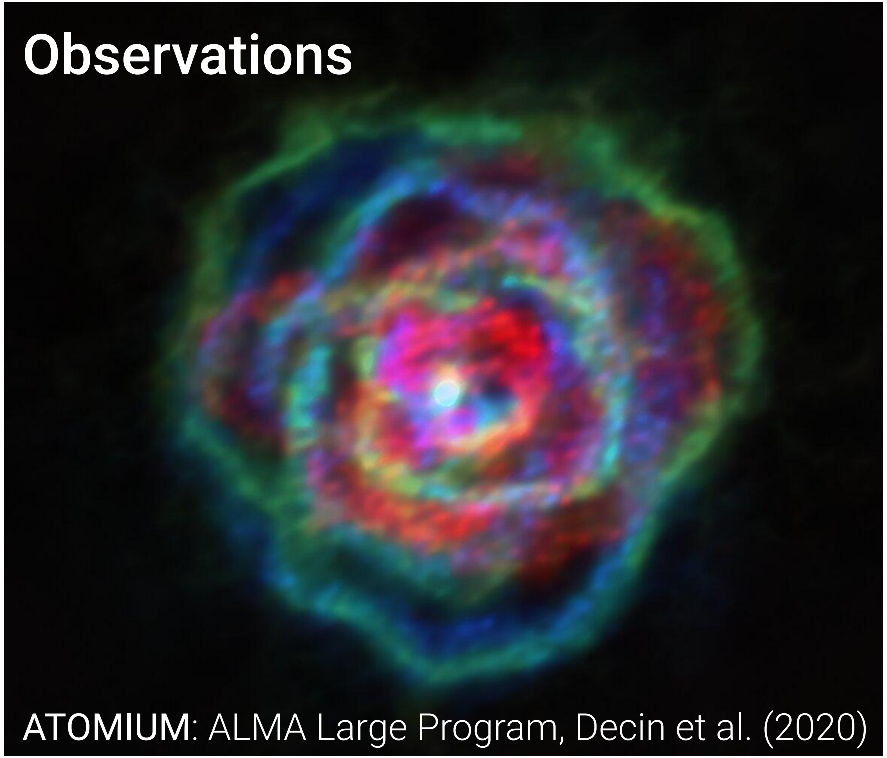

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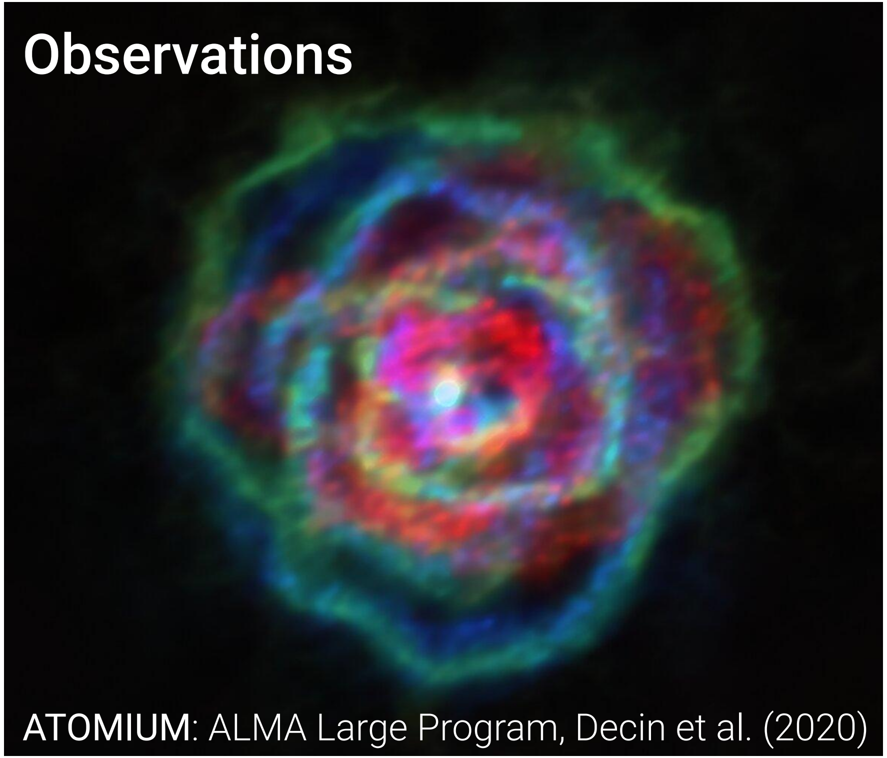
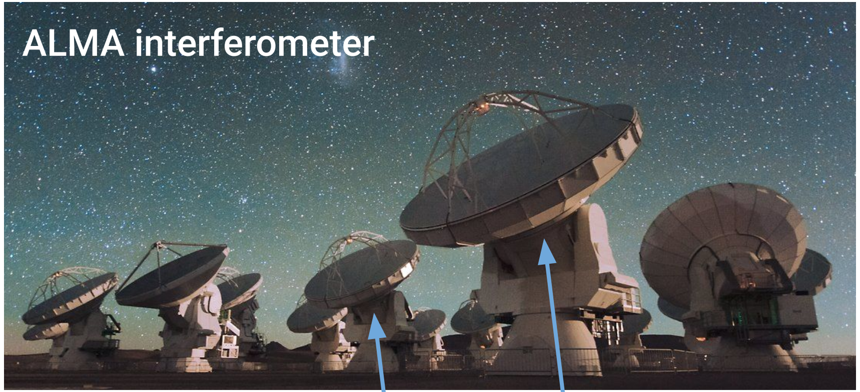


ATOMIUM: ALMA Large Program, Decin et al. (2020)



$$V(\nu, \boldsymbol{b}) = \langle E(\nu, \boldsymbol{x}_1) E(\nu, \boldsymbol{x}_2) \rangle$$

$$\boldsymbol{b} = \boldsymbol{x}_2 - \boldsymbol{x}_1$$

$$I(\nu, \boldsymbol{x}) = \mathcal{F}\{V(\nu, \boldsymbol{b})\}$$

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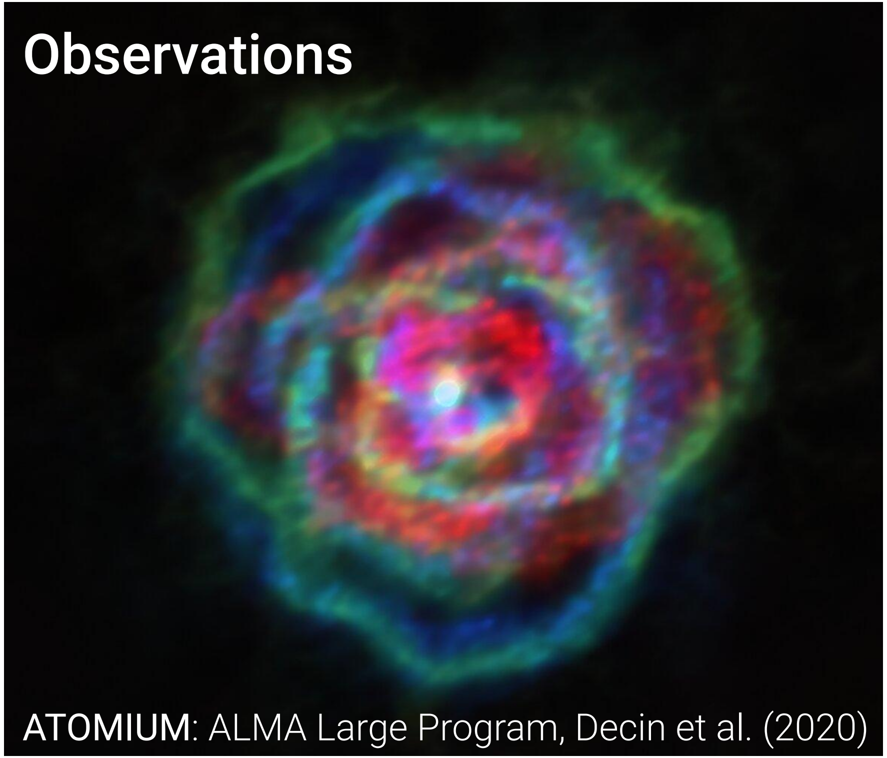

