

Signatures of Massive Star Formation in Simulations and Synthetic Observations

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Für mein Familie.

ZUSAMMENFASSUNG

Die Entstehung von massereichen Sterne beeinflusst die Entwicklung von Galaxien durch energiereiches Feedback in Form von ionisierender Strahlung, Sternwinden und Supernovaexplosionen maßgeblich. Auf Skalen von mehreren Parsecs zeigt dieses Feedback meist erst seine Wirkung, wenn die Sterne beginnen ihre dichten Geburtsregionen zu zerstreuen. In den anfänglichen Epochen sind massereiche Protosterne oft noch tief in dichtes Material eingebettet, wodurch sich die Ausdehnung großskaliger H II-Regionen verzögert. In dieser Phase kann das Erwärmen von Materie durch Strahlung sowie der Strahlungsdruck auf Gas und Staub besonders wichtig sein, da dies Fragmentation und Akkretion reguliert.

In dieser Arbeit betrachten wir die Entstehung und frühe Entwicklung massereicher Sterne und ihrer Entstehungsregionen bis zum Einsetzen (ultra-)kompakter H II-Regionen. Dazu berechnen wir strahlungs-(magneto)hydrodynamische Simulationen des gravitativen Kollapses isolierter, parsec-großer, turbulenter Kerne mit dem Code FLASH. Unsere Modelle enthalten ein Schema zum Berechnen für Strahlungsdruck auf Staub und Gas sowie ionisierende Strahlung. Wir verfolgen die Wasserstoffchemie selbstkonsistent, sodass sich die Eigenschaften kompakter H II-Regionen direkt aus den Simulationen ergeben. Wir führen eine Parameterstudie durch, in der wir das anfängliche Dichteprofil, den Virialparameter und die Metallizität variieren. Dadurch erhalten wir eine statistisch aussagekräftige Stichprobe, mit der sich isoliert studieren lässt, wie Anfangsbedingungen die Fragmentation, Akkretionsgeschichte, Feedback-Ausbruch und die Sternentstehungseffizienz beeinflussen.

Um Theorie und Beobachtungen zu verbinden, verarbeiten wir die Simulationen mit dem Strahlungstransfer-Code RADMC-3D weiter und erzeugen synthetische Staubkontinuum- Observationen sowie ALMA-ähnliche interferometrische Bilder mit CASA, die wir mit denselben Methoden analysieren wie in Beobachtungen. Dieses Vorgehen erlaubt es, Projektionseffekte, Unsicherheiten in der Staubtemperatur und interferometrische räumliche Filterung zu erfassen und beobachtbare Kerneigenschaften und deren Umgebung direkt mit intrinsischen physikalischen Größen zu verknüpfen. Durch die Kombination physikreicher Simulationen mit observationsnahen synthetischen Beobachtungen ermöglicht diese Arbeit einen fundierten Vergleich und liefert simulationskalibrierte Leitlinien für die Interpretation von aus Kontinuumsdaten abgeleiteten Kernmassen sowie derer Hüllenstruktur in Regionen massereicher Sternentstehung.

ABSTRACT

High-mass star formation strongly influences the evolution of galaxies through energetic feedback from ionising radiation, stellar winds, and supernovae. However, the feedback from these stars will only affect their environment on parsec scales or beyond, once they have dispersed their parental clumps. In the earliest phases, massive protostars can remain deeply embedded, delaying the expansion of large-scale H II regions. During this stage, radiative heating and radiation pressure on gas and dust may be particularly important in regulating fragmentation and accretion.

In this thesis, we investigate the formation and early evolution of massive stars and their host cores up to the onset of (ultra-)compact H II regions. We carry out radiation-(magneto)hydrodynamical simulations of the gravitational collapse of isolated, parsec-scale, turbulent cores with the FLASH code. Our models include a scheme for radiation pressure on dust and gas as well as ionising radiation, and we follow hydrogen chemistry self-consistently so that the properties of compact H II regions emerge directly from the simulations. We perform a controlled parameter study varying the initial density profile, virial parameter, and metallicity, providing a statistically meaningful sample to isolate how initial conditions shape fragmentation, accretion histories, feedback break-out, and the star formation efficiency.

To connect theory to observations, we post-process the simulations with the radiative transfer code RADMC-3D to generate synthetic dust-continuum maps and ALMA-like interferometric images with CASA, which we analyse with the same methods used for observational surveys. This forward-modeling approach quantifies biases from projection, dust-temperature assumptions, and interferometric spatial filtering, and connect observable core and envelope properties to intrinsic physical quantities. By combining a physics-rich simulation suite with survey-like synthetic observations, this thesis enables a rigorous comparison between simulations and synthetic observations and provides simulation calibrated guidance for interpreting continuum-derived core masses and envelope structure in high-mass star-forming regions.

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INTRODUCTION

Since the earliest civilizations, the night sky has inspired curiosity and provided a foundation for scientific inquiry. Yet, despite centuries of study, many of its most fundamental processes remain only partially understood. Among them, the formation of stars, and in particular the formation of massive stars ($M \gtrsim 8 M_{\odot}$), stands out as a key driver of galactic evolution.

Massive stars shape the morphology, dynamics, and chemistry of galaxies and dominate the energy and momentum budget of the interstellar medium, even though they represent only a minor fraction of stars by number (Zinnecker & Yorke, 2007). Through ionising radiation, stellar winds, protostellar outflows, and ultimately supernova explosions, they carve H II regions, drive expanding shells and bubbles, and stir the surrounding gas. In doing so, they regulate how efficiently gas can collapse into new generations of stars, while also enriching their environments with heavy elements that are incorporated into subsequent star formation (Tan et al., 2014).

Because this feedback is both intense and multi-channel, star formation connects scales from dense protostellar cores (< 0.1 pc) to galaxy-wide gas cycles (> 100 pc). On small scales, feedback reshapes cores and envelopes and can quench or redirect accretion. On larger scales, it disperses molecular clouds, triggers or suppresses further collapse in neighbouring regions, and contributes to the turbulent support of the ISM. These processes influence galactic dynamics (Bolatto et al., 2013) and set the initial conditions for planet formation. Figure 1 illustrates this complexity in the Cassiopeia molecular cloud complex, highlighting sites of massive star formation and bubble-like structures produced by stellar winds and supernova explosions.

Understanding how massive stars assemble their mass remains one of the central open problems in modern astrophysics. While low-mass star formation is broadly captured by the interplay of gravity, turbulence, and thermal pressure leading to fragmentation near the Jeans scale, massive star formation requires additional physics. Magnetic fields (Commerçon et al., 2011) and radiative feedback (Krumholz et al., 2009) become crucial, and the most massive protostars may begin nuclear burning while still accreting, so that accretion and feedback proceed simultaneously.

Enhancing our understanding of massive star formation remains challenging because the process is difficult to access both, observationally and numerically. Observationally, massive young stars are rare and therefore typically more distant, demanding high angular resolution. They form in the densest, most embedded regions, where extinction and optical depth limit many wavelengths, and their rapid evolutionary timescales further reduce the window in which key stages can be observed. Numerically, the problem spans extreme dynamic ranges in density and spatial scale while coupling gravity, turbulence, magnetic fields, radiation, and feedback, making comprehensive simulations computationally demanding. Together, these challenges motivate the detailed theoretical and numerical exploration of massive star formation and its observable signatures in this thesis.

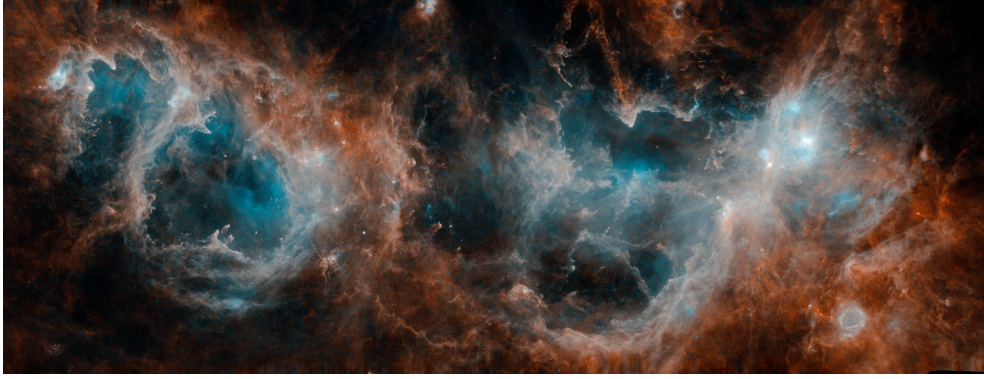


Figure 1: The W3/W4/W5 complex of molecular clouds in the northern constellation Cassiopeia, imaged by ESA's Herschel observatory. Observing the sky at far-infrared ($70\ \mu\text{m}$, in cyan) and submillimetre wavelengths ($100\ \mu\text{m}$, in orange) from 2009 to 2013. The image reveals regions of massive star formation, as well as bubbles carved by stellar winds and supernova explosions. *Credit: ESA/Herschel/NASA/JPL-Caltech*

The thesis is structured as follows. Chapter 2 introduces star formation from giant molecular clouds down to dense cores, reviews the basic theory of core collapse, and highlights the key processes that shape massive star formation. Chapter 3 presents the observational methodology, introducing interferometry and the surveys used throughout this thesis. Chapter 4 then describes the numerical simulations, and Chapter 5 outlines the post-processing pipeline. Chapter 6 motivates the research questions addressed in this work. The simulation analysis is presented in Chapter 7; Chapter 8 focuses on cores in simulations and synthetic observations; and Chapter 9 discusses radial envelope profiles. Finally, Chapter 10 summarises the results, draws the main conclusions, and provides an outlook for future work.

THE FORMATION OF STARS

2.1

GIANT MOLECULAR CLOUDS

Giant molecular clouds (GMCs) are the largest and most massive reservoirs of cold molecular gas within the interstellar medium (ISM), serving as the primary sites for star formation in the galaxies. Typically, GMCs contain $10^4 - 10^6 M_\odot$ of mass and can extend over tens of pc (Blitz, 1993). Their typical temperature is 10 K, with a mean hydrogen number density of $n_{\text{H}_2} \sim 100 \text{ cm}^{-3}$ (Solomon et al., 1987).

The internal structure of GMCs is highly complex and hierarchical, shaped by the interplay of several physical mechanisms including self-gravity, turbulence, magnetic fields, external pressure, and stellar feedback (McKee & Ostriker, 2007). Observations and simulations demonstrate that turbulence within GMCs establishes filamentary structures that fragment into denser clumps where stars are born (Larson, 1969; Hacar et al., 2023).

To estimate if a region within a GMC is gravitationally bound and capable of overcoming internal turbulent support to eventually collapse, the virial parameter, α_{vir} , is commonly employed:

$$\alpha_{\text{vir}} = \frac{2E_{\text{kin}}}{E_{\text{grav}}}, \quad (2.1)$$

where E_{kin} is the kinetic energy (dominated by turbulence and bulk motion) and E_{grav} the gravitational potential energy (Bertoldi & McKee, 1992). Structures with $\alpha_{\text{vir}} \leq 1$ are generally considered as gravitationally bound and are expected to collapse, while higher values indicates that the kinetic energy dominates and provides support against the collapse.

Beyond this classical expression, additional pressure terms also contribute to the cloud stability. Thermal pressure acts to counterbalance gravitational compression, maintaining internal equilibrium (Scoville & Hersch, 1979). Meanwhile, magnetic fields thread GMCs, exerting magnetic pressure and tension forces that influence gas dynamics and fragmentation supporting clouds against collapse and shaping filamentary structures (Crutcher, 1999). Ganguly et al. (2024) show that the classical virial parameter alone can be misleading, as additional pressure and surface terms substantially alter the effective virial balance. In their simulations, dense regions that seem bound from the standard virial parameter can still be supported or confined by magnetic and thermal surface terms, while low-density gas may often be stabilized by magnetic pressure.

Observations show that stars within GMCs are not formed in isolation but rather in groups, showing that stellar clusters originate from the same parental molecular cloud (Lada & Lada, 2003). A fundamental description of the stellar population within such clusters is the initial mass function (IMF). It defines the mass distribution

of stars within the cluster, first done by [Salpeter \(1955\)](#):

$$\xi(m)dm \propto \left(\frac{m}{M_\odot}\right)^{-2.35} \left(\frac{dm}{M_\odot}\right), \quad (2.2)$$

where $\xi(m)$ is the number of stars formed per unit mass interval, m the stellar mass. The classical form from [Salpeter \(1955\)](#) describes the high-mass end, following a single power-law with a slope of -2.35 for stars between $0.1 M_\odot$ to $10 M_\odot$. Later the profile was modified by [Kroupa \(2001\)](#) and [Chabrier \(2003\)](#), who introduced a more realistic shape for lower mass stars by flattening the IMF below about $0.5 M_\odot$. [Kroupa \(2001\)](#) proposed a segmented power-law with shallower slopes at low masses. [Chabrier \(2003\)](#) proposed a log-normal distribution at low masses which smoothly transitions to a Salpeter-like power-law at higher masses. These modifications better match observations of stellar populations in the Milky Way and other galaxies.

2.2

FROM CLOUDS TO CORES

GMCs exhibit a pronounced hierarchy of structure in both observations and simulations. Supersonic turbulence, self-gravity, magnetic fields, and external compression generate strong density contrasts and organize the gas into elongated overdensities (filaments) and more centrally concentrated condensations. A key advantage of this hierarchical description is that it provides a physical bridge between the global cloud reservoir and the local initial conditions for collapse: cloud-scale flows assemble a dense-gas network dominated by filaments; the densest parts of this network collect into parsec-scale clumps (often at filament junctions or along high-column-density ridges); and clumps fragment into cores that are the direct progenitors of protostars (e.g. [André et al., 2014](#); [Hacar et al., 2023](#); [Pineda et al., 2023](#)).

2.2.1

FILAMENTS

Filamentary structure is ubiquitous in molecular clouds and provides a natural morphology for connecting large-scale flows to smaller-scale gravitational fragmentation ([André et al., 2014](#); [Hacar et al., 2023](#)). In nearby clouds, filaments typically extend over $\sim 1 - 10$ pc and show a characteristic inner width of ~ 0.1 pc in *Herschel* column-density analyses (e.g. [Arzoumanian et al., 2011](#)). Filaments are generally not isolated, hydrostatic cylinders. They are embedded in larger-scale dynamics and can be continuously fed by their surroundings. Observationally, this coupling is suggested by the presence of velocity gradients consistent with mass loading onto filaments, indicating that filament evolution reflects the interplay between internal support (thermal, turbulent, magnetic) and ongoing accretion (e.g. [Palmeirim et al., 2013](#)).

A useful indicator of whether a filament can readily form dense condensations is its mass per unit length, M_{line} . For an isothermal, non-magnetized cylinder supported only by thermal pressure, the critical (thermal) line mass is

$$M_{\text{line,crit}} = \frac{2c_s^2}{G} \simeq 16 \left(\frac{T}{10 \text{ K}}\right) M_\odot \text{ pc}^{-1}, \quad (2.3)$$

where c_s is the isothermal sound speed, and G the gravitational constant ([Ostriker,](#)

1964). Thermally supercritical filaments ($M_{\text{line}} \gtrsim M_{\text{line,crit}}$) are expected to contract and fragment into a chain of dense condensations. In realistic environments, non-thermal motions, magnetic support, pressure and surface terms can substantially modify the effective stability boundary, so filament stability is best interpreted alongside kinematics and virial-based diagnostics (e.g. Bertoldi & McKee, 1992; Ganguly et al., 2024).

Herschel surveys provide empirical support for a filament-to-core connection: in nearby clouds, the majority of gravitationally bound (prestellar) cores are found along the densest filaments and preferentially within filamentary segments that are close to or above the critical line mass (Arzoumanian et al., 2011). In the Aquila Rift cloud complex, Könyves et al. (2015) identify gravitationally bound (prestellar) cores in *Herschel* far-infrared/ submillimetre maps and find that most are strongly associated with thermally supercritical filaments, consistent with core formation being favored in the densest, gravitationally unstable parts of the filament network.

2.2.2

CLUMPS

Filaments can serve as direct sites of core formation, but they may also act as channels that transport dense gas into more centrally concentrated, parsec-scale condensations (Gómez & Vázquez-Semadeni, 2014; Ma et al., 2023). These clumps are compact overdensities with typical sizes of $\sim 0.3 - 3$ pc (Smith et al., 2008), embedded within molecular clouds that contain sufficient mass to form stellar groups or clusters and typically fragment into multiple dense cores (Motte et al., 2018). They are frequently found within high-column-density ridges or at filament junctions (hubs), consistent with a hub–filament picture in which clumps represent local gravitational potential minima fed by converging filamentary flows (Myers, 2009; Hacar et al., 2023). Clumps do not need to be closed systems. They can continue to grow by accreting gas delivered by the surrounding filamentary network, which may influence their stability, fragmentation, and evolutionary timescales (e.g. Hennemann et al., 2012; Pineda et al., 2023).

The internal evolution and fragmentation of clumps depend on the balance between gravity and internal support (turbulence and magnetic fields), modified by thermal physics (including radiative heating) and by stellar feedback as star formation proceeds (e.g. McKee & Ostriker, 2007; Motte et al., 2018).

Observationally, the ATLASGAL Galactic-plane survey reports clumps with radii $R \sim 0.3 - 1$ pc, masses $M \sim 10^2 - 10^4 M_{\odot}$, and mean densities $n_{\text{H}_2} \sim 10^4 - 10^5 \text{ cm}^{-3}$, with densities in embedded cores reaching higher values (Urquhart et al., 2018). Similarly, ALMAGAL targets massive dense clumps with $M \sim 10^2 - 10^4 M_{\odot}$ and clump surface densities $\Sigma_{\text{clump}} \sim 0.1 - 10 \text{ g cm}^{-2}$ (Molinari et al., 2025) (see also Sec. 3.3). For clumps, the virial parameter (Eq. 2.1) serves as a commonly used measure of the balance between self-gravity and internal motions, in the absence of strong magnetic support. Urquhart et al. (2018) find that most massive star-forming clumps have α_{vir} around 1 and typically below ~ 2 even in evolved stages, and they report an overall decrease of α_{vir} toward higher masses. Magnetic fields can also provide additional support against gravity. Observations suggest typical field strengths of $\sim 10^1 - 10^3 \mu\text{G}$, so that magnetic forces can be dynamically important but often cannot prevent collapse on their own (Tan et al., 2014; J. Liu et al., 2020).

Clumps are not necessarily static reservoirs. In many regions they evolve dynamically as self-gravity drives global contraction while turbulence, magnetic fields, and

continued accretion shape the internal flow. In the inertial-inflow picture, supersonic turbulence produces large-scale converging flows that assemble dense structures and keep feeding them with gas, so turbulence can actively drive accretion rather than only opposing collapse (Padoan et al., 2020). Weis et al. (2022), who follow clumps forming in magnetized flows, find that clumps can be short-lived and that their effective confinement can be strongly influenced by external pressure (ram and thermal) acting at their boundaries. Early analysis likewise shows that external pressure is an essential part of the force balance of pressure-confined clumps and cores (Bertoldi & McKee, 1992).

2.2.3

CORES

During this dynamical evolution of clumps, the gas becomes increasingly structured, and the highest-density material is gathered into localized condensations (cores) that provide the immediate initial conditions for star formation. Dense cores are cold (~ 10 K) and compact ($\sim 0.01 - 0.1$ pc), with characteristic densities $n_{\text{H}_2} \sim 10^4 - 10^5 \text{ cm}^{-3}$, while centrally concentrated prestellar cores can reach central densities $\gtrsim 10^5 - 10^6 \text{ cm}^{-3}$ (e.g. Bergin & Tafalla, 2007; Könyves et al., 2015; Caselli et al., 2025). These overdensities can be identified in (sub-)millimetre dust continuum emission and/or dense-gas tracers (e.g. NH_3 and N_2H^+), which probe cold dense gas (e.g. Benson & Myers, 1989; Caselli et al., 2002). Because core identification depends on tracer choice, angular resolution, and source-extraction method, the term core is best understood as a practical, scale-dependent description of a local overdensity rather than a uniquely defined physical entity (e.g. André et al., 2014).

Even as clumps contract, their internal density field is often organized into filamentary substructure. High-resolution observations reveal pronounced substructure down to core scales, with narrow strands and kinematically coherent velocity components existing within the clump (Hacar et al., 2018; T. Liu et al., 2020). Dense cores often form within a subset of these filamentary substructures, where the gas becomes gravitationally unstable and fragments (e.g. Hacar et al., 2013; Henshaw et al., 2016). In this picture, core formation is linked to the fragmentation of the dense, filamentary substructure within clumps rather than to a single uniform collapse of the clump gas to a single core.

As a consequence, clumps typically fragment into a population of dense cores rather than forming a single object (e.g. Lada & Lada, 2003; Reipurth et al., 2014). Also, individual cores may then fragment further, so that binary and higher-order multiple systems can form. Reviews show that the frequency and properties of multiple systems depend on the stellar mass and environment, indicating that multiplicity is shaped by both, fragmentation and the subsequent dynamical evolution in denser regions (e.g. Duchêne & Kraus, 2013; Krumholz et al., 2014). The resulting distribution of core masses is the core mass function (CMF). It remains debated how directly the CMF maps onto the stellar IMF. In nearby clouds, reviews often summarize the observational result that the CMF has a broadly IMF-like shape but is shifted to higher masses by a factor of $\sim 2-3$, which is commonly interpreted as a characteristic core-to-star efficiency of $\sim 0.3 - 0.5$ (with substantial systematic uncertainties and possible environmental dependence) (e.g. Alves et al., 2007; André et al., 2010; Pouteau et al., 2023).

2.3

GRAVITATIONAL COLLAPSE AND PROTOSTAR FORMATION

We now turn to the physical conditions in dense cores and the circumstances under which they become gravitationally unstable, collapse, and form a protostar. Star formation begins when a core can no longer be supported against self-gravity and start to collapse. The early evolution is often close to isothermal, before heating and radiative feedback change the thermodynamics and lead to the formation of a protostar (e.g. [Stahler & Palla, 2004](#)).

2.3.1

RADIAL CORE STRUCTURE

Hydrostatic Isothermal Sphere

We start with the assumption of a static, spherically symmetric core in hydrostatic equilibrium. In this case, the inward gravitational force per unit volume is balanced by the outward pressure gradient, such that

$$\nabla P = -\rho \nabla \Phi, \quad (2.4)$$

where P is the pressure, ρ is the density, and Φ is the gravitational potential. For the spherical symmetric case the quantities depend on the radius r :

$$\frac{dP}{dr} = -\rho(r) \frac{d\Phi}{dr}. \quad (2.5)$$

Using Poisson's equation, $\nabla^2 \Phi = 4\pi G \rho$ and assuming spherical symmetry, the radial derivative of the gravitational potential can be expressed in terms of the enclosed mass $M(r)$ as

$$\frac{d\Phi}{dr} = \frac{GM(r)}{r^2}. \quad (2.6)$$

This gives the standard form for the hydrostatic equilibrium equation

$$\frac{dP}{dr} = -\frac{GM(r)\rho(r)}{r^2}, \quad (2.7)$$

where the enclosed mass can be written as

$$\frac{dM}{dr} = 4\pi r^2 \rho(r). \quad (2.8)$$

For an isothermal equation of state (EOS) the gas temperature and the sound speed c_s are constant, so that

$$P = c_s^2 \rho. \quad (2.9)$$

Inserting the derivative of Eq. 2.9 into Eq. 2.7 and with $\frac{1}{\rho} \frac{d\rho}{dr} = \frac{d \ln \rho}{dr}$ leads to

$$c_s^2 \frac{d \ln \rho}{dr} = -\frac{GM(r)}{r^2}. \quad (2.10)$$

We multiply with r^2 and differentiating with respect to r . Inserting Eq. 2.8 then results into

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d \ln \rho}{dr} \right) = -\frac{4\pi G}{c_s^2} \rho(r). \quad (2.11)$$

Now we want to derive a dimensionless equation. Doing so we define a dimensionless function $\psi(r)$ with

$$\rho(r) = \rho_0 e^{-\psi(r)} \quad (2.12)$$

where ρ_0 is the central core density, so that with $\ln \rho = \ln \rho_0 - \psi$ we can simplify

$$\frac{d \ln \rho}{dr} = -\frac{d\psi}{dr}. \quad (2.13)$$

Further we define a dimensionless radial coordinate ξ :

$$\xi \equiv \frac{r}{a} \quad \text{with} \quad a \equiv \frac{c_s}{\sqrt{4\pi G \rho_0}}. \quad (2.14)$$

With inserting $d/dr = (1/a) d/d\xi$ and the assumed density distribution from Eq. 2.12 into Eq. 2.11 we derive the isothermal Lane-Emden equation:

$$\frac{1}{\xi^2} \frac{d}{d\xi} \left(\xi^2 \frac{d\psi}{d\xi} \right) = e^{-\psi}. \quad (2.15)$$

Now we assume boundary conditions of a non-singular solution:

$$\psi(0) = 0 \quad \text{and} \quad \left. \frac{d\psi}{d\xi} \right|_{\xi=0} = 0. \quad (2.16)$$

We can therefore expand $\psi(\xi)$ about the origin in a Taylor series containing only even powers,

$$\psi(\xi) = A\xi^2 + B\xi^4 + \mathcal{O}(\xi^6). \quad (2.17)$$

Inserting this expansion into Eq. 2.15 and using $e^{-\psi} \approx 1 - \psi + \mathcal{O}(\psi^2)$ for $\xi \rightarrow 0$, leading to $A = 1/6$, which gives

$$\psi(\xi) \simeq \frac{\xi^2}{6}, \quad \rho(\xi) = \rho_0 e^{-\psi} \simeq \rho_0 \left(1 - \frac{\xi^2}{6} + \mathcal{O}(\xi^4) \right). \quad (2.18)$$

Thus $\rho \rightarrow \rho_0$ as $\xi \rightarrow 0$, results in a constant density plateau at the core center. For larger radii we assume $\psi(\xi) \approx A \ln \xi + B$. Inserting it into Eq. 2.15 gives $A = 2$ and thus

$$\psi(\xi) \sim 2 \ln \xi + \text{const.}, \quad \rho(r) \propto r^{-2}. \quad (2.19)$$

The hydrostatic isothermal sphere therefore has a constant density at the center with an outer power-law exponent of -2.

Dynamical Isothermal Collapse

A commonly used idealized picture for isothermal protostellar collapse is the “inside-out” scenario (Shu, 1977). In this model the core starts with a singular isothermal sphere with $\rho \propto r^{-2}$, and the collapse begins at the center. An expansion wave propagates outward at approximately the sound speed such that material inside this radius is in infall while the outer envelope remains close to its initial hydrostatic structure.

To describe dynamical evolution in the isothermal case, we start from the spherically symmetric Euler equation,

$$\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial r} = -\frac{1}{\rho} \frac{\partial P}{\partial r} - \frac{GM(r, t)}{r^2}, \quad (2.20)$$

together with the continuity equation,

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho v) = 0, \quad (2.21)$$

and the definition of the enclosed mass,

$$\frac{\partial M}{\partial r} = 4\pi r^2 \rho. \quad (2.22)$$

For an isothermal equation of state, $P = c_s^2 \rho$ with constant sound speed c_s , the pressure term can be written as

$$-\frac{1}{\rho} \frac{\partial P}{\partial r} = -c_s^2 \frac{\partial \ln \rho}{\partial r}. \quad (2.23)$$

The free-fall time is the characteristic timescale for a self-gravitating sphere in the absence of pressure and other forces. For a uniform-density sphere it is given by

$$t_{\text{ff}} \sim \sqrt{\frac{3\pi}{32G\rho}}. \quad (2.24)$$

In a region where the flow approaches free-fall onto an enclosed mass M , the infall speed can be estimated as

$$v(r) \approx -\sqrt{\frac{2GM}{r}} \propto r^{-1/2}. \quad (2.25)$$

For a steady, spherically symmetric inflow, mass conservation implies a radius-independent accretion rate

$$\dot{M} = 4\pi r^2 \rho(r) |v(r)|. \quad (2.26)$$

If $\dot{M}$ is approximately constant with radius, we derive

$$\rho(r) \propto \frac{\dot{M}}{r^2 |v|} \propto \frac{1}{r^2 r^{-1/2}} \propto r^{-3/2}. \quad (2.27)$$

Therefore, in an isothermal core where the inner region approaches free-fall and the accretion rate is approximately constant, one expects density profiles $\rho \propto r^{-1.5}$ in the inner region, while the outer envelope remains close to its initial hydrostatic structure with $\rho \propto r^{-2}$.

Bonnor-Ebert Sphere

A Bonnor-Ebert (BE) sphere (Ebert, 1955; Bonnor, 1956) generalizes the isothermal sphere picture as a pressure-confined, self-gravitating isothermal sphere with a finite central density truncated at a finite outer radius R_{out} defined by an external pressure

$$P(R_{\text{out}}) = P_{\text{ext}}. \quad (2.28)$$

This pressure boundary condition yields a core of finite size and mass. A BE core is stable only up to a critical central concentration. The critical configuration corresponds to a central-to-edge density contrast of

$$\frac{\rho_c}{\rho(R_{\text{out}})} \approx 14, \quad (2.29)$$

while more centrally concentrated (supercritical) configurations are unstable to gravitational collapse.

The BE density profile can be approximated by a plummer profile:

$$\rho(r) = \frac{\rho_0}{\left[1 + \left(\frac{r}{r_0}\right)^2\right]^{p/2}}, \quad (2.30)$$

which reproduces a flat inner region for $r \ll r_0$ and a power-law decline $\rho \propto r^{-p}$ for $r \gg r_0$. The exponent p is a free parameter that controls the outer power-law slope.

Temperature Profiles

For the previously discussed isothermal sphere, the temperature is constant with radius, $T(r) = T_0$. Following [Draine \(2011\)](#), we consider a central heating source of luminosity L_* embedded in an optically thin envelope. The absorbed power is set by the incident flux, $F \propto L_*/(4\pi r^2)$, while the emitted thermal power scales as $\propto \kappa_P(T) \sigma T^4$, where $\kappa_P(T)$ is the Planck-mean dust opacity (e.g. [Klepitch et al., 2023](#)). Assuming radiative equilibrium, we can write

$$\frac{L_*}{r^2} \propto \kappa_P(T) T^4. \quad (2.31)$$

The dust absorption opacity can be approximated by a power law $\kappa_\nu \propto \nu^\beta$ over the frequencies relevant for the thermal emission, where β is the dust emissivity. With the

$$\kappa_P(T) \equiv \frac{\int_0^\infty \kappa_\nu B_\nu(T) d\nu}{\int_0^\infty B_\nu(T) d\nu} \Rightarrow \kappa_P(T) \propto T^\beta, \quad (2.32)$$

we obtain

$$T(r) \propto \left(\frac{L_*}{r^2}\right)^{1/(4+\beta)} \propto r^{-2/(4+\beta)}. \quad (2.33)$$

Equation (2.33) shows that the temperature slope is set by the dust emissivity index β ,

$$T(r) \propto r^{-q}, \quad q \equiv \frac{2}{4+\beta}. \quad (2.34)$$

Typical values adopted for (sub-)mm dust emission are $\beta \sim 1 - 2$, with $\beta \simeq 1$ often used as a low- β reference case in disk or envelope applications and $\beta \gtrsim 1.5 - 2$ closer to ISM-like values (e.g. [Hildebrand, 1983](#); [Beckwith et al., 1990](#); [Draine, 2006](#)). Using Eq. (2.34), this corresponds to temperature slopes in the range $q \simeq 0.33 - 0.4$.

Connecting Intensity, Density and Temperature Profiles

Observationally, radial profiles are typically measured from (sub-)mm continuum intensity maps. Combined with an independent estimate of the temperature profile, these profiles can be used to infer the underlying density structure ([Adams, 1991](#); [Motte & André, 2001](#)).

For optically thin dust emission the (sub-)mm specific intensity at projected radius R is

$$I_\nu(R) = \int_{-\infty}^{+\infty} \kappa_\nu \rho(r) B_\nu[T(r)] dz, \quad (2.35)$$

where $r = \sqrt{R^2 + z^2}$ and z is the line-of-sight coordinate. Assuming κ_ν does not vary

with radius and adopting the Rayleigh–Jeans limit $B_\nu(T) \propto T$, we obtain

$$I_\nu(R) \propto \int \rho(r) T(r) dz. \quad (2.36)$$

For power-law profiles $\rho(r) \propto r^{-p}$ and $T(r) \propto r^{-q}$ this becomes

$$I_\nu(R) \propto \int_{-\infty}^{+\infty} r^{-(p+q)} dz \propto R^{-(p+q-1)}, \quad \text{for } p+q > 1. \quad (2.37)$$

Defining

$$I_\nu(R) \propto R^{-m}, \quad (2.38)$$

the projected intensity slope is therefore

$$m \simeq p + q - 1, \quad p \simeq m + 1 - q. \quad (2.39)$$

Relevant aspects for this thesis In practice, dense cores are not perfectly isothermal and are not supported by thermal pressure alone. Temperature gradients, non-thermal motions (turbulence), magnetic fields, rotation, and external pressure confinement can all modify the stability criterion and the resulting density profile. We therefore interpret these models above as idealized reference cases for comparison with the radial profile analysis in Chapter 9. Furthermore, the introduced Plummer-profiles are not only used to describe cores but are also commonly adopted to approximate clumps. Therefore, in our simulations presented in Paper I (Chapter 7), we adopt a similar Plummer-like profile for the initial density distribution, capturing a flat inner region and an outer power-law decline.

2.3.2

COLLAPSE TO A PROTOSTAR

The formation of low mass stars ($m \leq 2 M_\odot$) is well established, due to their lower luminosities, slower evolution, and observational accessibility in nearby star-forming regions. The standard model has been shaped by theoretical studies (Larson, 1969; Shu et al., 1987) and observations (e.g. Lada & Wilking, 1984), and is further reviewed in the context of filamentary initial conditions and multi-scale gas flows in Hacar et al. (2023); Pineda et al. (2023).

The model starts with the gravitational collapse of a dense core, when the core mass exceeds the Jeans mass, given by:

$$M_J \sim \left(\frac{5kT}{G\mu m_H} \right)^{3/2} \left(\frac{3}{4\pi\rho} \right)^{1/2}, \quad (2.40)$$

where k is the Boltzmann constant, T the temperature, μ the mean molecular weight, m_H the mass of a hydrogen atom and ρ the density. Following Sec. 2.3.1, the collapse begins from an approximately isothermal configuration, where a centrally concentrated density profile (typically a Bonnor-Ebert sphere) is developed. When it reaches densities around $n_{H_2} \sim 10^{10} \text{ cm}^{-3}$ the gas becomes optically thick and radiative cooling becomes inefficient. At this point the gas heats up due to compression, and goes into an adiabatic phase. When temperatures of $\sim 2000 \text{ K}$ are reached, H_2 begins to dissociate, absorbing energy and triggering a second collapse phase. A protostar is born.

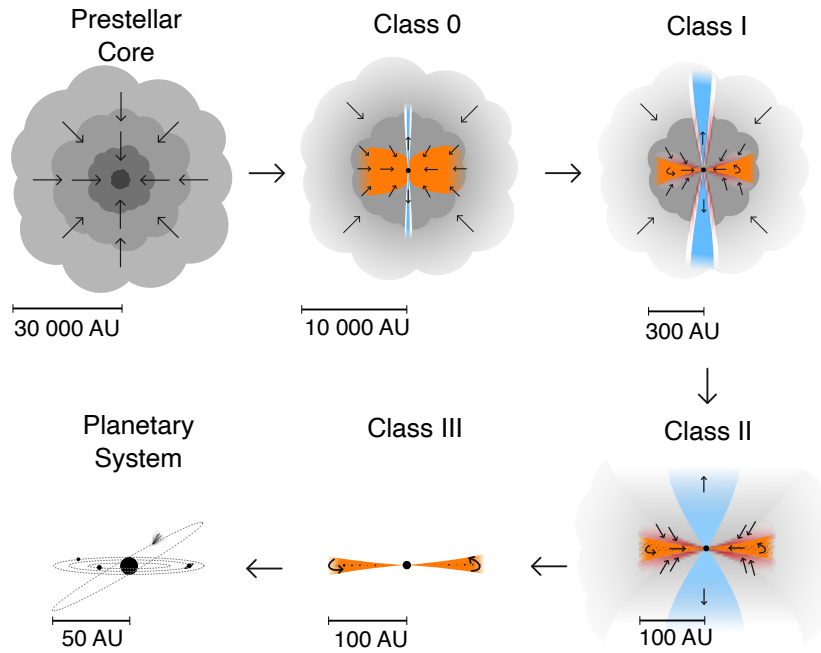


Figure 2: Evolutionary sequence of low-mass star formation. Schematic illustration of the of a collapsing core from a prestellar core to the Class 0, Class I, and Class II protostellar phases, followed by the Class III stage and the emergence of a planetary system. The diagram shows the infalling envelope, development of bipolar outflows, and growth and evolution of the circumstellar disk across these stages. Credit: [Persson \(2014\)](#)¹

The central protostar continues to grow in mass via accretion from the surrounding envelope through a circumstellar disk, which forms as a natural consequence of angular momentum conservation. These disks are now understood not only as reservoirs feeding material onto the star, but also as the sites where planets form, as revealed by high-resolution ALMA and near-infrared observations showing rings, gaps, spirals, and other substructures in young systems (e.g. [Pineda et al., 2023](#)). Protostellar systems also launch powerful bipolar outflows and highly collimated jets, driven magnetically from the inner disk regions. These outflows are essential for redistributing angular momentum and shaping the surrounding envelope.

The evolution of the system goes through different stages which can be distinguished by their spectral energy distributions (e.g. [Lada, 1987](#); [Greene et al., 1994](#); [Dunham et al., 2014](#)) and are illustrated in Fig. 2. In the Class 0 phase, the protostar is deeply embedded and its envelope contains most of the mass. At this stage, the protostar accretes mass through an accretion disk which drives magnetically launched collimated jets. As the system evolves into the Class I phase, cavities are formed in the envelope and the protostar heats up. It becomes visible in the infrared. By the Class II phase, the envelope has largely dissipated. The pre-main-sequence star is surrounded by a protoplanetary disk in which planet formation takes place, and the system becomes visible in the optical. In the Class III phase, most of the disk has dispersed, leaving a young pre-main-sequence star that may already host

¹https://figshare.com/articles/figure/Current_view_of_protostellar_evolution/654555?file=1589002

newly formed planets. The star continues its contraction, supported by gravitational energy, until the core temperature becomes high enough ($\sim 10^7$ K) for hydrogen fusion to begin (Stahler & Palla, 2004). At this point, a main-sequence star is born.

While the Class 0–III sequence and the disk–outflow model provide a useful framework for low-mass star formation, the picture becomes more diverse at higher stellar masses. Intermediate-mass stars ($m \sim 2\text{--}8 M_\odot$) are commonly studied as Herbig Ae/Be stars and their embedded progenitors (Waters & Waelkens, 1998; Brittain et al., 2023). These systems often show circumstellar disks and bipolar outflows that are broadly similar to those around low-mass protostars, but with higher luminosities. The higher luminosities can change how the inner disk is heated and how gas accretes onto the star (Natta et al., 2001). Toward the upper end of this mass range, intermediate-mass stars are also more often found in clustered environments (Testi et al., 1997).

In the following, we refer to stars with $m \leq 8 M_\odot$ as lower-mass stars.

2.4

MASSIVE STAR FORMATION

The formation of high-mass stars ($m \gtrsim 8 M_\odot$) underlies a higher complexity that distinguishes it from the formation of lower mass stars. Massive protostars evolve much faster and reach higher luminosities during their early stage of evolution providing strong feedback that influences their surroundings (e.g. Palla & Stahler, 1993; Keto & Wood, 2006). The classical spherical accretion model, which describes the formation of low-mass stars, gives challenges when applying it to massive stars. This is mainly due to the difference in the Kelvin-Helmholz (KH) timescale. The KH timescale indicates a phase during which a protostar balances radiative energy losses through gravitational contraction before nuclear reactions begin. It is given by

$$t_{\text{KH}} = \frac{GM^2}{RL}, \quad (2.41)$$

where G is the gravitational constant, M the mass, R the radius and L the luminosity of the protostar. For a protostar with $1 M_\odot$, the KH timescale is around $5 \cdot 10^7$ years. The timescale decreases significantly to about $6 \cdot 10^4$ years for a protostar with $15 M_\odot$, which shows the rapid increase in luminosity and contraction rate of higher mass stars (Iben, 1965; Hosokawa & Omukai, 2009). In comparison, the free-fall time, t_{ff} , (Eq. 2.24) defined as the time it takes for a gravitational collapse in absence of oppose forces, is largely independent of stellar masses and primarily depends on the core density. For typical core densities of $n_{\text{H}_2} \sim 10^4 \text{ cm}^{-3}$, the free-fall time results to about $4 \cdot 10^5$ years. Therefore, in the case of massive stars the free-fall time exceeds the KH timescale, $t_{\text{ff}} \gg t_{\text{KH}}$. This indicates that massive stars begin hydrogen burning while they are still accreting mass from their surrounding (Palla & Stahler, 1993). This early start of hydrogen burning phase results in a strong radiation pressure that oppose the gravitational collapse and prevent mass accretion (Kahn, 1974; Wolfire & Cassinelli, 1987). Early studies of a one-dimensional, spherical symmetric model predict that this radiation pressure could be strong enough to limit the final mass of a protostar to about $40 M_\odot$ (Kahn, 1974). These results suggested that the classical low-mass star formation model was not sufficient enough to explain the formation of high-mass stars and multi-dimensional models were developed to address the challenge of further mass growth despite strong

radiative feedback (Stahler & Palla, 2004). Recent simulations suggest that massive stars primarily accrete material through circumstellar disks, rather than via isotropic, spherical symmetric inflow. Accretion happens in the equatorial plane, thus radiation can easier escape along the lower-density pole regions. The directional escape of radiation reduces the radiation pressure acting against the infalling gas, allowing continued mass accretion. This is known as the "flashlight effect", introduced in the context of simulations done by Yorke & Sonnhalter (2002) and later by Krumholz et al. (2009); Kuiper et al. (2010). Additionally, mass accretion flows are often clumpy and filamentary rather than smooth. This irregular structure enables material to continue reaching the protostar even in the presents of strong radiative feedback (Kuiper et al., 2010).

2.4.1

STELLAR FEEDBACK

The formation of massive stars, typically with masses larger than $8 M_{\odot}$, involves several additional physical processes that must be taken into account.

At the earliest stages, massive young stellar objects (MYSOs) are observed as deeply embedded sources with compact circumstellar disks, collimated molecular outflows, and jets, reminiscent of the structures seen around low-mass protostars (Beuther et al., 2007; Cesaroni et al., 2007; Tan et al., 2014). As accretion proceeds, the luminosity of the central object increases and shocks in the infalling and outflowing gas become stronger. Shocks are regions where fast gas is abruptly slowed down, compressed, and strongly heated. Radiative heating from the protostar and dissipative heating in shocks both act on the surrounding material, and the dust and gas in the immediate vicinity are heated to temperatures of order 100 K or higher. This gives rise to so-called hot molecular cores, which are compact, dense, and warm regions with rich spectra and strong emission from a wide range of complex molecules (Osorio et al., 1999; Herbst & van Dishoeck, 2009). They are thought to trace one of the earliest embedded phases of massive star formation (Kurtz et al., 2000).

As the massive protostar evolves further, it emits intense ultraviolet (UV) radiation with photon energies exceeding 13.6 eV, which is the ionization threshold for hydrogen. This radiation ionizes the surrounding gas, creating H II regions, which are regions of ionized hydrogen (Spitzer, 1978). In the very earliest ionised phase, the ionised gas is confined to extremely small and dense hyper-compact H II regions (HC-H II) with sizes $\lesssim 0.05$ pc (Kurtz, 2005). As the ionised region grows, it expands into an ultra-compact H II region (UC-H II) with typical sizes of ~ 0.05 - 0.1 pc (Churchwell, 2002). Both HC- and UC-H II regions are usually observed as bright, compact radio continuum sources still embedded in dense molecular material. In these early phases, the thermal pressure of the ionised gas greatly exceeds that of the surrounding neutral medium. The resulting pressure gradients push material outwards and begin to carve cavities around the massive star. Over time, these H II regions can expand further, eventually reaching sizes of several parsecs. The compression of the surrounding gas can trigger further star formation (Zinnecker & Yorke, 2007). Expanding H II regions not only halt further mass accretion of the parental star but also of the stars in the vicinity and therefore limit on the overall star formation efficiency within the region and finally dispersing the parental cloud (Dale et al., 2013).

Additionally, stellar winds are an important aspect of the formation of massive

stars which not only influences the nearby environment but also larger scales. These winds are predominantly driven by radiation pressure and inject energy and momentum into their surrounding. Locally, stellar winds can regulate the accretion process leading to smaller final stellar masses (Gatto et al., 2017). They drive cavities helping radiation to escape. On larger scales, the injected energy can disturb the parental clump, drive turbulence and large-scale outflows. Moreover, more massive stars enrich the interstellar medium with higher amounts of metals - elements heavier than helium - through these winds, contributing to the chemical evolution of their host galaxy (Higgins et al., 2023).

Another feedback mechanism that influences the formation of (massive) stars are cosmic rays. Cosmic rays can be produced by stellar winds or supernovae but also from extragalactic sources. Unlike UV-photons, which are directly absorbed, cosmic rays can penetrate deeply into dense molecular clouds (Draine, 2011). They reach regions which are otherwise shielded from an external radiation field. Cosmic rays have a low level of ionization rate and therefore regulate the coupling of the gas with the magnetic field. Cosmic ray heating influences the thermal structure of the gas and may change the IMF. These effects can change the dynamics of the gravitational collapse and fragmentation (Padovani et al., 2009).

A further important feature in terms of massive star formation is magnetic fields. Magnetic fields can suppress fragmentation in massive clumps. This favors the growth of individual massive stars instead of a cluster of lower-mass stars (Commerçon et al., 2011). On the other hand, non-ideal magnetohydrodynamic effects, such as Ambipolar diffusion, Ohmic dissipation and Hall effect, reduce the tight coupling between magnetic fields and the collapsing gas, which allows the formation of circumstellar disks even in magnetized environments (Wurster et al., 2016; Masson et al., 2016). Magnetically launched bipolar outflows and jets can also be observed around massive stars (e.g. Beuther et al., 2002b; Purser et al., 2016). They play an important role in removing angular momentum and clearing cavities along the pole axis, which allows radiation to escape (e.g. Yorke & Sonnhalter, 2002; Kuiper et al., 2010; Menon et al., 2023).

At the end of its life, a massive star explodes as a supernova, releasing a high amount of energy, radiation and chemical enriched material into the ISM. The resulting shock waves can disperse the parental molecular cloud and may halt star formation in their direct environment (Cioffi et al., 1988), but they can also trigger new star formation by compressing and collecting gas in the surrounding ISM (e.g. Luisi et al., 2021). Beyond the local effects, supernovae shape the structure of the ISM and drive the chemical evolution on galactic scales (Mac Low & Klessen, 2004).

2.4.2

FORMATION THEORIES

Beyond the idealized inside-out scenario of Shu (1977) (see Sec. 2.3.1), several models have been proposed to explain how stars form and how they accrete their mass. The core accretion or core-fed model extends the low-mass star formation model to high-mass stars (McKee & Tan, 2003; Krumholz et al., 2005; Tan et al., 2014). In this framework, turbulence in a fragmenting clump lead to the formation of a centrally condensed massive core ($\sim 10^2 M_{\odot}$). This prestellar core is gravitationally bound and approximately isolated from its surroundings. Consequently, the mass available for accretion is largely determined by the prestellar core itself. This configuration allows a controlled, core-fed manner. Observationally, one of the main challenges of

this model is the limited direct evidence for massive prestellar cores. These cores have rarely been detected, even after extensive surveys (Motte et al., 2018).