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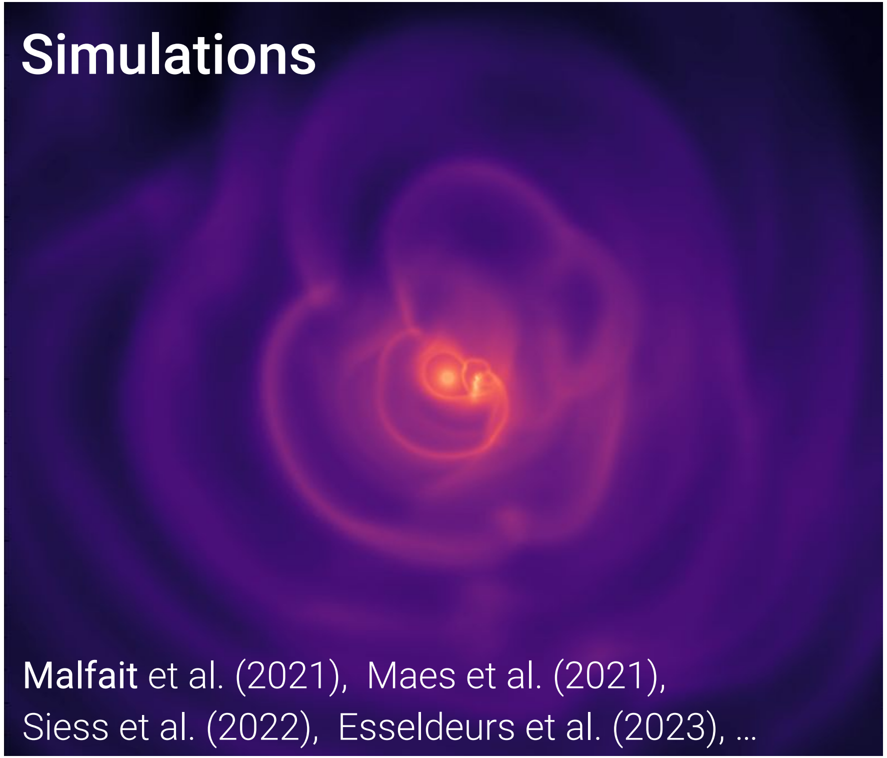

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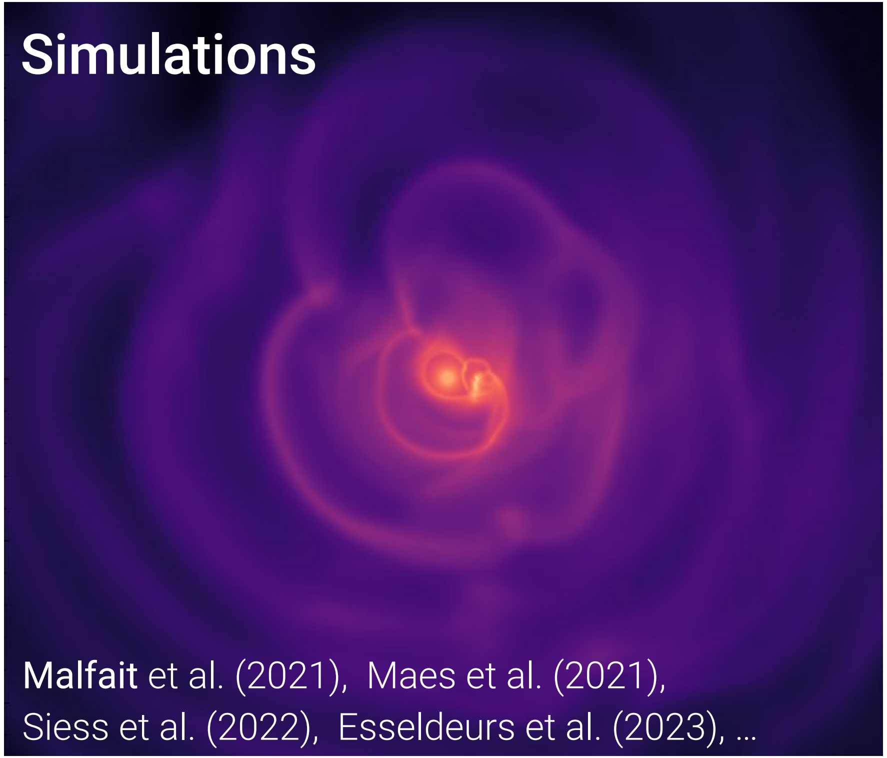
Stellar evolution: what? why? **how?**

Stellar wind model

- Hydrodynamics



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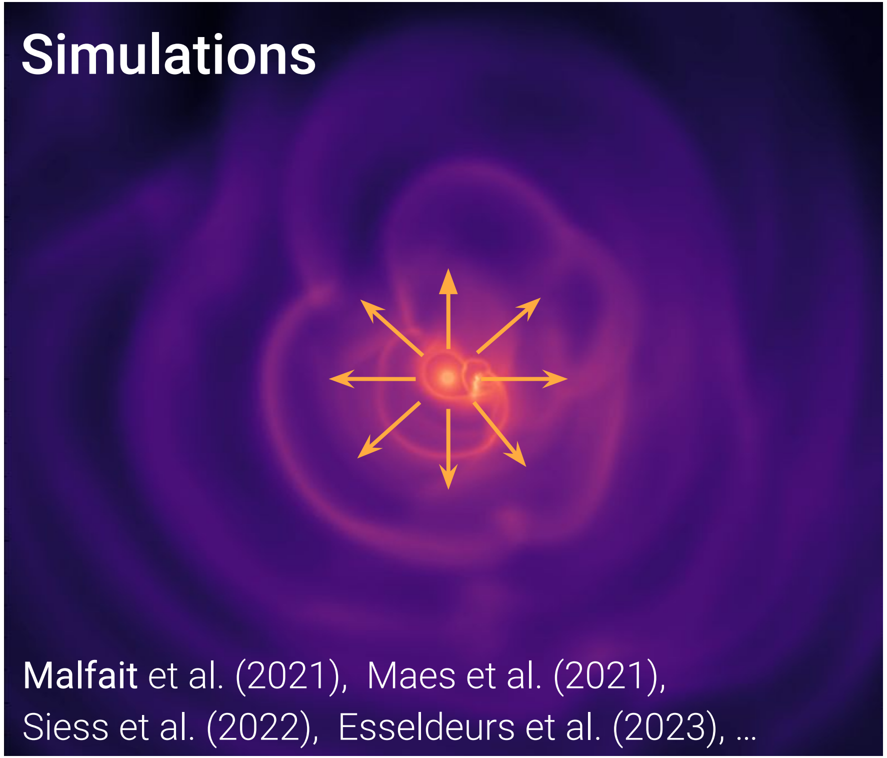
Stellar evolution: what? why? **how?**

Stellar wind model

- Hydrodynamics
- Radiation Transport

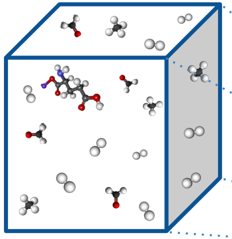


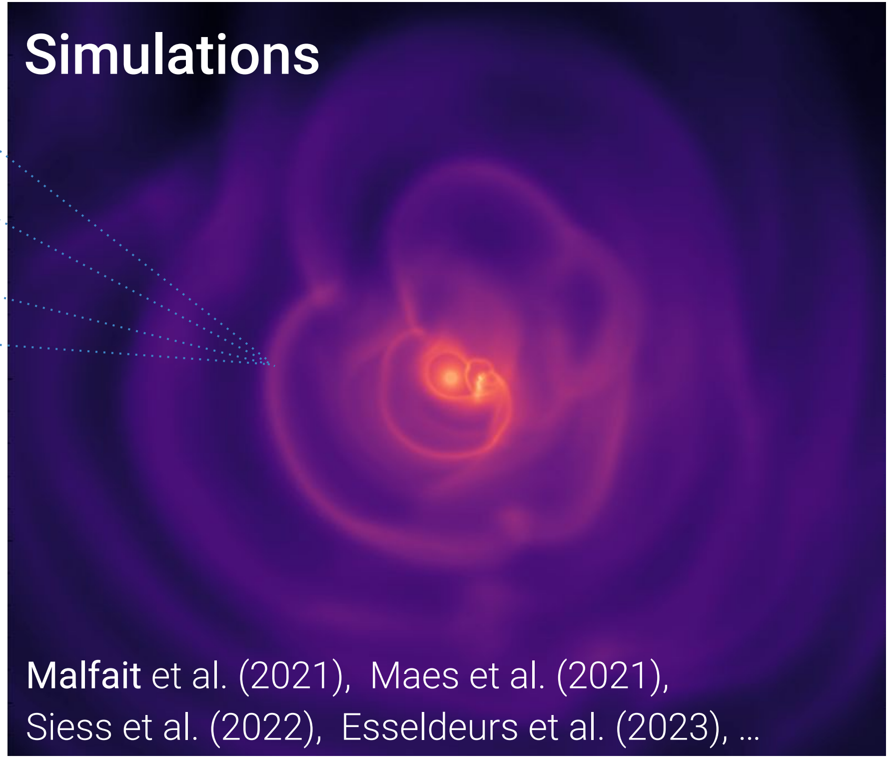
Context — A&A: from stellar winds to supernovae

Stellar evolution: what? why? **how?**

Stellar wind model

- Hydrodynamics
- Radiation Transport
- Micro-physics / chemistry
    - Quantum statistical state
    - Chemical kinetics





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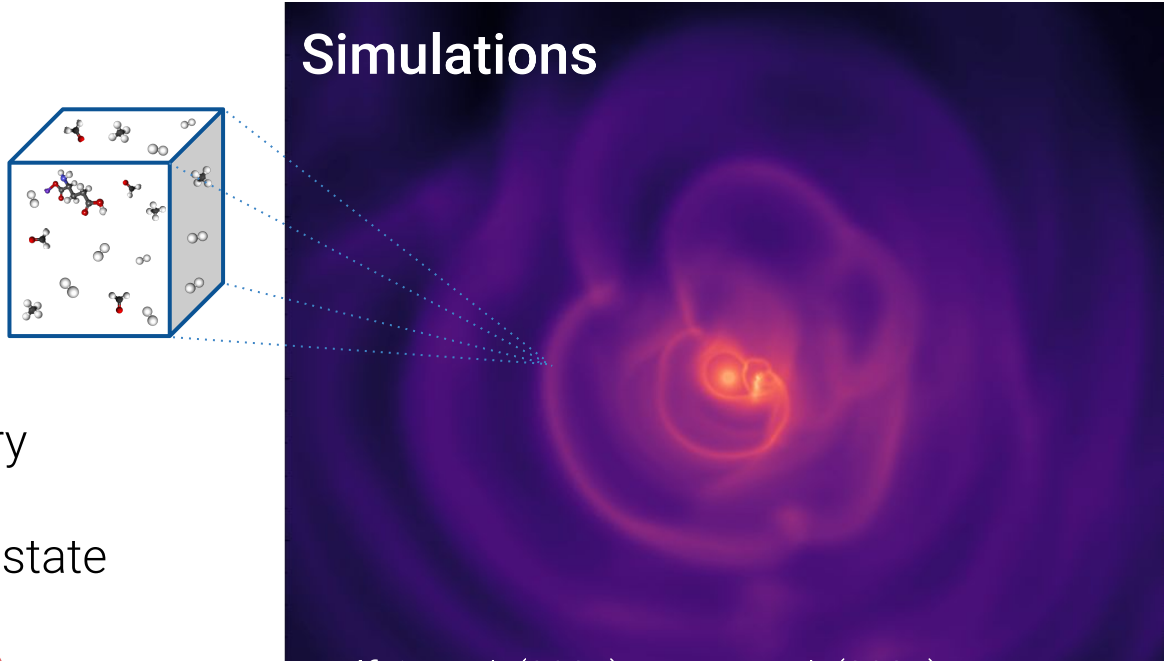
Stellar evolution: what? why? **how?**

Stellar wind model

- Hydrodynamics
- Radiation Transport (!)
- Micro-physics / chemistry
    - Quantum statistical state
    - Chemical kinetics (!)



Malfait et al. (2021), Maes et al. (2021),
Siess et al. (2022), Esseldeurs et al. (2023), …

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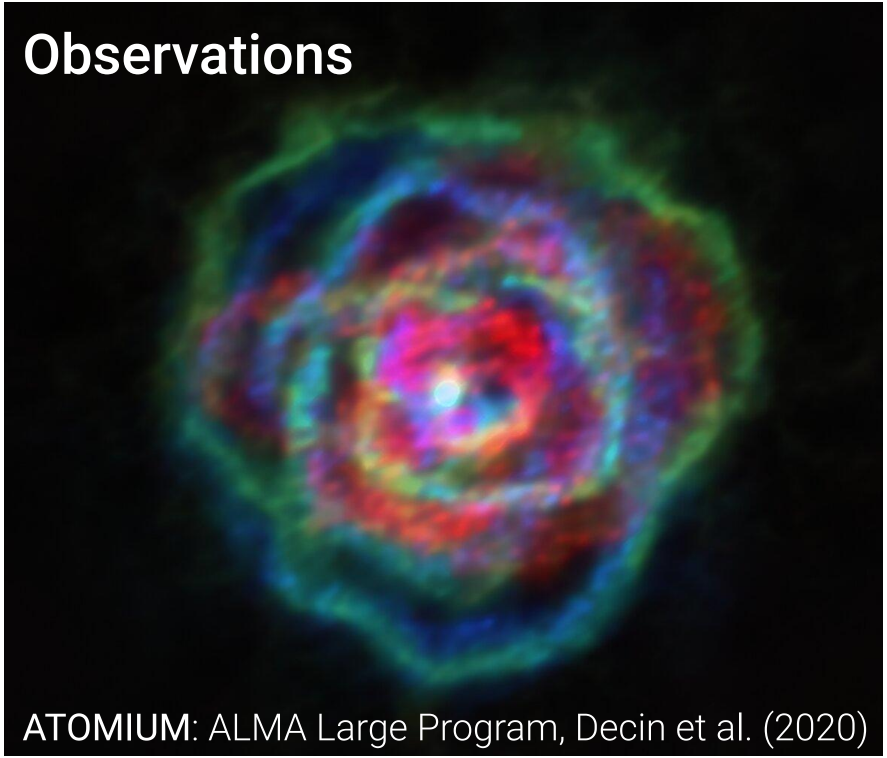