A contrasting model is the competitive accretion model, which incorporates a multi-scale, dynamic framework (Bonnell et al., 2001; Bonnell & Bate, 2006; Smith et al., 2009; Vázquez-Semadeni et al., 2019; Padoan et al., 2020). In this scenario, a protostar is initially formed as a low-mass object within a massive clump. Its mass reservoir is not limited by the prestellar core but can originate from the larger scale clump. All fragments within the clump compete for the available mass and those that accrete most efficiently grow more massive over time. Not all fragments will evolve into massive stars. This process is often referred to as clump-fed accretion. The model naturally explains the mass segregation observed in clusters, where the most massive stars are centrally concentrated. It also predicts that stellar masses are a dynamic outcome of the gas distribution, turbulence, and gravitational interactions, rather than being fully predetermined by the initial core.

A related concept that can limit the growth of the most massive protostar is fragmentation-induced starvation (Peters et al., 2010b; Girichidis et al., 2012). In this picture, a forming massive star is fed by a disc and/or filamentary inflow. If the inflowing structure contains sufficient amount of mass, it can fragment and form additional protostars. These companions accrete from the same gas stream and accrete material that would otherwise reach the central protostar. Consequently, the accretion rate onto the massive protostar is reduced and its growth can be halted even if the larger-scale reservoir still contains mass.

Recent models highlight the role of internal inflows driven by turbulent velocity fields on larger scales (Padoan et al., 2020). In this scenario, the mass reservoir of the clump is supplemented by stochastic accretion flows from the surrounding medium. Gas can flow along filaments and channels from the clump and even from the larger molecular cloud into protostellar cores. This mechanism explains how stars can gain mass beyond the initially available prestellar core mass. These multi-scale interactions show the complex coupling between core, clump, and cloud scales in determining the final mass and multiplicity of massive stars.

Relevant aspects for this thesis In this thesis, the focus is placed on the feedback of ionizing radiation and radiation pressure, as these represent the dominant mechanisms governing the early evolution of massive star-forming regions. Stellar winds are not included, since their impact during the early evolutionary stages is expected to be relatively minor compared to photoionization effects (Haid et al., 2018). Furthermore, magnetic fields, protostellar outflows, and cosmic ray feedback are neglected in the present simulations. Although these processes may influence the dynamics, fragmentation, and long-term evolution of molecular clouds, their inclusion would substantially increase the computational complexity. The adopted simplifications therefore allow us to isolate and examine the effects of ionizing feedback and radiation pressure in a controlled framework, while deferring the investigation of additional feedback channels to future work.

OBSERVATIONAL METHODOLOGY

High-mass star formation remains challenging to observe due to the short evolutionary timescales, large distances, and high extinction in their natal environments. Observations require both high angular resolution and sensitivity to cold dust and molecular gas. Over the past decades, several interferometric surveys have investigated the internal structure of giant molecular clouds and the early stages of massive star and cluster formation (e.g. [Beuther et al., 2002a](#); [Zhang et al., 2005](#); [Bontemps et al., 2010](#); [Csengeri et al., 2017](#); [Motte et al., 2018](#); [Sanhueza et al., 2019](#)). Such observations show that high-mass stars form in dense, clustered environments and that feedback processes such as ionizing radiation, outflows, and radiation pressure play a fundamental role in shaping their evolution. The advantages in observations have arisen due to millimeter and submillimeter interferometers, which can resolve dust continuum and molecular line emission on scales of a few ten to hundred astronomical units (au), even at large distances. One important instrument is the Atacama Large Millimeter/submillimeter Array (ALMA), which leads in both spatial resolution and sensitivity and enables the study of the earliest stages of high-mass star formation in unprecedented detail.

3.1

BASICS OF INTERFEROMETRIC IMAGING

In this section, we provide a short overview of the basic principles of interferometric imaging, which are required to understand the approach adopted for our synthetic observations.

An interferometer such as ALMA consists of several telescopes that observe the same part of the sky at the same time. The advantage of using multiple telescopes instead of a single one is that they can be placed far apart, which allows the array to mimic a telescope with a size comparable to their separation. In other words, an interferometer replaces one large telescope by many smaller telescopes spread over a larger area and working all together. In the case of ALMA, the telescopes are not based on mirrors (as in optical and infrared astronomical facilities), but are antennas that are sensitive to radio wavelengths. For this reason, interferometers like ALMA are usually referred to as radio interferometers.

An interferometer does not measure images directly. Instead, it measures the Fourier transform of the sky brightness distribution ([Thompson et al., 2017](#)). Each pair of antennas forms a baseline of length B (corresponding to the separation between the two antennas) and produces one complex number, called a visibility, at a single point in the (u, v) -plane. Physically, each baseline is most sensitive to a simple wave-like fringe pattern on the sky. The visibility is the complex amplitude of this pattern. Its modulus tells us how strong that spatial frequency is in the sky brightness, and its phase tells us where the corresponding structure is located on the sky.

By combining the visibilities from all baselines (i.e., all pairs of antennas), the interferometer samples many different spatial frequencies and thus traces the Fourier components of the sky brightness $I_\nu(x, y)$.

Because of this, an interferometer samples different spatial frequencies (i.e. different spatial scales) depending on how its antennas are distributed, or equivalently on the set of baseline separations. This is why interferometers act as “spatial filters”, i.e., they are sensitive to a limited range of spatial scales set by their baselines. The characteristic angular resolution is set by the longest projected baseline $B_{\max}$:

$$\theta_{\text{res}} \simeq \frac{\lambda}{B_{\max}}, \quad (3.1)$$

The maximum recoverable scale (MRS) of an interferometer is set by the shortest baseline $B_{\min}$. A commonly used empirical approximation is

$$\theta_{\text{MRS}} \simeq 0.6 \frac{\lambda}{B_{\min}}, \quad (3.2)$$

where the factor 0.6 is adopted from the ALMA (Cortés et al., 2025) and may differ for other telescopes and imaging setups. Long baselines therefore resolve compact structure, whereas short baselines are required to recover extended emission. Because the sampling of the (u, v) -plane is incomplete, the interferometer acts as a spatial filter. Emission on angular scales larger than θ_{MRS} is partially or fully resolved out. In addition, the inverse Fourier transform of the visibilities produces a so-called dirty image, the true sky brightness convolved with the synthesized beam, which has significant sidelobes. These sidelobes produce artifacts that must be removed by deconvolution or CLEANing algorithms to recover a faithful image of the sky.

During the CLEANing process the brightest emission peaks are iteratively identified, and the effect of the instrument’s response, the synthesized beam, is subtracted. From these CLEAN components, the sky image is reconstructed and, in a final step, convolved with an idealized Gaussian beam. This procedure yields the final CLEANed image. However, because an interferometer is limited by its shortest baseline, the maximum size of structures it can detect is finite, and emission from more extended regions may be filtered out.

Besides the limitations imposed by the (u, v) -coverage and the synthesized beam, the final image quality is also controlled by the thermal noise level in the data. The root-mean-square (RMS) noise decreases with increasing bandwidth and integration time, and it improves when more antennas (and therefore more baselines) are available. In practice, the noise level depends on the system temperature, the array configuration, the observing frequency, and the total on-source time.

3.2

THE ALMA TELESCOPE

The ALMA telescope is a powerful radio interferometer located on the Chajnantor Plateau in northern Chile (e.g. Wootten & Thompson, 2009). It consists of sixty-six antennas. Fifty-four 12 m dishes and twelve 7 m dishes that form the Atacama Compact Array (ACA). By combining signals from multiple antennas, ALMA has baselines ranging from ~ 15 m up to ~ 16 km, achieving angular resolutions down to $\sim 0.005''$ at its highest observing frequencies (Band 10, ~ 950 GHz) (Cortés et al., 2025).

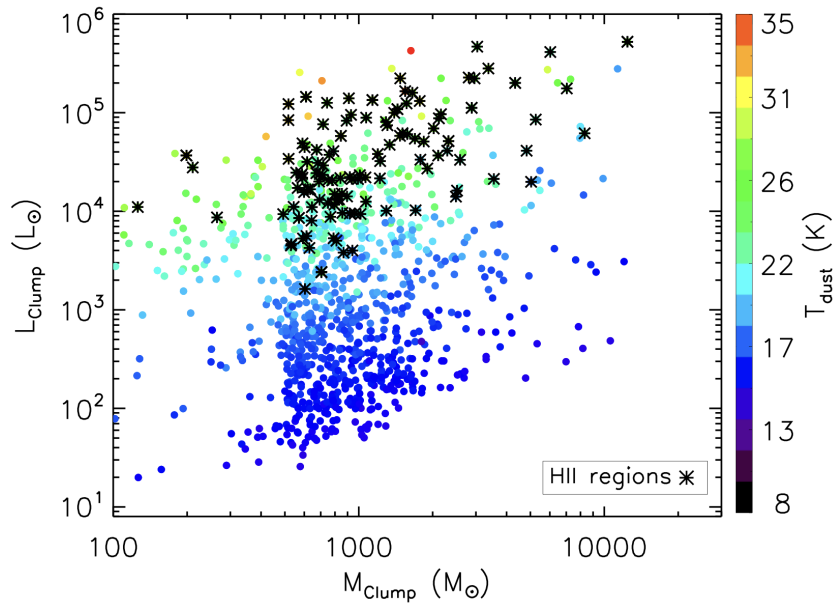


Figure 3: Bolometric luminosity, L_{bol} , versus clump mass, M_{clump} , for the 1017 selected clumps in the ALMAGAL survey. Points are color-coded according to the dust temperature T_{dust} . Asterisks mark Hi-GAL sources linked to H II regions identified in the CORNISH (Purcell et al., 2013) and CORNISH-S (Irahor et al., 2023) surveys. Credit: [Molinari et al. \(2025\)](#)

ALMA is designed to observe (sub-)mm wavelengths, where cold gas and dust emit most of their radiation. It currently offers ten receiver bands, covering frequencies from about 35 GHz to 950 GHz (wavelengths from ~ 9 mm to ~ 0.3 mm). The lower bands (e.g. Bands 1–3, ~ 35 –116 GHz) are well suited to study relatively extended, colder gas, low-frequency molecular lines, and continuum from more evolved disks and jets. Intermediate bands such as Band 6 (~ 211 –275 GHz, $\lambda \sim 1.3$ mm) and Band 7 (~ 275 –373 GHz, $\lambda \sim 0.8$ mm) are widely used to trace dense molecular gas (e.g. CO and its isotopologues, HCN, HCO^+) and dust continuum in star-forming regions, disks, and nearby galaxies. The highest-frequency bands (Bands 8–10, up to ~ 950 GHz) provide very high angular resolution and sensitivity to warm dust and highly excited molecular transitions, but are more strongly affected by atmospheric opacity.

Because of this broad frequency coverage and flexible array configurations, ALMA can observe a wide range of molecular line and dust continuum emission that traces the cold interstellar medium and star formation processes across many scales: from giant molecular clouds and massive clumps down to individual dense cores, disks, and jets (e.g. [Motte et al., 2018](#)).

3.3

ALMAGAL SURVEY

The ALMAGAL survey (ALMA Evolutionary Study of High-Mass Protocluster Formation in the Galaxy) provides high-resolution and high-sensitivity observations that enable a detailed study of massive star-forming regions across the Milky Way ([Molinari et al., 2025](#); [Sánchez-Monge et al., 2025](#)). By combining dust continuum

and molecular line observations at sub-arcsecond resolution, ALMAGAL allows the identification of embedded protostars, compact cores, and feedback signatures.

The survey makes use of the ALMA telescope to systematically study 1017 dense clumps. These clumps have typical masses around $1000 M_{\odot}$ (see Fig. 3), surface densities exceeding 0.1 g cm^{-2} , and distances up to 7.5 kpc. Observations are done at 1.38 mm (corresponding to $\sim 219 \text{ GHz}$) and include both dust continuum and molecular line emission.

To recover both compact and extended emission, ALMAGAL combines data from three array configurations: the ACA 7 m array and two 12 m array configurations (TM1 and TM2). This strategy provides a nearly uniform spatial resolution of 800-2000 au across the full distance range of the survey, enabling detailed studies of fragmentation and small-scale structure within high-mass star-forming clumps. The achieved mass sensitivity in the continuum ranges between 0.02 and $0.07 M_{\odot}$ per beam, depending on distance.

The first set of ALMAGAL publications already illustrates the wide range of analyses enabled by the combined continuum and line dataset. [Molinari et al. \(2025, ALMAGAL I\)](#) introduce the survey, its scientific goals, and target selection, while [Sánchez-Monge et al. \(2025, ALMAGAL II\)](#) describe the observational strategy, calibration, and data products. [Coletta et al. \(2025, ALMAGAL III\)](#) build the compact core catalogue and characterise the fragmentation and the mass and size distributions, as well as the evolutionary trends of the core population. [Mininni et al. \(2025, ALMAGAL IV\)](#) compare the morphology of the dust continuum and multiple molecular tracers using the histogram of oriented gradients method to identify which lines best trace the bulk dense gas. [Elia et al. \(2026, ALMAGAL V\)](#) relate the demographics and physical properties of the cores to clump-scale quantities such as mass, luminosity-to-mass ratio, and environment, while [Schisano et al. \(2025, ALMAGAL VI\)](#) analyse how the spatial distribution and clustering of dense cores evolve along the clump evolutionary sequence. Finally, [Wallace et al. \(2025, ALMAGAL VIII\)](#) use the continuum emission to characterise the hierarchical mass structure from clumps down to individual cores across the survey.

With the high sensitivity, angular resolution, and flexible array configurations, the ALMAGAL survey provides a statistically significant, high-resolution view of massive star-forming clumps across a wide range of evolutionary stages. These data are ideally suited for comparison with numerical simulations, enabling direct tests of theoretical models under realistic observational conditions.

Relevant aspects for this thesis In this thesis, we focus on the dust continuum emission observed by ALMA at 1.36 mm. The dust continuum is a direct tracer of the column density and mass distribution of the dense gas within star-forming clumps, as it originates from thermal emission of cold dust grains that are well coupled to the gas. Unlike molecular line emission, which depends on chemical abundances and excitation conditions, the continuum provides a robust probe of the underlying structure and morphology of the cloud.

NUMERICAL SIMULATIONS

Observations provide the fundamental constraints on how massive stars form, but they are often limited by spatial resolution and temporal cadence. These limitations make it difficult to disentangle the coupled effects of turbulence, self-gravity, radiation, magnetic fields, and feedback, since many of these processes operate simultaneously and leave overlapping signatures. Numerical simulations therefore play a central complementary role. They can model the relevant physics, as (magneto-)hydrodynamics, self-gravity, radiative transfer, and feedback from radiation pressure and ionization, in a controlled framework. By introducing physical ingredients step by step, simulations enable systematic tests of their relative importance and allow us to quantify how each process influences accretion, fragmentation, and ultimately the efficiency of star formation.

In the following, the FLASH code is introduced and the physical processes included in this work are explained.

4.1

FLASH 4

All simulations presented in this thesis are performed with the adaptive mesh refinement (AMR) code FLASH (Fryxell et al., 2000). FLASH provides a flexible framework in which different physical processes can be included via dedicated modules. In the following sections, the relevant physical modules used in this work are described in detail (hydrodynamics, self-gravity, chemistry and heating/cooling, and radiative transfer including radiation pressure).

Astrophysical simulations cover a wide range of spatial scales. For example, molecular clouds can span several parsecs, while accretion flows occur on scales of tens of AU. Resolving all of these scales with a uniform grid would be computationally inefficient and prohibitively expensive. FLASH therefore employs adaptive mesh refinement (AMR). The three dimensional computational domain is divided into cubic blocks, each containing 8^3 cells. Blocks can be dynamically refined by replacing one block with eight child blocks. Each child block has half the linear size of the parent block (thereby increasing the spatial resolution). Blocks can also be derefined by reverting this process, depending on local refinement criteria.

In the simulations, refinement is guided by the Jeans length,

$$\lambda_J = \left(\frac{\pi c_s^2}{G\rho} \right)^{1/2}, \quad (4.1)$$

which is required to be resolved by at least 8 grid cells following Truelove et al. (1997) in order to avoid artificial fragmentation. This strategy provides high resolution in regions of interest, such as collapsing protostars or dense filaments, while keeping a coarser grid in more diffuse regions.

FLASH organizes the AMR hierarchy using an octree data structure. The octree

stores the blocks in a tree-like arrangement. The root represents the full simulation domain, refined blocks become child nodes, and blocks that are not further refined form the leaves. This structure enables efficient access to blocks at different refinement levels and is also used by several physics modules in this work, in particular for the tree-based computation of self-gravity (Section 4.3) and for radiative transfer within the TreeRay framework (Section 4.5).

4.2

(MAGNETO)-HYDRODYNAMICS

In the regime of star formation, the gas can be treated as a continuous fluid and is modeled using the fluid approximation. This approach is valid when the mean free path of particles, λ , is much smaller than the characteristic scale of interest (Bodenheimer et al., 2007). For a primarily neutral gas, which dominates molecular clouds, the mean free path can be estimated as $\lambda = 1/(n\sigma)$, where n is the number density of neutral particles and σ is the scattering cross section. For typical molecular cloud conditions, with n of a few 100 – 1000 atoms per cm^3 and $\sigma \sim 10^{-15} \text{ cm}^2$, the mean free path is $\lambda \sim 10^{12} - 10^{13} \text{ cm}$. This is much smaller than the typical size of a molecular cloud, which is on the order of tens of parsecs ($10^{19} - 10^{20} \text{ cm}$), justifying the use of the fluid approximation (Bodenheimer et al., 2007).

For the gas evolution in FLASH we employ the entropy-stable magnetohydrodynamics (MHD) solver developed by Derigs et al. (2016). The ideal MHD equations are:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \quad (4.2)$$

$$\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot \left(\rho \mathbf{v} \otimes \mathbf{v} + \left(P + \frac{B^2}{8\pi} \right) \mathbf{I} - \frac{\mathbf{B} \otimes \mathbf{B}}{4\pi} \right) = \rho \mathbf{a}, \quad (4.3)$$

$$\frac{\partial E}{\partial t} + \nabla \cdot \left[\left(E + P + \frac{B^2}{8\pi} \right) \mathbf{v} - \frac{(\mathbf{B} \cdot \mathbf{v}) \mathbf{B}}{4\pi} \right] = \rho \mathbf{v} \cdot \mathbf{a} + \dot{U}, \quad (4.4)$$

$$\frac{\partial \mathbf{B}}{\partial t} - \nabla \times (\mathbf{v} \times \mathbf{B}) = 0, \quad (4.5)$$

$$\nabla \cdot \mathbf{B} = 0, \quad (4.6)$$

where ρ is the gas density, $\mathbf{v}$ is the velocity field, P is the pressure, $\mathbf{B}$ the magnetic field, E is the total energy density, $\mathbf{I}$ is the identity tensor, $\mathbf{a}$ represents external accelerations and $\dot{U}$ denotes the source terms from external heating and cooling processes (see Section 4.4). The total energy density is

$$E = U + \frac{1}{2} \rho v^2 + \frac{B^2}{8\pi}, \quad (4.7)$$

where U denotes the internal energy density. The system is closed with the ideal-gas equation of state

$$P = (\gamma - 1) U, \quad (4.8)$$

where γ is the adiabatic index.

Equation 4.2 is the continuity equation, which ensures mass conservation. Equation 4.3 is the momentum equation, describing how momentum changes due to pressure gradients and external forces. The third equation, Eq. 4.4, is the energy

equation which tracks the evolution of the total energy, including compressional heating and cooling through the $P \nabla \cdot \mathbf{v}$ term. Additional heating and cooling processes enter as source terms $\dot{U}$ (see Section 4.4). Eq. 4.5 is the induction equation of ideal MHD and Eq. 4.6 enforces a divergence-free magnetic field.

In the present work, the simulations are purely hydrodynamical and do not include magnetic fields and set $\mathbf{B} = 0$, which reduces the ideal MHD equations to the hydrodynamic equations.

A common approach to solve the (magneto)-hydrodynamic equations is the finite-volume-method (FVM) (Bodenheimer et al., 2007), which is a grid-based method also used in FLASH. The FVM has two important properties. First, the mass, momentum and energy are conserved. Second, it robustly handles discontinuities, such as shocks or ionization fronts. The idea is to divide the computational domain into controlled volumes, or cells, and compute the fluxes across the cell boundaries to evolve the conserved quantities. The general form of a conservation law can be written as

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{U}) = 0, \quad (4.9)$$

where $\mathbf{U}$ is the vector of the conserved variable (e.g., density and momentum) and $\mathbf{F}(\mathbf{U})$ is the flux vector. The FVM updates the cell-averaged value of $\mathbf{U}_j^n$ for cells j at timestep n over a time-interval Δt according to

$$\mathbf{U}_j^{n+1} = \mathbf{U}_j^n - \frac{\Delta t}{\Delta x} \left(\hat{\mathbf{F}}_{j+1/2}^n - \hat{\mathbf{F}}_{j-1/2}^n \right), \quad (4.10)$$

where $\hat{\mathbf{F}}_{j\pm 1/2}^n$ are the numerical fluxes through the cell interfaces. These fluxes are computed by solving local Riemann problems at each cell interface, which account for the discontinuity between the left and right states reconstructed from neighboring cells. The time stepping is controlled by the Courant–Friedrichs–Lewy (CFL) condition, which limits the timestep so that the fluid does not propagate more than a fraction of a grid cell in one step (usually set to 0.5). It can be further reduced to prevent the chemical abundances from changing too strongly within a single update (see Sec. 4.4).

4.3

SELF-GRAVITY

For self-gravity, the gravitational potential, Φ , is related to the gas density via Poisson’s equation,

$$\nabla^2 \Phi = 4\pi G \rho, \quad (4.11)$$

where G is the gravitational constant. The gravitational acceleration is then given by

$$\mathbf{g} = -\nabla \Phi. \quad (4.12)$$

Self-gravity is included in the simulations and is computed with a tree-based solver that operates on the Octree structure introduced in Section 4.1. A direct summation of gravitational interactions between all cells scales as $O(N^2)$ and is therefore not feasible for large simulations. The tree-based approach reduces the computational cost to $O(N \log N)$ (Wünsch et al., 2018). The smallest tree elements, the leaves, store the information needed for the gravity calculation. An opening-angle test decides whether a region is split into smaller parts (nearby) or treated as

one combined gravitational source (far away).

4.4

CHEMICAL NETWORK

To follow the coupled chemical and thermal evolution of the gas, the simulations use a simplified non-equilibrium chemistry model, the so-called NL97 network, following [Nelson & Langer \(1997\)](#) and [Glover & Mac Low \(2007\)](#); [Glover et al. \(2010\)](#). The network evolves seven species: molecular hydrogen (H_2), atomic hydrogen (H), ionized hydrogen (H^+), carbon monoxide (CO), singly ionized carbon (C^+), atomic oxygen (O), and free electrons (e^-). The reaction rates are taken from [Nelson & Langer \(1997\)](#). The implemented heating and cooling processes are described in [Walch et al. \(2015\)](#).

Each chemical species is updated by accounting for both transport with the flow and local chemical reactions. For species i with mass density ρ_i , we write

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{v}) = C_i(\rho, T, \dots) - D_i(\rho, T, \dots), \quad (4.13)$$

where the left-hand side describes how species, i , is carried with the gas flow, and the right-hand side gives the net change due to chemistry, where C_i is the formation rate and D_i is the destruction rate. Both terms depend on the local gas properties (e.g. density and temperature) and on the abundances of other species.

In the code, advection and chemistry are treated in two steps. First, each species is simply carried along with the gas flow,

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{v}) = 0, \quad (4.14)$$

and then the chemical reactions are applied locally in each cell by solving

$$\frac{d\rho_i}{dt} = C_i(\rho, T, \dots) - D_i(\rho, T, \dots). \quad (4.15)$$

The chemistry is computed together with the heating and cooling, so that the energy released or absorbed by reactions is added to the energy equation (see Eq. 4.4) as a source term.

The gas temperature is determined by heating and cooling processes that are evaluated consistently with the chemical state. In these simulations, the cooling includes collisional dissociation of H_2 , collisional ionization of H , metal line cooling, in particular from C^+ and O , recombination cooling of H^+ in ionized gas, and energy exchange by gas–dust coupling ([Walch et al., 2015](#); [Haid et al., 2018](#)). In fully ionized gas within forming H II regions, cooling by H^+ recombination dominates, while cooling by C^+ and O lines is negligible ([Haid et al., 2018](#)). The heating terms include heating from H_2 formation, heating associated with H_2 photodissociation, shock heating, heating from the release of gravitational potential energy, cosmic ray heating, photoelectric heating, and photoionization heating. Photoionization heating is included via the chemistry network (see [Haid et al., 2018](#)) and is described in more detail in Section 4.7. Dust heating and cooling are further described in Section 4.8.1.

We assume that gas and dust are perfectly mixed. The dust-to-gas mass ratio, f_d ,

depends on the gas metallicity, Z , and is given by

$$f_d = \frac{1}{100} \frac{Z}{Z_\odot}. \quad (4.16)$$

For solar metallicity, $Z = 1 Z_\odot$, the dust-to-gas mass ratio is 0.01. In this thesis, we consider three metallicities, $Z = 0.5, 1$, and $2 Z_\odot$. For each metallicity, we rescale the dust-to-gas ratio according to Eq. 4.16 and scale the initial metal abundances (i.e. all elements heavier than hydrogen and helium) by the same factor. The heating and cooling rates are not changed.

The rates of photon-driven reactions (e.g. photoionization, photodissociation and photoelectric heating) depend on dust attenuation and on self-shielding by H_2 and CO. We account for these effects using the `TREERAY/OPTICALDEPTH` module (Wünsch et al., 2018) (see Sec. 4.5.1). In this work, we set an external interstellar radiation field (ISRF) to zero, since the simulated cores are assumed to be strongly shielded and embedded in a dense environment. As a consequence, photoprocesses associated with an ambient background field are suppressed and the radiation relevant for chemistry and heating is dominated by internal sources and cosmic ray heating.

4.5

RADIATIVE TRANSFER

Radiative transfer (RT) is computed with the `TREERAY` framework and is treated in a grey, steady-state approximation without scattering (Wünsch et al., 2018; Klepitko et al., 2023). In this framework, the radiation intensity, I , along a propagation direction, $\hat{\mathbf{n}}$, follows

$$\hat{\mathbf{n}} \cdot \nabla I = -aI + j, \quad (4.17)$$

where a and j are the (Planck-weighted) extinction and emission coefficients, respectively. We write

$$a = \kappa_P \rho, \quad (4.18)$$

with ρ the gas density and κ_P the Planck mean dust opacity. Thermal emission is described by

$$j = \kappa_P \rho \frac{\sigma}{\pi} T_d^4, \quad (4.19)$$

where σ is the Stefan-Boltzmann constant and T_d is the dust temperature associated with the emitting material.

From the intensity, we compute the mean intensity, $\bar{J}$, and the radiative flux, $\mathbf{F}$, as

$$\mathbf{F} = - \oint_S I \hat{\mathbf{n}}_{\text{rad}} d\Omega, \quad (4.20)$$

$$\bar{J} = \frac{1}{4\pi} \oint_S I d\Omega, \quad (4.21)$$

where $\hat{\mathbf{n}}_{\text{rad}}$ is the radial unit vector on the unit sphere and $d\Omega$ is the solid angle element.

For the dust opacity we employ a Planck mean prescription based on Semenov et al. (2003) in the form used by Krumholz & Thompson (2012),

$$\kappa_P(T_d) = 10^{-1} \frac{\text{cm}^2}{100 \text{ K}^2 \text{ g}} \times \begin{cases} T_d^2 & \text{for } T_d < 150 \text{ K} \\ (150 \text{ K})^2 & \text{else} \end{cases}. \quad (4.22)$$

RT is implemented with a reverse ray-tracing approach. For each target cell, rays are cast in a set of discrete directions on the sky. In this work, $N_{\text{PIX}} = 48$ directions are used, distributed with the HEALPix algorithm (Górski et al., 2005). Along each ray, contributions from sources and absorbing material are accumulated, and the directional information is combined to obtain local radiation field quantities (e.g. $\bar{J}$ and $\mathbf{F}$) used by the subsequent physics modules. The tree-walk makes use of the Octree structure introduced in Section 4.1.

4.5.1

OPTICAL DEPTH AND SHIELDING

Attenuation of radiation along a line of sight is given by

$$I_\nu = I_{\nu,0} e^{-\tau_\nu}, \quad (4.23)$$

where $I_{\nu,0}$ is the source intensity at the frequency ν and τ_ν is the integrated optical depth from the source to the target cell.

In the simulations, optical depths and shielding information are computed with the TREERAY/OPTICALDEPTH module (Wünsch et al., 2018), which is based on the TREECOL method of Clark et al. (2012). For each cell, the distribution of the surrounding gas is sampled in discrete N_{PIX} directions. Along each direction i , the column densities (e.g. total hydrogen, H_2 , and CO) are estimated, using the Octree data structure to sample the surrounding gas. These column densities are then used to compute the dust attenuation factor, the H_2 and CO shielding coefficients and the effective three-dimensional visual extinction, $A_{V,3D}$. The three-dimensional visual extinction can be written as

$$A_{V,3D} = -\frac{1}{2.5} \ln \left[\frac{1}{N_{\text{PIX}}} \sum_{n=1}^{N_{\text{PIX}}} \exp \left(-2.5 \frac{N_{\text{H,tot},n}}{1.87 \times 10^{21} \text{ cm}^{-2}} \right) \right], \quad (4.24)$$

where $N_{\text{H,tot},n}$ is the total hydrogen column density in direction n . This form reflects that radiation is reduced exponentially when it passes through matter. In optically thin regions most photons get through, while in optically thick regions dense gas is strongly shielded.

The visual extinction and shielding coefficients provide the basis for the radiation treatments described in the following sections.

4.6

NON-IONIZING RADIATION

Non-ionizing radiation refers to photons with energies below the Lyman-continuum threshold ($h\nu < 13.6 \text{ eV}$).

In the TREERAY framework, non-ionizing radiation can enter as an uniform external interstellar radiation field (ISRF). Its attenuation is computed within the TREERAY/OPTICALDEPTH module (Sect. 4.5.1, Eq. 4.24). In this work, the strength of ISRF is set to zero, since the simulated cores are assumed to be strongly shielded and embedded in a dense environment.

In addition, non-ionizing radiation is produced by sources within the computational domain. The treatment of non-ionizing radiation from internal sources is implemented in the TREERAY/RADPRESSURE framework (Klepitchko et al., 2023). In this approach, every cell and sink particle can act as a source of non-ionizing radiation.

Integrating the transfer equation along each ray gives the directional-depended radiation intensity.

Non-ionizing radiation is absorbed by dust and contributes to dust heating (see Sec. 4.8.1).

4.7

IONIZING RADIATION

Ionizing radiation from massive stars is treated with the `TREERAY/ONTHESPOT` module (Haid et al., 2018; Wünsch et al., 2021). Along each ray, absorption of ionizing photons by gas is computed, and the resulting ionization and heating are coupled to the non-equilibrium chemistry network.

Ionizing photons are defined as Lyman-continuum photons with energies $h\nu \geq 13.6$ eV, which are capable of ionizing hydrogen. Each source is assumed to emit a blackbody spectrum with an effective temperature T_* . From this spectrum we determine the mean energy of ionizing photons, $h\bar{\nu}$, and the corresponding average excess energy, $h(\bar{\nu} - \nu_{\text{LyC}})$, where $h\nu_{\text{LyC}} = 13.6$ eV denotes the hydrogen ionization threshold.

We use the On-The-Spot approximation (Osterbrock, 1988). In this approximation, the photoionization heating rate per absorbed photon per unit volume can be written as (Haid et al., 2018)

$$\Gamma_{\text{ih}} = n_{\text{H}}^2 \alpha_{\text{B}} h(\bar{\nu} - \nu_{\text{LyC}}), \quad (4.25)$$

where n_{H} is the hydrogen number density and α_{B} is the case-B radiative recombination coefficient, accounting for all excited levels above the ground state. This heating typically raises the temperature of the ionized gas to $\sim 10^4$ K, generating pressure gradients that are directly coupled into the hydrodynamic equations. This leads to dynamical feedback such as the expansion of H II regions.

4.8

RADIATION PRESSURE

Radiation pressure (RP) describes the transfer of momentum from photons to gas and dust. In FLASH, this process is implemented in the `TREERAY/RADPRESSURE` module (Klepitko et al., 2023), which builds on the `TreeRay` radiative transfer framework and accounts for momentum transfer from both ionizing and non-ionizing radiation, as well as radiative heating from non-ionizing radiation.

4.8.1

DUST HEATING AND COOLING

Non-ionizing radiation is absorbed by dust and heats the grains. The dust temperature is determined by balancing absorption of the local radiation field with thermal emission. The heating rate due to absorption, $\Gamma_{\text{BB-heat}}$, and the cooling rate due to thermal emission, $\Lambda_{\text{BB-cool}}$, are given by

$$\Gamma_{\text{BB-heat}} = \rho \xi 4 \pi \kappa \bar{J}, \quad (4.26)$$

$$\Lambda_{\text{BB-cool}} = \rho \xi 4 \sigma \kappa T_{\text{dust}}^4, \quad (4.27)$$

where ξ is the dust-to-gas ratio, $\bar{J}$ is the mean radiation intensity, κ is the dust opacity, and T_{dust} is the dust temperature. The equilibrium dust temperature is obtained by solving $\Gamma_{\text{BB-heat}} = \Lambda_{\text{BB-cool}}$.

In addition to radiative heating, dust can gain energy from local non-radiative processes. Collisions with gas particles transfer energy to dust grains, which becomes increasingly important at high densities. Furthermore, the formation of molecular hydrogen, H_2 , on dust grain surfaces releases energy, a fraction of which is absorbed by the grains and contributes to their heating. If an interstellar radiation field (ISRF) is present, it can also provide additional heating to the dust. The dust temperature in turn influences the gas temperature through gas–dust coupling

4.8.2

MOMENTUM TRANSFER AND ACCELERATION

In our simulations, ionizing radiation transfers momentum to the surrounding gas and dust. The total ionizing radiation pressure within each computational cell is obtained by summing the contributions from three distinct processes.

The radiation field is represented by discrete photon packages, each characterized by a photon number rate, $\dot{N}_{\text{ph}} = \frac{F}{h\nu}$, an average photon energy, $\bar{E}_{\text{ph}}$, and a propagation direction, $\mathbf{u}_{\text{ph}}$. As a photon package traverses a computational cell of volume, dV , a fraction of its photons is absorbed depending on the local gas and dust properties. Each absorbed photon transfers a momentum of $\bar{E}_{\text{ph}}/c$ in the direction $\mathbf{u}_{\text{ph}}$.

The first contribution arises from the absorption of ionizing photons by dust, leading to a momentum deposition rate

$$\dot{\mathbf{P}}_{\text{UV,dust}} = \frac{\sigma_{\text{d}} n}{c} \dot{N}_{\text{ph}} \bar{E}_{\text{ph}} \mathbf{u}_{\text{ph}} dV, \quad (4.28)$$

where $\sigma_{\text{d}} = 1.5 \times 10^{-21} \text{ cm}^2$ per hydrogen atom is the dust absorption cross-section (at solar metallicity) and n the gas number density. The second contribution results from the absorption of ionizing photons by neutral hydrogen,

$$\dot{\mathbf{P}}_{\text{UV,H}} = \frac{\sigma_{\text{H}} n_{\text{H}}}{c} \dot{N}_{\text{ph}} \bar{E}_{\text{ph}} \mathbf{u}_{\text{ph}} dV, \quad (4.29)$$

where σ_{H} is the photoionization cross-section and n_{H} the neutral hydrogen number density.

Finally, we account for ionized hydrogen, which temporarily recombines and immediately gets ionized again by the incident ionizing photon flux. This is given by the recombination rate, which we also take into account to calculate the ionization balance:

$$\dot{\mathbf{P}}_{\text{UV,H}^+} = \frac{n_{\text{H}^+}^2 \alpha_{\text{B}} \bar{E}_{\text{ph}}}{c} \mathbf{u}_{\text{ph}} dV, \quad (4.30)$$

where n_{H^+} is the ionized hydrogen density and α_{B} the case-B recombination coefficient.

For completeness, the TREE-RAY/RAD-PRESSURE framework also provides the momentum deposition rate from non-ionizing photons acting on dust,

$$\dot{\mathbf{P}}_{\text{IR,dust}} = \frac{\mathbf{F}}{c} \rho \kappa \frac{1 - e^{-\tau}}{\tau} dV. \quad (4.31)$$

We note, that in this set of simulations, the RP momentum from non-ionizing

radiation is not included, as this capability was not yet implemented in the code at the time the simulations were performed. The dominant RP contribution is expected to arise from ionizing radiation, so the omission of non-ionizing RP should have only a minor effect. Non-ionizing radiation is therefore used only for dust heating.

The corresponding acceleration due to radiation pressure is given by

$$\mathbf{a}_{\text{RP}} = \frac{\dot{\mathbf{p}}}{\rho dV}, \quad (4.32)$$

which expresses the momentum transfer per unit mass.

4.9

SINK PARTICLES

Sink particles represent stellar objects in our simulation. We employ the sink implementation of [Dinnbier & Walch \(2020\)](#), where the motion of sink particles is modeled with a 4th-order Hermite integrator. Sinks are created only on the finest AMR level once a cell exceeds a density threshold, ρ_{thresh} , which depends on the minimum resolved Jeans length of $\lambda_J = 4\Delta x$ with

$$\rho_{\text{thresh}} = \frac{\pi c_s^2}{G \lambda_J^2} = \frac{\pi c_s^2}{G (4\Delta x)^2}. \quad (4.33)$$

([Truelove et al., 1997](#)) In addition, within an accretion radius $r_{\text{acc}} = 2.5\Delta x$, the gas must be infalling and gravitationally bound. The region must be a local minimum of the gravitational potential and contain no other sink ([Federrath et al., 2010](#)). Sinks are only allowed to form if the gas would collapse faster than it would be accreted by a nearby sink ([Clarke et al., 2017](#)). Each sink is treated as a single star whose radius and surface temperature evolve primarily with its accretion history using protostellar evolution model ([Klassen et al., 2012](#)). A more detailed description of how the luminosity is treated is provided in Paper I (see Sec. 7).

4.10

TURBULENCE

For the initial conditions, we generate a turbulent velocity field following [Walch et al. \(2012\)](#). We use a uniform grid of 128^3 cells and generate a random Gaussian velocity field in Fourier space using modes in the range $k_{\text{min}} = 1$ to $k_{\text{max}} = 64$, where $k = 1$ corresponds to $2\pi/L$ with L being the simulation domain size. For each wavevector $\mathbf{k}$ we assign a complex Fourier coefficient

$$\tilde{\mathbf{v}}(\mathbf{k}) = A(k) e^{i\phi(\mathbf{k})}, \quad (4.34)$$

with random phases sampled from a uniform distribution on $[0, 2\pi)$. We use Burgers turbulence by adopting a power spectrum

$$P(k) \equiv \langle |\tilde{\mathbf{v}}(\mathbf{k})|^2 \rangle \propto k^{-4}, \quad (4.35)$$

which implies $A(k) \propto \sqrt{P(k)} \propto k^{-2}$. The velocity field in real space is then obtained via an inverse Fourier transform,

$$\mathbf{v}(\mathbf{x}) = \mathcal{F}^{-1}[\tilde{\mathbf{v}}(\mathbf{k})], \quad (4.36)$$

The velocity field is rescaled (in cgs units) such that its RMS velocity is unity. Since the generated velocity field is normalised, different turbulent field strengths are obtained by multiplying the velocity field by the corresponding velocity dispersion. The velocity dispersion can be obtained from the virial parameter α_{vir} (see Eq. 2.1). For a sphere with uniform density, the one-dimensional velocity dispersion σ is related to α_{vir} via

$$\sigma = \left(\frac{\alpha_{\text{vir}} G M}{5r} \right)^{1/2}, \quad (4.37)$$

where M is the total core mass and r its radius. In this thesis, we consider $\alpha_{\text{vir}} = 0.2, 0.6$, and 1.2 . The initial conditions of the numerical simulations are discussed in detail in Paper I (see Sec. 7).

SYNTHETIC OBSERVATIONS

Connecting numerical simulations with real observations is a key challenge in modern astrophysics. Simulations provide detailed information about three-dimensional distributions of physical quantities such as gas density, temperature, velocity fields, chemical abundances, and radiation fields. However, these quantities cannot be observed directly. Real observations are inherently limited by telescope sensitivity, angular and spectral resolution, instrumental effects, LOS projection, and radiative transfer. To bridge this gap, synthetic observations have become an increasingly important tool.

Numerical simulations can be post-processed with radiative transfer codes to generate synthetic observables such as dust continuum emission, molecular line emission, or polarisation maps. These codes account for absorption, scattering, and thermal re-emission as radiation propagates through the medium, effects that would be prohibitively expensive to compute self-consistently within the simulations. In addition, telescope- and instrument-specific effects, including beam convolution, noise, and limited dynamic range, can be applied. This allows the production of synthetic maps that closely resemble real observations, as if the simulated system were placed on the sky.

The long-term aim of this work is to compare numerical simulations with observations from the ALMAGAL survey. In this thesis, we take the first steps toward this goal and focus on generating synthetic dust-continuum maps from the simulation outputs and applying observational effects so that the resulting maps resemble the ALMAGAL data products and can be compared to the underlying simulation properties (see Sec. 3.3).

5.1

RADIATIVE TRANSFER POST-PROCESSING

A variety of radiative transfer codes exist for post-processing numerical simulations. RADMC-3D (Dullemond et al., 2012) is widely used for dust and line radiative transfer, POLARIS (Reissl et al., 2016) specialises in polarised dust and line emission, TORUS (Harries et al., 2019) combines Monte Carlo radiative transfer with photoionisation modules, and tools such as LIME (Brinch & Hogerheijde, 2010) focus on non-LTE molecular line transfer on irregular grids. In this thesis, we use RADMC-3D to compute synthetic dust-continuum emission from our simulations. We restrict the analysis to thermal dust emission and do not model spectral lines, free-free radiation, or synchrotron components.

5.1.1

RADMC-3D SIMULATIONS

The radiative transfer calculations are based directly on the simulation outputs. For each snapshot, we provide the three-dimensional density field and the dust

temperature distribution as input to RADMC-3D. Since the dust temperature is already computed within the simulation, we do not solve for radiative equilibrium in RADMC-3D.

Dust-continuum emission depends on the dust opacity κ_ν . It describes how efficiently dust absorbs radiation per unit dust mass. The opacity depends on the dust properties (e.g. grain composition and size distribution) and on observing frequency. Different opacity prescriptions are used in the literature, from simple power-law descriptions (Hildebrand, 1983) to more detailed dust models for the diffuse ISM (Draine, 2003). In dense molecular environments, opacities that include grain growth and ice mantles are often adopted (e.g. Ossenkopf & Henning, 1994). In this thesis, we use the dust model of Weingartner & Draine (2001) with $R_V = 4.0$. This corresponds to an absorption opacity of $\kappa_{1.3\text{ mm}} = 0.32\text{ cm}^2\text{g}^{-1}$ per unit dust mass. For the millimetre continuum calculations presented here, we neglect scattering and include only absorption and thermal emission by dust.

Continuum maps are computed by solving the radiative transfer equation along lines of sight through the three-dimensional domain using ray tracing. We generate synthetic emission at $\lambda = 1.36\text{ mm}$ (ALMA Band 6) and place the simulated region at a distance of 3 kpc. Each snapshot is post-processed for three viewing directions, taking lines of sight along the simulation x -, y -, and z -axes, which yields three corresponding two-dimensional intensity maps per snapshot. These maps represent the idealised continuum emission before applying observational effects such as beam convolution and noise.

To match the ALMAGAL continuum observations described in Section 3.3, we generate synthetic dust-continuum maps in ALMA Band 6 at $\lambda = 1.36\text{ mm}$ and place the simulated region at a distance of 3 kpc. These maps are well suited for studying dense structures such as clumps and cores. At this wavelength, the emission is often optically thin, although the highest-column regions can become optically thick.

5.1.2

CASA SIMULATIONS

We simulate ALMA observations with the software CASA. We follow the observing and imaging approach used in the ALMAGAL survey (Sánchez-Monge et al., 2025). As input sky models, we use the two-dimensional RADMC-3D specific-intensity maps from the radiative-transfer step.

The input maps are ideal (noise-free) continuum images at the intrinsic simulation resolution. They contain all small-scale structure in the model clouds and represent the true sky brightness before any instrumental effects. For the CASA simulations, we use two input resolutions (RFL9 and RFL12), corresponding to RADMC-3D sky-model pixel sizes from 403 to 50 au, while keeping the same physical field of view. All CASA observing and imaging parameters described below (e.g. array configuration, weighting, and image pixel size) are kept fixed across RFL9 and RFL12 so that only the input model resolution changes. For RFL9, the sky-model pixel size is $0.134''$, corresponding to 403 au at a distance of 3.0 kpc. For RFL12, the pixel size is 50 au (i.e. $0.0167''$ at the same distance). The maps have 512×512 pixels in RFL9 and 4096×4096 pixels in RFL12, while the field of view is kept fixed at $\simeq 69''$ in both cases. The synthesized beam is $\sim 1200\text{ au}$, which corresponds to ~ 3 input pixels in RFL9 and ensures that the effective angular resolution is set by the beam rather than by the image grid.

We create synthetic ALMA visibilities (the interferometric measurements in

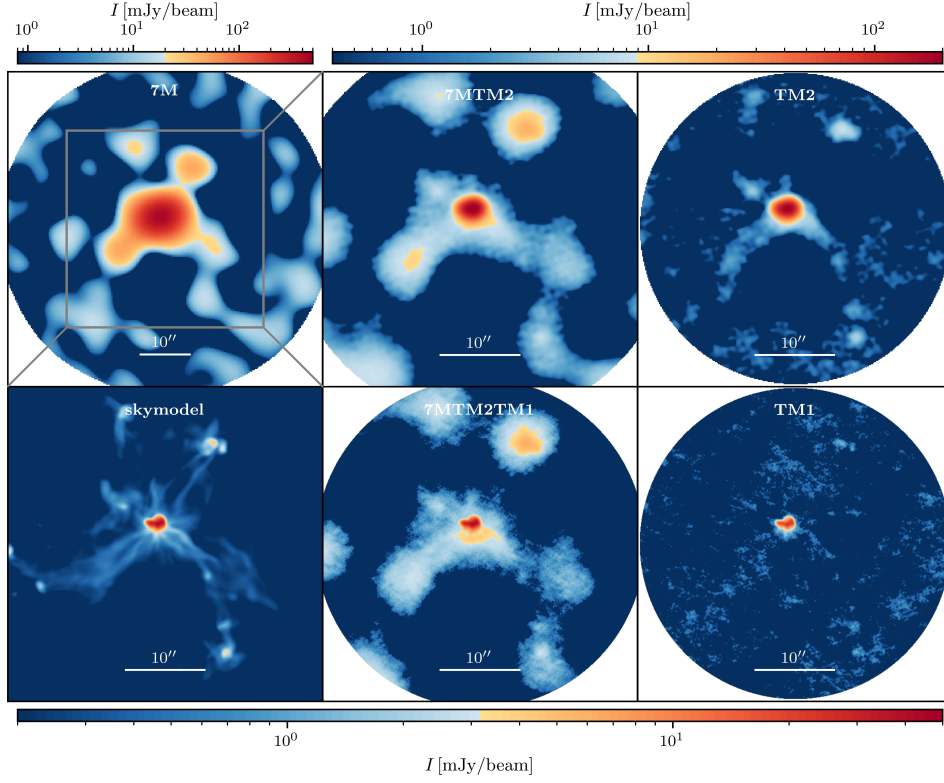


Figure 4: Intensity maps from different ALMA array configurations simulated with CASA. The top row shows the 7M array with a beam resolution of $\sim 18,360$ au (left), the combined 7MTM2 arrays (middle), and the TM2 configuration with a beam resolution of $\sim 3,850$ au (right). The bottom row shows the sky model (left), the fully combined 7MTM2TM1 image with a beam resolution of $\sim 1,200$ au (middle), and the TM1 map with a beam resolution of ~ 890 au (right).

the Fourier domain) with the `simobserve` task. We use three array configurations, matching those used in ALMAGAL: the 7 m array (`aca.cycle7.cfg`), a compact 12 m configuration (`alma.cycle7.2.cfg`), and an extended 12 m configuration (`alma.cycle7.5.cfg`). We also image combinations of these datasets (7M, TM2, TM1, 7M+TM2, and 7M+TM2+TM1).