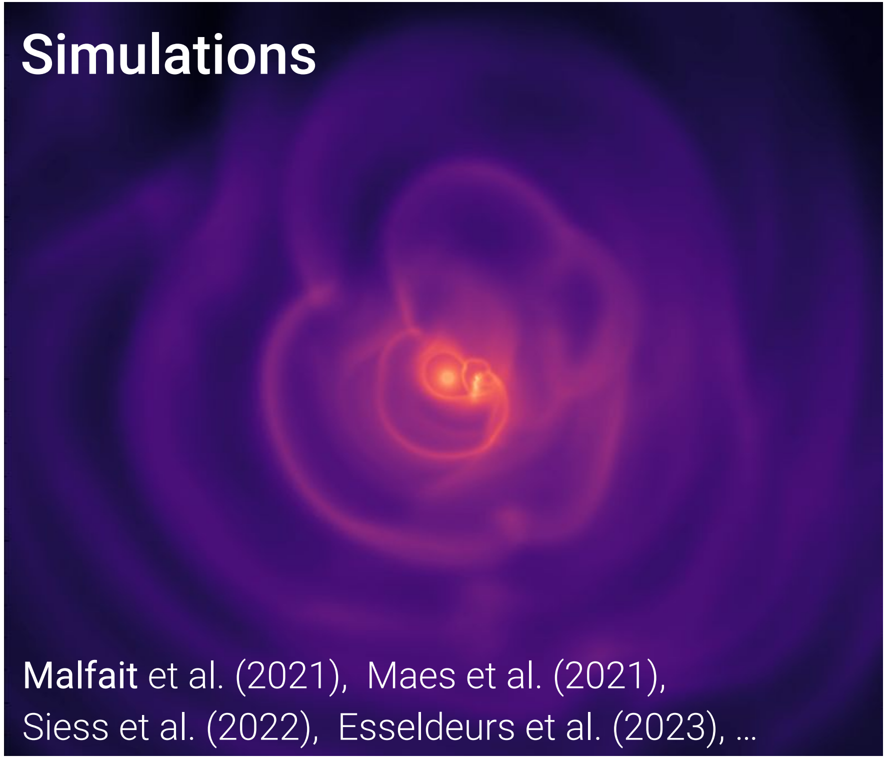

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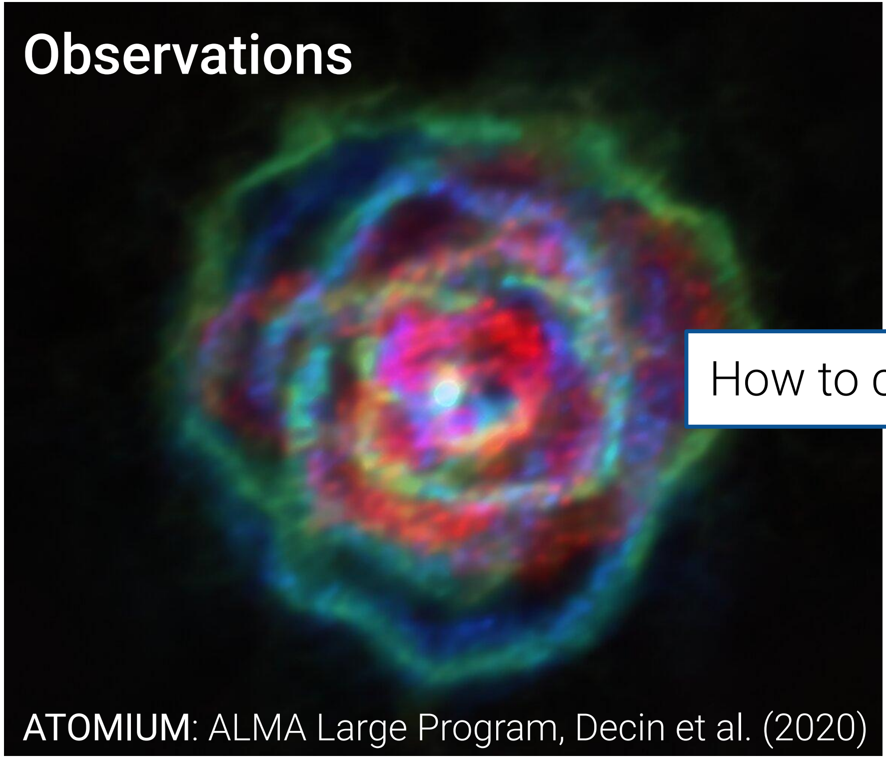
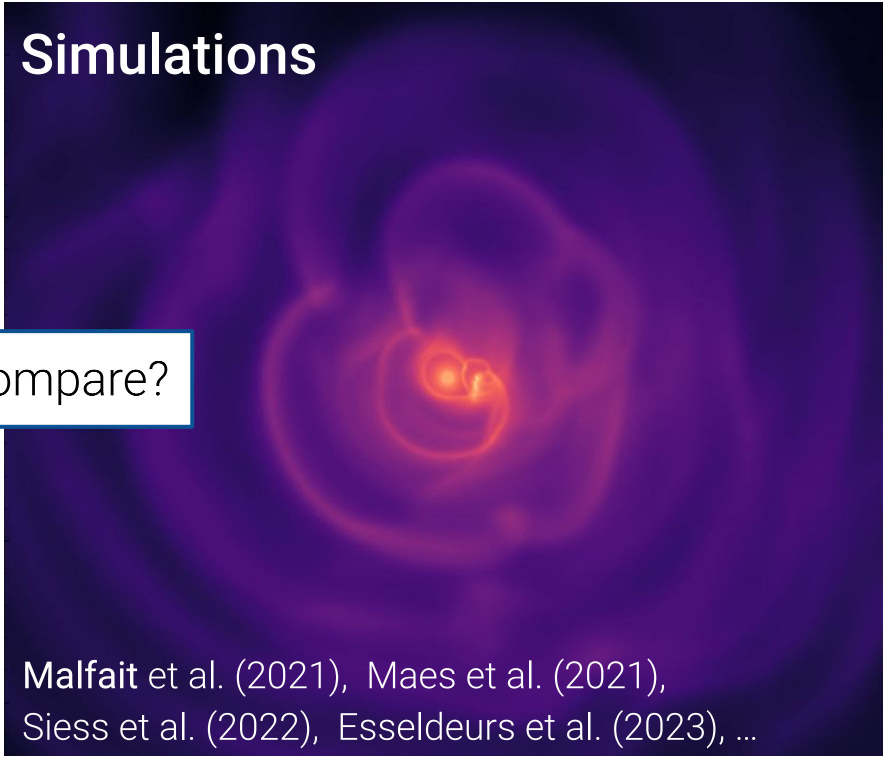


How to compare?



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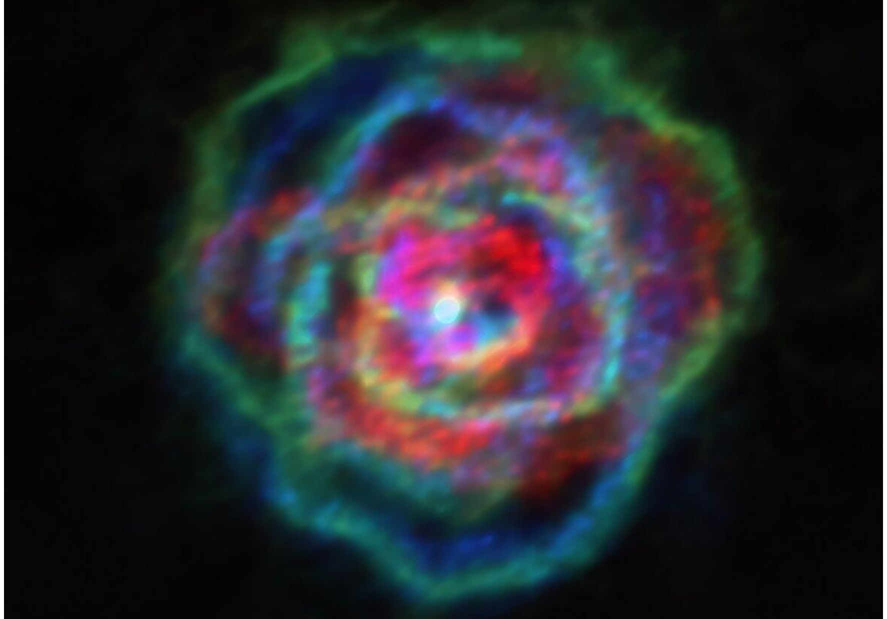
Stellar evolution: **what? why? how?**

Observations



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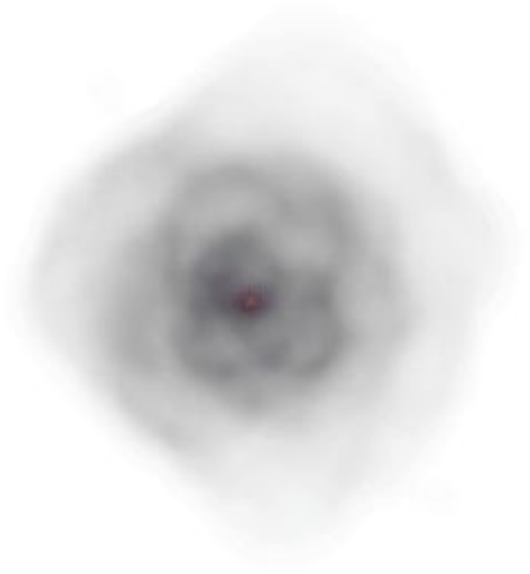
Reconstructions



FDC, Ceulemans, Decin, Danilovich, & Yates (2024)

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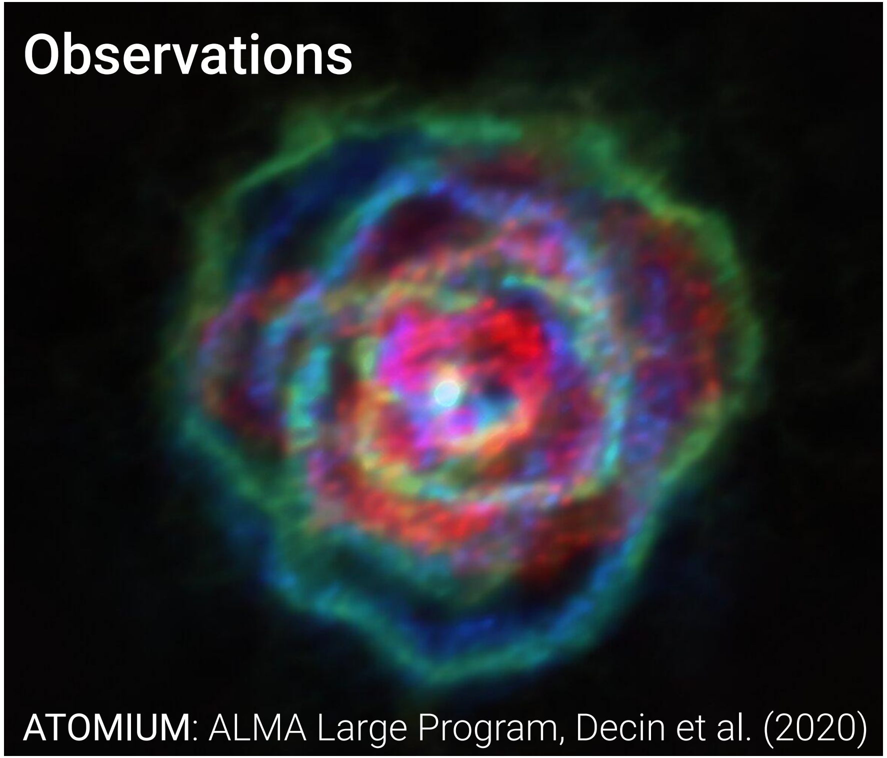

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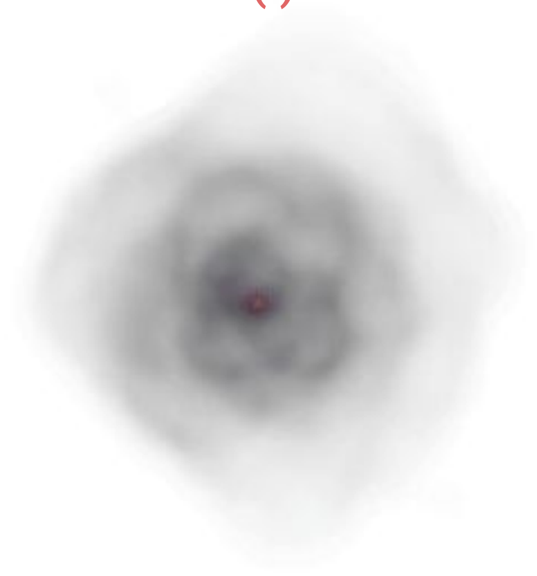

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Goals — Need for Probabilistic Numerics in A&A

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(!) **Fast / approximate, but quantifiably / tunably accurate models**

e.g. Radiation Transport, Chemical Kinetics

(!) **Large uncertainties on various input parameters**

e.g. spectroscopic data, chemical reaction rates

(!) **Highly degenerate inverse problems**

e.g. model reconstructions

Goals — Need for Probabilistic Numerics in A&A

Note

- **Typical problem scale** ($\sim 10^6 - 10^9$ particles, elements, …)

- **Many, very different components all working together**

  ⇒ uncertainties have to be propagated

- **Non-linear components**

Application 1 — Radiation Transport

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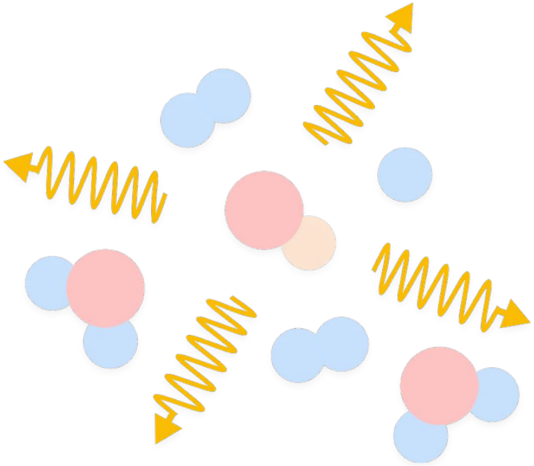
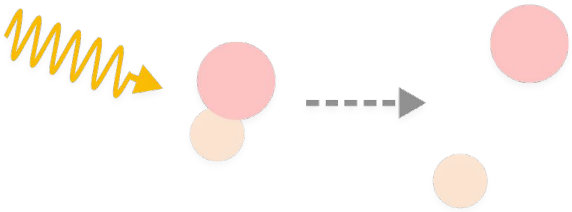
How would our models appear in observations?

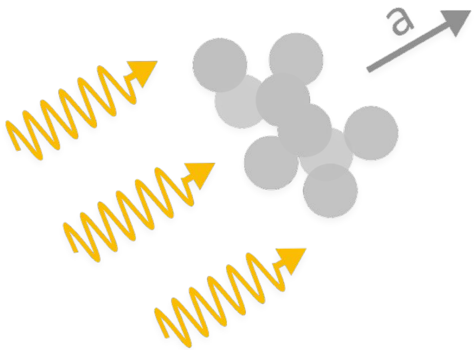
How much:



Radiative cooling?



Photochemistry?



Radiative pressure on dust?

Application 1 — Radiation Transport

Radiative Transfer equation

$$\hat{\boldsymbol{n}} \cdot \nabla I(\boldsymbol{x}, \hat{\boldsymbol{n}}) = \eta(\boldsymbol{x}, \hat{\boldsymbol{n}}) - \chi(\boldsymbol{x}, \hat{\boldsymbol{n}})\, I(\boldsymbol{x}, \hat{\boldsymbol{n}}) + \oint \mathrm{d}\hat{\boldsymbol{n}}' \; \Phi(\hat{\boldsymbol{n}}, \hat{\boldsymbol{n}}')\, I(\boldsymbol{x}, \hat{\boldsymbol{n}}')$$

emission absorption scattering

Application 1 — Radiation Transport

Radiative Transfer equation

$$\hat{\boldsymbol{n}} \cdot \nabla I(\boldsymbol{x}, \hat{\boldsymbol{n}}) = \eta(\boldsymbol{x}, \hat{\boldsymbol{n}}) - \chi(\boldsymbol{x}, \hat{\boldsymbol{n}})\, I(\boldsymbol{x}, \hat{\boldsymbol{n}}) + \cancel{\oint \mathrm{d}\hat{\boldsymbol{n}}' \; \Phi(\hat{\boldsymbol{n}}, \hat{\boldsymbol{n}}')\, I(\boldsymbol{x}, \hat{\boldsymbol{n}}')}$$

emission absorption scattering

optical depth

$$\tau(x_1, x_2) = \int_{x_1}^{x_2} \mathrm{d}x' \; \chi(x')$$

formal solution

$$I(x_2) = \int_0^{x_2} \mathrm{d}x' \; \eta(x')\, e^{-\tau(x', x_2)} + \mathrm{BC}$$

Application 1 — Radiation Transport as Regression

Radiative Transfer as a Bayesian Linear Regression problem

FDC, Ceulemans, Cockayne, Decin, & Yates (*MNRAS*, 2023)

"A&A intro to Probabilistic Numerics applied to Radiative Transfer"

(Actually 2 consecutive Bayesian Linear Regression problems, given χ and η)

optical depth
$$\tau(x_1, x_2) = \int_{x_1}^{x_2} \mathrm{d}x' \, \chi(x')$$

formal solution
$$I(x_2) = \int_{0}^{x_2} \mathrm{d}x' \, \eta(x') \, e^{-\tau(x', x_2)} + \mathrm{BC}$$