We simulate Band 6 continuum observations with a central frequency of $\nu_0 = 220$ GHz and a bandwidth of $\Delta\nu = 3$ GHz, resembling that of the ALMAGAL observations. We adopt an integration time of 10 s and a total on-source time of 180 s per configuration, equivalent to the ALMAGAL observations. We simulate an observation centred on source transit (hour angle = 0) and adopt 2019/06/21 as the reference observing date. The pointing centre is $\alpha_{J2000} = 16^{\text{h}}10^{\text{m}}00^{\text{s}}$ and $\delta_{J2000} = -35^{\circ}30'00''$.

We add thermal noise by letting CASA compute the system temperature T_{sys} (which sets the thermal noise level) from an atmospheric model (sky emission/opacity plus receiver noise) for Band 6, adopting a precipitable water vapour of $\text{PWV} = 1.7$ mm. The combined 7MTM2TM1 ideal image is noise-free, whereas all other images (7MTM2TM1, 7MTM2, TM1, TM2, 7M) are produced from the corresponding noisy measurement sets.

We image the simulated visibilities with CASA `tclean` using Briggs weighting with `robust=0.5`, a standard choice that balances angular resolution and sensitivity.

We restrict the imaging to the primary-beam region by applying `pbmask=pblimit=0.2`, i.e. we only analyse regions where the primary-beam response is at least 20%.

To keep a similar field of view for all products, we adjust the image size (in pixels) and pixel size as follows: 256×256 pixels with $0.268''$ pixels for 7 m-only images, 512×512 pixels with $0.134''$ pixels for TM2 and 7M+TM2, and 1024×1024 pixels with $0.067''$ pixels for TM1 and 7M+TM2+TM1.

We deconvolve the images using the CLEAN algorithm in a few simple steps. First, we run a shallow CLEAN with 100 iterations down to 0.1 mJy to obtain an initial residual image. Next, we build a CLEAN mask based on the signal-to-noise ratio ($\text{SNR} = I/\sigma$, where I is the pixel intensity and σ is the RMS noise): we include faint emission above a low-SNR threshold only when it is spatially connected to a high-SNR detection. We update this mask iteratively (up to five times) and relax the SNR thresholds in later iterations. Within each mask iteration, we continue CLEANing in blocks of 100 iterations down to a threshold of 1σ . We stop when the relative improvement in both the model flux and the residual noise level (estimated from the median absolute deviation, i.e. $\text{median}(|R - \text{median}(R)|)$ with R the residual image, falls below 2%. Finally, we apply primary-beam correction with `impbcor` and export the final images.

The final synthetic continuum maps include finite angular resolution, beam convolution, spatial filtering, and thermal noise. They can be analysed in the same way as the observed ALMAGAL continuum images.

Figure 4 shows the intensity maps for different array configurations in an example snapshot. The sky model matches the RADMC-3D input (bottom-left panel). The 7M image has the lowest beam resolution, corresponding to $\sim 18,360 \text{ au}$, but provides the widest field of view and is most sensitive to extended emission due to its short baselines (top left panel). The TM2 configuration improves the resolution to $\sim 3,850 \text{ au}$. Its longer baselines restrict the field of view while imaging structures more sharply (top right panel). The combined 7MTM2 image recovers both large-scale emission and intermediate spatial scales (top middle panel). The TM1 map reaches the finest resolution, $\sim 890 \text{ au}$, allowing compact features to be separated and individual cores to be identified (bottom right panel). The fully combined 7MTM2TM1 image (beam resolution $\sim 1200 \text{ au}$) combines information from all configurations, retaining sensitivity to extended emission while preserving compact structure (bottom middle panel). Compared to the sky model, some small-scale substructures are not captured, but most cores and emission peaks remain detectable.

THE RESEARCH

Massive star formation is governed by a tightly coupled set of physical processes that remain challenging to disentangle. In particular, radiative feedback is expected to play a central role: non-ionising heating can suppress fragmentation and reshape the accretion environment (e.g. [Krumholz et al., 2010](#); [Myers et al., 2013](#)), while ionising radiation from massive stars heats and evacuates their surroundings, drives cavities, and ultimately powers expanding H II regions (e.g. [Peters et al., 2010a](#); [Dale et al., 2013](#)). The importance of radiation pressure during the earliest stages is still debated, but it may further modify accretion and the evolution of embedded ionised regions (e.g. [Kuiper & Hosokawa, 2018](#); [Rosen et al., 2019](#); [Klepitko et al., 2023](#)). These uncertainties motivate a state-of-the-art numerical study that follows collapse, accretion, and feedback self-consistently.

A key objective of this thesis is to connect such simulations directly to observations. The initial conditions of our models are informed by the parameter range probed by the ALMAGAL survey ([Molinari et al., 2025](#)), establishing a natural synergy between simulations and data. We therefore run a controlled suite of simulations in which the initial density profile, virial parameter, and metallicity are varied systematically. The initial density profile strongly affects the global collapse and clump evolution ([Girichidis et al., 2011](#)), turbulence shapes the morphology and substructures ([Walch et al., 2010](#)), and metallicity regulates the thermal evolution during collapse via its impact on cooling ([Omukai et al., 2005](#)). This provides a unique basis to isolate the impact of each parameter on fragmentation, accretion, and star-formation efficiency in a way that is difficult to achieve observationally.

The simulations also offer a major advantage for synthetic observations. Because the dust temperature is computed self-consistently during the radiation-hydrodynamical evolution, radiative-transfer calculations (with RADMC-3D) can use physically consistent temperature fields mapped from the AMR grid, avoiding post-processed dust temperatures. Finally, being part of the ALMAGAL project enables us to process synthetic continuum maps through the same imaging and analysis pipeline used for the real survey, effectively treating the simulations as if they were ALMAGAL targets on the sky ([Sánchez-Monge et al., 2025](#)). This creates a direct, controlled comparison between observed and intrinsic quantities, allowing us to quantify biases, calibrate analysis methods, and provide practical guidelines for interpreting continuum cores (e.g. their masses and temperatures) and envelope structure in observational studies.

PAPER I - FEEDBACK AND SFE IN HIGH-MASS STAR-FORMING REGIONS

This paper presents numerical simulations of the isolated gravitational collapse of a $1000 M_{\odot}$ clump with an initial radius of 1 pc. A resolution study is carried out to assess how sensitive the results are to numerical refinement. The simulations then examine how ionizing radiation and radiation pressure influence the clump evolution. Finally, a suite of production runs explores a range of ALMAGAL-motivated initial conditions, enabling a systematic comparison of fragmentation behaviour and star formation efficiency.

7.1

PUBLICATION I

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Feedback and Star Formation Efficiency in High-Mass Star-Forming Regions

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ABSTRACT

To advance our understanding of massive star formation, it is essential to perform a comprehensive suite of simulations that explore the relevant parameter space and include enough physics to enable a comparison with observational data. We simulate the gravitational collapse of isolated, parsec-scale turbulent cores using the FLASH code, modelling stars as sink particles. Our simulations incorporate ionizing radiation and the associated radiation pressure from stellar sources, and non-ionizing radiation and its dust heating, along with self-consistent chemistry, to capture the properties of emerging ultra-compact HII regions. Dust, gas, and radiation temperature are computed independently. The initial conditions are informed by ALMAGAL observations. We assess stellar feedback, comparing ionizing radiation and radiation pressure. Ionizing radiation ultimately halts mass accretion on to sink particles, while direct radiation pressure enhances the expansion of HII regions. Heating from non-ionizing radiation suppresses fragmentation. We examine the effect of spatial resolution, finding that higher resolution leads to more sink particles which are situated in environments with higher densities. As a result, ionizing radiation remains trapped longer, allowing continued accretion and yielding a higher overall star formation efficiency (SFE). We explore the impact of varying initial conditions, including the core density profile, virial parameter, and metallicity. Our parameter study reveals that a flatter density profile, higher virial parameter, and increased metallicity promote fragmentation, potentially enhancing the SFE by slowing the growth of the most massive stars and delaying the onset of stellar feedback. Overall, we find SFEs between 35% and 57%. Stellar feedback dictates the final SFE.

Key words: software: simulations – hydrodynamics – radiative transfer – stars: massive – formation

1 INTRODUCTION

Star formation is a fundamental process, shaping both the large and small astronomical scales and simultaneously influencing galactic dynamics (Bolatto et al. 2013). One of the largest unresolved problems in modern star formation is the formation of massive stars (here defined as $>8 M_{\odot}$). The formation of low-mass stars ($<8 M_{\odot}$) is mainly governed by the interplay of gravity, turbulence, and thermal pressure leading to quasi-Jeans fragmentation; however, additional support against gravity is necessary for the formation of higher-mass stars (McKee & Tan 2003). Such support is thought to be provided primarily by magnetic fields (Commerçon et al. 2011, 2022; Mignon-Risse et al. 2021; Hennebelle & Inutsuka 2019) and radiative feedback (Krumholz et al. 2009). It is a fact that high-mass stars evolve faster and start nuclear burning before the mass accretion process is finished, so feedback and accretion happen at the same time (Hosokawa & Omukai 2009). Cores hosting massive star formation are very dense and have higher average temperatures (~ 20 K) than lower mass and less dense cores (~ 10 K) (Beuther et al. 2007). A

manifest of young massive stars is the presence of ultra-compact HII (UC-HII) regions which have sizes of ~ 0.1 pc and densities of around 10^4 cm^{-3} (Wood & Churchwell 1989; Churchwell 2002; Hoare et al. 2007).

The formation of high-mass stars is associated with very energetic feedback ((ionizing) radiation, radiation pressure, protostellar outflows and stellar winds). At the end of their lifespans supernovae feedback becomes important and influences the interstellar medium (ISM) on larger scales. Several numerical simulations have been performed to model feedback in the ISM e.g., the SILCC project (Walch et al. 2015; Peters et al. 2017; Rathjen et al. 2021, 2023), the TIGRESS simulations (Kim & Ostriker 2018; Kim et al. 2023) or the STARFORGE project (Grudić et al. 2021; Guszejnov et al. 2022).

However, the feedback from massive stars will only affect their environment on parsec scales or beyond once they have dispersed their parental molecular cloud core. Massive stars are initially deeply embedded, causing a delay between the birth of a massive star and the time from which it blows a larger-scale bubble. In this initial phase, radiation pressure (RP) on gas and dust becomes important (Rosen et al. 2019; Klepitko et al. 2023; Ali 2021). Kuiper & Hosokawa (2018) find that RP may reduce the mass accretion rate while stars

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Figure 1. Looking into the heart of a massive star-forming core. Volume rendering of our run RFL10 shown at $0.78 t_{\text{ff}}$. We render molecular hydrogen, H_2 , showing the cold gas distribution within the core. In addition, we show atomic hydrogen, H , and ionized hydrogen, H^+ in blue and red, respectively. The alpha channels are proportional to the logarithmic density. The volume rendering reveals a violent outflow accompanied by an expanding ultra-compact HII region with an asymmetric shape, supported by radiation pressure. The atomic gas (blue) surrounds the ionized gas (red), which fills the bubble.

are still forming and thus limits their final mass. Not only RP, but also radiative heating due to the absorption of ionizing (> 13.6 eV) and non-ionizing (< 13.6 eV) stellar radiation by the surrounding gas and dust is important in this phase (Rosdahl et al. 2013; Klepitko et al. 2023). Before an UC-HII region emerges, large scale protostellar outflows are commonly observed (Avison et al. 2021). Stellar isotropic winds and collimated protostellar outflows are assumed to reduce the mass accretion rate of the forming massive stars (Kuiper et al. 2015; Oliva & Kuiper 2023; Rosen 2022). However, these processes may not represent the ultimate mechanism responsible for halting accretion (Kuiper et al. 2016; Rosen & Krumholz 2020; Rosen 2022). The interplay of the different feedback processes plays an important role in setting the star formation efficiency in massive host cores, and there are still open questions regarding how they act in concert.

Moreover, the impact of the initial conditions on the formation process of massive stars as well as their mass evolution and spatial distribution is not well understood (e.g., Tan et al. 2014). In particular, key parameters such as density profile, virial parameter, and metallicity are expected to play crucial roles.

DENSITY PROFILE. The evolution of the cloud core strongly depends on the initial density profile (Boss 1987; Lomax et al. 2013). Existing numerical simulations commonly use density profiles that vary from a flat distribution to a very steep power-law profile. Using a core mass of $100 M_{\odot}$, Girichidis et al. (2011) compared four different density profiles (uniform, Bonnor-Ebert type and power law density profiles) with $\rho(r) \sim r^{-1.5}$ and $\rho(r) \sim r^{-2}$, while neglecting any type of radiation. They find that a steep density profile shows a rapid collapse and leads to a central high-mass star, while a flat core has

a longer collapse phase and several lower-mass stars are produced. In general, low-mass stars form later and also via disc fragmentation (Stamatellos et al. 2007), which requires sufficient resolution to capture. However, in the case of massive stars, disc fragmentation is a complex process that may also depend sensitively on radiative feedback, as different treatments of radiation can significantly influence disc stability and fragmentation behaviour (e.g., Rosen et al. 2016; Oliva & Kuiper 2020; Kuiper et al. 2010a). Additionally, magnetic fields, which are not included in this study, can provide additional support against gravitational collapse and reduce fragmentation by stabilizing discs and regulating angular momentum transport (Rosen & Krumholz 2020).

TURBULENCE/ VIRIAL PARAMETER. The initial turbulent velocity field dictates the morphology of the gas and dust during the initial core collapse (Walch et al. 2010). Especially the virial parameter is important for the fragmentation process (Girichidis et al. 2011).

METALLICITY. The metallicity in the natal star-forming environment impacts the thermal evolution of prestellar cores (Omukai et al. 2005). Metal lines provide efficient cooling, particularly in the hotter, lower-density regions influenced by stellar feedback (Schneider et al. 2003). However, at the higher densities typical of prestellar cores, dust cooling dominates and plays a crucial role in regulating the temperature. Therefore, decreasing metallicity generally implies a lower dust content, leading to less efficient dust cooling and consequently higher gas and dust temperatures. This increase in temperature raises the Jeans mass, reducing fragmentation, especially the formation of lower-mass stars (Chon et al. 2022; Klepitko et al. 2023). In the extreme case of Population III star formation, this process can result in

a top-heavy stellar initial mass function (IMF) (e.g., Whalen 2013; Latif et al. 2022).

In this paper, we investigate the influence of ionizing radiation and the associated radiation pressure (Klepitko et al. 2023) on the massive star formation process as well as the impact of the spatial resolution. Furthermore, we carry out a parameter study of high-mass star-forming regions, where we vary the virial parameter, density profiles, and metallicities. The parameter range study is informed by the ALMAGAL¹ observations, which is an ALMA large-scale programme and includes observations from over thousand high-mass star-forming regions (Molinari et al. 2025; Sánchez-Monge et al. 2025; Coletta et al. 2025). Thus, in a follow-up paper, we will confront observations and simulations.

This paper is structured as follows. First, we explain the numerical methods and initial conditions of the simulations in section 2, where we highlight the treatment of ionizing radiation and RP. In section 3, we introduce a fiducial run and show the importance of ionizing radiation and RP as well as the impact of numerical resolution on the cloud evolution. In section 4 we investigate the results of the parameter study, followed by a discussion in section 5 and conclude in section 6.

2 SIMULATION DETAILS

2.1 Numerical Methods

We use the adaptive mesh refinement (AMR) code FLASH 4.6 (Fryxell et al. 2000) to calculate (magneto-)hydrodynamical prestellar core collapse simulations. Hydrodynamics is solved using the entropy-stable scheme by Derigs et al. (2016). To follow the chemical evolution of the gas, we use a non-equilibrium chemical network that tracks the evolution of seven species on the fly (Glover & Mac Low 2007; Glover et al. 2010). These species are molecular, atomic, and ionized hydrogen as well as carbon monoxide, ionized carbon, oxygen, and free electrons (H_2 , H , H^+ , CO , C^+ , O , e^-). The network uses reaction rates based on Nelson & Langer (1997) and our implementation of all heating and cooling processes within is summarized in Walch et al. (2015). We assume that gas and dust are perfectly mixed. The dust-to-gas mass ratio, f_d , depends on the gas metallicity, Z , and is calculated by

$$f_d = \frac{1}{100} \frac{Z}{Z_\odot}. \quad (1)$$

We use a tree-based solver for self-gravity and diffuse radiation (Wünsch et al. 2018). TREERAY/OPTICALDEPTH is used to calculate the dust shielding as well as the self-shielding of molecular hydrogen and CO. Here, we neglect an external interstellar radiation field (ISRF) as the cores are highly shielded and supposedly embedded in a dense environment. Additionally, the radiative transport module TREERAY/ONTHESPOT deals with ionizing radiation from point sources (e.g. sink particles representing stars) in a reverse ray-tracing approach (Wünsch et al. 2021). The contributions of all cells and sink particles are mapped onto rays. We use 48 rays which are distributed according to the HEALPix algorithm (Górski et al. 2005). Along each ray, the absorption of ionizing radiation by gas and the resulting gas heating and ionization are calculated (Haid et al. 2018). For emission, we assume the On-The-Spot approximation (Osterbrock 1988).

The module TREERAY/RADPRESSURE described in Klepitko et al.

(2023) is used to treat non-ionizing radiation where every cell and sink particle is a source of non-ionizing radiation. The integration of each ray along its line of sight gives a radiative intensity. Taking the contribution of all integrated rays into account a radiative flux and a mean intensity is calculated. Non-ionizing radiation is absorbed by the dust and thus heats the dust (see below). The dust opacity, κ_p , depends on the metallicity and dust temperature, T_d , and is given by (see Semenov et al. 2003; Krumholz & Thompson 2012; Klepitko et al. 2023):

$$\kappa_p(T_d, Z) = 10^{-1} \frac{Z}{Z_\odot} \frac{\text{cm}^2}{100 \text{ K}^2 \text{ g}} \times \begin{cases} T_d^2 & \text{for } T_d < 150 \text{ K} \\ (150 \text{ K})^2 & \text{else} \end{cases}. \quad (2)$$

In this set of simulations the dust is heated according to the non-ionizing radiation intensity, but the RP momentum of non-ionizing radiation is not transferred to the dust. In contrast, TREERAY/RADPRESSURE calculates the RP of ionizing radiation onto gas and dust and transfers the corresponding momentum. The heating from ionizing radiation is also included and handled via the chemistry network (as described in Haid et al. 2018).

The temperatures of dust, gas, and radiation are calculated self-consistently by balancing various heating and cooling processes and thus, can differ from each other (see Fig. 2). We include cooling due to collisional dissociation of H_2 , collisional ionization of H and metal line cooling, in particular of C^+ and O (Walch et al. 2015). The cooling of the gas by dust-gas coupling is also treated. Hereby, the dust temperature is calculated self-consistently, assuming it to be in thermal equilibrium. (see e.g. Klepitko et al. 2023, their Sec. 4.6). In fully ionized gas within the forming HII regions, cooling by H^+ recombination dominates, while cooling by C^+ and O lines is negligible (Haid et al. 2018). For heating, we include H_2 formation and H_2 photodissociation, shock heating and heating due to the release of gravitational potential energy as well as heating by photoionization. For the latter, each star (see below) is assumed to emit a black body spectrum according to the stellar temperature T_{int} . It is used to calculate the mean energy of the ionizing photons, $h\bar{\nu}$, and their average excess energy, $h(\bar{\nu} - \nu_{\text{LyC}})$, where $\nu_{\text{LyC}} = 13.6 \text{ eV}$ is the threshold frequency for hydrogen ionization. The photoionization heating rate results in

$$\Gamma_{\text{ih}} = n_{\text{H}}^2 \alpha_{\text{B}} h(\bar{\nu} - \nu_{\text{LyC}}) \quad (3)$$

where n_{H} is the hydrogen number density and α_{B} is the radiative recombination rate (Haid et al. 2018).

The equilibrium dust temperature is calculated by taking into account different heating and cooling processes as collisional interactions of dust grains and gas, heating by an interstellar radiation field (here set to 0), heating from H_2 formation on grain surfaces, heating by thermal radiation and cooling via thermal emission (see Klepitko et al. 2023, for details).

Sink particles represent protostellar objects and are formed from the gravitational collapse of gas that meets certain criteria (Offner et al. 2009; Klassen et al. 2012; Klepitko et al. 2023). We use the sink particle implementation of Dinabier & Walch (2020), which uses a 4th-order Hermite integrator to model their motion. To create a sink particle, the following criteria must be fulfilled. Sink particles are formed when the density in a cell is greater than a certain sink density threshold, ρ_{thresh} . The sink density threshold is related to the smallest resolvable Jeans length at the maximum refinement level, which is set to $\lambda_{\text{J}} = 4\Delta x$ and can be calculated from

$$\rho_{\text{thresh}} = \frac{\pi c_s^2}{G \lambda_{\text{J}}^2} = \frac{\pi c_s^2}{G (4\Delta x)^2}, \quad (4)$$

where G is the gravitational constant and c_s is the speed of sound

¹ ALMA Large Program 2019.1.00195.L

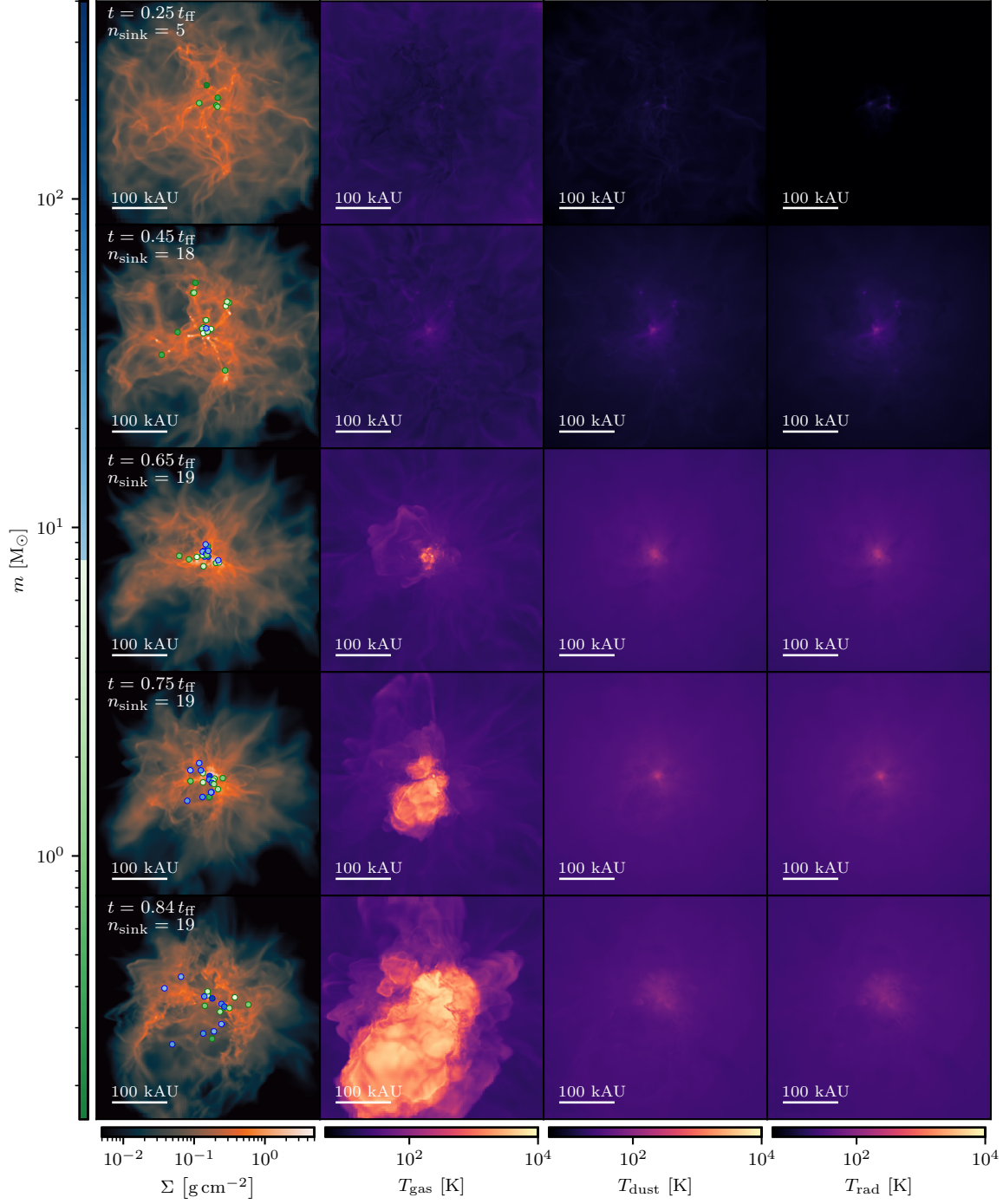


Figure 2. Time evolution of the fiducial run (from top to bottom). From left to right we show the projection in z -direction of the column density Σ and the mass-weighted temperatures of gas T_{gas} , dust T_{dust} , and radiation T_{rad} . Small circles represent sink particles. A green colour scheme represents lower-mass stars, while a blue colour scheme shows more massive sinks ($> 8 M_{\odot}$). After $\sim 0.4 t_{\text{ff}}$ (where $t_{\text{ff}} = 0.526$ Myr; see Table 1) massive sink particles are formed and drive an UC-HII region.

Initial Conditions

5

(Truelove et al. 1997). Within an accretion radius, $r_{\text{acc}} = 2.5\Delta x$ ($= 1000$ au for refinement level 9 in the FIDUCIAL run), the gas must be infalling and gravitationally bound. The region lies at a local gravitational potential minimum and does not contain other sink particles (Federrath et al. 2010). Additionally, a sink can only form from gas that collapses faster than it would accrete onto a nearby sink (Clarke et al. 2017).

Each sink particle is treated as a single star whose radius and surface temperature evolve primarily based on its mass accretion history, following the protostellar evolution model (Offner et al. 2009; Klassen et al. 2012). The model tracks the star's properties during the protostellar phase before transitioning to zero-age main sequence (ZAMS), where stars are modelled using the fitting functions of (Tout et al. 1996). The employed stellar evolution model does not depend on the metallicity. The treatment of the emitted feedback is described in Klepitko et al. (2023).

The emitted luminosity of the sink particles is distinguished into two parts, an internal luminosity, L_{int} , directly emitted from the star, and its accretion luminosity, L_{acc} , emitted by accretion events. For both luminosities, L_{int} and L_{acc} , we calculate the temperatures, T_{int} and T_{acc} , respectively, according to

$$T_{\text{int}} = \left(\frac{L_{\text{int}}}{\sigma 4\pi r_{\text{star}}^2} \right)^{1/4}, \quad (5)$$

$$T_{\text{acc}} = \left(\frac{L_{\text{acc}}}{f_{\text{filling}} \sigma 4\pi r_{\text{star}}^2} \right)^{1/4}, \quad (6)$$

where r_{star} is the stellar radius and f_{filling} is the fraction of the star's surface that accretes mass. The accretion luminosity is calculated with a hot spot accretion model and f_{filling} is set to 0.1 according to Calvet & Gullbring (1998). Based on the temperatures T_{int} and T_{acc} , we determine the fractions of ionizing radiation ($\gamma(T_{\text{int}})$ and $\gamma(T_{\text{acc}})$), and the complementary part of non-ionizing radiation ($[1 - \gamma(T_{\text{int}})]$ and $[1 - \gamma(T_{\text{acc}})]$). Ionizing radiation (UV radiation) are photons emitted in the Lyman continuum, ν_{LyC} . Therefore, the fraction of ionizing radiation is given by the luminosity emitted in the Lyman continuum divided by the bolometric luminosity.

$$\gamma(T_{\text{int}}) = \frac{\int_{\nu_{\text{LyC}}}^{\infty} \mathbf{d}\nu B_{\nu}(T_{\text{int}})}{\int_0^{\infty} \mathbf{d}\nu B_{\nu}(T_{\text{int}})}, \quad (7)$$

where B_{ν} is Planck's law of black body radiation. The fraction of ionizing radiation caused by the accretion luminosity is calculated in the same way. Therefore, for each sink particle, we can distinguish the luminosity of ionizing, L_{UV} , and non-ionizing, L_{IR} , radiation:

$$L_{\text{UV}} = \gamma(T_{\text{int}})L_{\text{int}} + \gamma(T_{\text{acc}})L_{\text{acc}}, \quad (8)$$

$$L_{\text{IR}} = L_{\text{int}} + L_{\text{acc}} - L_{\text{UV}}. \quad (9)$$

These luminosities are the sources for the radiative transfer described previously.

2.2 Initial Conditions

The initial core setups are designed to ensure the formation of massive stars as the cores collapse under self-gravity. These stars grow by accreting mass until their own feedback halts further accretion, ultimately determining their final mass.

The initial conditions for our study, including density profile, virial parameter and metallicity are motivated by observational data from the ALMAGAL survey of clumps and cores ((Molinari et al. 2025;

Name	ρ_0 [g/cm ³]	w	Z [Z _⊙]	σ [km/s]	α_{vir}	l_{ref}
FIDUCIAL	$2.86 \cdot 10^{-19}$	-2	1	71.7	0.6	9
RFL10	$2.86 \cdot 10^{-19}$	-2	1	71.7	0.6	10
RFL11	$2.86 \cdot 10^{-19}$	-2	1	71.7	0.6	11
RFL12	$2.86 \cdot 10^{-19}$	-2	1	71.7	0.6	12
α_{Low}	$2.86 \cdot 10^{-19}$	-2	1	41.5	0.2	9
α_{High}	$2.86 \cdot 10^{-19}$	-2	1	101.6	1.2	9
ZLow	$2.86 \cdot 10^{-19}$	-2	0.5	71.7	0.6	9
ZHigh	$2.86 \cdot 10^{-19}$	-2	2	71.7	0.6	9
FLAT	$1.16 \cdot 10^{-20}$	0	1	71.7	0.6	9
SHALLOW	$1.60 \cdot 10^{-19}$	-1.5	1	71.7	0.6	9

Table 1. Initial conditions of the performed simulations. From left to right, the columns show the run name, central density ρ_0 , powerlaw exponent of the initial core density profile w , core radius r , metallicity Z , velocity dispersion σ , virial parameter, α_{vir} and the maximum refinement level l_{ref} . With respect to the FIDUCIAL run, the yellow cells indicate the parameter changed in each row.

Sánchez-Monge et al. 2025; Coletta et al. 2025). This survey provides a representative sample of star-forming regions with measured physical properties, allowing us to select parameter values that reflect typical environmental conditions. By grounding our parameter choices in this observational dataset, we ensure that our simulations explore realistic regimes relevant to massive star formation.

All cores have a mass of $1000 M_{\odot}$ within a radius of 1 pc, which could be considered a typical setup for a massive star-forming core (Tan et al. 2014). The initial gas temperature is 20 K and the initial dust temperature of 2.7 K is immediately adjusted to the thermal equilibrium value in the first time step. The side length of the cubic box is 4 pc and the cores are surrounded by a low density ambient medium. The parameters we vary are the density profile, the virial parameter, and the metallicity (see Table 1).

2.2.1 Density Distribution

For the initial density distribution we use a Plummer-like density profile, i.e.

$$\rho(r) = \frac{\rho_0}{1 + \left(\frac{r}{r_0}\right)^w}, \quad (10)$$

where r is the core radius, ρ_0 the central density, w the density power-law, and r_0 the scale radius ($\sim 0.15 \text{ pc}$). Three different density power-laws are used, $w = 2$, $w = 1.5$, and $w = 0$, where $w = 0$ results in a constant density profile with $\rho = \rho_0$. Assuming a constant density distribution the core has a Jeans length of $r_j = 0.26 \text{ pc}$, resulting in a Jeans mass of $m_j = 18.1 M_{\odot}$. The core is pressure-confined by the environment; therefore, at the core boundary the density decreases by a factor of 100 while the temperature of the surrounding medium is increased to 2000 K.

Assuming a constant density $\bar{\rho}$, the free-fall time, t_{ff} , is the characteristic time it would take for a core to collapse purely under its own gravity. It is given by:

$$t_{\text{ff}} = \sqrt{\frac{3\pi}{32G\bar{\rho}}}. \quad (11)$$

In our simulations the free-fall time is $t_{\text{ff}} = 0.526 \text{ Myr}$. We normalize multiple time evolution plots to this t_{ff} .

2.2.2 Turbulence and Virial Parameter

For the initial turbulent velocity field, we generate a random Gaussian velocity field (Burkert & Bodenheimer 2000). It follows a power-law spectrum $P_k \propto k^{-4}$ (Burgers turbulence in 3D), while using the minimum and maximum wave numbers $k_{\min} = 1$ and $k_{\max} = 64$ in Fourier space, where $k = 1$ corresponds to $2\pi/4pc$. The velocity field is scaled to the desired root-mean-square velocity and mapped onto a uniform 128^3 grid.

To investigate the impact of turbulence on the cloud evolution we change the virial parameter, α_{vir} . The virial parameter is determined by the ratio of kinetic and gravitational energy. The velocity field is normalized; thus, we can derive different turbulent field strengths by multiplying with a chosen velocity dispersion. The velocity dispersion, σ , changes with the virial parameter according to

$$\sigma = \sqrt{\frac{\alpha_{\text{vir}} G M}{5r}}, \quad (12)$$

where M is the total core mass. We change the virial parameter from subvirial with a very low velocity dispersion ($\alpha_{\text{vir}} = 0.2$) to supervirial ($\alpha_{\text{vir}} = 1.2$).

2.2.3 Metallicity

The fiducial setup has solar metallicity ($Z = 1 Z_{\odot}$) with the according dust mass fraction, f_d (see Eq. 1). The abundances of metals in the gas-phase as well as f_d are reduced or increased linearly with Z to model different metallicities. This affects the ability of the gas to cool and shield. We vary the metallicity to $0.5 Z_{\odot}$ and $2 Z_{\odot}$ to mimic the conditions of massive star-forming cores towards the outer Milky Way disc and near the Galactic Centre.

3 ANALYSIS

3.1 Fiducial Run

We investigate the formation and early evolution of massive stars and their host cores up to the point where UC-HII regions are established (see Fig. 1). Here, we discuss the FIDUCIAL run.

3.1.1 General Evolution

We first present the time evolution (top to bottom) of the gas column density, Σ , and the mass-weighted temperatures of gas, dust, and radiation, T_{gas} , T_{dust} , and T_{rad} , respectively (see Fig. 2). The cloud core is initialized to collapse under its own gravity. Due to the interplay of gravitational and turbulent kinetic energy, substructures form and evolve into several filaments. The filaments converge at the central hub. The first sink particles are formed in this central hub, whereas later on sink particle formation also takes place in the outer parts of the filamentary structures.

At first, the temperatures of dust and gas show a similar morphology as Σ (see Fig. 2). The first sink particle is formed after $0.18 t_{\text{ff}}$ (see Eq. 11 and Table 1). As a result of the formation of sink particles and their growing feedback, the dust is heated by radiation. After $\sim 0.4 t_{\text{ff}}$ the first massive sink particles develop. From this point on, the dust temperature is dominated by the radiation temperature. In the inner region, the temperatures of gas, dust, and radiation are mostly in equilibrium. However, in the outer region, the temperature of the gas is still higher due to shock heating. Later, ionizing radiation from massive sink particles heats the gas and the UC-HII region forms

and expands. As a consequence, the gas temperature increases significantly. A phase diagram of the temperature evolution of gas, dust, and radiation temperature according to Fig. 2 is shown in Fig. A1.

3.1.2 Sink Particle Evolution

Figure 3 illustrates the properties of the sink particle population. The time evolution of the mass (top left panel), accretion rate (bottom left), luminosity (top right) and ionizing photon rate (bottom right) are plotted. The most massive sink particle (MMS), defined as the sink that is most massive at the end of the simulation, is shown in black. For better readability, the accretion rate, ionizing photon rate, and luminosity derived from sink particles in this work are smoothed using a moving average with a window size of 250 data points. The formation of sink particles takes place from $0.18 t_{\text{ff}}$ to $0.55 t_{\text{ff}}$. The first formed sink particle does not evolve into the most massive one. The MMS is built from the fourth particle, which forms after $0.22 t_{\text{ff}}$ and is located close to the centre of the core. The MMS reaches a final mass of $187.2 M_{\odot}$ at $0.8 t_{\text{ff}}$ (Fig. 3, top left panel). We note that the MMS does not necessarily correspond to a single star. Although we treat it as such in this work, it may host multiple stars, as we only take into account turbulent fragmentation and no further disc fragmentation. (see section 3.3 for more details). A binary (or multiple system) would most likely provide less feedback than a single star with the same mass. Additionally, Hosokawa et al. (2012) report that a protostar's radius may oscillate, and its averaged effective temperature should decrease with an accretion rate higher than $3 \times 10^{-3} M_{\odot}/\text{yr}$. Therefore, we might somewhat overestimate the properties and (ionizing) feedback from the massive sink particles.

Fragmentation plays a crucial role in our simulation. Turbulence drives fragmentation, leading to the formation of multiple stars, each contributing feedback against the infalling gas from the surrounding core. This feedback compresses the gas, halting accretion for some stars and enhancing it for others. As a result, the turbulent accretion process produces highly variable accretion rates. The interplay between local and global collapse ultimately leads to the formation of the MMS.

The average accretion rate of the MMS is $\sim 1 \times 10^{-3} M_{\odot}/\text{yr}$ and peaks at time $0.69 t_{\text{ff}}$ with $2.9 \times 10^{-2} M_{\odot}/\text{yr}$, just before the feedback begins to suppress further accretion (Fig. 3, bottom left panel). Between $0.56 t_{\text{ff}}$ and $0.61 t_{\text{ff}}$, accretion onto the MMS is partially prevented. Ionizing feedback from the sink itself pushes the gas away and locally stops accretion. However, the internal feedback from the MMS is not strong enough to completely stop further accretion. Because the global collapse continues, after $0.05 t_{\text{ff}}$, the gravitational energy is again stronger than the feedback and the local collapse continues.

In the top right panel of Fig. 3, the stellar and total luminosity is shown, while the total luminosity is just the sum of the stellar and the accretion luminosity. The stellar luminosity is the main contribution to the total luminosity. It increases continuously, and the MMS reaches $3.2 \times 10^6 L_{\odot}$. The accretion luminosity gives an additional noisy contribution to the total luminosity if accretion events are happening.

Some ionizing photons (bottom right panel) are already emitted before the first massive star is born because of the hot spot accretion. The ionizing photon rate, $\dot{N}_{\text{LyC}}$, gradually increases before sharply rising once the first sink particle reaches $8 M_{\odot}$. The MMS reaches a maximum value of $\dot{N}_{\text{LyC}} = 4 \times 10^{50} \text{ s}^{-1}$. For comparison, a typical O-type star with around $25 M_{\odot}$ would have an average value of $\dot{N}_{\text{LyC}} \sim 10^{49} \text{ s}^{-1}$ (Tielens 2005). During the aforementioned accretion pause

Fiducial Run

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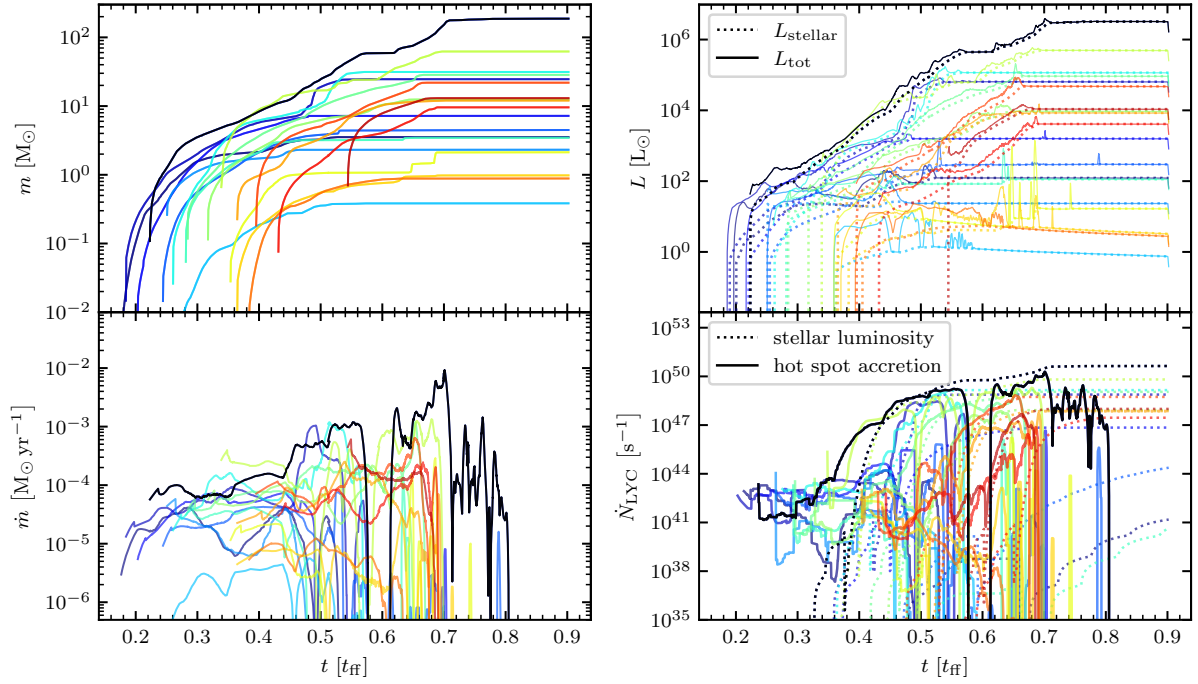


Figure 3. Properties of sink particles in time in the *FIDUCIAL* run. Top Left: Sink mass. Top Right: Luminosity (smoothed). Bottom Left: Accretion rate (smoothed). Bottom Right: Rate of emitted ionizing (Lyman Continuum) photons (smoothed). In total 20 sink particles are formed. The sink particle that ends up being most massive (MMS) is coloured in black.

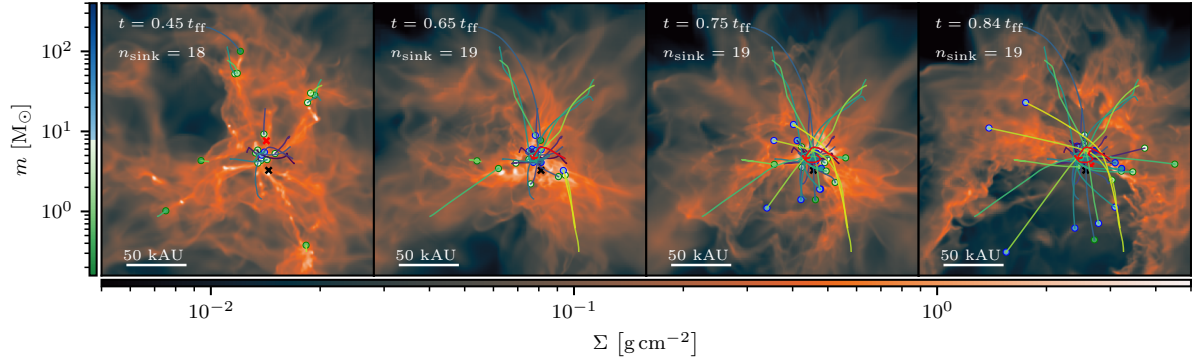


Figure 4. Time evolution of the column density of the *FIDUCIAL* run. The circles show the current position of the sink particles, similar to Fig. 2. The lines show the track of each sink particle, coloured as in Fig. 3. The geometric centre and the centre of mass are marked with black and red crosses, respectively. Sink particles that are formed in the outer region fall towards the central region and immediately escape the potential well due to high velocities.

of the MMS only ionizing photons from the star itself are emitted while accretion does not contribute any photons at this time.

3.1.3 Sink Particle Dynamics

Fig. 4 shows the movements of the sink particles in time on top of the column density. The colours of the tracks are the same as in Fig. 3. The sink particles that are formed in the outer region initially fall towards the centre. Because of their high radial velocities and a decreasing potential well depth, they almost immediately escape the

potential well again. When a substantial amount of ionizing photons is first emitted (the first stars become massive after $\sim 0.4 t_{\text{ff}}$), the dense gas near the central sink-forming hub first hinders the formation of an UC-HII region. In total 10 sink particles reach $> 8 M_{\odot}$ (see section 4). As soon as massive sink particles either move into or reside in lower-density regions because they have eaten most of their surrounding gas, the radiative feedback is more and more able to push the gas away from the centre. Thus, the UC-HII region around the massive sink particles expands and the cavity grows ($\sim 0.7 t_{\text{ff}}$). For some sink particles, accretion stops completely at this point,

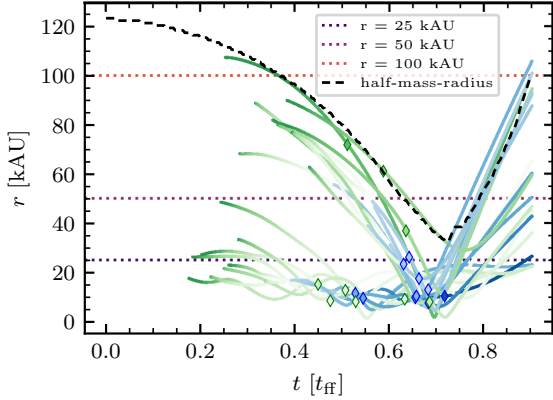


Figure 5. Evolution of the radial distribution of sink particles with respect to the geometric centre of the simulation box. The colour code shows the mass of the sink particles, while diamonds indicate when the sink particle has accreted 95% of its final mass. The black dashed line shows the half-mass-radius, which is the radius of the sphere in which half of the initial mass (here $500 M_{\odot}$) is located. The dotted lines indicate the radii used in Fig. 7. Sink particles that are formed near the geometric centre stay near the centre, while particles that are formed outside perform a V-shaped movement in terms of radius. The MMS is formed near the centre, while sinks with very low final masses are formed at larger distances. However, for intermediate final masses, sink particles can form near the centre or in the outer parts.

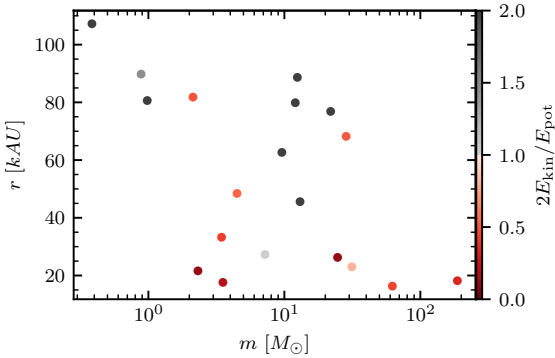


Figure 6. Radial distance of the sink particles at the formation time with respect to the geometric centre compared to their final mass. The colour shows if a sink particle is gravitationally bound (red) or unbound (grey) after $0.9 t_{\text{ff}}$ when the parental cloud is dispersed. 10 out of 19 sink particles remain gravitationally bound at this point. We find that it is more likely that a sink particle ends up staying bound if it has been formed close to the centre.

while the MMS sink particle is still sitting in a dense hub where its radiation is trapped and mass accretion is still ongoing. Nevertheless, the radiation from nearby massive stars (although less massive than the MSS), which live in somewhat more diffuse environments, keeps pushing gas out of their surroundings and starts to disrupt the inner hub. The MMS continues to accrete until $\sim 0.8 t_{\text{ff}}$. In the end, the remaining gas is dispersed.

The sink particles that accumulated high radial velocities at formation are now moving outwards. A more detailed analysis of the star formation rate and feedback is done in the following.

Fig. 5 shows the time evolution of the radial distribution of stars.