Application 1 — Radiation Transport as Regression

GP interpolate absorption χ and emissivity η with the same kernel κ

$$p(\chi) = \mathcal{N}(\mu_\chi, \Sigma_\chi)$$

$$p(\eta) = \mathcal{N}(\mu_\eta, \Sigma_\eta)$$

with **mean** functions

$$\mu_\chi(x) = \boldsymbol{\chi}^{\mathrm{T}} \mathbf{K}_\chi^{-1} \kappa(\boldsymbol{x}, x); \qquad \mathbf{K}_\chi = \kappa(\boldsymbol{x}, \boldsymbol{x}) + \boldsymbol{\Sigma}_\chi$$

$$\mu_\eta(x) = \boldsymbol{\eta}^{\mathrm{T}} \mathbf{K}_\eta^{-1} \kappa(\boldsymbol{x}, x); \qquad \mathbf{K}_\eta = \kappa(\boldsymbol{x}, \boldsymbol{x}) + \boldsymbol{\Sigma}_\eta$$

and **covariance** kernels

$$\Sigma_\chi(x_1, x_2) = \kappa(x_1, x_2) - \kappa(x_1, \boldsymbol{x}) \mathbf{K}_\chi^{-1} \kappa(\boldsymbol{x}, x_2)$$

$$\Sigma_\eta(x_1, x_2) = \kappa(x_1, x_2) - \kappa(x_1, \boldsymbol{x}) \mathbf{K}_\eta^{-1} \kappa(\boldsymbol{x}, x_2)$$

Application 1 — Radiation Transport as Regression

As a result, the intensity I and optical depth τ follow distributions

$$p(\tau) = \mathcal{N}(\mu_\tau, \Sigma_\tau)$$

$$p(I \,|\, \tau) = \mathcal{N}(\mu_{I|\tau}, \Sigma_{I|\tau}) \qquad \text{(given optical depth)}$$

with **mean** functions

$$\mu_\tau(x_1, x_2) = \int_{x_1}^{x_2} \mathrm{d}x' \; \mu_\chi(x') \qquad \text{(optical depth)}$$

$$\mu_{I|\tau}(x_2) = \int_{x_0}^{x_2} \mathrm{d}x' \; \mu_\eta(x')\, e^{-\tau(x', x_2)} \qquad \text{(formal solution)}$$

and **covariance** kernels

$$\Sigma_\tau(x_1, x_2) = \int_{x_1}^{x_2} \mathrm{d}x_1' \int_{x_1}^{x_2} \mathrm{d}x_2' \; \Sigma_\chi(x_1', x_2')$$

$$\Sigma_{I|\tau}(x_1, x_2) = \int_{x_1}^{x_2} \mathrm{d}x_1' \int_{x_1}^{x_2} \mathrm{d}x_2' \; \Sigma_\eta(x_1', x_2') \; e^{-\tau(x_1', x_1)} \, e^{-\tau(x_2', x_2)}$$

Application 1 — Radiation Transport as Regression

Using the results, given the optical depth τ

$$\mu_{I|\tau}(x_2) = \int_{x_0}^{x_2} \mathrm{d}x' \; \mu_\eta(x')\, e^{-\tau(x', x_2)}$$

$$\Sigma_{I|\tau}(x_1, x_2) = \int_{x_1}^{x_2} \mathrm{d}x'_1 \int_{x_1}^{x_2} \mathrm{d}x'_2 \; \Sigma_\eta(x'_1, x'_2)\; e^{-\tau(x'_1, x_1)}\; e^{-\tau(x'_2, x_2)}$$

From the law of **total expectation**

$$\begin{aligned} \mathbb{E}\left[I\right] &= \mathbb{E}_\tau\left[\mu_{I|\tau}\right] \\ &= \mu_{I|\hat{\tau}} \end{aligned}$$

and the law of **total variance**

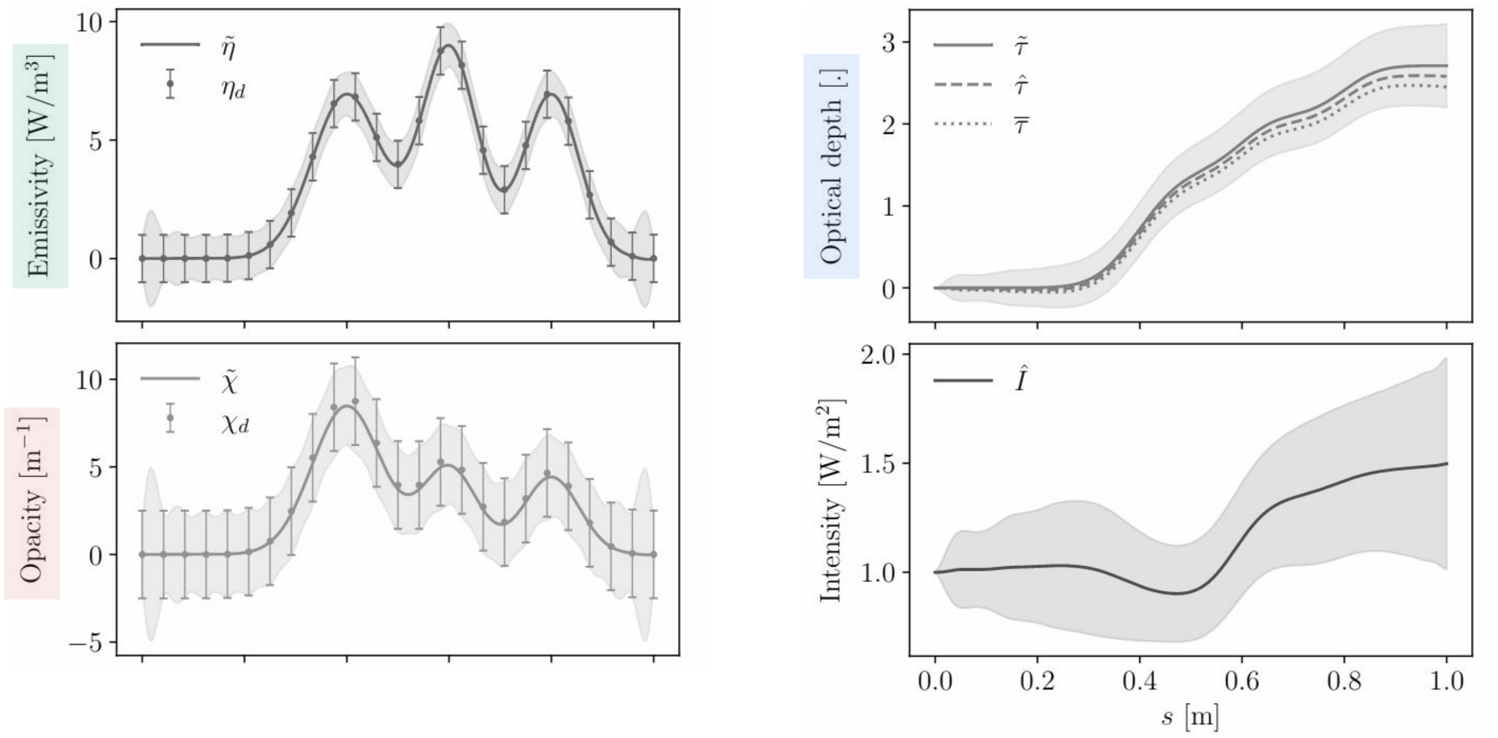
$$\begin{aligned} \mathbb{V}\left[I\right] &= \mathbb{E}_\tau\left[\Sigma_{I|\tau}\right] + \mathbb{V}_\tau\left[\mu_{I|\tau}\right] \\ &\leq \Sigma_{I|\bar{\tau}} + \mu^2_{I|\bar{\tau}} - \mu^2_{I|\hat{\tau}} \end{aligned}$$

Effective optical depths

$$\boxed{\begin{aligned} \hat{\tau} &= \tau - {}^1\!/_2\, \Sigma_\tau \\ \bar{\tau} &= \hat{\tau} - {}^1\!/_2\, \Sigma_\tau \end{aligned}}$$

Application 1 — Radiation Transport as Regression

Example



Application 1 — Radiation Transport as Regression

Added value of probabilistic numerics

(!) **Fast / approximate, but quantifiably / tunably accurate models**

e.g. creating reduced-order models by mapping GP to feature space

(!) **Modelling the impact of uncertainties on the input and discretisation**

Issue with current implementation

(!) **Large computational cost** $\rightarrow$ replace with iterative GP (cfr. Monday)

Application 2 — Chemical Kinetics

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How much of a particular atom or molecule is present at each point?