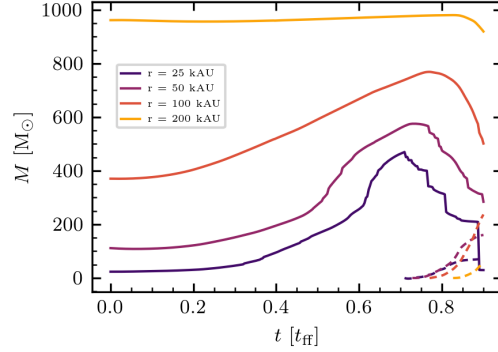


Figure 7. The solid line shows the mass evolution within spheres with different radii around the geometric centre (masses of gas and sink particles are considered). The dashed lines show the outflowing gas mass that is leaving these spheres due to feedback. First, the mass of the inner region of the cloud increases due to the gravitational collapse and later decreases again when either sink particles leave the region (sharp decreases) and/or feedback blows material out.

In particular, we plot the radial distances between the positions of each sink and the geometric centre of the simulation box. Particles that are formed near the central region stay near the centre until the remaining cloud is dispersed. Sink particles that are formed outside perform a V-shaped movement in terms of radius in time. They enter the central region and immediately leave again. The MMS is formed at 20 kAU from the centre. Generally, we find that sink particles with low final masses most likely form at larger distances, while sink particles with intermediate final masses form either near the centre or in the outer parts. The diamond-shaped symbols indicate the time that a sink particle accreted 95% of its final mass. It can be seen that the sink particle accretion is basically complete before the cluster begins to disperse at $\sim 0.7 t_{\text{ff}}$.

The black dashed line represents the radius of a sphere around the geometric centre, which contains half the mass of the initial cloud, i.e., the sphere within the half-mass-radius (HMR) contains $500 M_{\odot}$. The HMR is initially 123 kAU. During collapse, it decreases to 32 kAU and increases again as soon as the cluster is dispersed. All sink particles are formed within the HMR.

The evolution of the sink particle cluster is determined by N-body dynamics and the gravitational interaction of the sinks and the gas distribution. Overall, we show that not all sink particles remain in a gravitationally bound cluster. Fig. 6 depicts whether or not a sink particle is bound after $0.9 t_{\text{ff}}$. We find that 10 out of 19 sink particles end up in a gravitationally bound system. With a total SFE of 42 % (discussed in section 4) around 53 % of the sink particles remain bound in a cluster, which agrees with earlier studies (Adams 2000; Baumgardt & Kroupa 2007). If a sink particle is either very massive (here $> 25 M_{\odot}$) or formed close to the centre it is more likely that it stays in a bound system.

3.1.4 Gas Dispersal and Outflowing Mass

Stellar feedback drives outflows, resulting in the dispersal of the core. Fig. 7 shows the evolution of the total mass within spheres with different radii around the geometric centre. First, the mass at the centre increases due to the gravitational collapse. In the inner region ($r = 25$ kAU) almost all gas is accreted onto sink particles. After $\sim 0.7 t_{\text{ff}}$, feedback becomes dominant and starts to push the

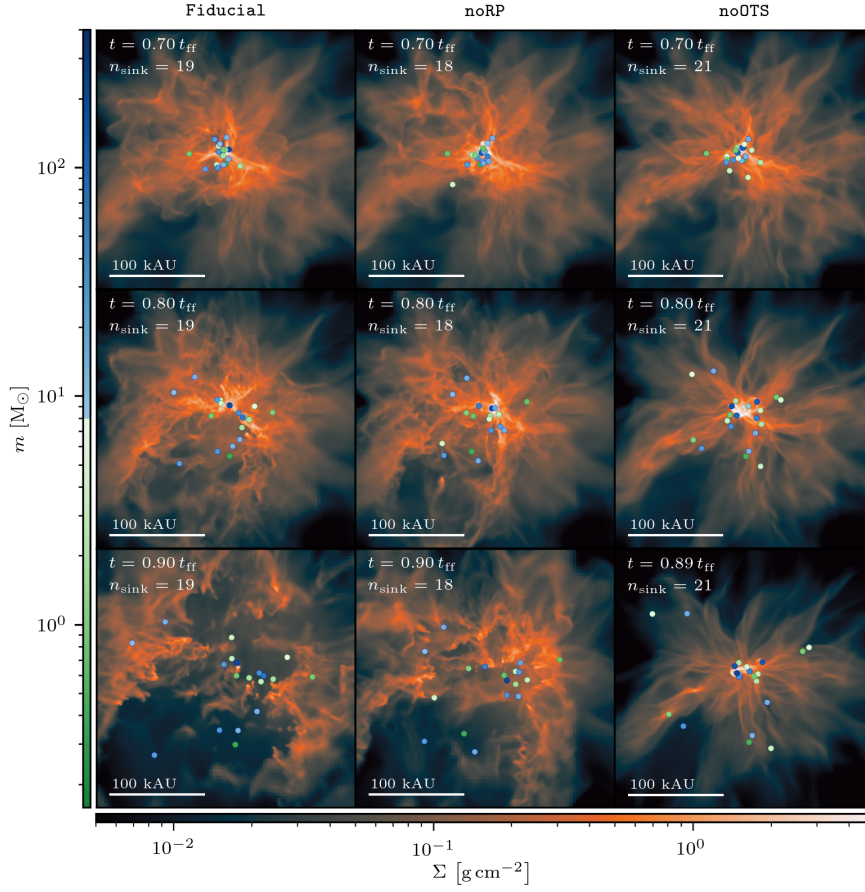


Figure 8. Time evolution (from top to bottom) of the column density of simulations with different feedback mechanisms. From left to right we plot the FIDUCIAL run (both ionizing radiation and radiation pressure are included), the simulation without radiation pressure from ionizing radiation (noRP) and the run without ionizing radiation at all (noOTS). Ionizing radiation becomes important as soon as sink particles reach $8 M_{\odot}$ and more. Radiation pressure of ionizing radiation transfers momentum to gas and dust and supports the grow of the HII region.

Name	ionizing radiation	non-ionizing radiation	ionizing rad. pres.
FIDUCIAL	x	x	x
noRP	x	x	
noOTS		x	

Table 2. List of runs investigating the impact of ionizing radiation and radiation pressure

gas out. Therefore, the mass begins to decrease near the centre. This also coincides with the time when the sink particles begin to move outwards (see Fig. 5, dotted lines indicates the radii used in Fig. 7). The dashed lines in Fig. 7 represent the gas mass, which leaves the boundary of the respective sphere. At a radius of 100 kAU over $230 M_{\odot}$ have been blown out of the sphere after $0.9 t_{\text{ff}}$. The decrease in mass occurs with a time delay at larger radii, indicating an inside-out expansion.

3.2 Impact of Ionizing Radiation and Radiation Pressure

In this section, we discuss the impact of ionizing radiation and radiation pressure from ionizing radiation on our core collapse scenario.

We compute three simulations with the same initial conditions but evolving them with different radiation physics (see Tab. 2). The first run is the FIDUCIAL run, which includes ionizing radiation and RP. Secondly, we run the simulation without RP (noRP). Then we neglect both, ionizing radiation and RP (noOTS). Heating by non-ionizing radiation from sinks and dust is always included (see sec. 2.1).

3.2.1 Morphological Evolution

In Fig. 8 the time evolution of the column densities is shown for the three simulations with different feedback mechanisms. The initial cloud collapse phase is similar for all simulations and noticeable differences only emerge once the sink particles become massive enough for feedback to become efficient (after $\sim 0.4 t_{\text{ff}}$; see Fig. 3). For this reason, the early evolution is not shown from Fig. 8. The first two columns in Fig. 8 (FIDUCIAL run and noRP) include ionizing ra-

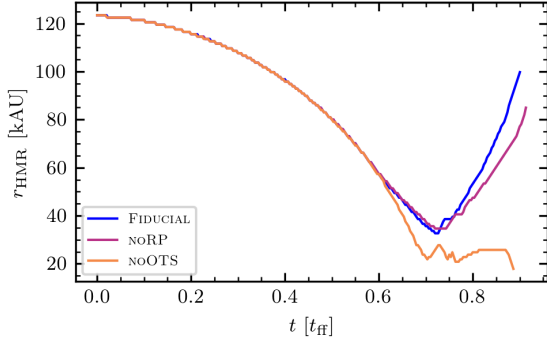


Figure 9. Evolution of the half-mass-radius, r_{HMR} , which is the radius of the sphere in which half of the initial mass ($500 M_{\odot}$) is located, showing the expansion of the cloud core. Ionizing radiation ultimately stops the core collapse and causes the cloud to re-expand. The extra momentum from RP accelerates the expansion.

diation. Ionizing feedback becomes significant once sink particles exceed $8 M_{\odot}$, ionizing the surrounding hydrogen within the Ström-gren radius and forming an UC-HII region. If no ionizing radiation is included (Fig. 8, last column, run noOTS), no gas is pushed outwards and the cloud still collapses when the simulation is stopped (also see Fig. 9).

3.2.2 Role of Radiation Pressure in UC-HII Expansion

When RP is included, the absorption of ionizing photons is associated with a momentum transfer. In particular, near the sink particles, the radiation energy density is high. As a result, the momentum input by RP pushes the gas away, which reduces the local density. Consequently, the recombination rate within the ionized gas is also reduced, since it depends on the square of the local gas density. Thus, the UC-HII region in the FIDUCIAL run can expand faster compared to noRP (see Fig. 8, bottom panels, and Fig. 9). The total number of ionizing photons, both, from stellar luminosity and from accretion events, is comparable for both runs, FIDUCIAL and noRP (see Fig. 10, bottom left), which indicates that the UC-HII region expansion may be promoted by RP. We note here that a different spatial distribution of (massive) sink particles may also contribute to a different shape of the UC-HII region in noRP.

3.2.3 Star Formation Efficiency and Accretion Rates

Previous studies show that ionization feedback is effective on suppressing star formation in giant molecular clouds (e.g. [Gee et al. 2016](#); [Kim et al. 2018](#); [Fukushima et al. 2020](#)). In runs FIDUCIAL and noRP, the feedback and pressure of ionizing radiation blow out the gas, thereby suppressing further mass accretion onto sink particles. This can be seen in Fig. 10, top left panel, where the slope of the SFE becomes flatter after $0.55 t_{\text{ff}}$ when the UC-HII region starts to grow. Feedback from massive sink particles is strong enough to finally fully prevent further accretion (Fig. 10, top right panel, showing the total mass accretion rate onto sinks), so that the SFE stays constant after around $0.8 t_{\text{ff}}$ for both runs, FIDUCIAL and noRP (Fig. 10, top left panel).

The mass accretion of the run noOTS is comparable to the FIDUCIAL run but does not decrease after $\sim 0.7 t_{\text{ff}}$ and stays roughly

Name	l_{ref}	Δx [au]	ρ_{thresh} [g/cm ³]
FIDUCIAL	9	400	3.67×10^{-17}
RFL10	10	200	1.48×10^{-16}
RFL11	11	100	5.88×10^{-16}
RFL12	12	50	2.35×10^{-15}

Table 3. Run name, maximum refinement level, the corresponding minimum cell size, and the sink threshold density for the runs in our resolution study.

constant at a few times $10^{-3} M_{\odot} \text{ yr}^{-1}$ even at late times (Fig. 10, top right panel). After the initial growth phase, the SFE of the run noOTS increases linearly and reaches ~ 0.65 during the simulation time, while there is no indication to stop further growth for longer simulation times (Fig. 10, top left panel). This indicates that ionizing radiation is the most efficient feedback mechanism in our simulations, assisted by RP.

The mass accretion of the MMS of run noOTS is slightly time-delayed but, in the end, the MMS grows even more massive than in the FIDUCIAL run, as there is no mechanism to stop further mass accretion (see Fig. 10, bottom right panel).

3.2.4 Thermal Impact and Fragmentation

Ionizing feedback (runs FIDUCIAL and noRP) leads to an increase of the mass-weighted temperature after $\sim 0.4 t_{\text{ff}}$ as soon as the first sink particle becomes massive and starts to emit ionizing radiation (see Fig. 11, left panel). In comparison, run noOTS shows a significantly cooler core with a gradually increasing average temperature. The difference in the temperature evolution affects the fragmentation process. The fragmentation process follows a similar pattern in all runs up to $\sim 0.4 t_{\text{ff}}$. As the temperature increases, the Jeans mass increases, and fragmentation becomes more demanding. This leads to a slightly lower final number of sink particles in the FIDUCIAL run and noRP (see Fig. 11, right panel). In run noOTS the formation process is quicker (until $\sim 0.47 t_{\text{ff}}$) but leads to the formation of more sink particles. Nevertheless, the number of high-mass sinks (dotted lines on the right panel) stays almost the same for all runs.

3.3 Resolution Study

We start from the FIDUCIAL run with a maximum spatial resolution of $\Delta x = 400$ au at refinement level 9 and increase the maximum refinement level in different simulations for the same initial conditions (see Tab. 3). We increase the refinement level to 10 (run RFL10), 11 (run RFL11), and 12 (run RFL12), which corresponds to an effective resolution of $\Delta x = 200$ au, $\Delta x = 100$ au, $\Delta x = 50$ au, respectively. For all simulations, the minimum refinement level is set to 5. This corresponds to a 128^3 base grid with a base resolution of $\sim 6,400$ au in the ambient medium.

3.3.1 Morphological Evolution with Resolution

Figure 12 shows the time evolution of the column density of the four runs with different resolutions (the increase in resolution is shown from left to right). The simulations RFL11 and RFL12 had to be stopped much earlier than the lower resolution runs due to limitations in the computing time.

The early evolution of the cloud (until $\sim 0.45 t_{\text{ff}}$) is similar for all runs, modulo the fact that more sink particles are formed with higher resolution. For later times, comparing runs RFL10 and FIDUCIAL, the cavity blown by stellar feedback forms a bit earlier and seems to be more pronounced with higher resolution.

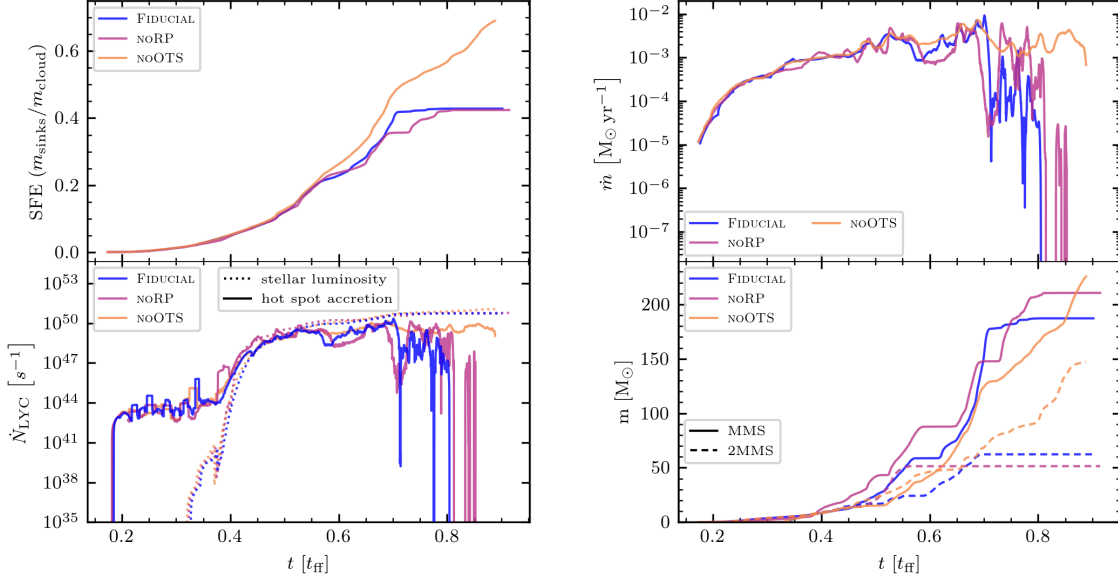


Figure 10. Top Left: Evolution of the star formation efficiency. Top Right: Total accretion rate (smoothed). Bottom Left: Total ionizing photon rate (smoothed). Bottom Right: Mass of the most massive sink (MMS) and the second most massive sink (2MMS). Ionizing radiation suppresses mass accretion and finally prevents the mass growth of sink particles completely. For runs without ionizing feedback, mass accretion onto sink particles is not prevented and the SFE increases until the simulation is stopped.

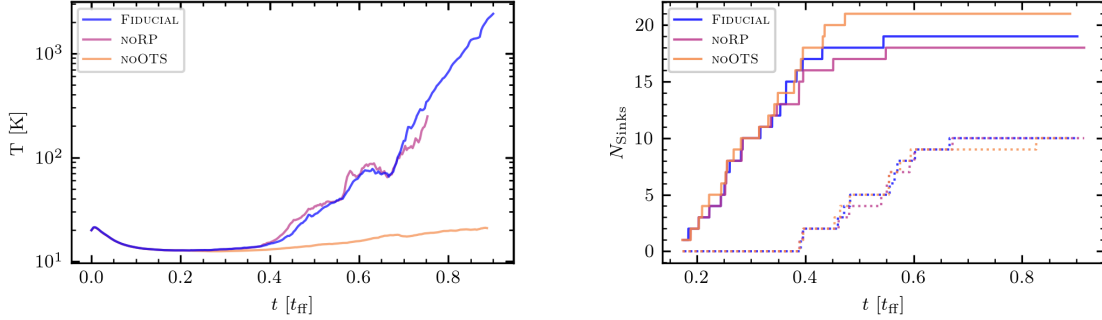


Figure 11. Left: Mass-weighted gas temperature of the whole simulation domain. Right: Number of sink particles, while the dotted line shows the number of high mass sinks with $\geq 8M_{\odot}$. Due to ionizing radiation, the temperature starts to heat up after $\sim 0.4t_{\text{ff}}$, while simulations without ionizing radiation have a constant shallow temperature increase. The increase in temperature results in a decrease in the number of lower-mass sink particles.

3.3.2 Impact of Resolution on Sink Statistics

The stars in our simulation are represented by sink particles. Several criteria are checked before sink particles are formed or allowed to further accrete gas from within the sink accretion radius (see section 2.1). One condition for the formation of sink particles is that the gas density within the accretion radius (2.5 cells on the highest refinement level) is greater than a certain density threshold, ρ_{thresh} (see eq. 4). It depends on the smallest resolvable Jeans length at the maximum refinement level. Table 3 lists the refinement level, the corresponding minimum cell size, and the sink threshold density for our resolution study.

During the initial collapse phase, the gas density is optically thin to infrared radiation and the core cools efficiently via dust thermal emission and behaves isothermally. When the gas density reaches $\rho \gtrsim 10^{-13} \text{g cm}^{-3}$, it becomes optically thick to infrared radiation.

The core cannot cool efficiently anymore and behaves adiabatically (Omukai et al. 2005). Therefore, for densities $> 10^{-13} \text{g cm}^{-3}$, the Jeans mass increases with increasing density and no more fragmentation should occur. Hence, only at such high densities would a sink particle represent a single star. In other words, we would only expect convergence with increasing resolution if a Jeans density of $\sim 10^{-13} \text{g cm}^{-3}$ could be resolved (e.g., Hubber et al. 2013). In our setup, this would require a refinement level of 15. However, when sink particles are formed at lower densities, they may represent binaries or even higher-order multiples. Therefore, for any maximum resolution used in this work, sink particles could represent single stars, binaries, or higher-order systems.

In the regime we resolve, it is expected that the number of sink particles, especially the number of lower mass sink particles, increases with higher spatial resolution. This is indeed the case (see Fig. 13, left

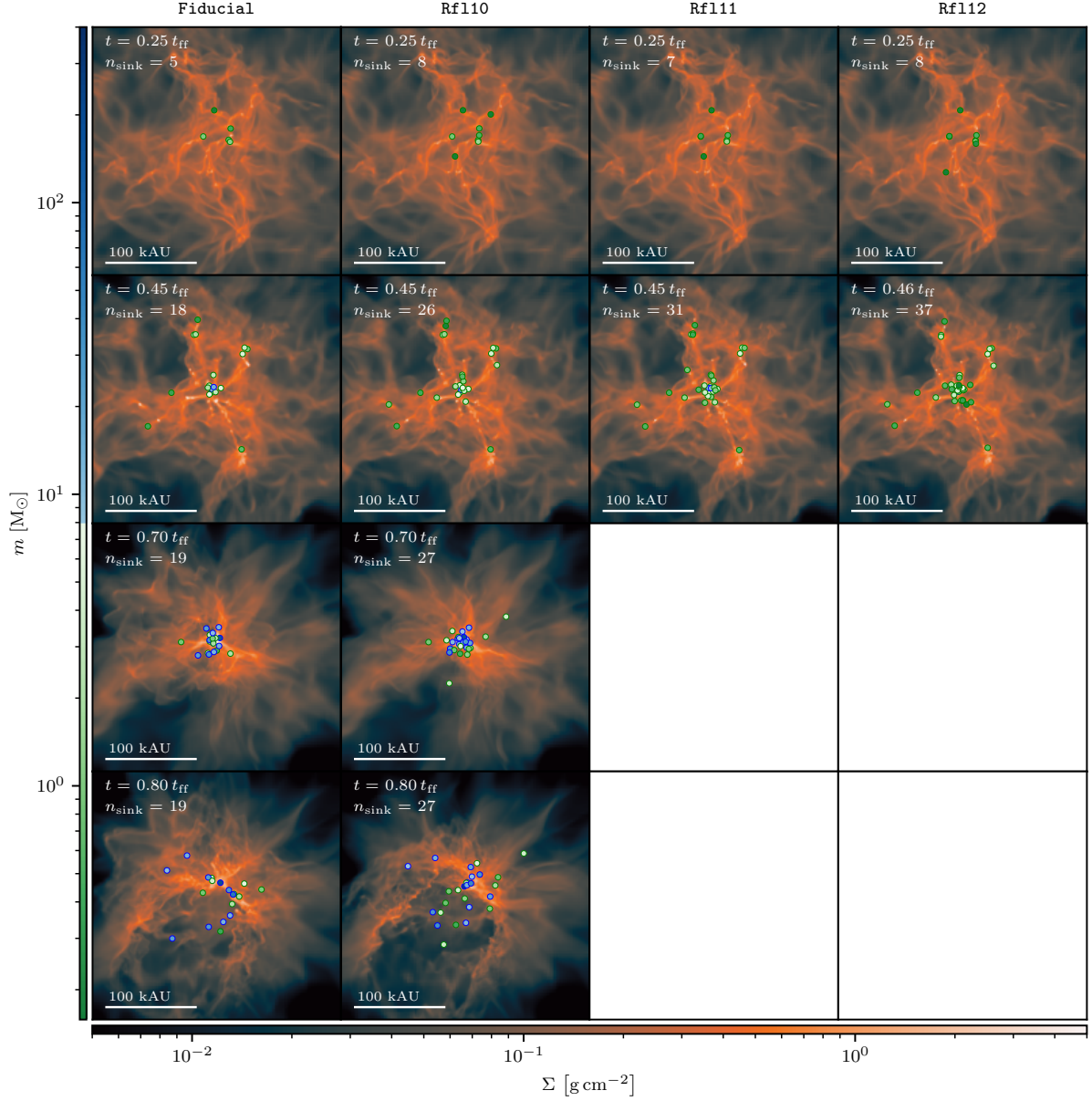


Figure 12. Evolution of the column density (from top to bottom) for different resolutions (from left to right). The higher the resolution, the more sink particles are created. The resolution has an impact on the evolution of the UC-HII region. Although the UC-HII region forms slightly earlier and appears to be more pronounced, the feedback is less efficient in regulating star formation with increasing resolution. Panels are blank for runs that were stopped at earlier times due to computational expense.

panel). Both, the number of low- and high-mass sink particles (sinks with more than $8 M_{\odot}$) increases (also see Fig. A3). Additionally, the cumulative sink mass function (Fig. 13, right panel) becomes slightly more bottom heavy with increasing resolution, at least at the time when $90 M_{\odot}$ have been accreted onto sinks (as shown by the solid lines). Later, the cumulative mass functions of the runs FIDUCIAL and RFL10 appear similar. However, overall, the lower resolution runs are lacking lower mass sink particles. We conclude that cloud fragmentation and sink formation are very sensitive to the numeri-

cal resolution in this regime, as expected. For a detailed analysis of the fragmentation process and the resulting sink mass distribution, it would be necessary to run simulations with higher resolution.

3.3.3 Resolution Effects on Accretion and SFE

As shown in Fig. 14, we find that all runs show a similar total mass accretion rate onto sinks until $\sim 0.7 t_{\text{ff}}$ (see bottom panel).

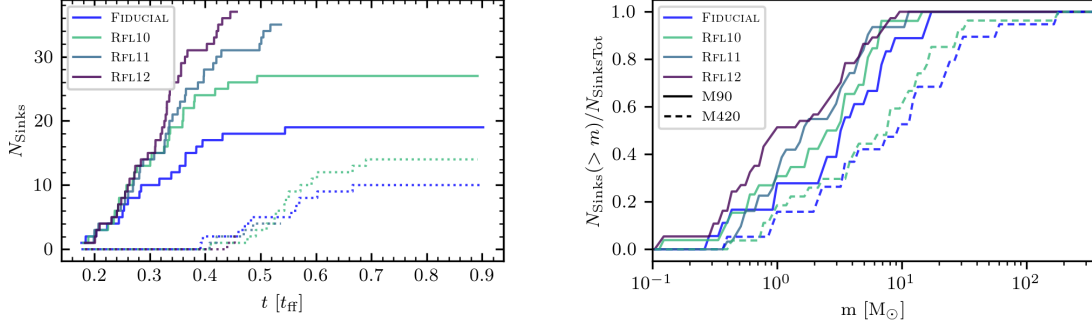


Figure 13. Left: Number of sink particles as a function of time (solid lines) and number of high mass sinks with $\geq 8 M_{\odot}$ (dotted lines). Right: Cumulative sink mass distributions, normalized to the respective total number of sink particles. Two different times are shown: when a total mass of $90 M_{\odot}$ has been accreted onto sinks (M90; solid lines) and when $420 M_{\odot}$ (M420; dashed lines) have been accreted, respectively. M420 can only be presented for runs FIDUCIAL and RFL10 since the higher-resolution runs had to be stopped earlier. Overall, runs with higher resolution show more fragmentation and the corresponding cumulative mass functions are slightly more bottom-heavy. For M420, there is no significant difference in the mass functions of FIDUCIAL and RFL10.

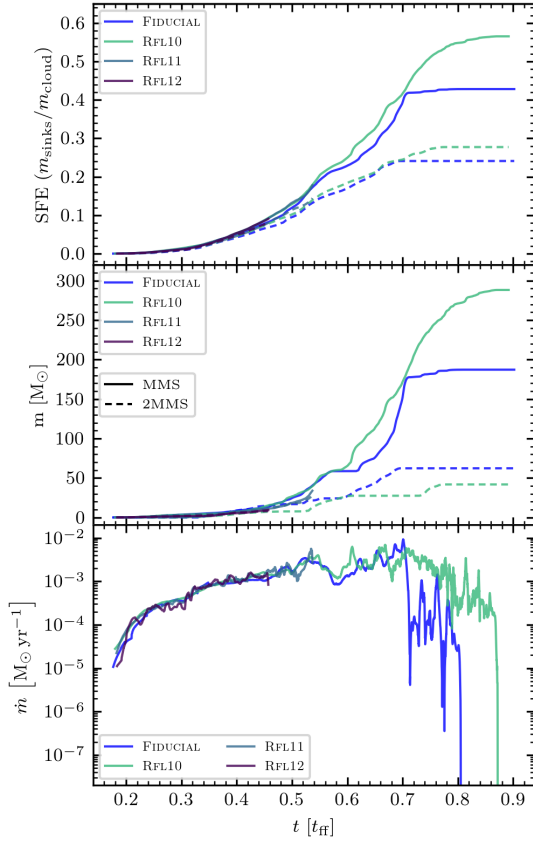


Figure 14. Top: Evolution of the star formation efficiency. Solid lines show the total SFE and dashed lines the total mass in companion stars (when the MMS is subtracted). Centre: Evolution of the mass of the most massive sink (MMS) and the second most massive sink (2MMS) in each simulation. Bottom: Total mass accretion rate onto sinks (smoothed). In the beginning all runs evolve in a similar manner. At later times, mass accretion continues for longer for higher resolution due to higher densities around the sinks. Thus, in run RFL10, the SFE and the mass of the most massive sink particle grow beyond the ones found in the lower resolution run (FIDUCIAL).

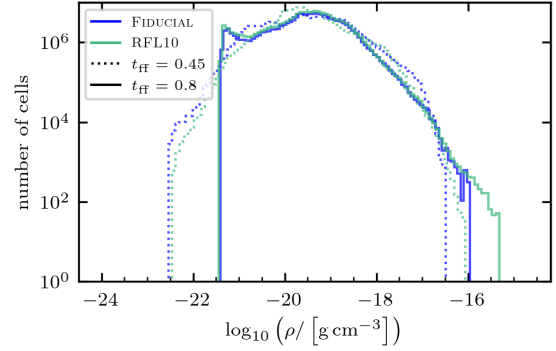


Figure 15. Density probability distribution functions (PDFs) within a sphere around the MMS with a radius of 10 kau . We compare runs FIDUCIAL (blue) and RFL10 (green) at two different times, $0.45 t_{\text{ff}}$ (dotted lines) and $0.8 t_{\text{ff}}$ (solid lines), respectively. Higher densities are resolved in the higher resolution case.

After this time, the total accretion rate of run FIDUCIAL decreases significantly, while RFL10 still accretes at a higher rate. This results in a similar SFE at early times (Fig. 14, top panel); however, while the SFE of the FIDUCIAL run stops at 0.42 after $\sim 0.7 t_{\text{ff}}$, the continued mass accretion in RFL10 leads to a higher final SFE of 0.56 (after $\sim 0.85 t_{\text{ff}}$). The SFE in companion stars, i.e., when subtracting the mass of the MMS from the total mass in sinks (dashed lines), we find that the SFE is similar for both FIDUCIAL and RFL10, with values of 0.24 and 0.27 , respectively. This means that the reason for the higher SFE in RFL10 is the increase in the mass of the MMS. The MMS in RFL10 ends up with $241 M_{\odot}$, which is higher compared to the FIDUCIAL run, where the most massive sink particle reaches $187.2 M_{\odot}$ (see 14, middle panel). However, the second most massive sink (2MMS) in both runs again have comparable masses, with the 2MMS of FIDUCIAL being slightly more massive than the one formed in run RFL10.

3.3.4 UC-HII Expansion

The MMS forms near the centre of the core and is surrounded by gas with high density as long as the sink particle is accreting. The density

probability distribution function (PDF) within a sphere with a radius of 10 kau around the MMS shows that RFL10 generally resolves higher densities compared to the FIDUCIAL run (see Fig. 15). Due to higher densities in RFL10 the recombination rate is higher, resulting in a decreased Strömgren radius and the UC-HII region is trapped for a longer period of time. During this time, the MMS is able to further accrete the mass and therefore becomes more massive. As soon as the feedback becomes strong enough to blow away the surrounding gas, the UC-HII region inflates, and further mass accretion is reduced and finally fully prevented.

Nevertheless, the general evolution of the core collapse and dispersal is similar for all runs with different resolutions. Therefore, $t_{\text{ref}} = 9$ is used to carry out a parameter study. At this resolution, it is possible to produce a statistically relevant sample of simulations, which will be later used as a basis for a comparison to the ALMAGAL observations.

4 PARAMETER STUDY

We perform a parameter study in which we vary the initial conditions (see sec. 2.2) of the collapsing core and investigate the resulting SFE and stellar feedback. Specifically, we compare simulations with different initial density profiles, virial parameters, and metallicities. The set of runs is summarized in Table 1.

4.1 Effects of the Initial Density Profiles

The initial density profile of the cloud cores affects their evolution. The evolution of the column density for each run is shown in Fig. 16. A *flatter* initial density profile (second and third column, runs SHALLOW and FLAT) results in a slower core collapse. Therefore, turbulence has more time to shape the cloud before it collapses under gravity, and more substructures are formed, where sink particle formation takes place. The densities at the edges of the cloud with a *flatter* density profile are higher compared to the FIDUCIAL run, thus turbulence leads to additional sink formation in the outer regions. The cloud collapse is less centrally condensed. Therefore, the MMS in the run FLAT is formed at a distance of around 100 kau from the centre.

Flatter density profiles lead to more fragmentation and thus to an increasingly high number of sink particles (see Fig. 17, left panel). In both runs, SHALLOW and FLAT, more high-mass stars are found, probably because feedback sets in later. Additionally, for a flat initial density profile (run FLAT) also the number of lower- and intermediate-mass sink particles increases. Therefore, the normalized cumulative sink mass distribution for run FLAT has, on the one hand, a dominant low mass end and, on the other hand, is also slightly shifted to be top heavy. Moreover, the slower core collapses of the runs SHALLOW and FLAT lead to a significant time delay in sink formation (see Fig. 18, bottom left panel). While the first sink particle in the FIDUCIAL run is formed after $0.17t_{\text{ff}}$, the runs SHALLOW and FLAT start with sink formation after $0.3t_{\text{ff}}$ and $0.43t_{\text{ff}}$, respectively (also see Fig. A4).

The *flatter* the initial density profile, the higher is the total SFE (see Fig. 18, top left panel). Due to the slower core collapse, the initial mass accretion rate is lower compared to the FIDUCIAL run (see Fig. 18, top right panel). However, the slower collapse also extends the time period in which the sink particles can accrete mass before ionizing feedback stops the mass growth. This results in a final SFE of 0.57 in run FLAT and 0.49 in run SHALLOW, which is higher than the SFE of the FIDUCIAL run with 0.42 (see Fig. 18, top left panel).

All three runs are dominated by one unique very massive sink particle. A flat initial density profile (run FLAT) leads to a MMS with a mass of $191 M_{\odot}$, which is even more massive than the MMS in the FIDUCIAL run, while the MMS in run SHALLOW only reaches $144 M_{\odot}$ (see Fig. 18, bottom right).

The time-delayed core collapse affects the temperature evolution of the core, which starts rising when the first sink particle reaches $8 M_{\odot}$ and starts to emit ionizing radiation, which heats the surrounding (see Fig. 19, left panel). At the reference time, $t_{\text{ref}} = t - t_{\text{m}}$, where t_{m} is the time when the first sink particle reaches $8 M_{\odot}$, the temperature is similar (around 15 K) for all three runs (see Fig. 19, right panel). There is a clear trend that slowly collapsing runs also have a slower temperature rise compared to the FIDUCIAL run but they catch up after $0.27 t_{\text{ff}}$.

4.2 Effects of the Initial Virial Parameter

The virial parameter gives the relation between the kinetic and gravitational energies of the initial core setup. A low virial parameter indicates that less turbulence disturbs the gravitational collapse, leading to the formation of fewer substructures during the collapse and vice versa (see Fig. 16). For a low virial parameter (run αLow with $\alpha_{\text{vir}} = 0.2$), the gravitational energy is dominant and the collapse is efficiently feeding the central hub where almost all sink particles are formed. The core is able to collapse faster than in run FIDUCIAL. In run αHigh with $\alpha_{\text{vir}} = 1.2$, the kinetic energy dominates and the cloud core collapses more slowly than in the FIDUCIAL run.

A low turbulent energy (run αLow) leads to a reduction of fragmentation and sink particle formation resulting in nine sink particles only, while the FIDUCIAL run consists of 19 sinks (see Fig. 17, left panel). A high velocity dispersion (run αHigh) leads to more fragmentation and 22 sink particles are formed. The formed sink particles in run αLow are very massive and thus the cumulative sink mass distribution is more top heavy (see Fig. 17, right panel). On the other hand, the shape of the mass distribution of αHigh and the FIDUCIAL run is similar.

The SFE in run αHigh increases slower than in the FIDUCIAL run, yet overall the star formation is only time-delayed and the SFE reaches a value of 0.4, which is slightly higher than in FIDUCIAL (see Fig. 18, top left panel). The final SFE of run αLow is reduced to 0.35. The ionizing photon emissivity from the few but very massive sinks increases faster compared to the FIDUCIAL run and quenches mass accretion earlier (see Fig. 18, top right panel and Fig. A5). The increased turbulence in run αHigh delays mass accretion onto (massive) sinks, leading to a lower ionizing photon rate (see Fig. 18, top right panel and Fig. A5). As a result, cloud disruption occurs later, extending the period during which sink particles can accrete mass, allowing the SFE to eventually catch up with the FIDUCIAL run (see Fig. 18, top left panel).

Compared to the MMS in the FIDUCIAL run ($187 M_{\odot}$), the MMS has a reduced mass for both runs αLow and αHigh with final masses of $127 M_{\odot}$ and $140 M_{\odot}$, respectively (see Fig. 18, bottom right panel). With a low virial parameter, gravity is more important and thus, the accretion rate of the MMS increases compared to the FIDUCIAL run (see Fig. 18, bottom left panel). However, the earlier stop of mass accretion in run αLow due to ionizing radiation feedback from the very massive sinks limits the MMS to grow more massive than the MMS in the FIDUCIAL run. On the other hand, in run αHigh the higher amount of turbulence hinders mass accretion onto the MMS.

For run αHigh , the numbers of low and intermediate mass sinks are similar to the FIDUCIAL run, but in total more massive sink particles (14 in total) are formed (see Fig. 18, bottom left panel). Thus, αHigh

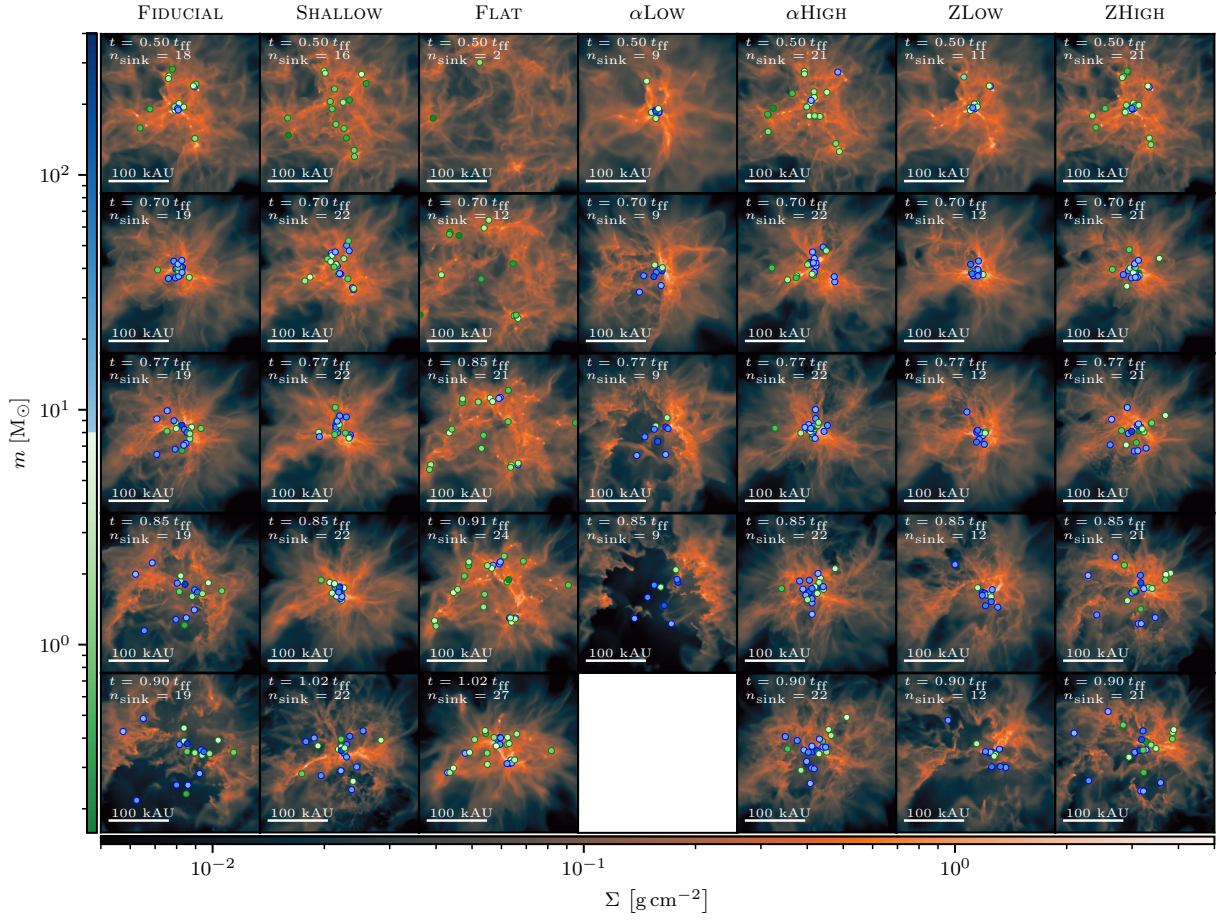


Figure 16. Time evolution (from top to bottom) of the column density distributions for different initial conditions according to tab. 1. The flatter the density profile (columns one, two, three), the slower the collapse. A lower virial parameter (fourth column) leads to a faster collapse while a higher virial parameter (fifth column) leads to more sub-structures. Lower metallicity leads to less fragmentation (sixth column) compared to higher metallicity (last column), which promotes fragmentation. Because Run α Low evolved more rapidly, the last panel is blank.

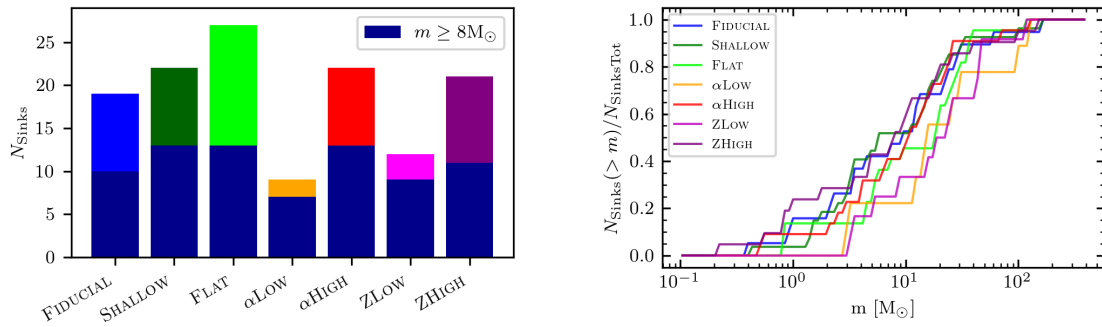


Figure 17. Left: Number of formed sink particles for the different runs. The dark blue parts indicate the number of high mass stars. Right: Cumulative sink mass distribution, normalized to the total number of formed sink particles of each run. Both plots represent the time when 95% of the final mass has been accreted onto sink particles. The flatter the initial density profile, the more fragmentation occurs. A low virial parameter as well as a low metallicity leads to fewer and very massive sink particles and the cumulative sink mass distribution is shifted towards top heavy. High virial parameter and metallicities have a minor impact on the fragmentation process and the cumulative sink mass distribution is comparable to the FIDUCIAL run.

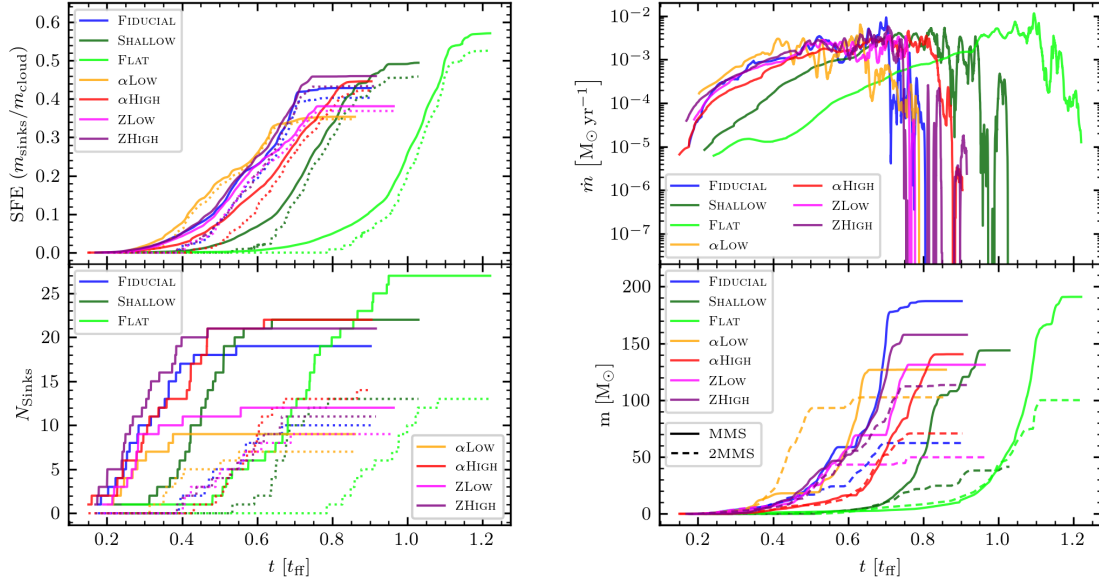


Figure 18. Top Left: Evolution of the star formation efficiency. The dotted lines represent the SFE of massive stars only. Top Right: Total accretion rate (smoothed). Bottom Left: Number of sink particles, while the dotted line shows the number of high mass sinks with $\geq 8 M_\odot$. Bottom Right: Mass of the most massive sink (MMS) and the second most massive sink particle (2MMS). Runs with flatter density profile collapse more slowly but in the end, they produce more fragments resulting in a higher SFE. The total accretion rate starts lower but accretion continues for longer. However, the mass of the MMS does not reach the one in the FIDUCIAL run. Low virial parameter and low metallicities lead to fewer sink particles with reduced SFE and a reduced mass of the most massive sink. A high virial parameter and high velocity dispersion evolves similar to the FIDUCIAL run, but the most massive sink particle is not as massive as in the FIDUCIAL run.

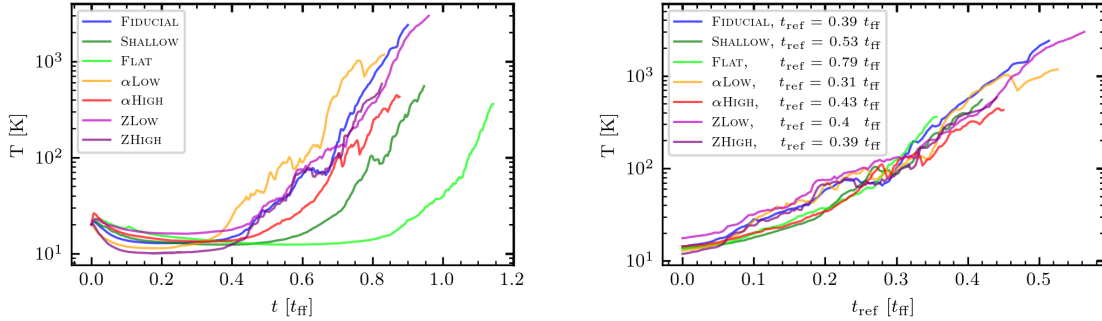


Figure 19. Left: Mass-weighted temperature of the whole simulation domain. Right: Mass-weighted temperature, with $t_{\text{ref}} = 0$ when first sink has $8 M_\odot$. The runs with a delayed core collapse (α HIGH, SHALLOW, and FLAT) also show a corresponding delay in the temperature evolution. Additionally, once a massive star has formed these cores heat up a bit more slowly but catch up with the other runs later on. The amount of metals affects the gas temperature due to more (ZHIGH) or less (ZLOW) dust cooling in the first $0.4 t_{\text{ff}}$.

ends up with more high mass sinks which, individually, are not as massive as in the FIDUCIAL run. In run α LOW, seven out of nine sink particles end up being massive.

The faster collapse in run α LOW results in a faster mass-weighted temperature increase, but the evolution is similar to the FIDUCIAL run (see Fig. 19, left panel). The slower collapse and slower star formation in run α HIGH is also reflected in the temperature evolution: when considering the increase in temperature after t_{ref} , run α HIGH is similar to the two runs with initially flatter density distributions (see Fig. 19, right panel).

4.3 Effects of Metallicity

The gas and dust metallicity has an impact on the evolution of (massive) clouds and cores. Metal lines and dust cool the gas and their absence may result in a suppression of fragmentation in lower metallicity environments (Omukai et al. 2005). In addition, dust grains shield ionizing photons in high-density filaments (e.g. Fukushima et al. 2020). At low metallicities, ionizing photons can penetrate further into higher-density gas where the star formation occurs and aid to disrupt the parental cloud. The temperature evolution of prestellar clouds changes with different metallicities (Omukai et al. 2005).