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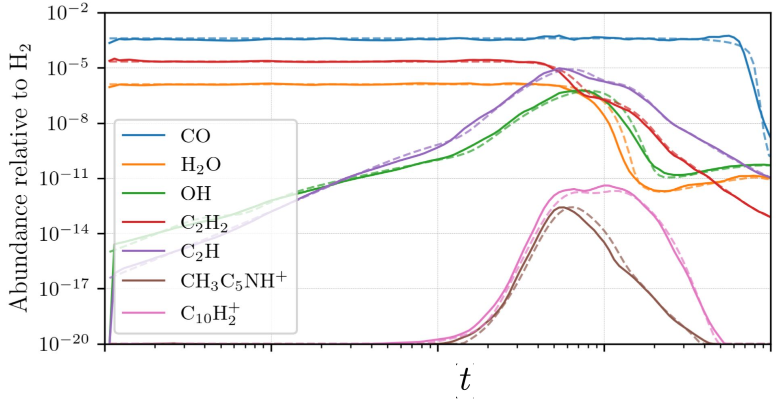
Described by a set of coupled non-linear ODEs,

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = \underbrace{\sum_{j\in F_i}\left(k_j \prod_{r\in R_j} n_r\right)}_{\text{production reactions}} - \underbrace{\sum_{j\in D_i}\left(k_j \prod_{r\in R_j} n_r\right)}_{\text{destruction reactions}}$$



~500 species

~5000 reactions

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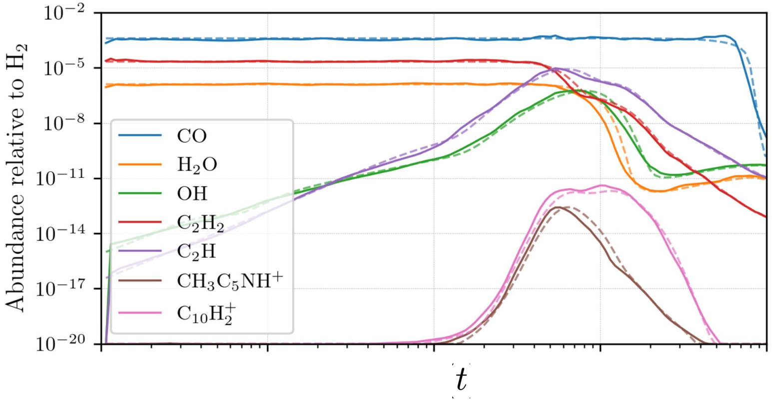


~500 species

~5000 reactions

… and this for every point in the simulation!

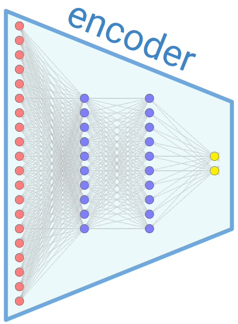
Application 2 — Chemical Kinetics Surrogate Model

In $\longrightarrow$ **out**

Classical dynamics

$$\boldsymbol{n}_0 \qquad \frac{\mathrm{d}n_i}{\mathrm{d}t} = A_{ij}n_j + B_{ijk}n_j n_k \qquad \boldsymbol{n}(\Delta t)$$

$\boldsymbol{n}_0$



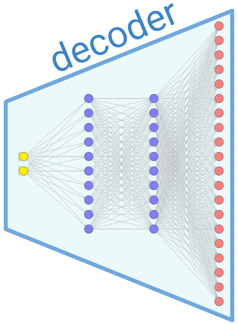
$\boldsymbol{z}_0$

Latent / surrogate dynamics

$$\frac{\mathrm{d}z_\alpha}{\mathrm{d}t} = \mathcal{C}_\alpha + \mathcal{A}_{\alpha\beta}z_\beta + \mathcal{B}_{\alpha\beta\gamma}z_\beta z_\gamma$$

`torchode` (Lienen & Günnemann 2022)

$\boldsymbol{z}(\Delta t)$



$\boldsymbol{n}(\Delta t)$

Maes, **FDC**, Van de Sande, & Decin (2024)

Application 2 — Chemical Kinetics

Potential **added value** of probabilistic numerics

(!) Modelling the impact of large uncertainties on reaction rates

(!) Modelling the impact of the dimensional reduction

(!) Inform dimensional reduction process

Application 3 — Bayesian model reconstruction

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How to create realistic 3D models based on (spectral line) observations?

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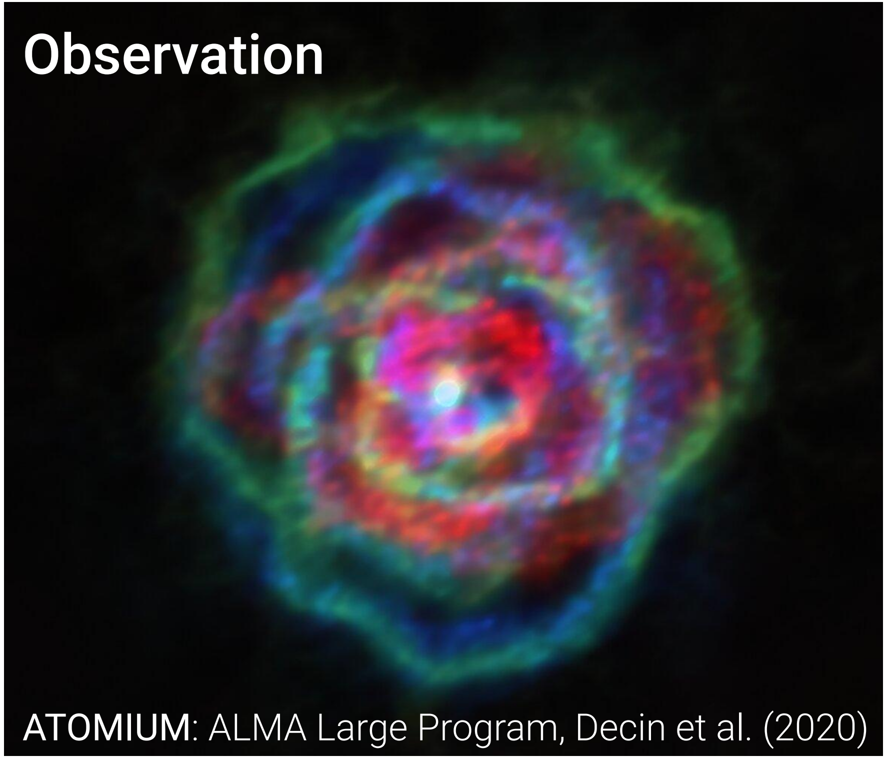
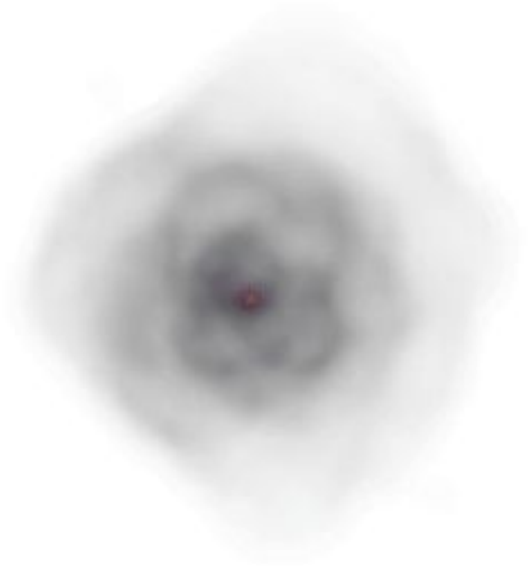