Starting with a lower initial metallicity, run ZLOW shows less

fragmentation and sink formation (see Fig. 16) than the FIDUCIAL run. Most sink particles are formed in the central region and the collapse is faster. Only 12 sink particles are formed out of which nine become massive (see Fig. 17, left panel). Therefore, the cumulative sink mass distribution of run ZLOW is shifted towards top heavy (see Fig. 17, right panel). However, the cloud with a higher initial metallicity (run ZHIGH) evolves similar to the FIDUCIAL run. In total, 21 sink particles are formed, while 11 grow massive. This is slightly higher compared to the FIDUCIAL run with 19 sink particles and 10 massive ones. However, the mass distribution of run ZHIGH is comparable to the one of the FIDUCIAL run.

During the first $0.25 t_{\text{ff}}$ the formation of sink particles of the run ZLOW is similar to runs ZHIGH and FIDUCIAL. After this time, fragmentation in ZLOW is more and more suppressed, while in run ZHIGH sink particle formation is accelerated (see Fig. 18, bottom left panel). The lower number of sink particles in run ZLOW leads to a reduction in the total SFE to 0.38, while run ZHIGH reaches ~ 0.46 , which is even higher than in the FIDUCIAL run (see Fig. 18, top left panel). The accretion rates of all three runs are initially similar (see Fig. 18, top right panel). However, mass accretion in run ZHIGH lasts longer compared to the FIDUCIAL run, causing the overall higher SFE. Nevertheless, the mass of the MMS ($158 M_{\odot}$) is still lower in run ZHIGH than in the FIDUCIAL run ($187 M_{\odot}$). The MMS in run ZLOW reaches only $131 M_{\odot}$.

The metallicity has an impact on the cooling of gas via dust. Higher metallicity leads to more efficient cooling and vice versa. The simulation starts with a gas temperature of 20 K, which is initially slightly cooled. During the first $0.4 t_{\text{ff}}$ the mass-weighted temperature of run ZHIGH is cooler (~ 10 K) than that of the FIDUCIAL run with ~ 13 K and run ZLOW with ~ 16 K (see Fig. 19, left panel). After $\sim 0.4 t_{\text{ff}}$, when the sinks become massive, the temperature increases in all runs. However, when considering the time evolution as normalized to t_{ref} , ZLOW still has a slightly increased temperature with respect to ZHIGH and FIDUCIAL until $t_{\text{ref}} \sim 0.32 t_{\text{ff}}$ (see Fig. 19, right panel).

5 DISCUSSION

5.1 Effects of the Initial Density Distribution

If the density distribution follows a power law ($\rho \sim r^{-1.5}$ or $\rho \sim r^{-2}$) the gravitational collapse leads to one central massive star. This is in agreement with previous work (Girichidis et al. 2011; Rosen et al. 2019; Klepitko et al. 2023). However, even with an initially uniform density distribution, only one very massive sink particle (with mass $M_{\text{MMS}} \sim 2 \cdot M_{2\text{MMS}}$) is formed, which dominates the gravitational potential. Consistent with our simulations, Girichidis et al. (2011) find that an initially uniform density leads to sink formation in filaments in the outer regions. However, in Girichidis et al. (2011), the first sink particle that forms always evolves into the most massive one. In our simulations, the MMS is not necessarily the first formed sink particle (see Fig. A4). This might be the result of stellar feedback, which is not included in the simulations of Girichidis et al. (2011).

5.2 Effects the Initial Virial Parameter

Dale (2017) find a decreasing SFE for cores with an increasing virial parameter (from $\alpha_{\text{vir}} = 0.7$ to 1.5) simulating a larger-scaler setup than ours of a $10^4 M_{\odot}$ cloud core within a radius of 5 pc. Also, Krumholz & McKee (2005) reports that the star formation rate

decreases with an increasing virial parameter. However, in our study the overall SFE increases with the virial parameter (see Fig. 18, top left), which is again a result of stellar feedback. The subvirial core undergoes a fast global collapse with high accretion rates and photon emissivity, in agreement with Rosen et al. (2019)² and Krumholz & McKee (2005). The resulting higher source luminosities (intrinsic plus accretion) lead to high radiative heating rates and an efficient warm-up of the core (see left panel of Fig. 19), which suppresses fragmentation. However, high accretion rates result in more massive sinks and their high photon emissivities destroy the cloud faster causing lower SFEs. On the other hand, a higher level of turbulence leads to more turbulent fragmentation (also seen by Rosen et al. (2019)). As a result, a higher number of massive sinks is formed but they are less massive on average. The lower-mass MMS leads to less radiative heating, and the core is cooler than in the FIDUCIAL run or in the low α_{vir} case. Additionally less massive sinks have a lower photon emissivity, thus star formation proceeds for a longer time.

5.3 Effects of Metallicity

Metals cool the gas, which favours fragmentation (Omukai et al. 2005). In particular, dust cooling promotes the fragmentation within star forming clumps and cores. Simulations of star formation in the early universe show a tendency to result in a top-heavy IMF at lower metallicities ($10^{-4} Z_{\odot}$ and $10^{-5} Z_{\odot}$) (Clark et al. 2008; Dopcke et al. 2011; Whalen 2013; Latif et al. 2022). However, Bate (2009, 2019) suggest that at near-solar metallicities, the overall properties of stars, including the IMF, are relatively insensitive with metallicity, supporting the idea that the IMF is largely universal. Previous studies (Tanaka & Omukai 2014; Matsukoba et al. 2022) show that the fragmentation of accretion discs is enhanced in the metallicity range of $10^{-2} Z_{\odot} - 10^{-5} Z_{\odot}$. However, in this study, we do not resolve disc fragmentation and also use higher metallicities ($0.5 Z_{\odot} - 2 Z_{\odot}$). For higher metallicities radiation pressure might become more important (Fukushima et al. 2020) and therefore, pushing gas outwards. Chon et al. (2021) reports that metallicities greater than $0.1 Z_{\odot}$ may limit the mass accretion of massive stars through the formation of low-mass companions. Overall, the SFE tends to increase with higher metallicity, which is shown in (Fukushima et al. 2020; He et al. 2020; Ali 2021), and can also be seen in our results.

5.4 Trends in Star Formation Efficiency

The overall SFE in our simulations is 35% to 57% depending on the initial conditions. The lowest SFE (35%) is reached in run αLow with a lower virial parameter compared to the FIDUCIAL run. We see a clear increase in SFE (from 0.42 to 0.57) with an increasing central gas density surface from the FIDUCIAL run with $\Sigma = 0.1 \text{ g cm}^{-2}$ ($\hat{=}$ $480 M_{\odot} \text{ pc}^{-2}$) to run FLAT with $\Sigma = 0.39 \text{ g cm}^{-2}$ ($\hat{=}$ $1800 M_{\odot} \text{ pc}^{-2}$). Therefore, a more rapid collapse does not necessarily lead to a higher SFE.

Our SFE is perhaps slightly higher than expected (see discussion of code limitations on the SFE below). However, previous results show a strong dependence of the SFE on the core surface density and the density profile. For example, in low surface density clouds with $\Sigma = 0.01 \text{ g cm}^{-2}$ ($\hat{=}$ $48 M_{\odot} \text{ pc}^{-2}$), Geen et al. (2018) find that the SFE can range from 6 to 23% depending on the initial conditions. Higher

² Note that the simulations of Rosen et al. (2019) study cores with a similar gas surface density; however, the cores are smaller and less massive, and therefore the simulations afford a higher effective spatial resolution of 20 au.

SFEs (up to 21 % and 32%) are found in clouds with $\Sigma \sim 2.1 \text{ g cm}^{-2}$ ($\hat{=} 10^4 \text{ M}_\odot \text{ pc}^{-2}$)³ (Howard et al. 2017; Grudić et al. 2018) and steep density profiles (Rahner et al. 2019, SFE $\geq 50\%$). For an initial gas surface density of 0.28 g cm^{-2} ($\hat{=} 1300 \text{ M}_\odot \text{ pc}^{-2}$), Kim et al. (2018) report a SFE of 51% while the SFE in Raskutti et al. (2016) reaches over 60 % with only 0.05 g cm^{-2} ($\hat{=} 250 \text{ M}_\odot \text{ pc}^{-2}$). Fukushima & Yajima (2021) report that if the surface density reaches 0.02 g cm^{-2} ($\hat{=} 100 \text{ M}_\odot \text{ pc}^{-2}$) ionizing feedback becomes increasingly inefficient in regulating mass accretion due to the deep gravitational potential well and thus the SFE increases.

5.5 Feedback Effects

5.5.1 Ionizing Radiation

Stellar feedback is known to reduce the SFE. Ionizing radiation is a main feedback mechanism, which limits the final SFE and is crucial to model HII regions (Geen et al. 2015; Dale 2017; Haid et al. 2018). We use the approximation of a black body spectrum to model the ionizing photon fraction without considering the stellar atmosphere, which might lower the ionizing photon rate (Kurucz 1979; Kuiper et al. 2020). The SFE is very sensitive to the ionizing photon emissivity (Dobbs et al. 2022), which we also see in our simulations. A fast increase in the ionizing photon rate results in a short mass accretion period and thus lower SFE. Olivier et al. (2021) shows that it might be useful to take into account UV attenuation by dust in HII regions to not overestimate the ionization rate. Furthermore, FUV radiation which can photo-dissociate H_2 and CO and cause photo-electric heating is not included yet and can suppress star formation (Inoguchi et al. 2020; Fukushima & Yajima 2022). However, in a follow-up code development paper of FLASH (Rathjen et al. 2025) a self-consistent adaptive ISRF is implemented. They find that, compared to photoionization, the IRSF is not that important for regulating star formation on scales of several hundred parsec.

5.5.2 Radiation Pressure

Radiation pressure is important to include in numerical simulations on different scales even if it is not the dominant feedback mechanism (Peters et al. 2017; Rosen & Krumholz 2020; Klepitko et al. 2023). Especially the interplay of photo-ionization and RP seems to be important at later stages and may limit the final mass of high-mass stars (Kuiper & Hosokawa 2018). In addition, RP supports the growth of the HII region (Ali et al. 2018; Ali 2021). RP from non-ionizing radiation, which is not included in our simulations, might become increasingly important at higher resolutions in higher density regions (Kuiper & Hosokawa 2018). Neglecting the acceleration due to non-ionizing radiation pressure could lead to an underestimation of feedback effects during the early stages, potentially allowing somewhat higher accretion rates and final stellar masses than would be expected if this mechanism were included.

Kuiper & Hosokawa (2018) report that on smaller scales the radiation feedback caused by dust thermal emission is most effective in suppressing mass accretion onto a massive protostar. However, Kuiper & Hosokawa (2018) are resolving mass accretion through a disc onto a protostar because of the use of a spherical grid. They also use a fixed dust opacity of $\kappa_{\text{dust}} = 4 \times 10^4 \text{ cm}^2 \text{ g}^{-1}$ in the FUV regime, which is much higher than our typical dust opacity, which

depends on the dust temperature and is calculated self-consistently (see equation 2 and Fig. A1; typically we have Planck mean opacities between $10 - 10^3 \text{ cm}^2 \text{ g}^{-1}$). With the resolution of our FIDUCIAL run ($\sim 400 \text{ au}$) we are not able to resolve the accretion disc around a massive star (see also Sec. 3.3). Resolving the accretion disc around the MMS might limit its final mass and thus, also its radiative feedback. With a resolution of $\sim 20 \text{ au}$, Klepitko et al. (2023) and Rosen & Krumholz (2020) also conclude that RP alone is not able to suppress mass accretion.

Looking at GMC scales, Kim et al. (2018) (fiducial model with $M = 10^5 \text{ M}_\odot$ and $R = 20 \text{ pc}$) says that ionizing feedback has a greater impact on cloud destruction than RP and only considering RP leads to a higher SFE, which is in agreement with our results. The larger the scales considered, the lower the average density, and the less impactful is the feedback by RP on dust (Krumholz 2018). However, they also emphasize that the effects of both feedback mechanisms are not linear and act in concert. By calculating direct RP from a star, resolving the dust sublimation front (between $100 - 1000 \text{ au}$) can play an important role (Kuiper et al. 2010b; Krumholz 2018) in not overestimating the escape fraction of ionizing radiation and thus the efficiency of RP. In our simulation, according to Krumholz (2018), we only resolve the dust sublimation radius for the very massive sinks ($> 40 \text{ M}_\odot$). However, we also see that neglecting RP does not change the overall SFE. Thus, we speculate that reducing the efficiency of RP by using a subgrid model that describes the effects of dust sublimation would not strongly affect the SFE.

In addition to RP, radiative heating by non-ionizing photons is important and leads to a higher Jeans mass, which results in fewer and more massive stars (Krumholz et al. 2007; Peters et al. 2010; Rosdahl & Teyssier 2015; Howard et al. 2017; Hennebelle et al. 2020, see also Sec. 3.2). (Bate 2009) show that radiative heating reduces small-scale fragmentation and shifts the IMF towards higher masses, which helps explain why the IMF appears to be universal.

5.5.3 Protostellar Outflows

Stellar outflows from both low- and high-mass protostars can regulate mass accretion during star formation. Observations show that these outflows can remove material and angular momentum from the protostellar environment, carve cavities in the infalling envelope, and disrupt accretion flows (e.g. Maud et al. 2015; Kuiper et al. 2016). By ejecting gas from the system, they reduce the reservoir available to the forming star and inject turbulence into the surrounding medium, and thereby lowering the SFE (Kuiper et al. 2015; Kölligan & Kuiper 2018; Rosen & Krumholz 2020; Rohde et al. 2021; Commerçon et al. 2022; Oliva & Kuiper 2023). In our simulations, protostellar outflows are not yet included which might lead to an overestimate of the accretion rates and final stellar masses. Outflows from massive sink particles could also hinder mass accretion onto the MMS and might limit its mass (Tanaka et al. 2018).

5.5.4 Stellar Winds

Also, stellar winds might regulate the SFE. These winds can reach velocities of thousands of kilometres per second and carry mass and momentum into the circumstellar medium (e.g. Puls et al. 2008). By removing material from accretion flows and clearing gas from the immediate vicinity of the star, stellar winds have the potential to reduce accretion onto very massive stars (Rosen 2022; Krumholz et al. 2014). However, Haid et al. (2018) find that stellar winds dominate over ionizing radiation only under conditions where the

³ The column density threshold for massive star formation suggested by Krumholz & McKee (2008) is 1 g cm^{-2} or $4.7 \times 10^3 \text{ M}_\odot \text{ pc}^{-2}$.

gas is already heated to 10^4 K. Moreover, hydrodynamic simulations suggest that stellar winds can generate cavities and bubbles that further disrupt star-forming clouds on larger scales (Geen et al. 2015; Dale et al. 2014). On smaller scales, line-driven disc ablation might play a role in preventing mass accretion onto massive stars (Kee & Kuiper 2019).

5.6 Magnetic Fields

In addition to the feedback mechanisms, magnetic fields are an important factor in star formation, influencing fragmentation and accretion processes (Hull & Zhang 2019; Crutcher 2012). By providing additional support against gravitational collapse and regulating angular momentum transport, magnetic fields reduce fragmentation and lower accretion rates onto protostars. Several studies show that magnetic fields can affect both, the final stellar masses and the overall SFE (e.g., Krumholz & Federrath 2019; Rosen & Krumholz 2020; Hennebelle et al. 2022; Mignon-Risse et al. 2021; Myers et al. 2014; Seifried & Walch 2015). Therefore, including magnetic fields in our simulation would most likely lower the accretion rates, stellar masses and SFE.

(Kuiper et al. 2015) emphasize that the mass accretion period and thus the final mass in sink particles highly depend on the lifetime of the circumstellar accretion disc and the surrounding material, which can be influenced by the processes mentioned above.

5.7 Resolution Limitations

In our simulations, the run with a spatial resolution of ~ 200 au produces a more massive sink than the run with a resolution of ~ 400 au. The higher resolution allows us to resolve higher gas densities, which in turn affects the propagation of ionizing radiation. Since the recombination rate scales with the square of the density, ionizing photons are absorbed more efficiently at higher densities, effectively trapping the radiation for longer and delaying the expansion of the UC-HII region. This delay gives the sink more time to accrete additional mass before feedback-driven disruption of the cloud halts further accretion. In our simulations, each sink particle represents a single star. The fiducial spatial resolution of ~ 400 au is not high enough to resolve the internal structure of massive stars or very close companions. This means that some sink particles probably contain several unresolved stars. Treating them as single objects increases the effective accretion, so that gas that would in reality be divided among multiple stars instead accretes onto a single sink, raising its accretion rate and final mass (Bate 2009; Federrath et al. 2010). At the same time, the artificially high mass of these sinks results in a stronger radiative feedback, which can heat and disperse surrounding gas more efficiently, halting accretion earlier and suppressing further fragmentation (Krumholz et al. 2009; Kuiper et al. 2010b; Rosen et al. 2016). These two effects act in opposite directions: unresolved multiplicity tends to boost accretion, while stronger feedback tends to limit it. In our simulations, the enhanced accretion dominates during the early phases, leading to more massive stars. As the most massive sinks grow, their intensified feedback becomes increasingly effective at heating and dispersing the surrounding gas, which can slow or shut down further accretion and reduce subsequent star formation (Peters et al. 2010; Myers et al. 2013). Our simulations resolve turbulent fragmentation, but lack additional disc fragmentation, which might result in too massive stars, an overestimation of stellar feedback and a lack of lower-mass companion stars.

When simulations on a larger scale are performed, sink particles

usually represent several stars or a star cluster. In this case, subgrid models that sample the stellar IMF are used (Rathjen et al. 2023; Kim et al. 2023). Using a coarser resolution than ours (~ 7000 au) Cournoyer-Cloutier et al. (2021) find that including a massive star binary fraction in clusters may have an impact on the dynamics of the forming star cluster. However, from observations Enokiya et al. (2021) sees a correlation between the number of massive stars in a region and the corresponding column density. In our simulation 11 massive sink particles are formed at a column density of around 1 g cm^{-2} which is in agreement with Enokiya et al. (2021).

5.8 Massive Star Formation Scenarios

There are several theories about how a massive star forms and how it accretes mass. The theory of a core collapse scenario suggests that a star is formed from a single clump that already contains most of the final stellar mass of the forming star (McKee & Tan 2003). Less than half of the clump mass is supposed to end up in one massive star. This cannot be seen in our simulations, as our sink particles do not have an isolated mass reservoir and still accrete mass from their surroundings while moving towards the centre of the simulation domain. However, the competitive accretion model (Bonnell et al. 2001) says that the gas which is eventually accreted by a forming massive star is initially not necessarily gravitationally bound to the star. The formed stars share a mass reservoir and compete to accrete. This scenario can be found in our simulations. In addition, Padoan et al. (2020) propose the internal inflow model, where most of the final mass of a star reaches the star due to a random velocity field from larger scales and not due to its gravitational potential. Although they simulated a $(250 \text{ pc})^3$ box, this can also be seen on smaller scales in our simulation. Dense gas clumps move towards the most massive sink, where they are accreted. However, the clump motion can be caused by both turbulence and gravity; in our simulations, it is not clear that turbulence dominates the clump motion.

6 CONCLUSIONS

This work studies (massive) star formation in isolated collapsing turbulent cores with an initial mass of $1000 M_\odot$ and a radius of 1 pc with the hydrodynamic AMR code FLASH. A novel scheme to treat the radiative transfer of ionizing radiation and radiation pressure from ionizing radiation as well as heating by non-ionizing radiation is included. The temperatures of gas, dust, and radiation are calculated self-consistently. We investigate the collapse, star formation, and evolution of the cores until UC-HII regions are established and star formation is mostly complete.

We analyze in detail the evolution of the FIDUCIAL run, a core with solar metallicity, a moderately steep density profile, and a virial parameter of 0.6. In total 19 sink particles are formed, while 10 become massive. Initially, the dust temperature follows the gas temperature morphology because of gas-dust coupling. Once sink particles form, radiative feedback heats the dust and the dust temperature primarily governed by the radiation temperature. Due to turbulence, the accretion rates of sink particles are highly variable. The combination of the local and global collapse leads to the formation of the most massive sink, the so-called MMS. The MMS forms near the centre and is only the 4th sink particle that forms and dominates the cluster due to its mass. The density around the MMS is typically so high that ionizing radiation is trapped, while mass accretion is still ongoing. Ionizing feedback from other massive sinks, located in less dense

environments, launches an expanding HII region, which finally disrupts the central hub around the MMS. Then, the trapped ionizing feedback from the MMS escapes, further powers the HII region, and finally disrupts the parental cloud.

We compare the feedback mechanism of ionizing radiation and radiation pressure. Ionizing radiation sets an upper limit on the mass accretion. Without ionizing feedback, sink particles do not stop accreting mass during the simulated time period. We find that the momentum, which is transferred to the gas by direct radiation pressure from ionizing radiation, supports the growth of the HII region. Radiative heating from non-ionizing radiation is essential, as it suppresses fragmentation while the core warms up.

Our resolution study shows that increasing resolution leads to an increasing number of (lower-mass) sink particles. At the same time, sink particles are formed at higher densities, thus ionizing feedback of the MMS is trapped for a longer time period, and thus the MMS has more time to accrete mass. As a result, the total SFE increases with resolution.

Finally, we investigate the impact of different initial conditions. All simulations are dominated by one very massive sink particle, which is most likely not the sink particle that forms first. The flatter the density profile, the slower the collapse. However, the final number of sink particles as well as the SFE increase for flatter core profiles. With a low virial parameter, gravity is more dominant than kinetic motions. This leads to a faster core collapse that produces fewer but very massive sink particles which have a high ionizing photon emissivity leading to a decrease in the overall SFE. With an initially high virial parameter, turbulence is more dominant and the core collapse is time delayed. More substructures are produced, resulting in a slightly increased number of sink particles that have a lower average mass, resulting in a higher SFE. Lower metallicity leads to reduced dust cooling, resulting in higher average temperatures during the initial collapse phase and in the suppression of fragmentation. Fewer but massive sink particles are formed, while in total the SFE decreases. A core with a higher metallicity can more efficiently cool the dust, resulting in more fragmentation and a higher SFE. However, the SFE is very sensitive to the environment of the most massive stars. The longer massive stars are embedded and the formation of an UC-HII region is suppressed, the higher the overall SFE. Therefore, in our simulation a faster core collapse does not necessarily result in a higher SFE, as feedback plays a key role in determining the overall SFE.

The advanced and more realistic temperature calculation in our simulations provides an ideal test bed to compare with observations of high-mass cores such as observed in the ALMAGAL project. The comparison with observations will be presented in a follow-up paper.

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DATA AVAILABILITY

The data underlying this article will be shared on reasonable request to the corresponding author.

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APPENDIX A: ADDITIONAL FIGURES

We show a phase diagram of the temperature evolution for gas, dust and radiation temperature in the FIDUCIAL run (see Fig. A1). The gas temperature is initially warmer than the dust and radiation temperature. However, after $\sim 0.2 t_{\text{ff}}$, most of the gas and dust are in equilibrium. Later, the dust temperature follows the radiation temperature. When the sinks become massive, ionizing radiation is emitted and the gas temperature increases to up to 10^4 K in regions with a gas

density between $10^{-22} \text{ g cm}^{-3}$ and $10^{-17} \text{ g cm}^{-3}$. At the same time, the dust and radiation temperatures warm up. At $0.70 t_{\text{ff}}$ the central hub around the MMS becomes very dense ($\sim 10^{-16} \text{ g cm}^{-3}$) and warms before it is dispersed by ionizing feedback.

Fig. A2 shows a temperature phase diagram of gas, dust, and radiation of two runs in the resolution study (run FIDUCIAL and RFL11) at $0.53 t_{\text{ff}}$. Using a higher resolution (run RFL11) leads to a higher density threshold for sink particles (see also section 3.3) and therefore higher densities can be resolved. These higher densities reach higher gas, dust, and radiation temperatures compared to the FIDUCIAL run even before ionizing radiation sets in.

Fig. A3 shows the number of sink particles for two different stages. First, when $90 M_{\odot}$ are in sink particles and second, when 90% of the final mass has been accreted. Due to computational costs, runs RFL11 and RFL12 were stopped before they reached the second time. However, already when $90 M_{\odot}$ have been accreted onto sinks we can see that an increasing resolution leads to the formation of more sink particles. Stage two (95%) indicates that, especially, the number of low-mass sinks increases with higher resolution. Nevertheless, comparing both stages shows that when $90 M_{\odot}$ are accreted onto sink particles the fragmentation process is almost complete and only one additional sink particle is formed in both, runs FIDUCIAL and RFL10.

In Fig. A4 we show the fraction of mass that has been accreted onto the MMS, normalized by the total mass accreted by all sink particles for the runs of the parameter study. The first sink particles in each run do not necessarily evolve into the MMS. Only in runs ZLOW and FLAT the first sink particle also evolves into the MMS. The time when the first sink particle in each simulation becomes massive is marked with a star. Triangles indicate when the MMS reaches $8 M_{\odot}$. In all runs the MMS is overall not the first sink particle that becomes massive.

Fig. A5 shows the total ionizing photon rate for the runs in the parameter study. The ionizing photon rate highly depends on the mass growth of the sink particles (see Fig. 18). High mass accretion rates and an early formation of massive sink particles generally lead to a rapid increase of the ionizing photon rate. Therefore, the ionizing photon rate increases faster for the run αLow compared to the FIDUCIAL run while the time-delayed evolution of the runs αHigh , SHALLOW, and FLAT results in a time-delayed rise of the total ionizing photon rate. Although the time evolution of the ionizing photon rate varies, it eventually converges across all runs as the stellar luminosity becomes the dominant factor.

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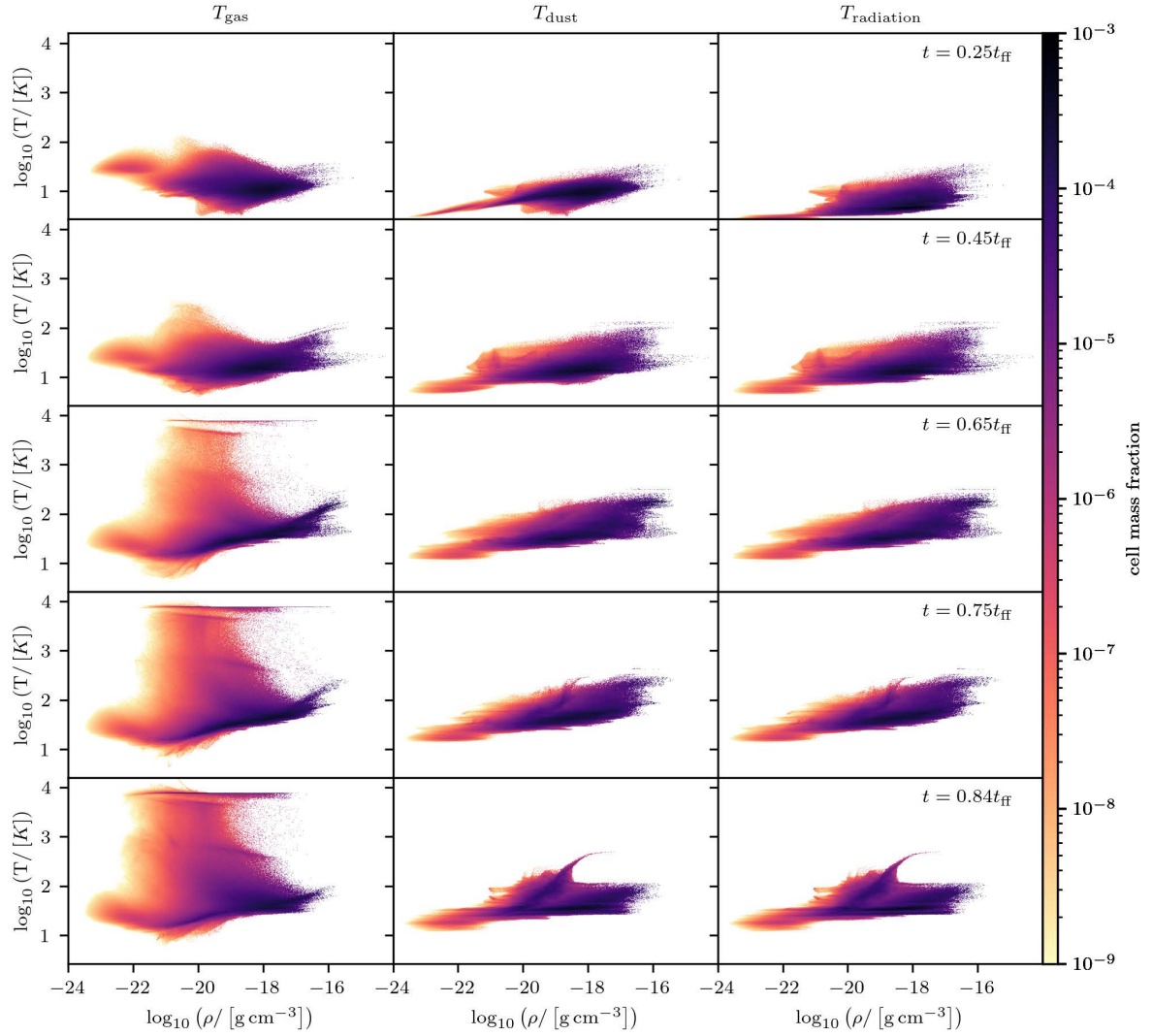


Figure A1. Phase diagram of the temperature evolution (from top to bottom) for gas, dust and radiation temperature (left to right) in the FIDUCIAL run. At the beginning the radiation temperature is colder than the dust and gas temperature. After $\sim 0.4 t_{\text{ff}}$ the dust and radiation temperature behave similar. The gas temperature rises (up to 10^4 K) as soon as sink particles become massive (after $\sim 0.4 t_{\text{ff}}$). As a result, the dust and radiation temperature become warmer. The very dense region ($10^{-16} \text{ g cm}^{-3}$) at $0.70 t_{\text{ff}}$ shows the region around the MMS, before ionizing feedback disperses the dense central hub.

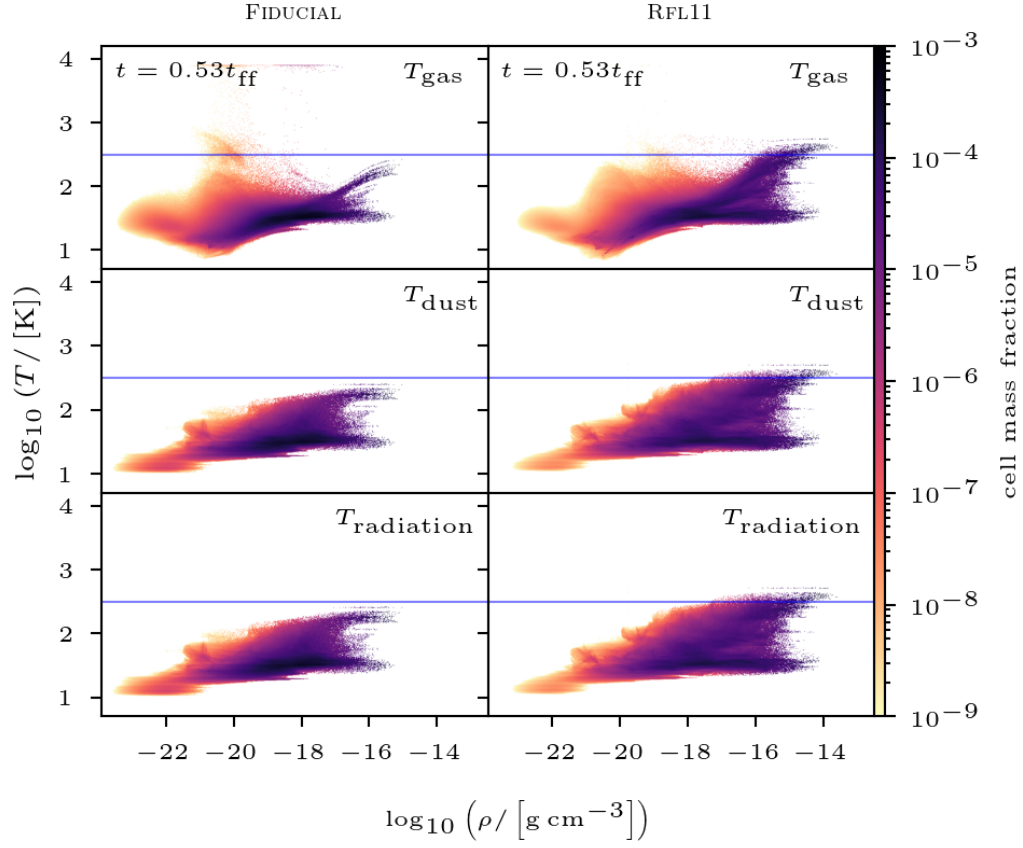


Figure A2. Phase diagram of the temperature for gas, dust and radiation temperature (top to bottom) for the runs FIDUCIAL (left panels) and RFL11 (right panels). Blue lines help for better comparison. A higher resolution (run RFL11) resolves higher densities and dense cells can be heated up to higher temperatures compared to the FIDUCIAL run.

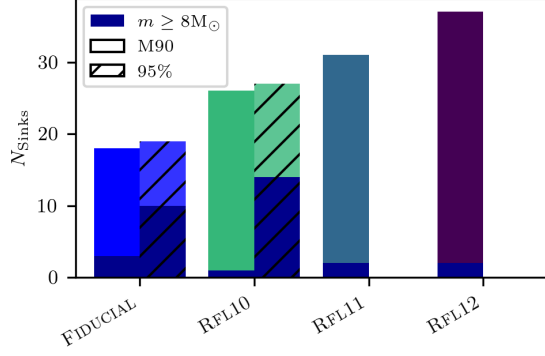


Figure A3. Number of sink particles at two different stages, when $90 M_{\odot}$ and 95% of the final mass has been accreted, shown by the non hatched and hatched region, respectively. Runs RFL11 and RFL12 never reach this stage due to computational costs. The dark blue area shows the number of high-mass stars. The total number of low- and high-mass sink particles increases with higher resolution.

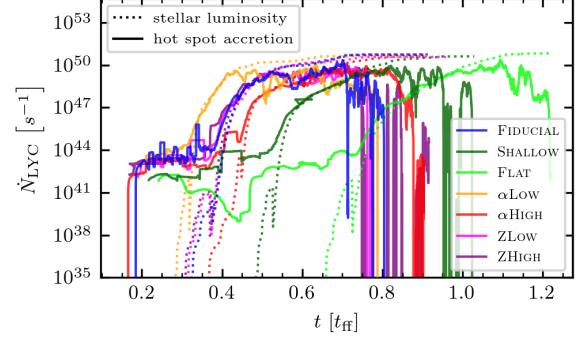


Figure A5. Total ionizing photon rate (smoothed) from hot spot accretion (solid lines) and stellar luminosity (dotted lines) for the runs in the parameter study. In run α Low the ionizing photon rate increases faster compared to the fiducial run, while it is time delayed for run α High and runs with shallower density profiles (SHALLOW and FLAT). Later, the ionizing photon rate from stellar luminosity is comparable for all runs.

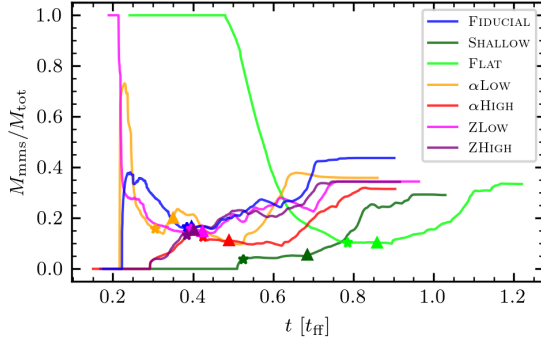


Figure A4. Fraction of the accreted mass onto the MMS normalized by the total accreted mass. The stars indicate when the first sink particle in the simulation reaches $8 M_{\odot}$ and the triangles show when the MMS becomes massive. Only for two runs (ZLow and FLAT) the first sink particle evolve into the most massive one. For every run the MMS is not the first sink which becomes massive.

PAPER II - MASSES AND TEMPERATURES OF DENSE CORES

We analyse two simulations from Paper I and post-process snapshots with RADMC-3D to generate synthetic 1.36 mm dust-continuum maps along three different line-of-sight. Using CASA, we convert these maps into synthetic ALMA images with ALMAGAL-like configurations and define cores around sink particles with a fixed radius of 1500 au to enable direct comparisons between simulation quantities and observational measurements. We then quantify how numerical resolution, viewing geometry, different temperature-estimation methods (a clump-based luminosity-to-mass, L/M , prescription, an L/M +flux model, and a supervised machine-learning approach), and interferometric flux recovery affect the masses inferred from continuum data.

8.1

PUBLICATION II

Birka Zimmermann, Álvaro Sánchez-Monge, Stefanie Walch, Gary Fuller

Linking simulations and observations of star-forming regions I. Masses and temperature of ALMAGAL-like cores. Submitted to A&A, aa59518-26, February 2026

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Linking simulations and observations of star-forming regions

I. Masses and temperatures of ALMAGAL-like cores

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ABSTRACT

Context. Stars form inside dense cores and clumps deeply embedded in (massive) star-forming complexes. These dense cores and clumps are commonly probed through (sub-)millimetre observations, with their physical properties derived from measured fluxes and sizes that may be affected by factors such as limited spatial resolution, interferometric filtering, or projection effects.

Aims. By comparing numerical simulations with synthetic observations of (massive) star-forming clumps, we aim to quantify how reliably core masses and temperatures can be inferred from ALMA-like continuum data.

Methods. We analyse radiation–hydrodynamic simulations of collapsing $1000 M_{\odot}$ clumps, post-processed with RADMC-3D and CASA to generate synthetic ALMA-like images that reproduce the observational properties of the ALMAGAL Large Program. In our analysis, cores are defined as spherical regions (circular, in 2D projection) around numerical sink particles, enabling a simple comparison of the mass estimated from the 3D simulation, from idealised RADMC-3D emission maps, and from synthetic ALMA images. We also quantify how resolution, projection, and viewing angle affect core and sink masses, and test three dust-temperature estimators (clump-scale L/M , a L/M +flux model, and a supervised machine-learning-based estimate).

Results. Projection effects cause the line-of-sight integrated mass within a core radius of 1500 au to exceed the corresponding spherically enclosed mass by factors of 2–3. The empirical L/M temperature prescription, used in some observational works to determine core masses, follows the global thermal evolution but misses the core-to-core scatter, producing individual core mass errors of a few. We show that improved estimates can be achieved when local flux information is taken into account. Preliminary tests of a machine-learning-based estimate with a gradient-boosting model further suggest potential improvement. Synthetic ALMAGAL-like images recover the global core structure, while residual flux-reconstruction uncertainties introduce additional mass errors of up to a factor ~ 3 and limit reliable minimal detectable core-mass estimates to $\gtrsim 0.3 M_{\odot}$, comparable to the ALMAGAL core mass completeness limit of $0.23 M_{\odot}$. Finally, from the relation between sink and core masses seen in the simulations, we derive an empirical relation that provides the expected sink mass for a given projected core mass.

Conclusions. Synthetic observations calibrated on simulations provide a practical framework to interpret core catalogues such as the one derived within the ALMAGAL project. We show that this comparison can be used to derive more robust constraints on massive dense core formation. Combining temperature uncertainty, projection, and flux-reconstruction effects, individual ALMA continuum-derived core masses in our simulations are typically uncertain by a factor of ~ 3 –5. Dust-temperature estimates and flux reconstruction are the main limiting factors: a single clump-scale L/M -based temperature prescription is not sufficient, and the presented data-driven machine-learning approach appears to be the most promising route to reduce these biases.

Key words. stars: formation – ISM: clouds – stars: massive – methods: numerical – techniques: interferometric

1. Introduction

High-mass stars and stellar clusters play a central role in shaping the interstellar medium through their ionising radiation, winds, and supernovae (e.g. Zinnecker & Yorke 2007; Tan et al. 2014; Motte et al. 2018). Yet the physical processes that govern their formation remain poorly constrained. A key step towards understanding high-mass star formation is to characterise the dense cores embedded in massive, collapsing clumps, since their masses, temperatures, and evolution set the initial conditions for individual stars and multiple stellar systems.

Large interferometric surveys such as ALMAGAL (ALMA Evolutionary Study of High-Mass Protocluster Formation in the

Galaxy, see Molinari et al. 2025; Sánchez-Monge et al. 2025) are designed to address this problem observationally. ALMAGAL targets more than a thousand dense clumps across the Milky Way, spanning a broad range of environments and evolutionary stages, and providing (sub-)millimetre continuum and line data at typical spatial resolutions of order 10^3 au. These data enable statistical studies of fragmentation, core growth, and feedback, among others, and are expected to serve as a benchmark for theoretical models of high-mass star and stellar cluster formation. The first set of ALMAGAL publications (see e.g., Coletta et al. 2025; Mininni et al. 2025; Elia et al. 2025; Schisano et al. 2025; Wallace et al. 2025) uses the ALMA continuum emission

at 1.3 mm to identify dense cores and determine properties such as their mass, size and density.

Interpreting such continuum observations is, however, non-trivial. For instance, core masses inferred from dust continuum emission at millimeter wavelengths depend on the assumed dust temperature, opacity, and geometry (e.g., Hildebrand 1983; Beuther et al. 2007; André et al. 2014), and are further affected by line-of-sight (LOS) projection effects and interferometric filtering (e.g., Offner et al. 2012; Seifried et al. 2017; Koepferl et al. 2017; Padoan et al. 2023; Nucara et al. 2025). In practice, the dust temperature of individual cores is rarely measured directly. Within ALMAGAL, so far, an empirical prescription assigns a single temperature to all cores in a region (or clump) based on its luminosity-to-mass ratio (L/M), taken as a proxy for their evolutionary stage (Coletta et al. 2025). This approach captures the global heating history, but it cannot account for core-to-core temperature variations driven by local accretion, clustering, feedback, and geometry. Such temperature mismatches introduce systematic biases in the inferred core masses (e.g., Malinen et al. 2011; Traficante et al. 2023). Additional uncertainties arise from flux reconstruction in interferometric imaging and from the fact that continuum cores are intrinsically projected entities contaminated by foreground and background material (e.g., Offner et al. 2012).

Numerical simulations provide a complementary way to quantify and interpret these biases on core and clump scales (e.g., Rosen et al. 2020; Padoan et al. 2023; Lobreuil et al. 2025). When such simulations are post-processed with radiative transfer tools, the resulting synthetic observations become a powerful tool for interpreting real data and for guiding the development of numerical models (e.g., Haworth et al. 2018). When they are additionally imaged with realistic telescope configurations (e.g., mimicking ALMA observations), these synthetic datasets can be analysed in exactly the same way as real observations, while the underlying “true” core properties remain known. The post-processing and comparison of 3D simulation data and 2D synthetic observations offers a controlled laboratory to calibrate temperature prescriptions, assess the impact of projection and flux reconstruction, and link observed continuum cores to their underlying stellar content.

In this paper, we use the radiation–hydrodynamic simulations of Zimmermann et al. (2025) as a testbed to confront simulations and synthetic observations of high-mass star-forming clumps. We focus on two runs that differ only in numerical resolution and post-process each snapshot with the radiative transfer code RADMC-3D (Dullemond et al. 2012). Synthetic ALMA observations that mimic ALMAGAL cores are then calculated with CASA (CASA Team et al. 2022). Cores are defined around individual sink particles with a fixed physical radius, allowing a direct one-to-one comparison between simulated structures and their observational counterparts.

Our aims are twofold: (i) on the theoretical side, to quantify how numerical resolution and projection effects bias core and sink masses, as well as the clump-scale core mass fraction; and (ii) on the observational side, to evaluate several dust-temperature estimators and how, together with flux reconstruction, they affect continuum-based core masses. The paper is organised as follows. In Sect. 2, we briefly introduce the numerical simulations, and describe the process of construction of the synthetic observations. In Sect. 3, we analyse core and sink masses, projection effects, and the evolution of the core mass fraction. In Sect. 4, we investigate different dust-temperature estimators and their impact on mass estimates. In Sect. 5, we provide a compact “recipe of warnings” and quantitative guidelines for interpreting

observational dense core catalogues, like that of ALMAGAL, and in Sect. 6 we summarise our main findings.

2. Simulations and synthetic observations

2.1. Numerical simulations

The simulations used in this work are described in detail in Zimmermann et al. (2025); here we summarise only the main aspects. The simulations follow the collapse of a massive clump with the adaptive mesh refinement (AMR) code FLASH (Fryxell et al. 2000), using an entropy-stable (magneto-) hydrodynamics scheme (Derigs et al. 2016). Gas and dust are treated as perfectly mixed with a fixed dust-to-gas mass ratio of 0.01. A non-equilibrium chemical network evolves seven species (H_2 , H , H^+ , CO , C^+ , O , e^-) with reactions from Nelson & Langer (1997) and updates from Glover et al. (2010).

Self-gravity and radiative transfer are handled with the tree-based TREERAY scheme (Wünsch et al. 2018, 2021). The TreeRay/OpticalDepth module (Wünsch et al. 2018) accounts for dust shielding as well as the (self-)shielding of molecular hydrogen and CO, while TreeRay/OnTheSpot (Haid et al. 2018; Wünsch et al. 2021) models ionising radiation from sink particles using the on-the-spot approximation (Osterbrock 1988). In these runs, radiation pressure from ionising photons onto gas and dust is calculated, and the corresponding momentum is transferred via TreeRay/RadPressure (Klepitko et al. 2023). This model also includes the heating of dust from non-ionising photons. The stellar feedback (ionising and non-ionising luminosities) follows the sink accretion histories as described in Klepitko et al. (2023).

Sink particles represent individual stars and are created self-consistently following the method of Dinnbier & Walch (2020). The density threshold for sink formation is tied to the local Jeans length at the maximum refinement level,

$$\rho_{\text{thresh}} = \frac{\pi c_s^2}{G \lambda_J^2} = \frac{\pi c_s^2}{G (4 \Delta x)^2}, \quad (1)$$

where c_s is the local sound speed, G the gravitational constant, and Δx the smallest cell size (Truelove et al. 1997). Additional checks ensure that the gas is gravitationally bound and collapsing, that the location is a potential minimum, and that it lies outside the accretion radius of existing sinks. Each sink is evolved with a fourth-order Hermite integrator, and its radius and effective temperature follow the accretion-dependent protostellar evolution models of Offner et al. (2009). Note, that at our resolution, a sink particle does not necessarily represent a single star, but rather a protostar together with its disk and inner envelope. This interpretation is appropriate, as the observational data resolve structures on similar spatial scales (~ 1200 au).

The initial conditions of the simulations are chosen to be representative of ALMAGAL clumps (see e.g., Molinari et al. 2025). The computational domain is a $(4 \text{ pc})^3$ box containing a $1000 M_\odot$ clump within a radius of 1 pc at solar metallicity. The clump follows a Plummer-like density profile with an outer slope of -2 and has a virial parameter of $\alpha_{\text{vir}} = 0.6$, ensuring global collapse. The initial gas temperature is 20 K; the dust temperature is set to 10 K and is rapidly brought into thermal equilibrium. No external interstellar radiation field is included, as the region is deeply embedded. In this work, we use two runs from the resolution study performed in Zimmermann et al. (2025) that share the same global setup but differ in maximum refinement level, $l_{\text{ref}} = 9$ and 12 (hereafter RFL9 and RFL12, respectively),

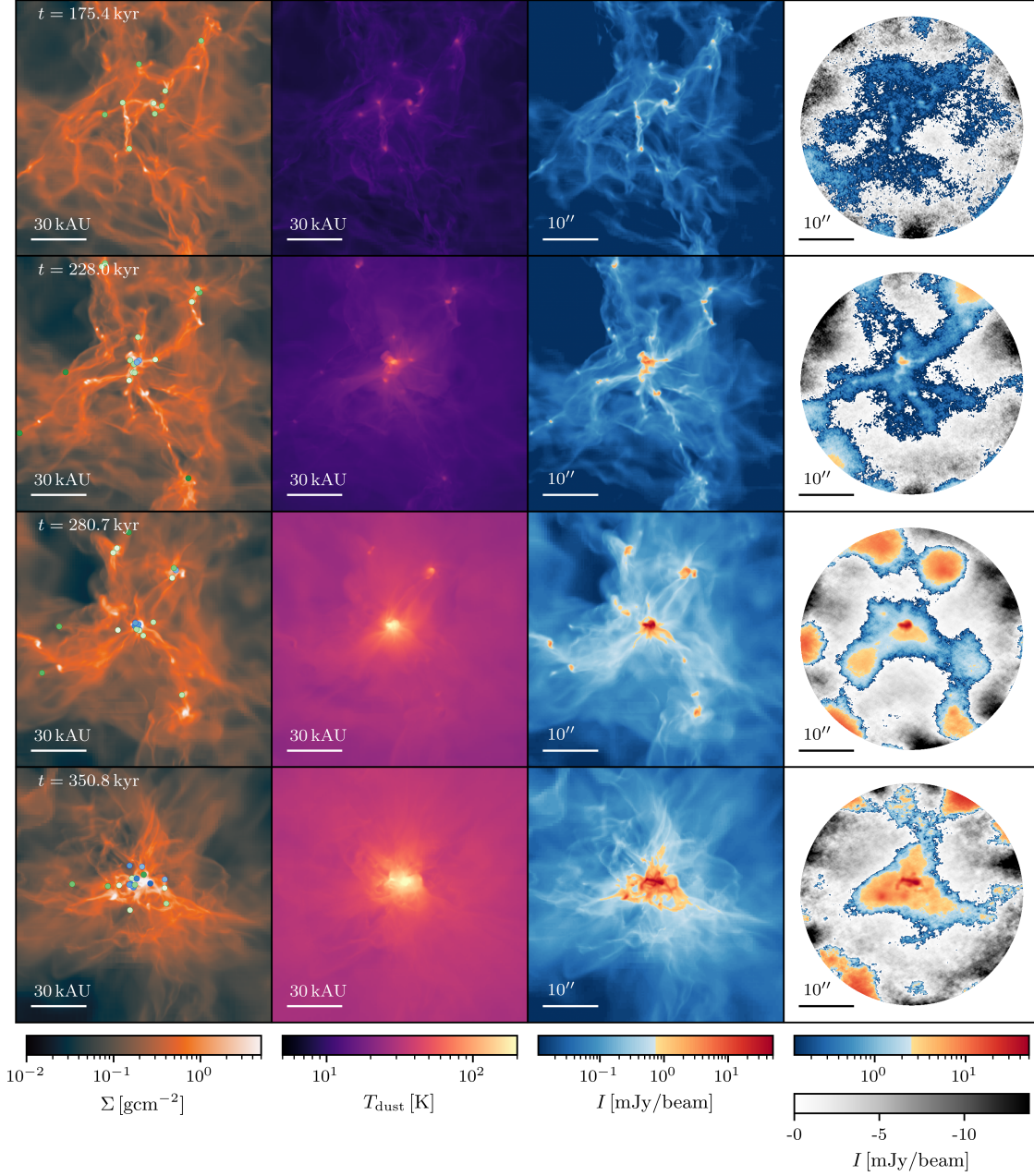


Fig. 1: Time evolution of run RFL9. The first two columns show the intrinsic simulation outputs: column density and dust temperature. The third column shows flux maps obtained through post-processing with RADMC-3D at $1362.7\,\mu\text{m}$ and a distance of 3 kpc, and the final column presents synthetic ALMA observations generated with CASA, taking into account the interferometric response.

corresponding to minimum cell sizes of 400 and 50 au, respectively.

In the following analysis, we make use of snapshots that cover the entire early evolution of the clump, from the onset of collapse to the stage where stellar feedback disrupts the cloud. The temporal evolution of RFL9, showing column density, dust temperature, and the corresponding RADMC-3D (see also Sec. 2.2.1) and ALMA (see also Sec. 2.2.2) post-processed maps

(from left to right), is presented in Fig. 1. Here, the first sink particles form after ~ 93 kyr. The sink population grows rapidly during the subsequent global collapse phase. Ionising radiation first appears once the most massive sink reaches $8\,M_{\odot}$, typically at $t \approx 240$ kyr, after which the thermal and density structure of the clump begin to deviate from pure gravitational collapse. As the H II region expands, it eventually disrupts the parent clump at $t \approx 370$ kyr, at which point most of the dense gas is dispersed.

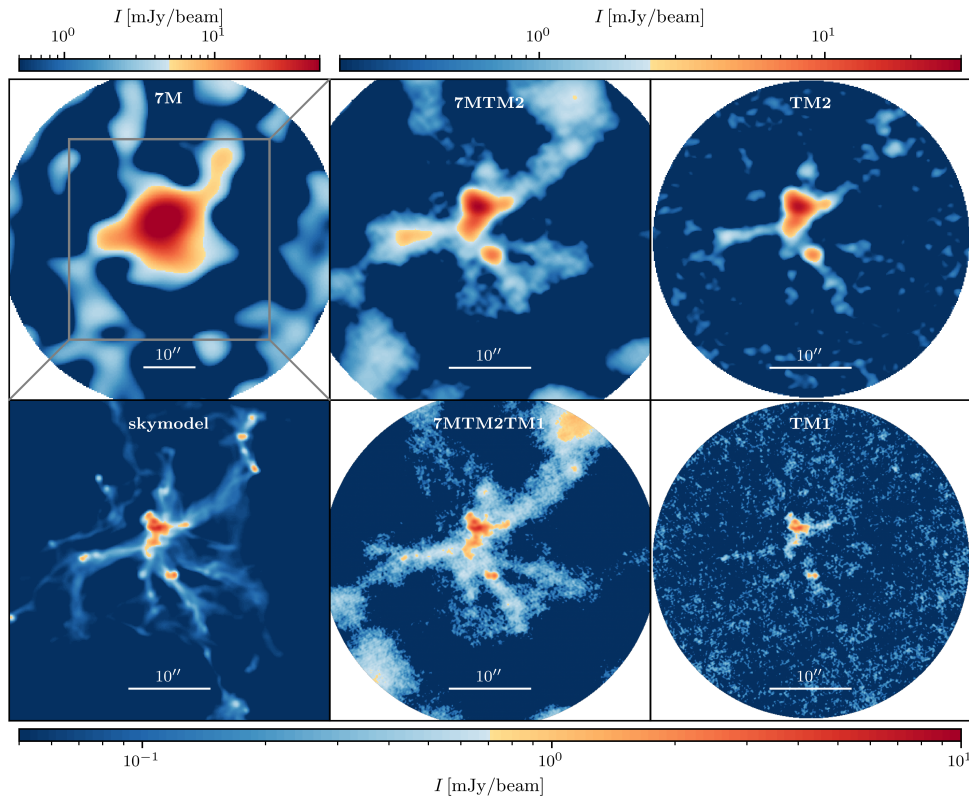


Fig. 2: Flux distributions from different ALMA telescope array configurations simulated with CASA at 230 kyr, shown for the LOS along the z -direction. Top row: 7 m array (left; geometric mean resolution $6.1''$, 18 360 au), combined 7 m+TM2 arrays (middle; $1.4''$, 4 340 au), and TM2 alone (right; $1.3''$, 3 850 au). Bottom row: sky model (left), combined 7 m+TM2+TM1 configuration (middle; $0.41''$, 1 220 au), and TM1 alone (right; $0.30''$, 890 au). The combination of short and long baselines is required to recover both compact cores and extended emission.

These characteristic evolutionary stages (the onset of sink formation, onset of ionisation, eventual cloud disruption) provide the temporal context for the synthetic observations and the trends presented in later sections.

2.2. Radiative transfer and synthetic observations

The numerical simulations described in Sect. 2.1 serve as a testbed to confront simulations with observations. The ultimate goal is to compare with real observational data from the ALMAGAL survey (Molinari et al. 2025). In this work, we compare the simulation outputs with their corresponding synthetic observations. To achieve this, we post-process the simulations using radiative-transfer techniques (see Sect. 2.2.1) and simulate the telescope configurations used in the ALMAGAL project (see Sect. 2.2.2), mimicking the conditions of real observations.

2.2.1. RADMC-3D post-processing

To produce synthetic dust continuum emission maps, we post-process our simulation snapshots with RADMC-3D (Dullemond et al. 2012) to compute the intensity by integrating the radiative transfer equation along rays through the three-dimensional grid, accounting for dust absorption and thermal emission and neglecting scattering. For the post-processing, we

provide RADMC-3D with the dust temperature computed self-consistently in the simulation, as well as the corresponding gas and dust density distribution.

With these precomputed fields, we generate synthetic dust continuum emission maps at 1.36 mm for cloud located at a distance of 3 kpc. This corresponds to the wavelength used in the ALMAGAL project to study the continuum emission from cold, dense dust in massive clumps. For the dust opacity we adopt the Weingartner & Draine (2001) model with $R_V = 4.0$, corresponding to an absorption opacity of $\kappa_{1.3\text{ mm}} = 0.32 \text{ cm}^2 \text{ g}^{-1}$ per unit dust mass. Each 3D simulation snapshot is post-processed for three LOS along the x , y , and z axes, yielding three 2D continuum maps at 1.36, mm.

2.2.2. ALMA (CASA) post-processing

We simulate ALMA band 6 continuum observations using the software CASA (Common Astronomy Software Applications CASA Team et al. 2022), following the observing and imaging philosophy adopted in the ALMAGAL project (see Sánchez-Monge et al. 2025).

We initiate the process using noise-free two-dimensional RADMC-3D specific-intensity maps as input sky brightness models. Synthetic interferometric visibilities are generated for these sky models using the task `simobserve`. We consider

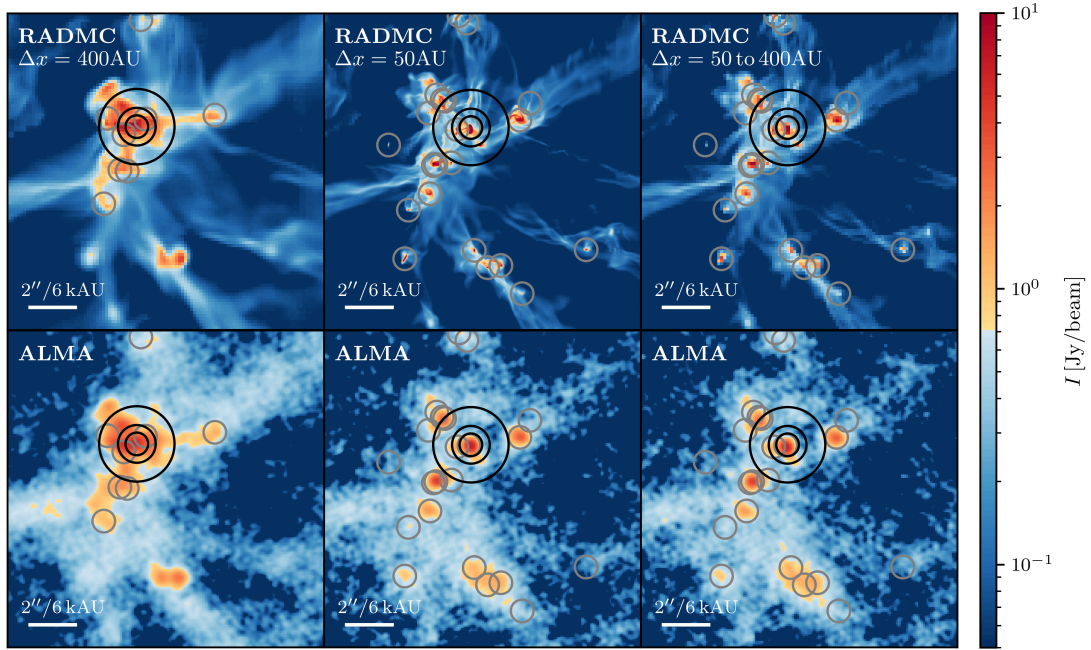


Fig. 3: Synthetic RADMC-3D emission (top panels) and ALMA-imaged counterparts (bottom panels) at $t = 230$ kyr, shown for the LOS along the z -direction. From left to right: native resolution 400 au (RFL9); native resolution 50 au (RFL12); and initial resolution 50 au. Only for the right-hand panels, the RADMC-3D output is first downsampled to a common grid of 400 au, and the ALMA images are then generated from these downsampled maps. Gray circles indicate the sink particle (core) locations. Black circles mark physical radii of 1500 au, 2500 au, and 5000 au, centred on the most massive sink particle. Higher intrinsic simulation resolution resolves more substructure and produces more sharply defined cores. Even after downsampling, the high-resolution run retains fine structure that the lower-resolution simulation cannot reproduce. The ALMA maps are limited by an effective resolution of ~ 1200 au, but the RFL12-based downsampled ALMA images (bottom right) still show more clearly defined cores than the lower-resolution case. The intrinsic simulation resolution sets which features remain visible and how well the cores are delineated.

three different telescope configurations, corresponding to those used in the ALMAGAL project: 7 m (ACA or 7M), compact 12 m (TM2), and extended 12 m (TM1, see Sánchez-Monge et al. 2025, for more details). For the spectral setup, we set the central observing frequency at $\nu_0 = 220$ GHz (i.e., ALMA band 6) and use a total bandwidth $\Delta\nu = 3$ GHz, equivalent to the frequency and effective bandwidth of the ALMAGAL continuum observations. We use the same on-source integration times as in the ALMAGAL observations for the different arrays (i.e., between 2 and 4 minutes). The phase center of the synthetic observations is set at $\alpha_{J2000} = 16^h10^m00^s$, $\delta_{J2000} = -35^\circ30'00''$, mimicking the coordinates of a southern-hemisphere source. Finally, thermal noise is added using the CASA atmospheric plus receiver model for band 6, adopting a precipitable water vapour PWV = 1.7 mm.

Imaging of the synthetic visibilities is performed using the `tclean` task. We use a Briggs weighting (`robust=0.5`) and restrict the imaged region to the 20% level of the primary-beam area via `pbmask=pblimit=0.2`. Primary-beam correction is applied to the final images. Deconvolution follows an ALMAGAL-style iterative masking procedure (see Sánchez-Monge et al. 2025), in which CLEANing masks are updated based on signal to noise emission and residual-noise estimates until convergence. First, we run a shallow CLEAN with only 100 iterations to obtain an initial partially-CLEANed image. Next, we use this first image to build a CLEANing mask based on the signal-to-noise ratio ($\text{SNR} = I/\sigma$, where I is the pixel intensity

and σ is the rms noise). The mask includes those regions with emission above a user-defined low-SNR threshold only when it is spatially connected to a user-defined high-SNR detection. We automatically and iteratively update this mask (up to five times) and relax the SNR thresholds in later iterations. Within each mask iteration, we continue CLEANing in blocks of 100 iterations down to a threshold of 1σ . We stop when the relative improvement in both the model flux and the residual noise level (estimated from the median absolute deviation) fall below 2%. Once the iteration process is finished, the final continuum images are generated. As a last step, we apply primary-beam correction with the task `impbcor`, and export the final images into FITS format. This iterative process is performed to generate images of individual configuration arrays (i.e., 7M, TM2 and TM1), as well as images of combined arrays (i.e., 7M+TM2, 7M+TM2+TM1). These images correspond to the science products generated within the ALMAGAL project.

Figure 2 shows the flux distributions obtained with the different ALMA array configurations for a representative snapshot of run RFL9. The bottom-left panel displays the sky model, corresponding to the original RADMC-3D input. The 7M image (top-left) has the coarsest resolution ($\sim 18,360$ au). Its short baselines provide the largest field of view and good sensitivity to extended emission, but blend multiple cores into broad structures. The TM2 configuration (top-right) improves the resolution to $\sim 3,850$ au, resolving individual features more clearly at the cost of reduced sensitivity to large-scale

emission. The 7M+TM2 image (top middle) recovers both extended and intermediate-scale structures. TM1 (bottom-right) reaches the highest resolution (~ 890 au), resolving compact cores but filtering out much of the envelope. The fully combined 7M+TM2+TM1 image (bottom-middle, with ~ 1200 au) incorporates the strengths of all arrays, capturing both compact sources and extended emission. Although some filamentary structure is lost relative to the input map, the main cores and emission peaks remain detectable.

2.3. Core identification and properties

In this study, we examine the temperature and mass of individual cores, and compare their values from numerical simulations with the corresponding parameters that can be derived from synthetic observations. Throughout this work, we assume that each sink particle in every simulation snapshot represents a core with a radius of 1500 au. As a consequence of this fixed radius, the identified cores may spatially overlap. We note that in this work, we aim at comparing the properties of cores rather than to perform an exhaustive core-identification analysis, as would be required for comparison with observational core-finding strategies, which is left for a later publication.

Based on that, the (projected) sink positions define the core locations in the simulations and synthetic observations, ensuring a direct one-to-one comparison between the simulated structures and their observational counterparts. As shown in Fig. 3, the sink locations coincide with the peaks of emission in the post-processed RADMC-3D and ALMA images. Before comparing the properties of the cores from synthetic images and numerical observations, we remove objects that do not represent detectable dense cores. For instance, some sinks have very low enclosed masses because ionising radiation clears their inner envelopes. Others may simply form with intrinsically low-mass envelopes. Such objects are not expected to be detectable in post-processing and would introduce non-representative errors. We therefore include only cores with more than $0.1 M_{\odot}$ of gas within a 1500 au-radius sphere around the sink particle. Moreover, the smaller field of view of the synthetic ALMA observations (see Sect. 2.2.2), compared to the field of view of the numerical and RADMC-3D maps, result in some of the simulated cores to be located outside the ALMA field of view, and therefore excluded from the analysis.

Synthetic dust-continuum observations generated with RADMC-3D and CASA allow us to estimate the masses of dense cores and protostellar envelopes. Under the assumption that the dust emission is optically thin, the total mass can be estimated directly from the observed flux density:

$$m = \frac{I_{\nu} D^2}{f_d \kappa(\nu) B_{\nu}(T_d)}, \quad (2)$$

where I_{ν} is the measured flux density, D is the distance to the source (set to 3 kpc), f_d is the dust-to-gas mass ratio (set to 1/100), $\kappa(\nu)$ is the dust opacity at the observing frequency ($\nu = 230$ GHz, $\kappa(\nu) = 0.32 \text{ cm}^2 \text{ g}^{-1}$, taken from Weingartner & Draine (2001)), and $B_{\nu}(T_d)$ is the Planck function evaluated at the dust temperature T_d (Hildebrand 1983).

2.4. Definitions of masses and temperatures

For clarity, we summarise the different mass and temperature parameters used throughout the paper in Table 1. In the simulations, we distinguish between the sink mass, m_{sink} , the spherically enclosed gas mass within radius r , m_{3D} , and the projected

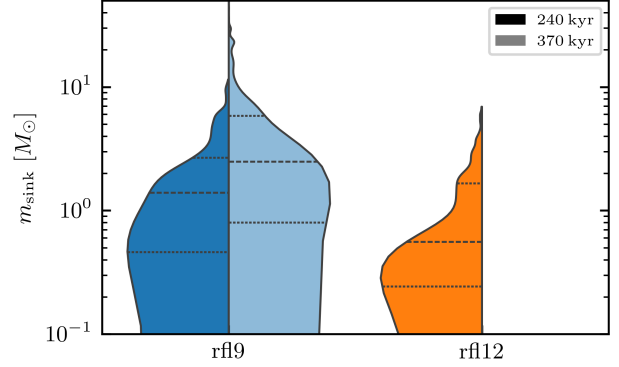


Fig. 4: Sink masses for all sinks at each snapshot up to 240 kyr (blue) and 370 kyr (orange). Higher resolution (RFL12) systematically results in lower individual sink masses.

mass along the LOS, m_{2D} . We additionally consider a purely geometrical cylindrical mass, m_{cyl} , defined within a cylinder of radius r and height $2r$. From the RADMC-3D and ALMA emission maps, we derive core masses, m_{RADMC} and m_{ALMA} , using Eq. 2 with different dust-temperature estimates.

The “true” core dust temperature, $T_{\text{sim,rad}}$, is defined as the mass-weighted dust temperature along the LOS within the core radius in projection (2D). The quantity $T_{\text{sim,avg}}$ denotes the mass-weighted average of $T_{\text{sim,rad}}$ over the core, providing a single representative temperature per core. In addition, we consider several observational temperature estimates (see more in section 4.1.2): (i) $T_{L/M}$, the empirical temperature assigned from the clump luminosity-to-mass ratio following Coletta et al. (2025); (ii) a combined $T_{L/M+F}$ model that depends on both the clump L/M and the flux of each core; and (iii) T_{ML} , a supervised machine-learning estimate trained on $T_{\text{sim,avg}}$. These definitions are used consistently in the following sections.

3. Determination and analysis of core masses

In this section we analyse how the numerical resolution and geometrical projection affect the mass distribution around forming stars (sink particles) in our simulations. We then analyze the core masses derived from the RADMC-3D and ALMA synthetic images in relation to the actual values from the numerical simulations, using the mass and temperature definitions introduced in Sect. 2.4.

3.1. Impact of the numerical resolution

The study of cloud fragmentation and sink-particle formation in numerical simulations depends on the simulation’s resolution. From Zimmermann et al. (2025), we know that the number of sink particles increases with increasing resolution, but the total mass in sinks and the corresponding star formation efficiency is comparable across all runs up to $0.45 t_{\text{ff}}$ (≈ 240 kyr; see Zimmermann et al. 2025, Fig. 13-left panel, and Fig. 14-top panel). In this work, we analyze two sets of simulations, with different resolutions: RFL9, with a minimum cell size of 400 au and used for the main analysis in this work, and a higher-resolution run, RFL12, which reaches 50 au. Both achieve spatial resolutions significantly higher than the ~ 1200 au resolution of the ALMAGAL observations.

Table 1: Definitions of mass and temperature used in this work

Variable	Description of the variable
Masses	
m_{sink}	Sink (stellar) mass from numerical simulation
$m_{3\text{D}}$	Core mass (from simulation) within a sphere of radius r_{core} (in 3D)
$m_{2\text{D}}$	Projected mass (in 2D) along the LOS within a circle of radius r_{core} (from simulation)
m_{cyl}	Mass within in a cylinder of radius r_{core} and height $2r_{\text{core}}$ (from simulation)
m_{RADMC}	Mass derived using the flux of the RADMC-3D continuum map
m_{ALMA}	Mass derived using the flux of the synthetic ALMA continuum image
m_{core}	Generic core mass (context-dependent)
m_{clump}	Clump mass (from the simulation) within the adopted clump radius (see Sect. 3.5)
Temperatures	
$T_{\text{sim,rad}}$	Mass-weighted dust temperature along the LOS (from simulation)
$T_{\text{sim,avg}}$	Mass-weighted average of $T_{\text{sim,rad}}$ (simulation)
$T_{\text{L/M}}$	Temperature from the clump's L/M prescription (see Sect. 4.1.1)
$T_{\text{L/M+F}}$	Temperature from the L/M +flux model (see Sect. 4.1.2)
T_{ML}	Temperature from machine-learning model (see Sect. 4.1.3)
$T_{\text{flux,m2D}}$	Temperature required to reproduce $m_{2\text{D}}$ from the observed flux

Figure 4 shows the distribution of sink masses for the RFL9 and RFL12 runs at two different evolutionary stages: the onset of ionizing radiation at 240 kyr (left) and the point at which the H II region disrupts the clump at 370 kyr (right). Note that simulation RFL12 did not reach the later stage due to computational limitations. As indicated in Zimmermann et al. (2025), higher-resolution runs systematically have lower average sink masses compared to the lower-resolution runs. This trend arises because finer spatial resolution in the numerical simulations enables the gas to reach higher densities, allowing smaller-scale fragmentation to be resolved. As a result, the simulations produce a larger number of sinks with lower individual masses while maintaining a similar total stellar mass.

We explore now the effects of different numerical resolutions in the synthetic images. Figure 3 shows the synthetic RADMC-3D emission maps (top panels) and the corresponding ALMA synthetic images (bottom panels) for the two simulation runs: RFL9 (400 au; left) and RFL12 (50 au; middle and right). The top-right panel shows the RADMC-3D image from the high-resolution RFL12 run, down-sampled to a 400 au grid, i.e., equivalent to the low-resolution RFL9 run. This down-sampled RADMC-3D image is then post-processed to produce a synthetic ALMA image directly comparable to the synthetic ALMA image of the low-resolution RFL9 run (see bottom-left panel). Even after downsampling, the higher-resolution simulation RFL12 retains a finer substructure level of detail that the lower-resolution run cannot capture, demonstrating that the intrinsic simulation resolution sets the level of detail in the predicted emission, even when post-processed and downsampled to a lower resolution. The synthetic ALMA images shown in

the bottom panels have an effective angular resolution set by the synthesized-beam FWHM of ~ 1200 au. The pixel size of 400 au only specifies the image sampling and corresponds to ~ 3 pixels across the beam, not to a 400 au resolving power. At this lower resolution, the smallest structures from the numerical simulations are smoothed out. Nevertheless, cores originating from the higher-resolution run (RFL12) remain sharper and more centrally concentrated, whereas those from the lower-resolution run (RFL9) appear more diffuse. This shows that, even after accounting for telescope limitations, the intrinsic simulation resolution still strongly influences the observable appearance of protostellar cores and their immediate environment.

These differences are directly reflected in the averaged radial (Fig. 5). The vertical lines in these profiles correspond to the radii highlighted in Fig. 3. The profile centers are defined by the sink locations, which are not necessarily located at the center of a cell. Each simulation and RADMC profile begins at a radius determined by the effective resolution of that run. The ALMA images reach larger radii than the original RADMC images because the pixel grid is larger, not because the angular resolution is higher. The higher-resolution run (RFL12) reaches higher central column densities and shows a steeper radial decline in column density than RFL9 (top panel of Fig. 5). At larger radii ($\gtrsim 5$ kau), the profiles are comparable. The peak temperatures of both runs are similar (see the middle panel of Fig. 5). However, as in the column-density profiles, run RFL12 shows an earlier decline of temperature with radius. In the lower-resolution run, the temperature decrease sets in at larger radii, but the overall radial slope is comparable between the two simulations.

The RADMC-3D flux profiles show a pronounced central peak at small radii (see the bottom panel of Fig. 5). In the high-resolution RFL12 run, this peak is approximately a factor of two higher than in RFL9. In contrast, the lower-resolution run RFL9 exhibits a broader and more blended envelope structure, leading to a lower central maximum but a more extended flux tail toward larger radii. The corresponding ALMA profiles show systematically reduced peak intensities. Although the ALMA flux peaks are similar for both resolutions, their radial profile generally reflects the underlying RADMC-3D structure: the lower-resolution run exhibits a broader central peak and a more extended outer tail than the high-resolution case.

3.2. Geometrical effects

From an observational perspective, only the projected mass can be detected through dust continuum emission. Figure 6 presents the enclosed mass within a radius of 1500 au for the different simulation's resolutions. For each run, the right half of the violin represents the projected mass, $m_{2\text{D}}$, while the left half corresponds to the spherically enclosed mass, $m_{3\text{D}}$. Across all simulations, $m_{2\text{D}}$ is systematically higher than the true spherical mass, which occurs due to contamination from foreground and background material along the LOS. Although individual sink masses decrease with increasing resolution (see Figure 4), the corresponding $m_{3\text{D}}$ increases slightly, representing the opposite effect. This indicates that, at least in these simulations, the spherically enclosed mass is not necessarily a precise proxy for the true protostellar mass, as it primarily reflects the dense gas and dust in the immediate vicinity rather than the stellar component itself (see also Sect. 3.3). Overall, $m_{2\text{D}}$ show a similar distribution for both runs, even though the individual sink masses differ.

Figure 7 illustrates the time evolution of the mean ratio between the projected and spherical masses, $m_{2\text{D}}/m_{3\text{D}}$, for different numerical resolutions. Up to ~ 240 kyr, the ratio remains nearly

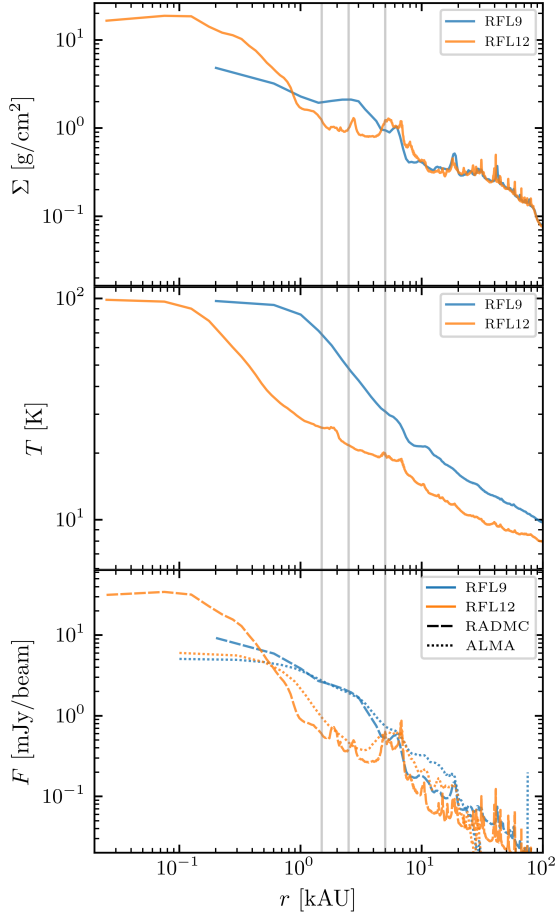


Fig. 5: Averaged radial profiles of the column density (top panel), the gas temperature (middle panel) and continuum flux (bottom panel) centered on the most massive sink particle at $t = 230$ kyr. The flux profiles are obtained from both the RADMC-3D images and the corresponding ALMA images, while the temperature and column density profiles are taken directly from the simulation. Results are shown for two spatial resolutions: RFL9 (400 au) and RFL12 (50 au). The vertical lines show the reference radii (from left to right 1.5, 2.5 and 5 kAU) from Fig. 3. The higher-resolution run (RFL12) shows a higher central column density and a more rapidly decreasing temperature toward larger radii. RADMC-3D fluxes generally peak higher than the ALMA fluxes, particularly at small radii and for the higher-resolution model. In contrast, the lower-resolution run (RFL9) produces a lower central flux peak but a broader outer tail in the radial flux distribution.

constant at values of 2–3, indicating that the projected mass, m_{2D} , systematically overestimates the true spherical mass, m_{3D} , by a factor of two to three during the early stages of collapse. Once ionizing radiation begins to affect the clump ($\gtrsim 240$ kyr), the ratio increases slightly, and it rises more strongly as the H II region expands (~ 340 kyr). This may be due to a decrease in m_{3D} within the ~ 1500 au vicinity as gas is blown out, while m_{2D} increases because more material disrupted by the H II region falls along the line of sight and is therefore included in the 2D projected mass. By ~ 370 kyr, the H II region driven by the most massive sink has disrupted the clump entirely.

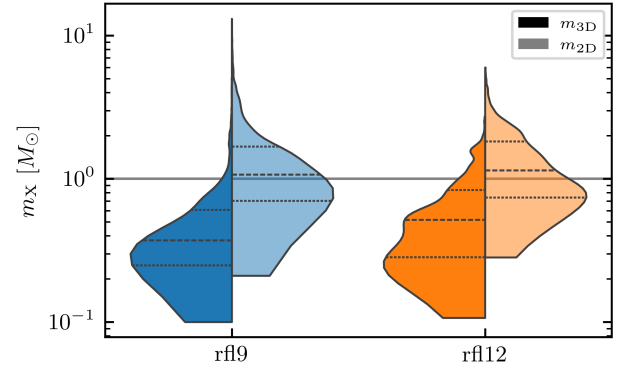


Fig. 6: Enclosed mass within a 3D (left halves) or 2D radius (right halves) of 1500 au up to 240 kyr for run RFL9 (blue) and RFL12 (orange). The projected mass, m_{2D} , is systematically higher than the spherical mass, m_{3D} , due to the contribution of material in the foreground and background. Higher numerical resolution leads to slightly higher 3D core masses as higher densities can be resolved.

To disentangle the contribution of foreground and background contamination from the purely geometric difference between a cylinder and a sphere, we compute the mass enclosed within a cylindrical volume with a radius of 1500 au and a height of 3000 au (see Fig. 7). In this setup, the cylinder is treated purely geometrically, ignoring additional contributions from material along the LOS, so that the comparison isolates the effect of the shape alone. The ratio of cylindrical mass to the spherical mass is nearly constant, with the cylindrical mass exceeding the true spherical mass by approximately 20 %. The ratio increases when the parental cloud is disrupted at late times.

We focus on the early stages of massive star formation as probed by dust continuum observations. We therefore exclude the more advanced evolutionary phases, where ionised gas dominates the emission, from the remainder of our analysis. In the early phase considered here, projection effects lead to m_{2D} exceeding m_{3D} by a factor of $\sim 2 - 3$.

3.3. Sink mass vs. core mass

We now compare the m_{2D} core masses (projected along the z -axis) to the corresponding sink masses. Figure 8 shows the time evolution of the ratio between each sink mass and its surrounding core mass m_{2D} . All sink–core pairs follow a broadly consistent trend. At early times, the inferred core mass is larger than the sink mass for most pairs. As accretion proceeds, the sink mass grows more quickly than the core mass, leading to a crossing point after about 50 kyr after the formation of the sink, beyond which the sink mass dominates for all pairs.

A similar trend is found when comparing to m_{3D} , which provides the most direct estimate of the intrinsic mass (not shown). From Sec. 3.2 we know that $m_{2D}/m_{3D} \approx 2 - 3$. Accordingly, the crossing point occurs earlier, at ~ 45 kyr.

Figure 9 shows the ratio of core mass to sink mass as a function of sink mass. Here, we consider cores at the three viewing angles for all time steps. m_{2D} s show a general decrease with increasing sink mass (top panel). In the early evolutionary stages, when sink masses are still low, the projected core mass typically exceeds the sink mass. At this stage, the envelope still contains most of the available material, and the sink has only be-

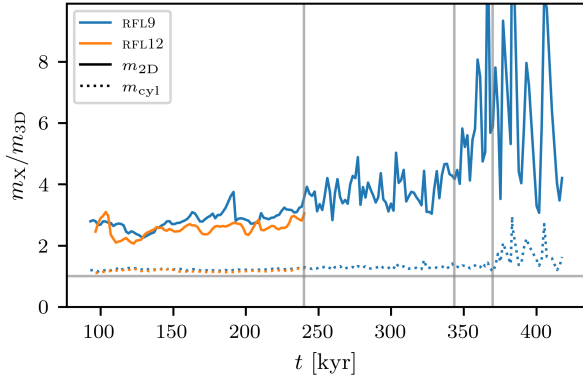


Fig. 7: Time evolution of the mean ratio of m_{2D}/m_{3D} (solid lines) and m_{cyl}/m_{3D} (dotted lines) for different numerical resolutions. In the RFL9 run, the m_{2D}/m_{3D} ratio remains nearly constant at ~ 2.9 until ~ 240 kyr, after which it increases to ~ 3.3 when ionizing radiation first appears. Once the expanding H II region begins to disrupt the parental cloud at ~ 370 kyr, both ratios rise sharply. The RFL12 run terminates earlier owing to computational limitations; in this case, the m_{2D}/m_{3D} ratio remains approximately constant at ~ 2.6 until ~ 240 kyr. The cylindrical estimate is closer to the real 3D mass. It systematically overpredicts the enclosed mass by a factor of ~ 1.2 .

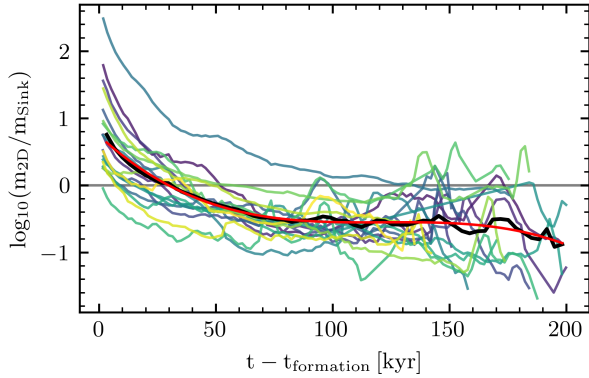


Fig. 8: Evolution with time since sink formation of the projected core mass, normalised by the corresponding sink mass. The grey line marks the one-to-one relation where both masses are equal. All sink–core pairs follow a similar trend: at the time of formation, the projected core mass exceeds the sink mass, but this relation rapidly inverts as accretion proceeds. The subsequent fluctuations around the relation likely arise from projection effects and variations in the local density structure.

gun to accrete. As evolution progresses, both the envelope and the sink continue to gain mass, but the sink grows more rapidly. Consequently, the ratio of projected core mass to sink mass decreases, and the projected masses begin to underestimate the more evolved sinks. Overall, we find an almost linear anticorrelation between the core and sink masses, with certain scatter. The fact that the core-to-sink mass ratio does not follow a perfect unity line indicates that a given sink mass does not correspond to a unique core mass, reflecting the diversity of accretion histories and core environments.

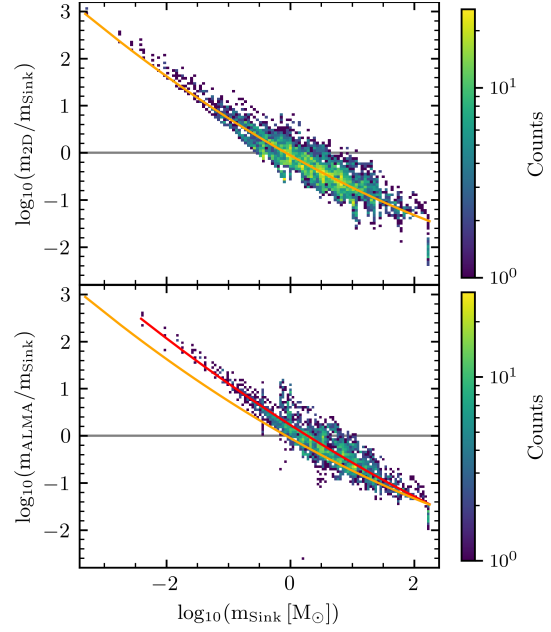


Fig. 9: *Top*: Projected simulation masses within a radius of 1500 au around each sink plotted against the corresponding sink mass. *Bottom*: ALMA masses within a radius of 1500 au around each sink, normalised by the corresponding sink mass, plotted against the sink mass. In both panels, the horizontal line indicates where the masses are equal. In the early evolutionary stages (when sink masses are still low), the core mass exceeds the sink mass, whereas at later times this trend reverses.

From our simulations, we derive an empirical fit that provides the expected sink mass for a given projected core mass (see orange line in the top panel of Fig. 9):

$$\log_{10}(m_{\text{sink}}) = -2.6 + \sqrt{8 + 20 \log_{10}(m_{2D})}. \quad (3)$$

A similar relation of the ALMA-recovered core masses (see also Sect. 3.4) is shown in the bottom panel of Fig. 9, which is empirically fitted by the expression:

$$\log_{10}(m_{\text{sink}}) = -2 + \sqrt{-1.56 + 25 \log_{10}(m_{\text{ALMA}})}. \quad (4)$$

The overall trend is similar to that of the simulation m_{2D} core masses, though the ALMA cores tend to exhibit systematically higher projected masses (see Sec. 3.4 for a detailed discussion). The fitted relation for the simulation cores is shown in orange, while the corresponding fit for the ALMA cores is plotted in red.

3.4. Core masses: Simulations vs. RADMC-3D vs. ALMA

We now assess how accurately the simulated core masses can be recovered from the post-processed RADMC-3D and ALMA images, provided the temperature is known (see Sect. 4 for the effect of different temperature estimates). In the following, we use either the mass-weighted LOS temperature, $T_{\text{sim,rad}}$, or the mass-weighted core temperature, $T_{\text{sim,avg}}$ (see Sect. 2.4 for their definitions).

Because the RADMC-3D maps provide idealised emission with the same resolution as the numerical simulation, the core

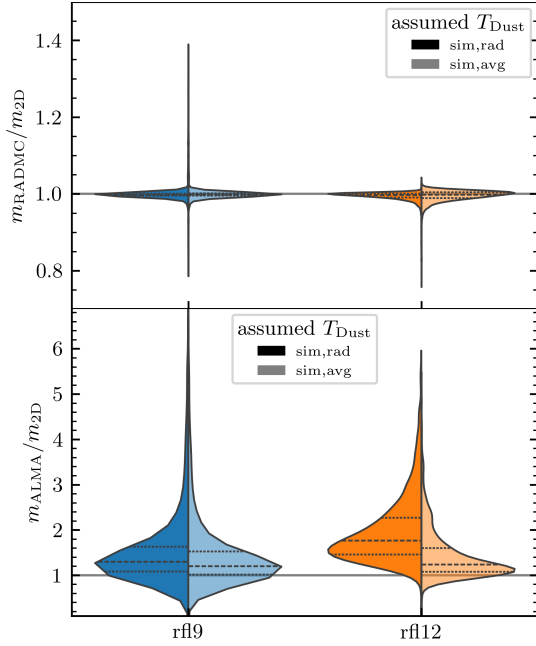


Fig. 10: Ratio of reconstructed core masses to the true 2D masses for idealised RADMC-3D emission maps (top) as well as for synthetic ALMA observations (bottom), each for RFL9 and RFL12. For both cases, cores are reconstructed using either the mass-weighted LOS temperature ($T_{\text{sim,rad}}$, blue) or the mass-weighted average temperature ($T_{\text{sim,avg}}$, orange). While RADMC-3D maps reproduce the true masses almost perfectly, interferometric filtering in ALMA introduces significant deviations.

masses in RFL9 run can be recovered with a high accuracy using either $T_{\text{sim,rad}}$ or $T_{\text{sim,avg}}$ (see top panel of Fig. 10). For this run, using a single averaged temperature per core makes virtually no difference. In contrast, the more centrally concentrated cores in the RFL12 run show slightly larger deviations when $T_{\text{sim,avg}}$ is used instead of the per-pixel temperature, reflecting their steeper temperature gradients (see also the radial profiles in Fig. 5).

The post-processed ALMA images, with a coarser resolution of ~ 1200 au, added noise and interferometric artifacts, have less sharply defined cores than in the idealised RADMC-3D maps. As a result, the flux distribution is smoother, and $T_{\text{sim,rad}}$ becomes a more accurate description of the intrinsic core structure. However, $T_{\text{sim,rad}}$ to infer core masses leads to a systematic overestimation (see bottom panel of Fig. 10), which increases with simulation resolution from a median mass ratio factor of 1.26 in RFL9 to 1.73 in RFL12. This trend is expected, as the high-resolution simulations resolve structures down to ~ 50 au, whereas the ALMA synthetic observations are limited to ~ 1200 au. Using a single representative temperature per core produces better mass estimates: for run RFL9 the improvement is modest from 1.26 to 1.17, but for the higher resolution run RFL12, the single-temperature approach yields significantly more accurate results, improving the median mass ratio from 1.73 to 1.2. As a consequence, using a single temperature rather than a full temperature profile is sufficient as long as the inner structure of the core is not resolved.

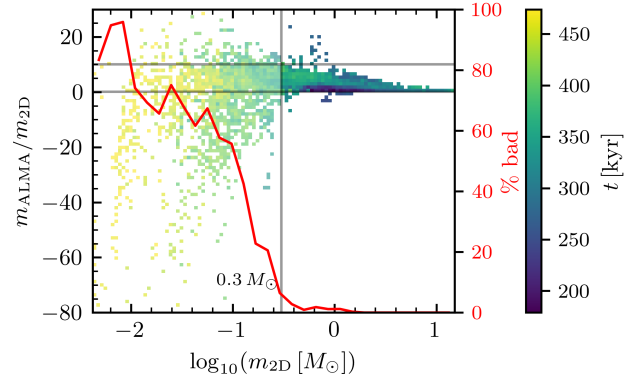


Fig. 11: Ratio of ALMA-derived core masses to the projected simulation masses, $m_{\text{ALMA}}/m_{2\text{D}}$, for all cores in run RFL9 and for all snapshots, plotted against the intrinsic projected core mass $m_{2\text{D}}$. The colour scale shows the evolutionary time. Horizontal grey lines mark the limits $m_{\text{ALMA}}/m_{2\text{D}} = 0.1$ and 10, which define “bad” cores with catastrophic mass under- or overestimates. The red curve (right-hand axis) shows the number fraction of such bad cores per mass bin. The vertical grey line at $0.3 M_{\odot}$ marks the adopted lower limit for reliable core-mass recovery. Note that all cores are shown here without any selection cuts and all time steps are included (see colour bar).

3.4.1. Reliable mass range of ALMA cores

To assess the mass range over which ALMA can reliably recover core masses, we compare the ALMA-derived masses, m_{ALMA} , of all identified cores in run RFL9 with their projected simulation masses, $m_{2\text{D}}$. Figure 11 shows the ratio $m_{\text{ALMA}}/m_{2\text{D}}$ as a function of $m_{2\text{D}}$, together with the fraction of “bad” cores, defined as those with mass errors larger than a factor of ten ($m_{\text{ALMA}}/m_{2\text{D}} < 0.1$ or > 10). At low masses, the scatter is extremely large, and the catastrophic-error rate is high, indicating that ALMA cannot reliably measure these cores. In this range, the estimated ALMA core masses can have unphysical, negative values. These negative masses occur when interferometric noise and filtering effects drive the measured core flux below zero. The failure rate decreases rapidly with increasing mass and flattens at values of $\lesssim 5\%$ above $m_{2\text{D}} \approx 0.3 M_{\odot}$. In this regime, the mass ratios cluster much more tightly, and most ALMA-derived core masses deviate from the true values by only factors of a few. This mass threshold is consistent with the core-mass completeness level of $0.23 M_{\odot}$ estimated by Coletta et al. (2025) for the ALMAGAL project. We therefore adopt $0.3 M_{\odot}$ as a conservative lower limit for reliable core-mass estimates in these simulations.

3.5. Cluster and clump properties

Following the ALMAGAL work by Elia et al. (2025), we examine how the total core population evolves relative to the parental clump mass. For this, we define the clump as a sphere of radius 0.5 pc, comparable to the ALMAGAL primary beam and the HiGAL clumps studied in the ALMAGAL project (see Elia et al. 2025), and sum all cores whose centres lie within this region. The clump mass, m_{clump} , is taken directly from the simulation. The corresponding core formation efficiency, CFE, is defined as

$$\text{CFE} = \frac{\sum m_{\text{core}}}{m_{\text{clump}}}. \quad (5)$$

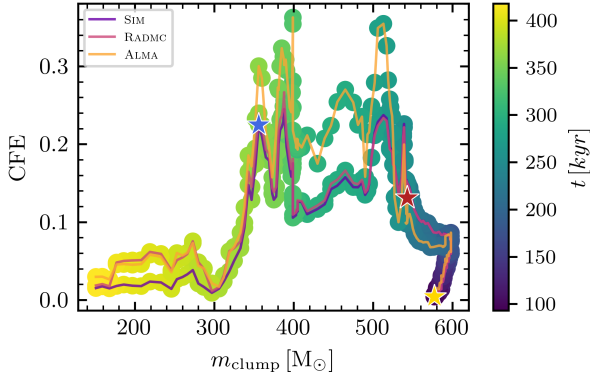


Fig. 12: Core formation efficiency vs clump mass, colour-coded by time. The curves trace the evolution from global collapse, through active core formation, to final clump dispersal. The yellow star marks the formation of the first core (93 kyr). The red star indicates the onset of ionizing radiation (240 kyr), and the blue star marks clump dispersal (370 kyr).