Reconstruction

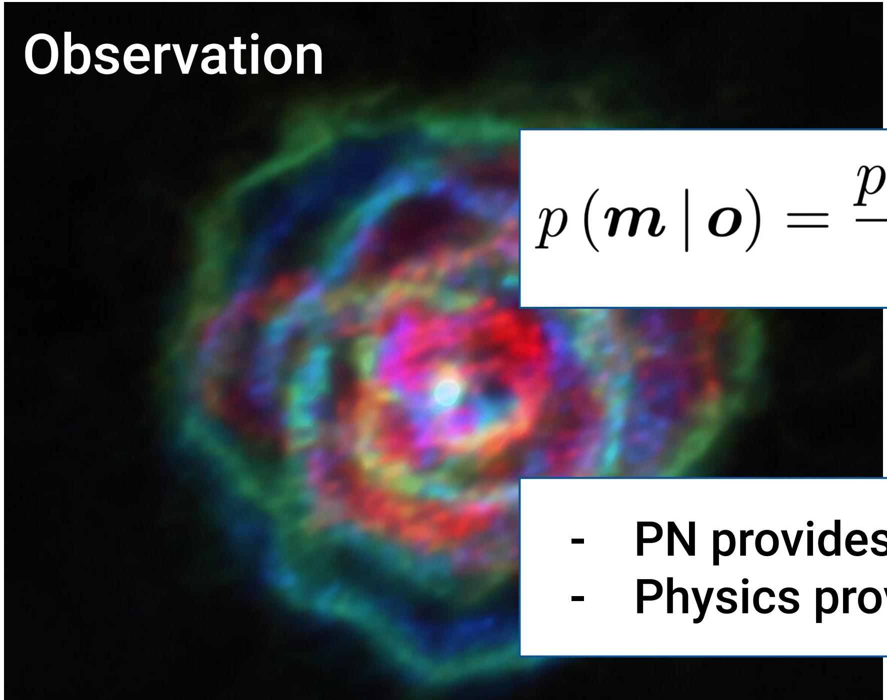


FDC, Ceulemans, Decin, Danilovich, & Yates (2024)

Application 3 — Bayesian model reconstruction

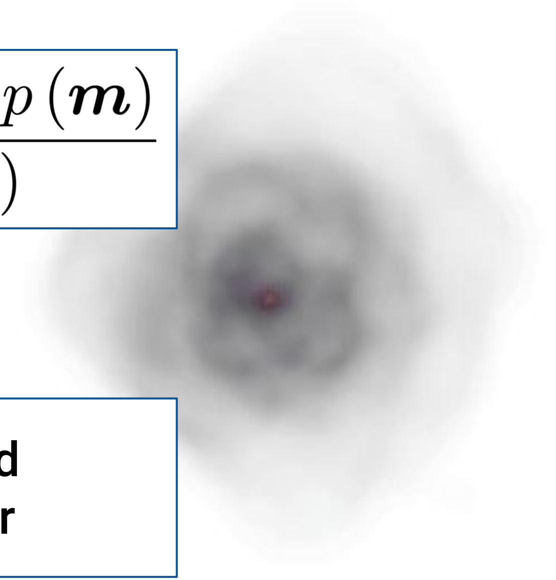
How to create realistic 3D models based on (spectral line) observations?

Observation



ATOMIUM: ALMA Large Program, Decin et al. (2020)

Reconstruction



$$p\left(\boldsymbol{m}\,|\,\boldsymbol{o}\right) = \frac{p\left(\boldsymbol{o}\,|\,\boldsymbol{m}\right)p\left(\boldsymbol{m}\right)}{p\left(\boldsymbol{o}\right)}$$

- **PN provides likelihood**
- **Physics provides prior**

FDC, Ceulemans, Decin, Danilovich, & Yates (2024)

Application 3 — Bayesian model reconstruction

Potential **added value** of probabilistic numerics

(!) **Modelling the large degeneracy**

(!) **Better idea of likelihood including model uncertainties**

Summary — Probabilistic Numerics in A&A

- **Fast / approximate, but quantifiably / tunably accurate models**

  e.g. Radiation Transport, Chemical Kinetics

- **Large uncertainties on various input parameters**

  e.g. spectroscopic data, chemical reaction rates

- **Highly degenerate inverse problems**

  e.g. model reconstructions

Thank you!

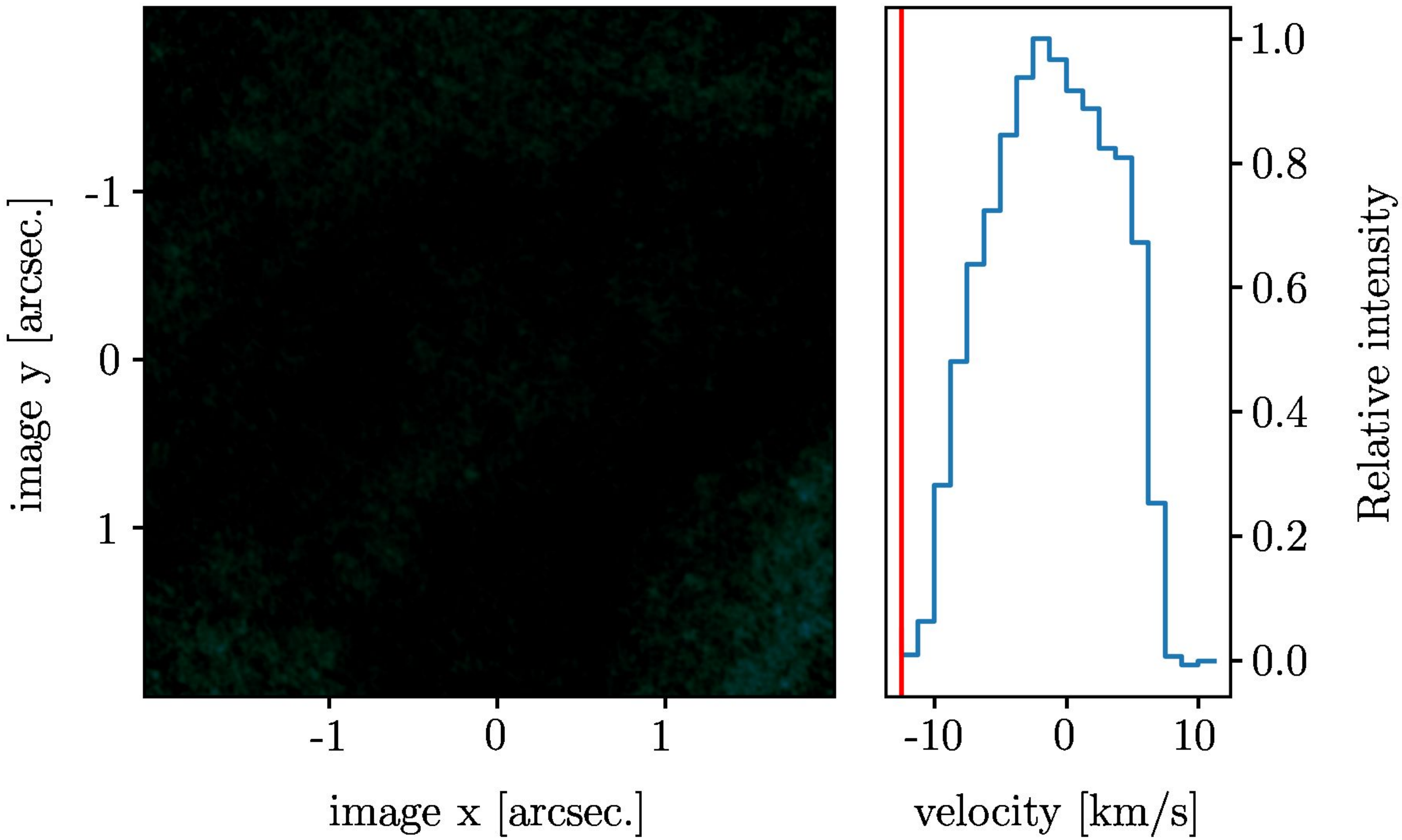
Want to collaborate? Please get in touch!

Frederik De Ceuster (frederik.deceuster@kuleuven.be)

in collaboration with

Thomas Ceulemans, **Silke Maes**, **Marie Van de Sande**, Jon Cockayne, Leen Decin, Jeremy Yates, Taïssa Danilovich, Mats Esseldeurs, Jolien Malfait, Shiqi Su, Mark Wilkinson, Tjonnie G.F. Li, …

Backup — Observations



Backup — Observations