Figure 12 shows the evolution of the CFE as a function of clump mass, with the core masses determined from the numerical simulations simulation, the RADMC-3D maps, and the synthetic ALMA images, and colour-coded by time. Generally, CFE evolves from right to left. During the early global collapse, the clump mass within 0.5 pc increases as material flows inward, while only a few cores are present. Once more sink particles form, the clump mass decreases as gas is accreted onto sinks and removed from the gas phase, whereas the total mass in cores continues to rise as new cores and sinks form. The red star indicates the onset of ionising radiation at 240 kyr. At later times, when ionising radiation disrupts the cloud (corresponding to 370 kyr, and indicated with a blue star), both clump and core masses decline. The RADMC-3D core masses closely follow the path described by the core masses calculated in the numerical simulations. The ALMA-derived core masses, despite showing a larger scatter and modest systematic offsets, still reproduce well the overall evolutionary trend.

Figure 13 shows the time evolution of the core mass fraction. During the early collapse phase, this fraction increases almost linearly; the fitted relation is

$$\text{CFE}(t) = \begin{cases} 8.9 \times 10^{-4} t - 0.088, & t < 240 \text{ kyr}, \\ \text{nonlinear evolution}, & t \geq 240 \text{ kyr}. \end{cases}$$

In this regime, before ionizing radiation becomes important, the linear relation implies that the current clump mass can be reconstructed from the total mass in cores. However, once ionizing feedback sets in, the evolution becomes highly nonlinear, and the core mass fraction declines as the expanding H II region disperses the clump. The FLASH and RADMC-3D curves agree very well. The ALMA curve follows the same qualitative trend but shows deviations at the factor-of-few level, consistent with the mass-recovery uncertainties discussed above.

4. Interpretation of synthetic observations: temperatures and masses

4.1. Dust temperature estimates

The core mass estimate strongly depends on the dust temperature (see Eq. 2). In the simulations, the dust temperature is directly

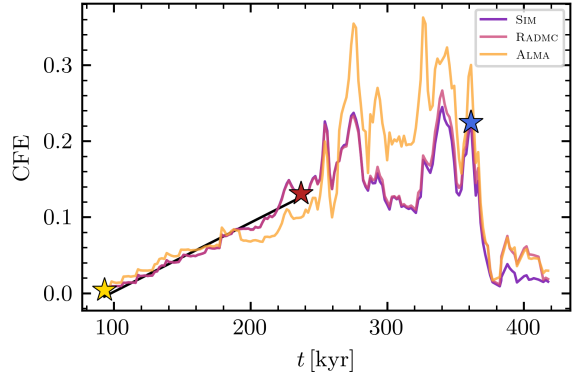


Fig. 13: Time evolution of the core formation efficiency estimated from the simulations, RADMC-3D, and ALMA. The yellow star indicates the first core formation. During the early collapse phase, CFE increases almost linearly; the black line shows a fit to this linear regime with a slope of 8.9×10^{-4} . The fraction begins to fluctuate once ionizing feedback from the first massive stars becomes important (red star) and eventually declines as the expanding H II region disperses the surrounding clump (blue star).

available for every cell, allowing us to compute a mass-weighted temperature distribution along the LOS with perfect spatial coverage. In real observations, however, the dust temperature cannot often be measured directly, and different methods and strategies need to be used. In the following we present and discuss three different methods to estimate the dust temperature.

4.1.1. Luminosity–mass relation temperature model

Within ALMAGAL, Coletta et al. (2025) estimate the core temperature based on the luminosity-to-mass ratio (L/M) of the parent clump (following the results by Molinari et al. 2016), which serves as a proxy for its evolutionary stage. The prescription defines three different regimes, summarised in Table 2. According to this prescription, a low L/M ratio ($\leq 1 L_{\odot}/M_{\odot}$) is expected to correspond to an early, cold phase dominated by accretion and lacking significant internal heating sources, representing prestellar clumps with an assumed temperature of 20 K (see Table 2). Intermediate values ($1 < L/M \leq 10 L_{\odot}/M_{\odot}$) correspond to clumps in a more evolved stage, where several protostars have already formed and start heating their surroundings, with an assumed temperature of 35 K. Finally, high L/M ratios ($> 10 L_{\odot}/M_{\odot}$) characterise the most advanced evolutionary phase, associated with luminous, embedded protostars and the emergence of H II regions. The empirical description assumes an increase of temperature with L/M .

This empirical prescription can be evaluated in our numerical simulations. The evolution of the clump's L/M ratio in the fiducial run is shown in Fig. 14. The L/M ratio begins to rise once the first sink particle forms (see yellow star in Fig. 14), marking the onset of protostellar activity (i.e., accretion and heating by radiative feedback). The appearance of ionizing radiation is indicated by the red star, and corresponds to $L/M \approx 10 L_{\odot}/M_{\odot}$, consistent with the empirical relation. A pronounced dip at $t \approx 300$ kyr corresponds to a temporary halt in the accretion onto the most massive sink particle in our simulations. Once accretion resumes, L/M increases again. After the cloud begins to disperse due to the expanding H II region (see blue star), the

Table 2: Core temperatures estimated from the clump’s L/M

$(L/M)_{\text{clump}} [L_{\odot}/M_{\odot}]$	$T_{\text{core}} [\text{K}]$	N_{cores}
≤ 1	20	1059
$1 < L/M \leq 10$	35	570
> 10	$21.1 \cdot (L/M)^{0.22}$	2081

Notes. Core temperatures assumed in the empirical L/M prescription for different evolutionary stages (see Coletta et al. 2025), and the corresponding number of cores in the RFL9 run with valid (positive) mass estimates (see Sect. 3.4.1).

value of L/M decreases. We note that in our simulations, although mass is expelled from the central region in these later evolutionary stages, which would by itself increase L/M , the total luminosity within the domain drops as accretion halts and radiation escapes through the disrupted cloud. Figure 14 marks $L/M = 1$, the transition between the 20 K and 35 K temperature regimes in the observational prescription. The dashed line marks $L/M = 10$, where the prescription enters the power-law regime, and it closely coincides with the onset of ionizing radiation in the simulation (red star).

Figure 15 (top panel) shows the mass-weighted average core temperature as a function of L/M , colour-coded by core mass. Overall, the simulations reproduce the global temperature trend used in Coletta et al. (2025) (see red line in Fig. 15 top panel). However, the simulations also reveal a significant intrinsic scatter. For a given L/M , individual cores span a wide range of temperatures. This variation arises because the thermal state of a core is determined not only by the global radiative environment of the clump but also by local conditions such as accretion luminosity, density, and optical depth. The results from the simulations also show that more massive cores are systematically warmer, reflecting enhanced accretion heating and stronger internal radiation fields. The bottom panel of Fig. 15 shows that the core temperature is not only related to the clump-wide L/M value but also correlates with the core continuum flux. This motivates a more flexible temperature model that depends on both quantities (see Sect. 4.1.2).

4.1.2. L/M –flux temperature model

Based on the results shown in the bottom panel of Fig. 15, we aim at describing the dust temperature T of each core as a function of the clump luminosity-to-mass ratio L/M (a proxy for the evolutionary stage) and its observed flux F (a proxy for its local radiation intensity or compactness). For that, we define first a global dependence of the dust temperature with L/M following previous work (see Molinari et al. 2016; Coletta et al. 2025) and the results of our numerical simulations (see Fig. 15). Based on this, we adopt the following as the baseline temperature relation:

$$T_{\text{base}}(L/M) = \begin{cases} 20 \text{ K}, & L/M < 0.8, \\ 21.1 (L/M)^{0.22} \text{ K}, & L/M \geq 0.8. \end{cases} \quad (6)$$

Similarly, the results shown in the bottom panel of Fig. 15 show that the characteristic flux level associated with a given L/M seems to follow a power-law relation that can be described as

$$F_{\text{base}}(L/M) = 3.37 \cdot 10^3 (L/M)^{0.32}. \quad (7)$$

Then, we can express the temperature as a perturbation from the baseline temperature given in Eq. 6, where the perturbation

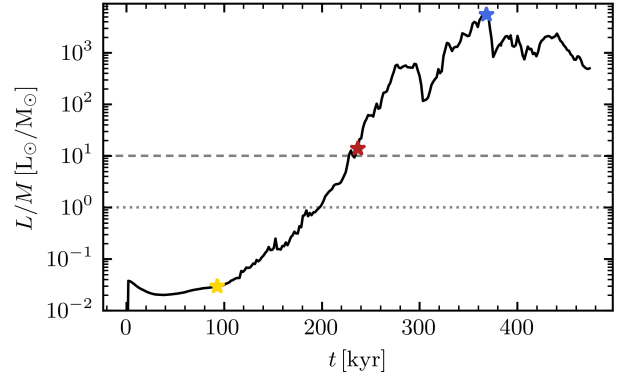


Fig. 14: Time evolution of the luminosity-to-mass ratio (L/M) in the FIDUCIAL run. The luminosity is obtained by integrating the spectral energy distribution produced with RADMC-3D, while the mass is directly taken from the simulation. Both luminosity and mass are measured within the same region used for the RADMC-3D images, corresponding to a cubic box with a side length of 1 pc centered on the cloud. Horizontal lines indicate the transition thresholds for the three temperature regimes: below the dotted line, a fixed temperature of 20 K is assumed; between the dotted and dashed lines, 35 K; and above the dashed line, a power-law temperature relation is applied. The yellow star marks the formation of the first sink particle, the red star indicates the onset of ionizing radiation, and the blue star denotes the stage when the cloud begins to be disrupted.

depends on the deviation of the observed flux from its expected baseline value (see Eq. 7). In its logarithmic form, this expression, including the perturbation factor, reads

$$\log_{10} T = \log_{10} T_{\text{base}}(L/M) + \beta [\log_{10} F - \log_{10} F_{\text{base}}(L/M)], \quad (8)$$

which can be written equivalently in linear form as

$$T(L/M, F) = T_{\text{base}}(L/M) \left(\frac{F}{F_{\text{base}}(L/M)} \right)^{\beta}. \quad (9)$$

The exponent β controls how strongly the temperature responds to flux variations at fixed L/M . We adopt $\beta = 0.47$ from our fit. Figure 15 shows the baseline $T(L/M)$ relation in red, together with flux-offset tracks at fixed L/M . The dark-red curve corresponds to $\log_{10}(F/F_{\text{ref}}) = +0.5$ and the orange curve to $\log_{10}(F/F_{\text{ref}}) = -0.5$.

This L/M +flux model captures the intuitive idea that L/M sets the global temperature scale of the clump, while the local flux provides a secondary adjustment reflecting local variations in radiation intensity or compactness. In Sect. 4.1.4 we show that this simple extension already provides a substantial improvement over using $T_{\text{base}}(L/M)$ alone.

4.1.3. Machine-learning temperature model

As an exploratory step for a new temperature determination approach, we have used a supervised machine-learning model to predict dust temperatures from a small set of observable quantities. This exercise is intended as a proof of concept rather than a fully developed method for observational use, and we therefore limit the description to the basic setup and performance.

Our model is trained directly on the simulated core catalogue, where the true dust temperature corresponds to the mass-weighted, LOS averaged value $T_{\text{sim,avg}}$ for each core. We adopt

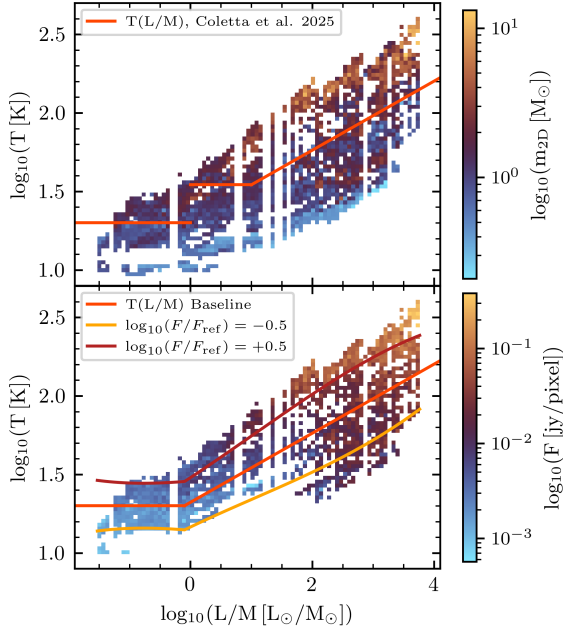


Fig. 15: Mass-weighted average core temperature as a function of the luminosity-to-mass ratio (L/M), colour-coded by the core mass (top panel) and by the ALMA continuum flux (bottom panel). Not all simulated cores have ALMA counterparts because of the limited interferometric field of view. In the top panel, the red line shows the temperature– L/M relation adopted from Coletta et al. (2025). In the bottom panel, the central curve shows the improved baseline temperature– L/M relation, and the two additional curves mark the fitted positive and negative deviations obtained from the flux–temperature response model (Sect. 4.1.2).

a Gradient Boosting Regressor (Friedman 2001), a decision-tree ensemble method that builds a prediction model by adding many small decision trees in sequence, where each tree learns to correct the errors made by the previous ones. By iteratively fitting these residuals, the method captures complex, non-linear dependencies and feature interactions without imposing a fixed analytical form.¹

We combine four physically motivated input quantities: (i) the luminosity-to-mass ratio (L/M) of the clump, (ii) the local (dust) continuum flux at 1.36 mm of the core, (iii) the projected distance of the core from the centre of the cloud/cluster, and (iv) the empirical L/M -based temperature estimate $T_{L/M}$. These quantities jointly encode information about both global and local heating processes: L/M traces the global evolutionary stage, the flux and $T_{L/M}$ characterise the local environment and a physically motivated baseline, and the radial distance of the core to the centre of the cloud/cluster captures systematic radial temperature gradients and geometric dilution. The Gradient Boosting model is trained to predict the logarithm of the dust temperature, $\log_{10} T_{\text{dust}}$, using 20% of the simulated cores and evaluated on the remaining 80%. Even with this limited training fraction, for the test set, the model reproduces approximately 93 % of the

variance in the simulated temperature distribution and achieves an root mean squared error of 0.092 dex in $\log_{10} T_{\text{dust}}$ (corresponding to a multiplicative error of ~ 1.24 , i.e. $\sim 24\%$).

4.1.4. Model accuracy in temperature retrieval

We now compare the three temperature estimates ($T_{L/M}$ as described in Sect. 4.1.1, the $T_{L/M+F}$ as described in Sect. 4.1.2, and the machine-learning based T_{ML} as described in Sect. 4.1.3) to the mass-weighted average core temperatures from the simulation, $T_{\text{sim,avg}}$. We use the coefficient of determination (R^2) to quantify how well the predicted temperatures reproduce the variance of the simulated values. Higher R^2 values indicate more accurate models, with $R^2 \approx 1$ reflecting near-perfect agreement between model predictions and the simulation data.

Figure 16 shows the ratio of each estimated to simulated core temperatures as a function of $T_{\text{sim,avg}}$. The top panel demonstrates that the L/M method systematically overestimates the temperatures of cold cores ($T_{\text{sim,avg}} \lesssim 50$ K) and underestimates those of warm cores, yielding an overall $R^2 = 0.43$. This pronounced temperature-dependent bias highlights the limitations of using a single global L/M indicator to characterise the thermal state of individual cores. The middle panel shows that the combined L/M +flux model substantially reduces the overall scatter and softens the strong temperature-dependent bias present in the pure L/M prescription. The data cluster far more tightly around unity, increasing the overall R^2 to 0.83. Some residual structure remains, but the distribution is markedly more concentrated than for the simple L/M method. The bottom panel displays the machine-learning model, which provides the most accurate reconstruction of the simulated temperatures. The ratios remain tightly concentrated around unity across the entire temperature range, and the residual scatter is small. The resulting $R^2 = 0.96$ indicates excellent agreement between the estimates and the simulation values.

Overall, our analysis shows that supervised machine learning offers an effective route toward accurate dust-temperature estimation, especially when trained on realistic simulations. Fully exploring its capabilities in observational contexts will be an important direction for future works.

4.2. Consistency between flux and temperature estimates

In addition to using accurate dust temperature estimates (see Sect. 4.1), the determination of core masses also requires good measurements of the dust continuum flux emission (see Eq. 2). In the following, we examine the accuracy of the ALMA observations to recover the original fluxes, as well as the consistency between the fluxes and temperatures used in the mass derivation.

For this, we start by exploring whether the fluxes of the cores in the RADMC-3D maps are accurately recovered in the synthetic ALMA observations. Figure 17 shows the ratio of the ALMA flux of each core to its corresponding RADMC-3D flux as a function of the RADMC-3D flux. Overall, most points cluster around the unity line, indicating that interferometric filtering preserves the global flux scaling for most cores. At low fluxes ($\lesssim 2$ mJy), ALMA tends to slightly overestimate the emission relative to RADMC-3D, whereas the scatter increases at intermediate fluxes (~ 1.5 – 12 mJy), which may arise from a combination of noise, beam convolution, and image artifacts likely produced by partially resolved-out structures not properly recovered in the interferometric images.

¹ We use the GradientBoostingRegressor implementation in scikit-learn (Pedregosa et al. 2011); see <https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.GradientBoostingRegressor.html>.

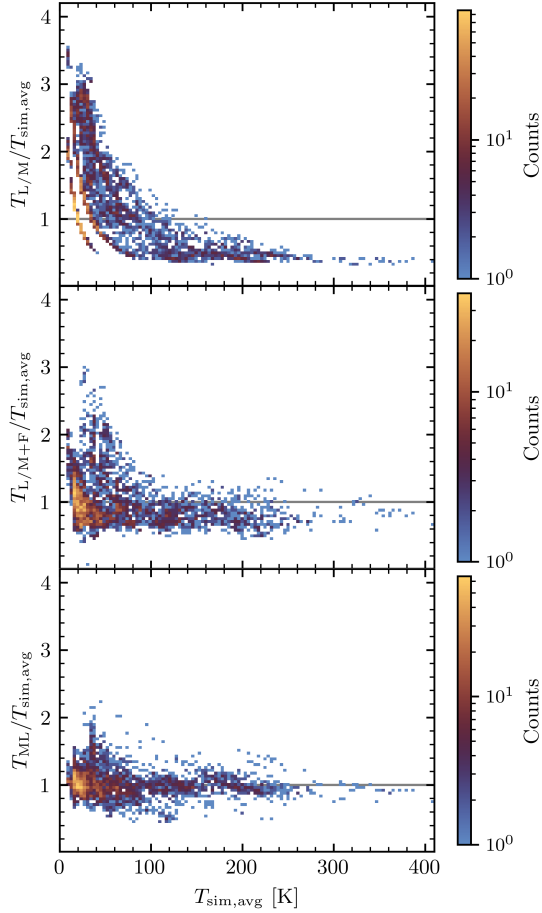


Fig. 16: Ratio between estimated and simulated mass-weighted core temperatures as a function of T_D . *Top:* $T_{L/M}/T_{\text{sim,avg}}$. *Middle:* $T_{L/M+F}/T_{\text{sim,avg}}$ for the L/M +flux model. *Bottom:* $T_{\text{ML}}/T_{\text{sim,avg}}$ for the machine-learning model. The horizontal line indicates equal temperatures. The empirical L/M method systematically overestimates the temperatures of cold cores and underestimates those of warm cores. Including flux information reduces this bias and scatter, while the machine-learning model recovers the simulated temperatures with minimal residual trends.

Since both the flux and the temperature are needed to compute the mass of a core, any change in the measured flux will automatically change the inferred mass for a given dust temperature. To isolate the effect of flux reconstruction, we invert the flux–mass relation and calculate the dust temperature $T_{\text{flux,m2D}}$ that would be required in order to recover the true core mass from the simulation using the both the measured (noise-affected) ALMA fluxes and the (ideal) RADMC-3D fluxes. Figure 18 compares $T_{\text{flux,m2D}}$ to the mass-weighted temperatures from the simulation. The top panel shows the reference case in which the temperatures have been calculated using the (ideal) RADMC-3D fluxes. In this case, both the flux and the true core mass are known from the simulation, and the inferred temperatures match the simulation temperatures extremely well, with the distribution tightly clustered around unity (with median and mean ratios of 1.00 and 1.03, respectively). This confirms that when the flux is accurately recovered, the mass estimated from the flux and temperature is reliable. The bottom panel shows the correspond-

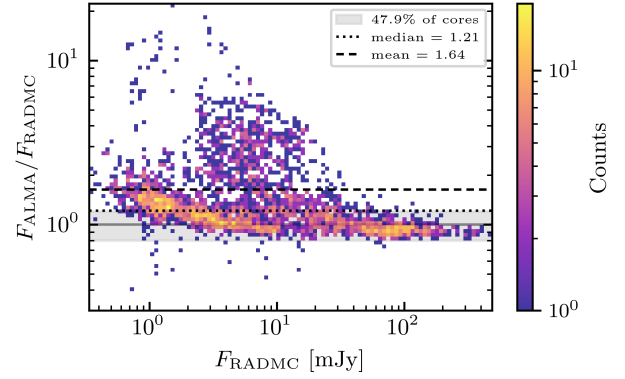


Fig. 17: Total fluxes of the synthetic ALMA cores compared to those derived directly from the RADMC-3D images. The grey line indicates the one-to-one relation. Overall, the ALMA fluxes reproduce the RADMC-3D fluxes well. At low fluxes, ALMA cores tend to exhibit slightly higher values than their RADMC-3D counterparts, while at intermediate flux levels the scatter increases, likely due to interferometric filtering and noise.

ing result using the ALMA fluxes. Similar to the previous case, most cores lie close to the unity line, indicating that the temperatures implied by the ALMA fluxes are broadly consistent with the intrinsic core temperatures. However, the elevated median and mean ratios (1.2 and 1.6, respectively) indicate a systematic tendency for the ALMA fluxes to be somewhat higher than the RADMC-3D fluxes or to miss some extended emission, depending on the configuration. A non-negligible fraction of cores shows significantly higher ratios, corresponding to cases with large ALMA-to-RADMC-3D flux discrepancies.

4.3. Core mass recovery using different temperature estimators

In this section, we assess how accurately the different temperature prescriptions recover the true core masses. For this, we compare the reconstructed masses to the intrinsic 2D masses (m_{2D}) for both resolution runs: RFL9 and RFL12. Figure 19 presents these mass ratios for the identified cores in both the idealised RADMC-3D maps (top panels) and the synthetic ALMA observations (bottom panels). In both cases, we test the three temperature models presented in Sect. 4.1, corresponding to the standard L/M approach, the improved L/M +flux method, and the machine-learning based model (ML).

For the RADMC-3D emission maps, where the fluxes are ideal and noise-free, the standard L/M method systematically underestimates the core masses, with median ratios $m_{\text{RADMC}}/m_{2D} \simeq 0.8$ for RFL9 and 0.85 for RFL10. The $L/M + F$ approach, however, provides a notably more accurate reconstruction with median ratios of 1.2 (RFL9) and 1.05 (RFL10), demonstrating its ability to account for variations in dust temperature more effectively than the standard L/M prescription. The machine learning approach yields the most accurate results for both runs, producing m_{RADMC}/m_{2D} values tightly clustered around unity. In the synthetic ALMA images, by contrast, the three temperature estimators yield broadly comparable m_{ALMA}/m_{2D} statistically across all cores, with modest differences in the distribution shapes and median values in the range 1.1 – 1.3.

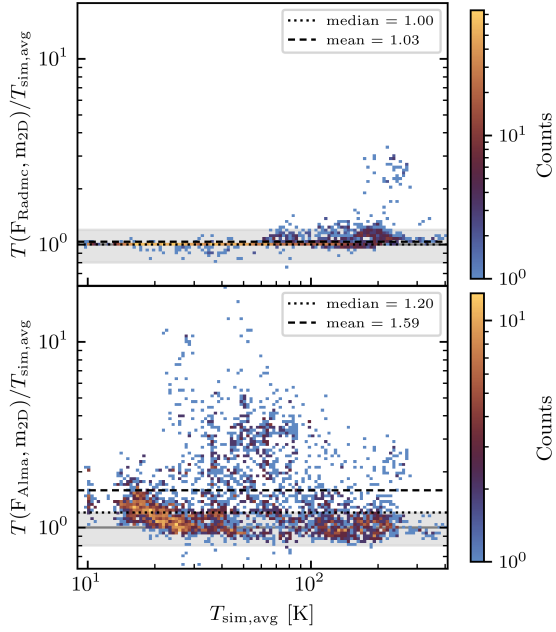


Fig. 18: Ratio between the dust temperature inferred from the post-processed flux and simulation mass, $T_{F,m2D}$, and the mass-weighted average core temperature from the simulation, $T_{sim,avg}$, plotted as a function of $T_{sim,avg}$ for RADMC-3D (top panel) and ALMA cores (bottom panel). The dotted and dashed horizontal lines indicate the median and mean of $T_{F,m2D}/T_{sim,avg}$, respectively. For the RADMC-3D cores the derived temperatures agree very well with the simulation temperatures. Most ALMA cores lie near to the unity line, but a non-negligible fraction shows significantly higher ratios.

We now compare temperature and mass biases for core masses derived from the three temperature prescriptions (Fig. 20). The top row shows the idealised RADMC-3D case, while the bottom row shows the synthetic ALMA analysis. In each panel the temperature bias (estimated temperature relative to the simulation value) is plotted against the corresponding mass bias (derived core mass relative to the projected simulation core mass), with colour indicating the projected simulation core mass.

For temperatures estimated from the L/M relation (left column), both RADMC-3D and ALMA exhibit the expected anti-correlation: underestimated temperatures lead to overestimated core masses, and vice versa. The most massive cores preferentially populate the regime of underestimated temperatures and overestimated masses. While the trend is tight in RADMC-3D, the ALMA results show substantially larger scatter in mass bias at fixed temperature bias.

Including the flux term ($L/M+F$; middle column) yields a more compact distribution around the one-to-one relations in the RADMC-3D case, but it also changes the mass dependence. Lower-mass cores tend to have underestimated temperatures with correspondingly overestimated masses, whereas higher-mass cores are recovered more accurately. The ALMA cores follow the same overall behaviour, again with noticeably increased scatter. However, the more massive cores now have a mass bias close to unity.

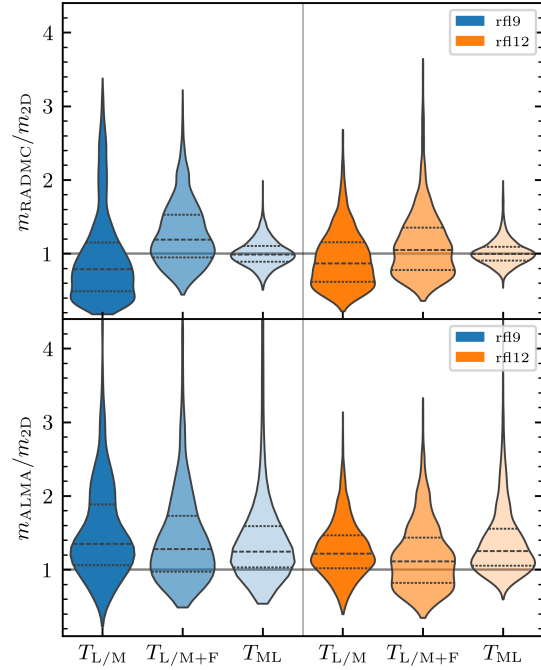


Fig. 19: Ratio of reconstructed core masses to the true 2D masses for RFL9 and RFL12. The panels show masses derived from the idealised RADMC-3D maps (top) and from ALMA maps (bottom). In both cases, core masses are reconstructed using either the L/M temperature estimate alone (dark colour), the combined L/M +flux temperature estimate (medium colour), or the machine-learning approach T_{ML} (bright colour). For the RADMC-3D case (top), the L/M method underestimates the core masses, whereas the L/M +flux method yields more accurate results and T_{ML} performs best. For the m_{ALMA} (bottom), all three temperature estimates perform similarly in a statistical sense.

Finally, the machine-learning model (right column) provides the best overall agreement in temperature. In RADMC-3D this translates into mass ratios clustered close to unity, whereas in the ALMA case the lowest-mass cores remain systematically overestimated even when the temperature bias is small.

The observational effects, such as noise, filtering, and imperfect flux recovery, dominate the mass uncertainties and reduce the sensitivity to the choice of temperature prescription. As shown above, inaccurate flux reconstruction directly propagates into mass errors, even when the temperature estimate is accurate. Consequently, a correct flux recovery is essential for a reliable mass determination in interferometric observations.

5. The observer's guide to the study of cores

In this section, we summarise the main aspects and caveats to consider when interpreting interferometric dust-continuum observations of star-forming clumps and cores, similar to those performed in the ALMAGAL project (see Molinari et al. 2025; Sánchez-Monge et al. 2025), based on our comparison between simulations and synthetic observations.

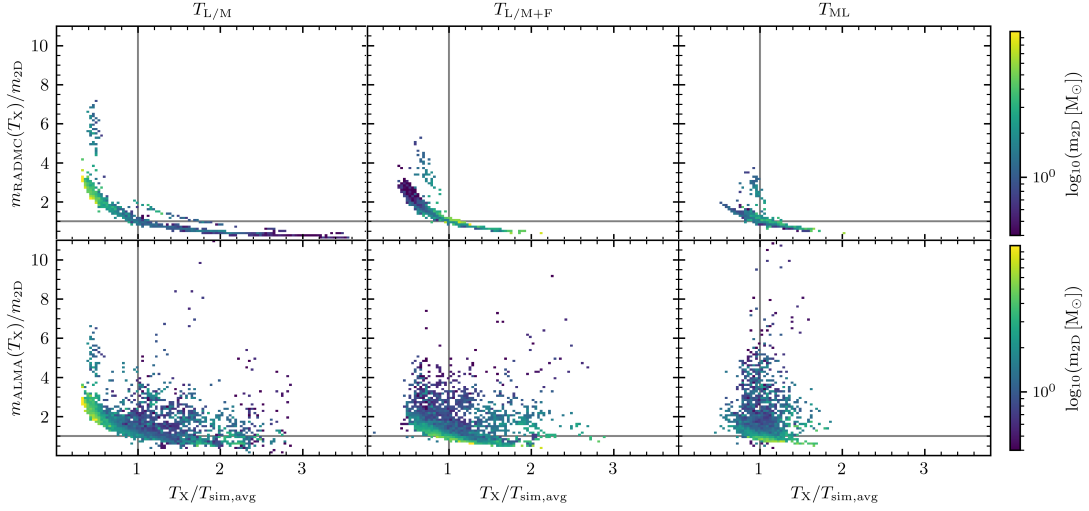


Fig. 20: Two-dimensional histograms comparing the temperature and mass biases of core masses derived with RADMC-3D (top row) and with the synthetic ALMA analysis (bottom row). From left to right, we use temperatures estimated from L/M , from L/M plus flux ($L/M+F$), and from the machine-learning (ML) model. The x-axis shows the temperature bias (estimated temperature relative to the simulation temperature), while the y-axis shows the corresponding mass bias (derived core mass relative to the projected simulation core mass). The colour scale indicates the projected simulation core mass (logarithmic). Grey lines mark equality. Overall, the ALMA cores show larger scatter in mass bias than the RADMC-3D cores. For the L/M method, RADMC-3D shows that an underestimated temperature relative to the simulation leads to an overestimated derived mass, and vice versa. ALMA cores show a similar trend. Including the flux term ($L/M+F$) in RADMC-3D yields a more compact distribution around the one-to-one relation, but it also alters the mass dependence. Lower-mass cores now preferentially show underestimated temperatures with correspondingly overestimated masses, whereas higher-mass cores are recovered comparatively well. ALMA cores shows a similar trend, though with noticeably more scatter. The ML model provides the best overall temperature agreement. However, in the ALMA case the lowest-mass cores remain systematically overestimated even when the temperature bias is small.

- **Projection effects in the core mass determination:** Our simulations show that 2D projected core masses systematically exceed the corresponding 3D spherical masses (see Sect. 3.2 and Fig. 6). The major contribution to this mass excess is the presence of additional material along the LOS (i.e., in the foreground or background of the core), rather than from geometric effects when projecting a 3D spherical core into a 2D circle (see Fig. 7).
- **Sink (stellar) masses and core masses:** Our simulations show that the core mass has a general decrease with increasing (stellar) sink mass (see Sect. 3.3 and Fig. 8). At earlier stages, cores are dominated by massive envelopes with small sink masses, while at later stages, sinks have accreted most of the available material contained in the envelope. Despite inferring stellar masses directly from core masses may be highly uncertain, we have defined an empirical relation between the sink (stellar) mass and the corresponding core mass (see Fig. 9, Eqs. 3 and 4) based on our simulations.
- **Global clump properties do not uniquely determine the core population:** Based on our simulations, before ionising feedback sets in, the core mass fraction (also known as core formation efficiency, CFE) increases approximately linearly with time (consistent with observational findings, see Elia et al. 2025), and the clump mass can be inferred from the total core mass. Once feedback becomes important, this relation breaks down and no clear correlation between clump-scale properties and the underlying core population remains (see Sect. 3.5 and Figs. 12 and 13).
- **L/M clump-based temperatures do not accurately describe core temperatures:** Even though the clump L/M traces the global thermal evolution and the onset of ionizing feedback (see Fig. 14), core temperatures span more than one order of magnitude at a fixed L/M . The empirical L/M prescription (see e.g., Molinari et al. 2016; Coletta et al. 2025) can underestimate or overestimate individual core temperatures by factors of $\sim 2 - 3$ (see Sect. 4.1.1 and Fig. 15).
- **Core flux information improves L/M clump-based temperature estimates:** The L/M clump-based temperature estimate for a core can be improved by incorporating the measured dust continuum flux of each core into a simple $L/M+F$ model (see Sect. 4.1.2, Eq. 9). This substantially reduces the scatter in the recovered temperatures (see Fig. 16) and increases the coefficient of determination from $R^2 = 0.43$ for the L/M -only estimate to $R^2 = 0.83$ for $L/M + F$. Temperature prescriptions that combine clump-scale (L/M) and core-scale (flux) information are therefore preferred. Preliminary studies of a machine-learning model suggests further improvements in the core temperature determination with $R^2 = 0.96$ (see Sect. 4.1.3 and Fig. 16), but its application to real observations still requires further investigation.
- **Mass recovery also depends on flux reconstruction:** Imperfect recovery of the core fluxes (e.g., due to artifacts or noise in interferometric observations) introduces additional errors in the mass determination for individual cores of up to a factor ~ 3 , even when the dust temperature is known with perfect accuracy (see Sect. 4.2, Figs. 17 and 18).

5.1 How wrong can core masses be?

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5.1. How wrong can core masses be?

Based on the comparison between numerical simulations, RADMC-3D emission maps, and synthetic ALMA images, the following quantitative biases may be expected when deriving core masses from (sub-)millimetre continuum interferometric observations.

- **Projection effects:** The (projected) core mass, m_{2D} , exceeds the true spherical core mass, m_{3D} , due to foreground and background contamination from cloud/clump material. This results in core masses overestimated by a factor 2 – 3.
- **Temperature uncertainty:** True core temperatures span a broad range that is not captured by a single clump-averaged L/M value. If the core temperature is underestimated by a factor of 2 (e.g. 20 K instead of 40 K), the mass is overestimated by a factor of 3 – 7. If the temperature is overestimated by a factor of 2, the mass is underestimated by a factor of ~ 2 . Typical errors in the core mass estimate based only on temperature uncertainties are usually about a factor 2 – 5.
- **Interferometric filtering:** Instrumental effects from interferometers like ALMA may typically overestimate the core mass by a factor $\sim 1 - 2$ due to incorrect flux reconstruction.

Combining all dominant uncertainties, we find that individual ALMA continuum-derived core masses may typically be uncertain by a factor of $\sim 3 - 5$ up to 10 for extreme cases.

6. Summary

We use radiation–hydrodynamic simulations, radiative-transfer post-processing, and synthetic ALMA imaging to quantify how reliably dense-core properties can be inferred from ALMAGAL-like continuum observations of massive star-forming clumps.

We find that geometric effects alone introduce a substantial mass bias, with projected core masses systematically exceeding (at the level of a factor $\sim 2-3$) the corresponding 3D spherical masses due to foreground and background contamination. Correct flux reconstruction and dust temperature estimation are the other main sources of uncertainty in continuum-based core masses. Imperfect flux recovery, e.g., due to interferometric filtering and atmospheric noise, introduces additional mass biases of up to a factor of ~ 2 for individual cores, even when the temperature is known. For ALMAGAL-like observations, we find a minimum reliably detectable core mass of $\gtrsim 0.3 M_{\odot}$. Regarding core temperatures, the empirical clump-scale L/M -derived temperature prescription, used in some observational works, captures the global thermal evolution but fails to represent the large core-to-core temperature scatter. As a result, it biases the recovered projected core masses, in particular for the most massive cores. Including the ALMA-measured core flux in a simple L/M +flux model significantly improves the temperature estimates, and a supervised machine-learning model trained on the simulations performs best in our tests. We also explore the relation between the sink and core mass in the simulations, and derive an empirical relation that provides the expected sink mass for a given projected core mass. Finally, at clump scales, the simulations reveal a tight, nearly linear growth of the core mass fraction during the early pre-feedback phase, followed by strong fluctuations and a decline once ionising radiation disrupts the clump. Synthetic observations reproduce these qualitative evolutionary trends and the overall behaviour of the core mass budget, even though individual core masses remain uncertain at the factor-of-few level.

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Appendix A: Effects of viewing angle

To characterise the geometry of the mass distribution, we investigate the fractional contributions of the projected mass components along the three coordinate axes. The ternary diagram in Fig. A.1 shows the normalised projected masses $m_{2D,X}/\Sigma m$, $m_{2D,Y}/\Sigma m$, and $m_{2D,Z}/\Sigma m$, with $\Sigma m = m_{2D,X} + m_{2D,Y} + m_{2D,Z}$. Around 50% of the cores cluster near the centre of the diagram, which corresponds to comparable contributions from all three projection directions. The remaining data are distributed in an extended structure in the diagram, indicating that the mass distribution around the other 50% of the cores is not isotropic and/or that these cores themselves might have elongated structures, with a preferred direction. This is consistent with an elongated, filamentary morphology rather than a spherical one. Such anisotropic structures arise naturally in a turbulent medium, where material is funneled along filamentary channels that can occur in any direction.

The higher-mass cores span a range of positions in the diagram. A small number appears closer to the $m_{2D,Z}/\Sigma m$ vertex, indicating cases where the projected mass is more strongly concentrated along the Z direction. However, the most massive cores are located near the central region of the diagram, where the three projected components contribute in more comparable proportions. Lower-mass cores are more broadly scattered and show a correspondingly wider range of projection ratios. The distribution suggests a variety of geometric structures of the cores.

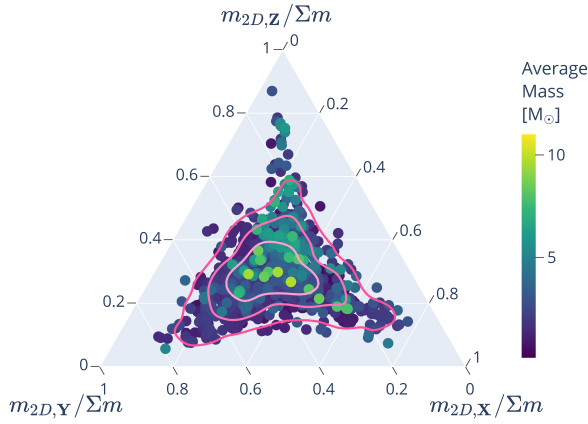


Fig. A.1: Ternary diagram showing the relative contributions of the 2D projected mass components derived from the simulation along the X , Y , and Z coordinates. Each point represents a mass configuration, where the three coordinates correspond to $m_{2D,X}/\Sigma m$, $m_{2D,Y}/\Sigma m$, and $m_{2D,Z}/\Sigma m$, such that their sum is unity. Points located near a vertex indicate a projection dominated by a single spatial direction, whereas points near the centre of the triangle correspond to nearly isotropic mass distributions. The colour scale corresponds to the average mass associated with each configuration. Contours indicate the regions containing 50 %, 80 %, and 95 % of the cores.

8.2

SUPPLEMENTARY MATERIAL TO PAPER II

8.2.1

NUMERICAL RESOLUTION AND ITS IMPACT ON SYNTHETIC OBSERVATIONS

Here we present a detailed analysis of how the numerical resolution of the simulations affects the resulting synthetic observations. While the paper shows only RFL9 and RFL12, we extend the analysis here to the full set of refinement levels—RFL9, RFL10, RFL11, and RFL12, corresponding to spatial resolutions of $\sim 400, 200, 100$, and 50 au, respectively.

A recurring challenge in linking simulations to continuum observations is that the observational beam smooths structure on scales comparable to, or larger than, the characteristic sizes of protostellar envelopes and fragments. It is therefore tempting to assume that, as long as the final synthetic maps are convolved to the observational resolution, the intrinsic numerical resolution of the simulation becomes secondary. However, in practice, the simulation resolution determines which density peaks form in the first place, how centrally concentrated cores become, and how gas flows through filaments onto protostars. These differences imprint themselves on the emergent dust continuum emission and can survive realistic post-processing and beam convolution.

Simulation pixel resolution and ALMA beam resolution

When comparing numerical simulations to interferometric continuum observations it is essential to distinguish between (i) the intrinsic spatial resolution of the simulation, (ii) the sampling of synthetic images (pixel size), and (iii) the true observational resolution set by the synthesized beam.

In the simulations, the smallest resolved physical scale is set by the minimum AMR cell size Δx at the highest refinement level. In this thesis, we consider refinement levels corresponding to minimum cell sizes in the range $\Delta x = 50\text{--}400$ au. This intrinsic numerical resolution controls how strongly gas can collapse, fragment on small scales and form sink particles and therefore affects the resulting density and temperature structure before any radiative-transfer post-processing is applied.

Synthetic 1.36 mm continuum maps are produced with radiative transfer and stored on a regular image grid with a chosen pixel size. This pixel resolution only determines how finely the final intensity field is sampled and does not reintroduce unresolved physics.

The true angular resolution of the ALMA images is set by the synthesized beam FWHM. For the observations used in this thesis we adopt the measured beam parameters $B_{\text{maj}} = 0.43''$ and $B_{\text{min}} = 0.39''$. Assuming a source distance of 3 kpc the beam FWHM is 1276×1171 au (major $\times$ minor). A common way to express the resolution with a single number is the geometric-mean beam size,

$$B_{\text{gm}} = \sqrt{B_{\text{maj}} B_{\text{min}}} = 0.40'', \quad (8.1)$$

corresponding to ~ 1200 au at 3 kpc.

While the beam determines the actual resolving power, the pixel (cell) size of the ALMA image determines how well the beam is sampled. A common choice in interferometric imaging is to use approximately 3-5 pixels across the beam FWHM along each axis (Sánchez-Monge et al., 2025). If the ALMA images are sampled

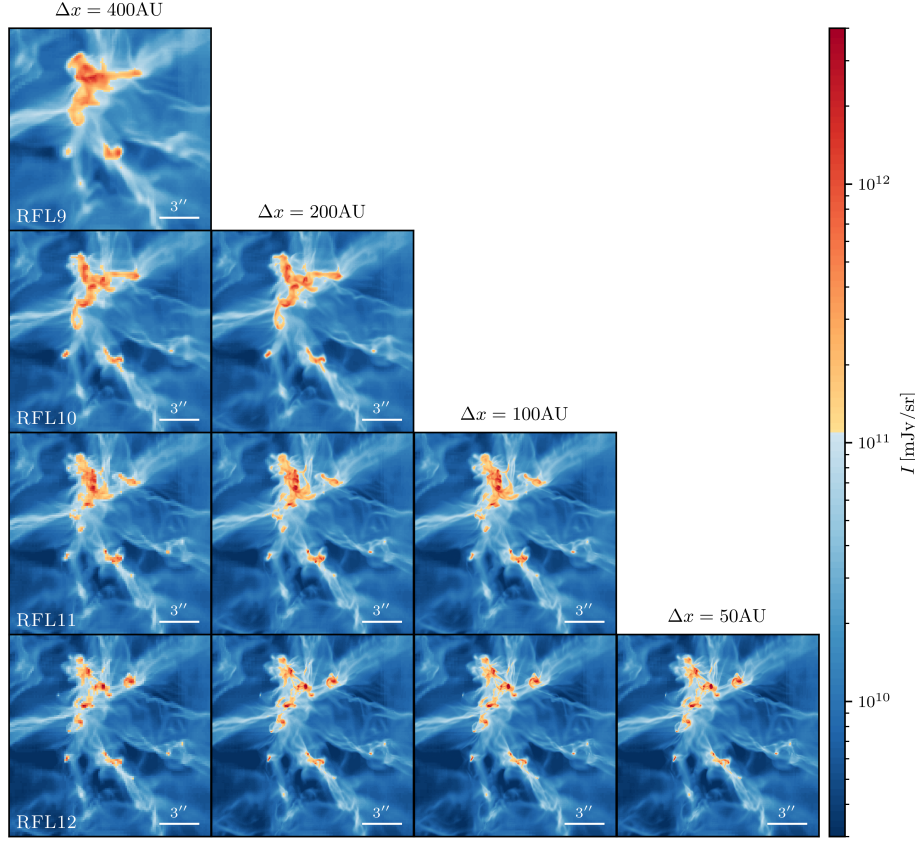


Figure 5: Flux maps derived from RADMC-3D at $t = 230$ kyr. Rows show increasing numerical refinement levels (from top to bottom: RFL9–RFL12), while columns show different sampled spatial resolutions (from left to right: 400, 200, 100, and 50 AU). The diagonal from the top left to the bottom right corresponds to images shown at their native numerical resolution. Images to the left of this diagonal are downsampled to coarser resolutions. At a given sampled resolution, the downsampled images are visually similar across refinement levels, while simulations with higher initial numerical refinement retain finer substructure that is not present in intrinsically lower-resolution runs.

with a pixel size of 400 au pix^{-1} , the sampling of our beam is 3 pixel/beam. Thus, 400 au pix^{-1} corresponds to a near-minimal but still acceptable sampling. Using finer pixel sizes (200, 100, and 50 au pix^{-1}) increases the sampling to ~ 6 , 12, and 24 pixels per beam, respectively, without changing the true angular resolution.

Separating intrinsic simulation resolution from image sampling

To separate the effect of the intrinsic simulation resolution from purely technical effects of image sampling, we perform controlled experiments in which the RADMC-3D post-processed images are resampled to coarser pixel sizes before further analysis. The key point is that two operations are fundamentally different: (i) running the simulation at lower resolution, which limits achievable density contrasts, suppresses small-scale fragmentation, and modifies accretion geometries and histories; and (ii) downsampling an already high-resolution radiative-transfer image, which reduces spatial information in the output but does not remove the small-scale physics that shaped the density and temperature field during the simulation.

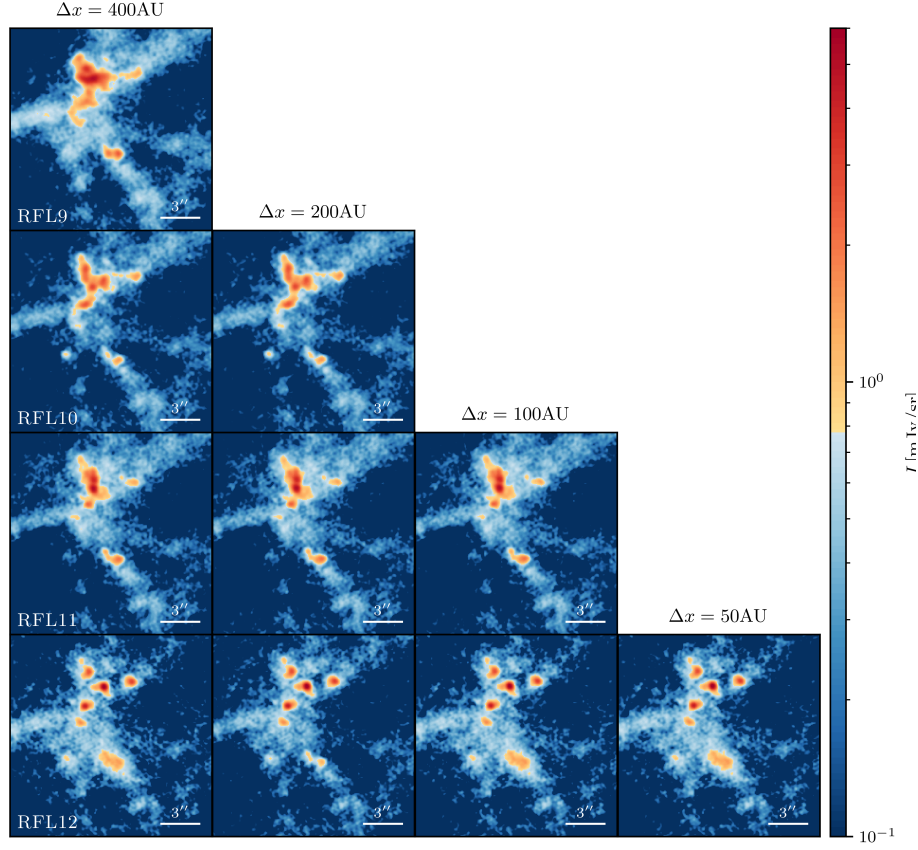


Figure 6: Flux maps derived from the same RADMC-3D images shown in Fig. 5 ($t = 230$ kyr), after post-processing with CASA to model ALMAGAL observations. Rows correspond to increasing numerical refinement levels (from top to bottom: RFL9–RFL12), while columns show different sampled spatial resolutions (left to right). At the ALMA resolution of $\sim 1200\text{au}$, the image structure is mainly set by the simulation’s intrinsic resolution, while prior downsampling of the RADMC-3D maps has only a minor effect.

The RADMC-only resolution matrix (see Fig. 5) visualises this distinction. Along the diagonal, each refinement level is shown at its native numerical resolution. Moving leftward within a given row shows the same underlying simulation emission downsampled to coarser sampling (400, 200, 100, 50 au). At a given sampling, maps based on higher-refinement simulations still show substantially more internal structure, even when down-sampled, than maps from intrinsically lower-resolution runs.

Persistence after synthetic ALMA imaging

Fig. 6 repeats the same procedure as for Fig. 5 after synthetic imaging designed to mimic ALMAGAL observing conditions, i.e. at an effective beam scale of ~ 1200 au for our adopted distance. This step includes interferometric response and imaging effects and therefore tests whether telescope limitations erase the numerical-resolution signature.

Two conclusions follow directly from this figure. First, the dominant control parameter is the simulation refinement level, not the downsampling performed before ALMA imaging. At fixed ALMA resolution, the qualitative appearance of

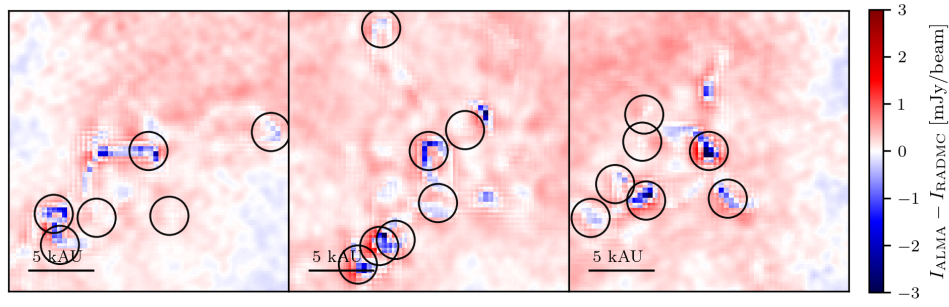


Figure 7: Difference between the flux images derived with RADMC-3D and ALMA, centered on the most massive sink of run RFL9 at $t = 230$ kyr. Circles show the cores with a radius of 1500 au. The ALMA flux is slightly higher in the low-density medium between the cores, likely due to noise. Pixels close to the core centres can show ALMA fluxes up to $\sim 3 \text{ mJy beam}^{-1}$ lower than the corresponding RADMC-3D pixels. Toward the edges of the cores, the ALMA flux can be higher.

compact emission peaks (their sharpness, multiplicity, and contrast relative to the filamentary background) varies primarily with the original numerical refinement level. By contrast, whether the RADMC images were first downsampled to 400, 200, 100, or 50 au before ALMA imaging makes comparatively little difference. This implies that observational post-processing largely preserves, rather than homogenises, the imprint of the simulation’s intrinsic resolution.

Second, beam convolution smooths small-scale structure but does not fully eliminate morphological differences. As expected, the ~ 1200 au beam suppresses the very smallest fragments and reduces the dynamic range. Nevertheless, higher-resolution runs still tend to produce more sharply defined compact structures and more distinct sub-peaks within clustered regions, while lower-resolution runs appear more diffuse and blended. This matters because the analysis (core detection, flux extraction, assignment of sizes, and the interpretation of multiplicity) depend on peak contrast and on how separable neighbouring components remain after convolution.

8.2.2

FLUX DIFFERENCE BETWEEN RADMC AND ALMA IMAGES

To better understand how interferometric imaging affects the core flux measurements we use throughout Paper II, we compare the pixel-by-pixel continuum flux in the idealised RADMC-3D maps to the flux recovered in the synthetic combined 7MTM2TM1 ALMA image at $t = 210$ kyr. Figure 7 shows the resulting difference map, with circles indicating the 1500 au core apertures. In the more diffuse, low-density medium between the cores, the ALMA map shows higher flux values of $\sim 0.1\text{--}0.3 \text{ mJy beam}^{-1}$, consistent with noise and imaging artefacts. However, within the 1500 au cores the centres often show negative residuals (with ALMA up to $\sim 3 \text{ mJy beam}^{-1}$ below RADMC-3D), while toward the edges of the same cores the residuals can become positive. This indicates that the interferometric response and the imaging do not only add noise, but can also change the recovered flux distribution within the core area.

This matters because in our analysis the flux of a core is not taken from a single pixel, but integrated within a fixed radius of 1500 au centred on the sink position. Thus, the core flux used throughout Paper II is measured over exactly the region highlighted in Fig. 7. If negative residuals in the core centre are compensated by

positive residuals toward the core edge, the total core flux can still agree reasonably well between ALMA and RADMC-3D. This is consistent with the overall good agreement seen in the core-integrated flux comparison (see Paper II in Sec. 8, Fig. 17). However, if the flux near the core edge is higher and covers a larger area, the aperture-integrated flux can become higher for the ALMA cores even if it is lower in the very centre. Conversely, if the central region shows strong negative residuals over a substantial fraction of the core, the integrated ALMA core flux can end up lower than the RADMC-3D value. Cores that show only small residuals across most of the aperture can still end up with a slightly higher ALMA flux because noise and reconstruction artefacts add positive fluctuations to the integrated signal.

PAPER III - RADIAL PROFILES OF DENSE CORES

In this paper we analyse radial profiles of dense cores in radiation-hydrodynamic simulations and their synthetic observables. We use simulation data for the gas density and dust temperature from Paper I and synthetic continuum maps from Paper II (RADMC-3D and ALMA). Cores are defined around sink particles following the core definition introduced in Paper II. We characterise the radial structure with power-law fits to median profiles in the range $r = 800 - 5000$ au and quantify the fit quality using the coefficient of determination (R^2). Deviations from a single power law are captured with an inner-to-outer slope ratio, where p_{inner} is fitted over $800 - 1200$ au and p_{outer} over $1200 - 5000$ au. We first benchmark the method for the most massive sink in one representative snapshot and track the evolution of the fitted slopes over time. We then present population statistics of radial core-envelope profiles across all sinks, relating the inferred slopes and slope ratios to sink and core masses and comparing intrinsic (3D), projected (2D), and flux-based diagnostics.

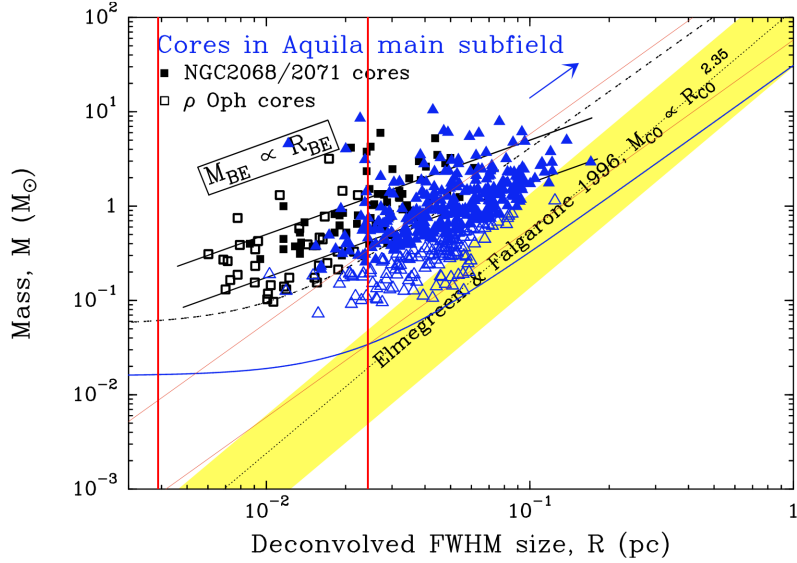


Figure 8: The mass-size relation of observationally identified cores. Filled triangles denote candidate prestellar cores, while open triangles indicate the remaining starless cores in Aquila (Herschel). Squares show literature prestellar core samples in ρ Ophiuchi and NGC 2068/2071 (e.g. [Motte et al., 1998](#)). Black solid lines show critical Bonnor-Ebert spheres at $T = 7$ and 20 K; the yellow band indicates the CO clump mass-size relation ([Elmegreen & Falgarone, 1996](#)). The dashed and blue curves show representative 5σ detection limits for ground-based (sub-)mm surveys and Herschel/SPIRE $250 \mu\text{m}$ observations, respectively. Red diagonal lines mark constant mean column densities (10^{21} and 10^{22} cm^{-2}). The Figure is adapted from [Könyves et al. \(2010\)](#). The vertical red lines mark the radial range adopted for our profile fitting, $r = 800\text{--}5000$ AU.

Figure 8, adapted from Könyves et al. (2010), shows the mass-size relation of starless cores in Aquila from Herschel observations and includes prestellar cores from (sub-)mm continuum surveys of ρ Ophiuchi and NGC 2068/2071. For the highest-resolution *Herschel* bands, the angular resolution corresponds to physical scales of roughly $\sim 800 - 2,200$ au, depending on the cloud distance. Könyves et al. (2010) report core sizes of $\sim 0.005 - 0.1$ pc, i.e., $\sim 1000 - 20,600$ au. The vertical red lines indicate our adopted fitting window, showing that the upper limit of 5000 au lies well within the range of observed core sizes.

9.1

PUBLICATION III

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Linking simulations and observations of star-forming regions

II. Radial profiles of ALMAGAL-like cores

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ABSTRACT

Context. Radial power-law profiles of dust-continuum emission are widely used to characterize the physical structure of dense cores and their envelopes, yet the connection between observed 2D intensity slopes and the intrinsic 3D density structure remains uncertain.

Aims. We compare numerical simulations of (massive) star-forming clumps with synthetic observations. Our goal is to quantify how reliably radial power-law slopes characterize core envelopes and how much of the intrinsic 3D core structure can be recovered from the 2D structure of synthetic ALMA-like continuum data.

Methods. Using radiation-hydrodynamic FLASH simulations, we extract sink-centred radial profiles of molecular hydrogen and dust temperature in 3D and their projected 2D counterparts. We post-process the simulations with RADMC-3D and generate ALMAGAL-like Band 6 maps with CASA. We measure power-law slopes over a range of 800–5000 au (and with separate inner and outer fits), restricting the analysis to well-fit, actively accreting cores.

Results. Around actively accreting sinks, the density slopes of the core envelope cluster around $p_{3D} \approx 2.4$. These slopes show no significant dependence on the initial parental clump profile, probing clump profiles of $\rho_{clump} \propto r^{-2}$ and flat. Massive sinks ($\geq 8 M_{\odot}$) show a tendency to steeper slopes, but also broader distributions of slopes and profile shapes. The projected column-density slopes are typically shallower by a factor of ~ 3 and exhibit substantial scatter due to foreground and background material. The median 3D temperature slope is $q_{3D} \approx 0.40$, which is the same value commonly assumed in observations. Continuum-based slopes show systematic offsets: RADMC-3D intensity profiles are steeper than the corresponding column-density slopes, whereas ALMA-like profiles are flatter and display the largest scatter. Applying the standard conversion between intensity and density slopes systematically underestimates p_{3D} , with median ratios of ~ 0.73 for RADMC-3D and ≈ 0.48 for ALMA-like maps.

Conclusions. Radial slopes provide useful summary statistics for accreting cores, but inferring intrinsic 3D density profiles from observed continuum slopes is biased and highly scattered, particularly in massive, non-spherical environments.

Key words. stars: formation – ISM: clouds – stars: massive – methods: numerical – techniques: interferometric

1. Introduction

Understanding how massive stars assemble their mass remains a central problem in star formation. Massive protostars form in dense, clustered environments where gravity, turbulence, magnetic fields, radiation, and stellar feedback interact over a wide range of scales. Observationally, the immediate surroundings of young massive stars are often probed via (sub-)millimetre dust continuum emission and molecular line tracers, which provide access to column densities, temperatures, and kinematics in the protostellar envelope and core. In this context, ALMAGAL (the ALMA evolutionary study of high-mass protocluster formation in the Galaxy) targets a statistically sample of 1013 candidate high-mass star-forming clumps across the Galactic disk (Molinari et al. 2025; Sánchez-Monge et al. 2025; Coletta et al. 2025). The survey observes 1.38 mm dust continuum together with a broad suite of molecular lines with a minimum resolution of ~ 1000 au. One key open question is how the radial structure of these envelopes evolves during the growth of the central object,

and to what extent observable diagnostics recover the intrinsic three-dimensional density structure.

A common empirical approach is to characterize envelopes through radial profiles (e.g. Motte & André 2001; Shirley et al. 2000). In idealized models, centrally concentrated cores are often approximated by power-law density distributions, $\rho(r) \propto r^{-p}$, which map onto projected column-density profiles and continuum-intensity profiles under simplifying assumptions. Such parameterizations are attractive because they offer a compact description of structure and can be compared across sources and evolutionary stages.

In the massive-star regime, ionizing radiation can start to influence the inner envelope once the central object becomes sufficiently massive, potentially altering the density and temperature structure and thus the inferred profile shapes (van der Tak et al. 2000). However, real massive-star-forming regions are far from spherical. Filaments, accretion streams, discs, multiplicity, and feedback-driven cavities introduce strong asymmetries (e.g. Motte et al. 2018; Hacar et al. 2018; Pineda et al. 2020). Pro-

jection effects, temperature gradients, and interferometric filtering further complicate the link between a core's intrinsic density structure and what is inferred from continuum observations. As a result, it is not obvious in which case a single power-law description is meaningful, how sensitive inferred slopes are to viewing angle and angular resolution, or how robustly continuum-based density profile slopes trace the underlying gas distribution.

Numerical simulations that self-consistently follow the evolution of massive stars provide a controlled framework to address these issues (Krumholz et al. 2009; Kuiper & Hosokawa 2018; Rosen & Krumholz 2020). Radiation-(magneto-)hydrodynamic simulations can track collapse, fragmentation, accretion, and feedback in three dimensions, while post-processing with radiative transfer and synthetic interferometric observations enables direct comparisons to observational diagnostics. In Zimmermann et al. (2025), in the following Paper I, we introduced a suite of radiation-hydrodynamic simulations of clustered massive star formation, and in Zimmermann et al. (subm. 2026), in the following Paper II, we developed a synthetic-observation pipeline (including RADMC-3D radiative transfer and CASA/ALMA imaging) together with a core definition tied to sink particles. Building on this framework, the present work quantifies the radial structure around forming stars and connects intrinsic 3D profiles to projected and continuum-based diagnostics.

Specifically, we address three questions: (i) when is a single power law a useful approximation to the radial envelope structure, and when do departures from a single slope motivate an inner/outer description (Motte & André 2001; Beuther et al. 2002); (ii) how does the mapping between intrinsic 3D density slopes and projected column-density and intensity slopes behave for different evolutionary stages; and (iii) do cores associated with massive sinks have systematically different profile slopes and shapes than those around lower-mass sinks?

This paper is organized as follows. In Sect. 2 we summarize the simulations, the synthetic-observation pipeline, and the extraction and fitting of radial profiles in 3D and 2D. In Sect. 3, we benchmark the method on a representative snapshot around the most massive sink and track the time evolution of profile slopes and inner-to-outer slope ratios through the onset of ionizing feedback. In Sect. 4, we present population statistics across all sinks, relating intrinsic and projected slopes to sink and core properties and quantifying how slopes inferred from synthetic continuum maps compare to the underlying density and column-density structure. In Sect. 5 we discuss our results, and in Sect. 6 we summarize the main conclusions and their implications for interpreting observed radial profiles in massive star-forming regions.

2. Methods

For the analysis, we use the radiation hydrodynamic simulations introduced in Paper I and the synthetic-observation pipeline described in Paper II. Below we summarise the numerical setup, post-processing, and core-definition approach adopted for this work.

2.1. Numerical simulations

We use simulations which are performed with the adaptive mesh refinement code FLASH (Fryxell et al. 2000) with a resolution of $\Delta x = 400$ au. Gas dynamics are solved with the entropy-stable (magneto-)hydrodynamics scheme of Derigs et al. (2016). Dust is assumed to be dynamically and thermally coupled to the gas

and is perfectly mixed, adopting a constant dust-to-gas mass ratio of 0.01. For the chemical evolution of the gas we use a non-equilibrium network including seven species (H_2 , H , H^+ , CO , C^+ , O , e^-) using the network of Nelson & Langer (1997) with the updates compiled by Glover et al. (2010).

Gravity and radiative effects are treated within the TREERAY module (Wünsch et al. 2018, 2021). Dust extinction and molecular (self-)shielding for H_2 and CO are included through TreeRay/OpticalDepth (Wünsch et al. 2018). Ionising feedback from stars is modelled with TreeRay/OnTheSpot (Haid et al. 2018; Wünsch et al. 2021), which applies the on-the-spot approximation (Osterbrock 1988). Momentum input from ionising photons and dust heating by non-ionising radiation are modeled TreeRay/RadPressure (Klepitko et al. 2023). The ionising and non-ionising luminosities are linked to the sink accretion following Klepitko et al. (2023).

Stellar objects are represented by sink particles that form self-consistently as described in Dinbbier & Walch (2020). The creation threshold is tied to resolving the local Jeans length on the finest grid, such that

$$\rho_{\text{thresh}} = \frac{\pi c_s^2}{G(4\Delta x)^2}, \quad (1)$$

with c_s the sound speed and Δx the smallest cell size (Truelove et al. 1997). Sink formation further requires a collapsing, bound region at a local potential minimum and not within the accretion radius of an existing sink. The sink movement is modeled with a fourth-order Hermite integrator, and their radii and effective temperatures follow the accretion-dependent protostellar models of Offner et al. (2009). The accretion radius of the sink is $2.5 \times \Delta x = 1000$ au. In our simulation the sink luminosity is split into stellar internal luminosity and accretion luminosity. At the given resolution in our simulation, each sink rather might be a protostar plus disk than necessarily an individual star, which is similar to what ALMAGAL resolves (~ 1000 au) (Molinari et al. 2025; Sánchez-Monge et al. 2025).

The simulated clumps are designed to resemble massive clumps observed in ALMAGAL. The simulation domain is $(4 \text{ pc})^3$ with a maximum resolution of 400 au. The clump has a mass of $1000 M_\odot$ within a radius of 1 pc at solar metallicity. The initial density follows a Plummer-like profile with an outer slope of -2 for the FIDUCIAL run (which is used for the main analysis) and a flat density profile for run FLAT. The virial parameter is set to $\alpha_{\text{vir}} = 0.6$. The initial gas temperature is 20 K and the dust temperature is 10 K. No external interstellar radiation field is applied as the environment is deeply embedded and expected to be fully shielded.

2.2. Synthetic Observations

We obtain dust-continuum intensities at 1.36 mm using RADMC-3D (Dullemond et al. 2012). With the dust temperatures and associated density distribution we calculate the radiative transfer along rays through the three-dimensional grid, including thermal emission and absorption by dust while ignoring scattering. We place the source at a distance of 3 kpc. Dust opacities are taken from Weingartner & Draine (2001) for $R_V = 4.0$, adopting $\kappa_{1.3 \text{ mm}} = 0.32 \text{ cm}^2 \text{ g}^{-1}$ per unit dust mass. For each snapshot we produce maps along three line of sights (LOS) in x -, y -, and z -directions.

We use the noise-free RADMC-3D continuum maps as input sky models for synthetic ALMA Band 6 observations generated with CASA (CASA Team et al. 2022). Interferometric visibilities are simulated with `simobserve` for the fully combined

2.3 Extraction and fitting of radial profiles

ALMAGAL-like dataset (7M+TM2+TM1), which is the configuration used in this work with a beam resolution of 1,200 au. We adopt $\nu_0 = 220$ GHz and a total bandwidth of $\Delta\nu = 3$ GHz, and match the on-source integration time to the ALMAGAL observations (e.g. 2–4 minutes). The CASA atmosphere plus receiver model for Band 6 is used to add thermal noise, assuming a precipitable water vapour of 1.7 mm.

2.3. Extraction and fitting of radial profiles

We identify cores with the (projected) position of sink particles, following the procedure introduced in Paper II.

In 3D, we analyse the molecular hydrogen density, ρ_{H_2} , and the dust temperature, T_{dust} , as functions of spherical radius around each core centre. In 2D, we analyse the corresponding projected quantities, the molecular column density, Σ_{H_2} , and a density-weighted, projected dust temperature, T_{proj} . In addition, we use the post-processed simulations with RADMC-3D and CASA to extract radial profiles of the continuum flux.

For a radial profile $y(r)$ around a core, we assume

$$y(r) \propto r^{-p}, \quad (2)$$

and perform a linear fit in log-log space. For the main radial profiles, we adopt a fitting range of $r = 800\text{--}5000$ au.

To assess deviations from a single power law, we additionally fit separate power laws in an inner, p_{inner} , (800 – 1200 au) and an outer, p_{outer} , (1200 – 5000 au) region. The ratio of the inner and outer slopes, s , quantifies changes in the radial behaviour between the two regimes:

$$s = \frac{p_{\text{inner}}}{p_{\text{outer}}} \quad (3)$$

We note that additional sink particles can lie within this radial distance, such that the measured profiles do not necessarily belong to isolated cores. Nevertheless, all profiles are computed with respect to the selected core centre, and the derived slopes therefore characterise the local environment around that sink, which may include the effects of clustering.

For the radial profiles, we use the median as the profile estimator. Compared to the mean, the median is less sensitive to intermittent substructure (e.g. filaments, shocks, or localised peaks) and therefore provides a more robust characterisation of a typical power law slope at a fixed radius.

To quantify the goodness of fit, we compute the coefficient of determination, R^2 , from the residuals in log space:

$$R^2 = 1 - \frac{\sum (z - z_{\text{pred}})^2}{\sum (z - \bar{z})^2}, \quad (4)$$

where z_{pred} is the best-fit prediction and $\bar{z}$ is the mean of z over the fitted points.

For the RADMC-3D images and the ALMA post-processed maps, we extract radial flux profiles using the same power-law fitting procedure as for the projected simulation quantities. This enables a controlled comparison between the intrinsic density structure and its corresponding post-processed continuum flux.

3. Case study: radial profiles around the most massive sink

In this section, we first benchmark the radial-profile method on a representative snapshot around the most massive sink (MMS).

Table 1: Definitions of fitted slopes and slope ratios

Variable	Description of the variable
Profile Slopes	
q_{3D}	Fitted slope of the median spherical profile of the dust temperature
q_{2D}	Fitted slope of the median density weighted dust temperature
p_{3D}	Fitted slope of the median spherical density profile of molecular hydrogen
p_{2D}	Fitted slope of the median column density profile of molecular hydrogen
p_{RADMC}	Fitted slope of the median intensity profile of the RADMC-3D continuum map
p_{ALMA}	Fitted slope of the median intensity profile of the ALMA continuum map
$X \in \{3D, 2D, \text{RADMC}, \text{ALMA}\}$	
s_X	Ratio of the inner-to-outer slope (see eq. 3)
R_X^2	Goodness-of-fit (coefficient of determination) of the power-law fit (see eq. 4)

We then track the time evolution of the fitted slopes to quantify how the radial structure changes as the system evolves and ionizing feedback becomes important.

3.1. Morphology and radial profiles in a benchmark snapshot

Figure 1 shows, from top to bottom, the density-weighted dust temperature, T_{proj} , the molecular hydrogen column density, Σ_{H_2} , the RADMC intensity maps, I_{RADMC} , and the ALMA intensity maps, I_{ALMA} , at $t = 210$ kyr. By this time, 17 of the 19 sink particles have formed. Two sinks have already become massive ($m > 8, M_{\odot}$), but ionizing feedback has not yet affected the clump. All panels are centred on the MMS, marked by the red star. From left to right, the three LOS are shown.

The dust temperature is primarily regulated by radiative heating from the sink particles. As a result, the projected dust temperature, T_{proj} , is relatively smooth and appears close to radially symmetric, with only weak deviations introduced by local density substructure (see Fig. 1, top row).

The column-density maps, Σ_{H_2} , reveal pronounced substructures, including accretion channels and compact overdensities. These features vary with viewing direction, indicating that the most massive sink might be embedded in a clustered, non-spherical environment rather than a strictly spherical envelope (see Fig. 1, second row). The morphology seen in the column-density maps is reproduced well in the RADMC-3D intensity maps, where the substructure remains clearly visible (see Fig. 1, third row). By contrast, the ALMA maps include interferometric imaging effects and have a coarser effective resolution (see Fig. 1, bottom row). The simulation resolves scales down to ~ 400 au, whereas the ALMA beam corresponds to ~ 1200 au. As a result, much of the small-scale substructure is smoothed out and is no longer detectable in the ALMA images.

The corresponding radial profiles around the MMS, based on the maps shown in Fig. 1, are presented in Fig. 2: the median radial 3D dust-temperature profile (top left) and the corresponding median radial density-weighted dust-temperature profile (top right); the median radial spherical density profile (middle left) and the corresponding median radial column-density

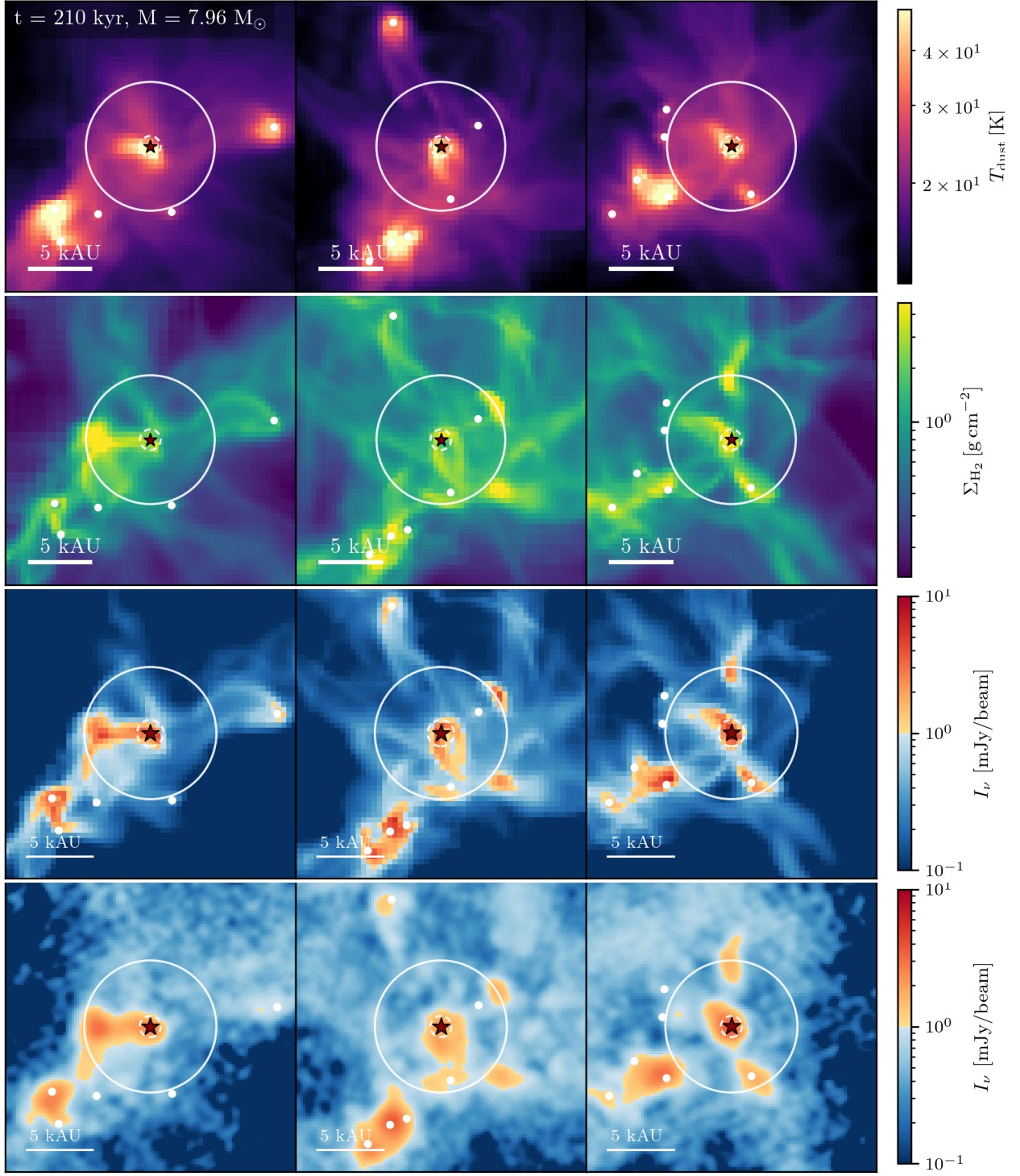


Fig. 1: From top to bottom: density-weighted dust temperature, H_2 column density, RADMC intensity maps, and ALMA intensity maps, centred on the most massive sink (red star), shown for three lines of sight (left to right: x -, y -, and z -directions). The fitting region for the radial profiles is indicated by circles: the inner solid circle marks an inner radius of 800 au, and the outer solid circle marks an outer radius of 5000 au. White dots denote other sink particles.

3.2 Time Evolution of Radial-Profile Slopes

profiles for the three LOS (middle right); and the median radial intensity profiles derived from the RADMC-3D (bottom left) and ALMA (bottom right) maps. The inner and outer slopes are not shown for projected quantities to avoid overcrowding the plots. The 3D temperature profile is well described by a single power law with index $q_{3D} = 0.61$. However, the inner profile is steeper, with $q_{inner} = 0.83$, while the outer profile is flatter, with $q_{outer} = 0.55$. The central temperature reaches ~ 70 K. For the density-weighted temperature profile, the central temperature is lower, ~ 50 K, indicating that the high temperatures are confined to the very inner region and that density weighting reduces the inferred temperature by also accounting for cooler, denser material. The corresponding power-law indices are therefore smaller, with $q_{3D} \approx 0.30 - 0.41$. The dust temperature profiles are further discussed in Section 4.6.

The 3D density profile is relatively stable and can be well described by a single power-law exponent over the fitted range, with $p_{3D} = 1.81$. This is substantially steeper than the projected slopes, which fall in the range $p_{2D} = 0.32 - 0.64$ depending on the line of sight. The three p_{2D} profiles show some scatter between the different projections, reflecting non-radial substructure and line-of-sight projection effects visible in the maps. Nevertheless, within the fitting range the profiles remain close to a power law, so fitting a global slope provides a useful quantitative measure for comparing viewing directions and linking the projected structure to the underlying 3D distribution.

Comparing the column-density profiles with the RADMC-3D intensity profiles shows that the RADMC-3D profiles are more stable across the different LOS (see Fig. 2, bottom left panel). Since the continuum intensity depends on both dust column density and dust temperature, a relatively smooth temperature field driven by protostellar heating can reduce the contrast of small-scale density structures in the intensity maps. The resulting power-law slopes are $p_{RADMC} \approx 0.87 - 0.97$, which are systematically steeper than those inferred from the projected column-density profiles ($p_{2D} = 0.32 - 0.64$). The ALMA profiles, in turn, exhibit a more extended inner plateau owing to the coarser angular resolution, and their fitted slopes fall between p_{RADMC} and p_{2D} values, with $p_{ALMA} = 0.65 - 0.88$ (see Fig. 2, bottom right panel).

3.2. Time Evolution of Radial-Profile Slopes

We now move from the single benchmark snapshot to the time evolution of the fitted radial density slopes around the most massive sink (see Fig. 3). Tracking p_{3D} over time shows that, during the early evolution, the median 3D profile is well described by a nearly constant power-law index of 2.4 (see Fig. 3, top right panel). Sink particles can emit ionizing radiation from the accretion process even before they become massive (see Paper I, Fig. 3, bottom-right panel). After ~ 210 kyr, the sink particle that later becomes the MMS exceeds $8 M_{\odot}$. However, ionizing radiation does not produce dynamical feedback until ~ 290 kyr. The MMS then undergoes an accretion halt between ~ 300 and 340 kyr, during which the fitted slope becomes highly variable, and the goodness of fit decreases, as indicated by a decline in R^2 . Once accretion resumes, when global infall is winning over the dispersing effects of the ionizing radiation feedback from the MMS, the slope stabilizes again and the fit quality improves. When the H II region begins to expand after ~ 370 kyr, the slope again becomes highly variable and R^2 drops again, indicating that a single power law no longer provides an adequate description once feedback starts to dominate the structure.

In projection, the early evolution of p_{2D} is also approximately constant but shows some scatter, both between different LOS and within each individual LOS over time (see Fig. 3, top left panel). Shortly after the most massive sink becomes massive (~ 240 kyr), p_{2D} increases slightly, even though no comparable change is seen in p_{3D} . During the accretion halt ($\sim 300 - 340$ kyr), p_{2D} decreases slightly, and the corresponding R^2 also declines, but both remain comparatively smoother than in 3D. This behaviour suggests that foreground and background material along the LOS can partially mask intrinsic changes in the underlying 3D profile.

p_{RADMC} and p_{ALMA} broadly follow the temporal trends of p_{2D} (see Fig. 3, bottom panels). They increase slightly as ionizing radiation sets in, decrease during the accretion halt, rise again once accretion resumes, and finally decline as the H II region expands. However, p_{RADMC} remains systematically steeper than p_{2D} . p_{ALMA} evolves more smoothly, consistent with beam smearing and the lower effective resolution of the interferometric maps. Overall, the results suggest that sustained accretion corresponds to phases where the radial profiles are well described by a single power law, whereas during accretion halts or strong feedback the slope becomes unstable and the fit deteriorates.

For the global analysis of profiles around all sinks, it is useful to restrict the sample to phases where the corresponding sink is still accreting since, in these intervals, a single power-law slope typically provides a more robust characterization of the radial structure.

3.3. Deviations from a single power law

To quantify deviations from a single power law and to track changes in the radial structure over time, we also compare the inner and outer power-law slopes obtained from the broken power-law fits (see also section 2). The ratio $s = \frac{p_{in}}{p_{out}}$ provides a compact measure of how the profile shape differs between the central region and the envelope: $s > 1$ indicates a relatively steeper inner profile, whereas $s < 1$ corresponds to a flatter inner region compared to the outer envelope.

For the most massive sink, we evaluate the median inner-to-outer slope ratio in two evolutionary phases: an early, pre-ionization epoch (0–220 kyr) and a later epoch (220–370 kyr) spanning the onset of ionization up to the disruption of the core by the expanding H II region. In 3D, the median ratio is close to unity in the early phase, $s_{3D} \approx 1.0$, and decreases to ≈ 0.6 in the later epoch (see Fig. 4, top right). In projection, the median ratio shows a similar but more pronounced shift: $s_{2D} \approx 1.3$ during 0–220 kyr, dropping to ≈ 0.7 during 220–370 kyr (see Fig. 4, top left). The flux-based ratios follow the same qualitative evolution, decreasing from ≈ 1.8 to ≈ 0.7 for the RADMC-3D intensity profiles and from ≈ 1.0 to ≈ 0.5 for ALMA (see Fig. 4, bottom panels). The systematic change in the inner-to-outer slope ratio in both 2D and 3D suggests that the onset of ionizing radiation, even if the trapped H II region has not yet begun to expand, is associated with a genuine structural change in the core–envelope profile.

The combination of steeper fitted slopes in the second epoch (see Fig. 3) and a decreasing inner-to-outer slope ratio (see Fig. 4), suggests a change in the shape of the radial profiles rather than a uniform steepening at all radii. While the overall profile becomes steeper on average, the drop from $s > 1$ to $s < 1$ indicates that the inner region becomes comparatively flatter than the envelope. In other words, the profiles evolve from being more

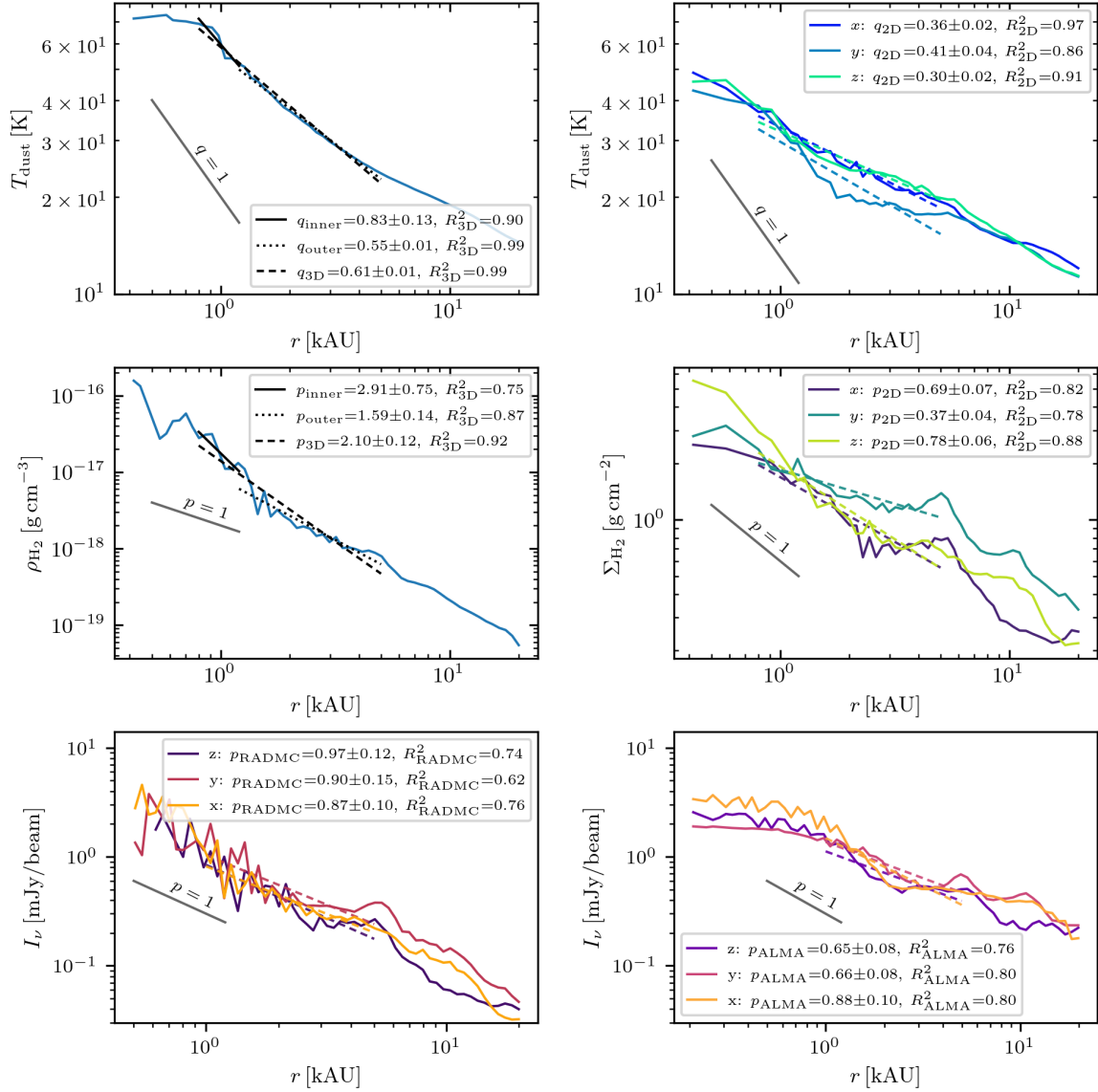


Fig. 2: Median radial profiles around the most massive sink: the 3D dust temperature (q_{3D} ; top left) and density-weighted dust temperature (q_{2D} ; top right); the spherical density profile (p_{3D} ; middle left) and column-density profile (p_{2D} ; middle right); and the intensity profiles from the RADMC-3D (p_{RADMC} ; bottom left) and ALMA (p_{ALMA} ; bottom right) maps. All profiles correspond to the maps shown in Fig. 1. The best-fitting global slope, p , is indicated by a dashed line. For p_{3D} , the inner and outer slopes from the broken power-law fit are shown as solid and dotted black lines, respectively. The grey line shows a reference slope of $q = 1$ or $p = 1$. The p_{3D} profile is relatively stable and can be well described by a single power law over the fitted range. Although the three p_{2D} profiles differ somewhat due to non-radial substructure and line-of-sight projection effects, a power-law approximation still provides a useful characterisation within the fitting region. The ALMA profiles show a more extended inner plateau owing to the coarser resolution. Overall, the RADMC-3D intensity profiles are the steepest, followed by ALMA, and then the column-density profiles.

centrally peaked relative to their outer parts, to a weaker central concentration compared to a steeper power-law in the envelope.

Several effects could cause this behaviour. One possible explanation is the increasing influence of ionizing feedback. Even before a fully developed expanding H II region disrupts the core, radiative heating raises the gas pressure in the vicinity of the most massive sink and can partially broaden the inner region. Such pressure-driven expansion would tend to flatten the in-

ner profile by redistributing material from the centre to slightly larger radii, while the transition to the surrounding envelope becomes sharper. In this picture, the inner-to-outer slope ratio decreases because the inner slope becomes more shallow whereas the outer profile appears steeper.

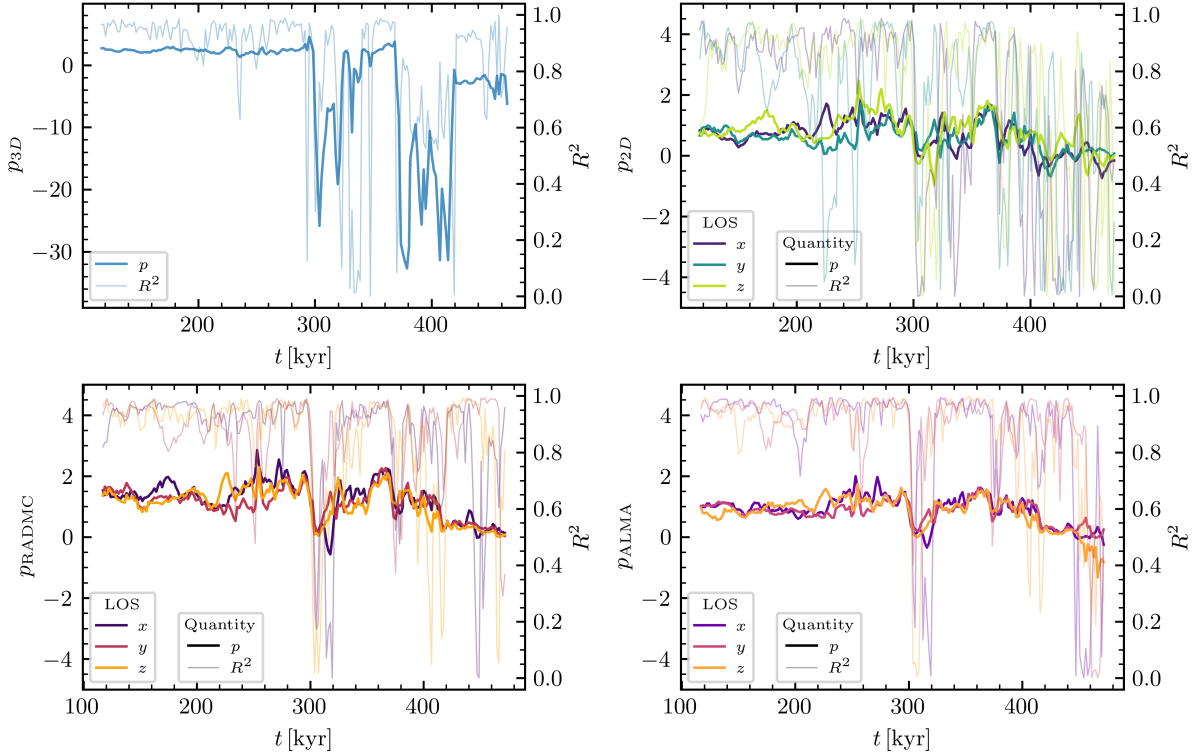


Fig. 3: Time evolution of the inferred radial power-law slope p (left axis) and the corresponding goodness-of-fit R^2 (right axis) around the most massive sink, measured from the median 3D gas density (top left), the median column density (top right), and the median intensity profiles from the RADMC-3D (bottom left) and ALMA (bottom right) flux maps. During the early evolution the slopes remain approximately constant, indicating a stable, centrally concentrated structure. The slope becomes markedly more variable and R^2 decreases during the accretion halt (~ 300 – 340 kyr) and again once the HII region expands ($\gtrsim 370$ kyr), indicating that a single power law no longer provides a sufficient estimation in the feedback-affected phase. p_{2D} , p_{RADMC} and p_{ALMA} follow the same overall trends. p_{RADMC} is systematically steeper than p_{2D} , while p_{ALMA} appears smoother due to beam convolution and the lower effective resolution.

4. Population Statistics of Radial Core Envelope Profiles

We now turn from the detailed benchmark around the MMS to a global analysis of radial profiles across the full core (sink) population. Table 2 lists the number of cores which are used in the analysis for the full sample and for subsets restricted to $R_X^2 > 0.9$, actively accreting sinks, or both.

Table 2: Number of cores (sinks) in the total sample and in the restricted subset, selected by radial-profile goodness-of-fit and/or actively accreting sinks.

Quantity	total number	$\dot{M}_{\text{Sink}} > 0$	$R_X^2 > 0.9$	$\dot{M}_{\text{Sink}} > 0, R_X^2 > 0.9$
p_{3D}	3,400	1,627	1,945	1,268
p_{2D}	10,200	4,881	2,683	2,261
p_{RADMC}	10,200	4,881	3,462	2,951
p_{ALMA}	7,956	3,477	2,653	1,895
q_{3D}	3,400	1,627	2,071	1,303
q_{2D}	10,200	4,881	7,956	3,196

4.1. Dependence on sink properties

First, we relate p_{3D} and p_{2D} , as well as p_{RADMC} and p_{ALMA} , to the corresponding sink properties (see Fig. 5). Only slopes with a corresponding $R_X^2 > 0.9$ are included. As a function of sink mass (see Fig. 5, top row), p_{3D} shows a weak decreasing trend (from ~ 2.6 to ~ 2.3) but becomes highly variable once sinks grow massive ($M_{\text{sink}} \gtrsim 8 M_\odot$). In contrast, p_{2D} increases slightly with sink mass (from ~ 0.7 to ~ 1.2). The RADMC slopes exhibit a similar mild increase with M_{sink} (from ~ 0.9 to ~ 1.5), whereas the ALMA slopes remain approximately constant at ~ 0.5 with noticeably larger scatter, showing an increase only for $M_{\text{sink}} \gtrsim 10 M_\odot$ to ~ 1.0 .

When plotted against the sink mass-accretion rate (see Fig. 5, right panels), p_{3D} (blue line) is broadly consistent with being constant at ~ 2.3 but displays substantial scatter at higher $\dot{M}_{\text{sink}}$. Notably, the negative values of p_{3D} that appear plotting against the sink mass are largely absent when the data are viewed as a function of the accretion rate. This suggests that these extreme slopes are not a generic feature of massive sinks, but instead occur preferentially once accretion has largely ceased. For massive objects, the absence of ongoing accretion is consistent with a phase in which ionizing feedback becomes dominant and dynamically reshapes the immediate envelope of the sink/core due to the expansion of an H II region. Such feedback-driven recon-

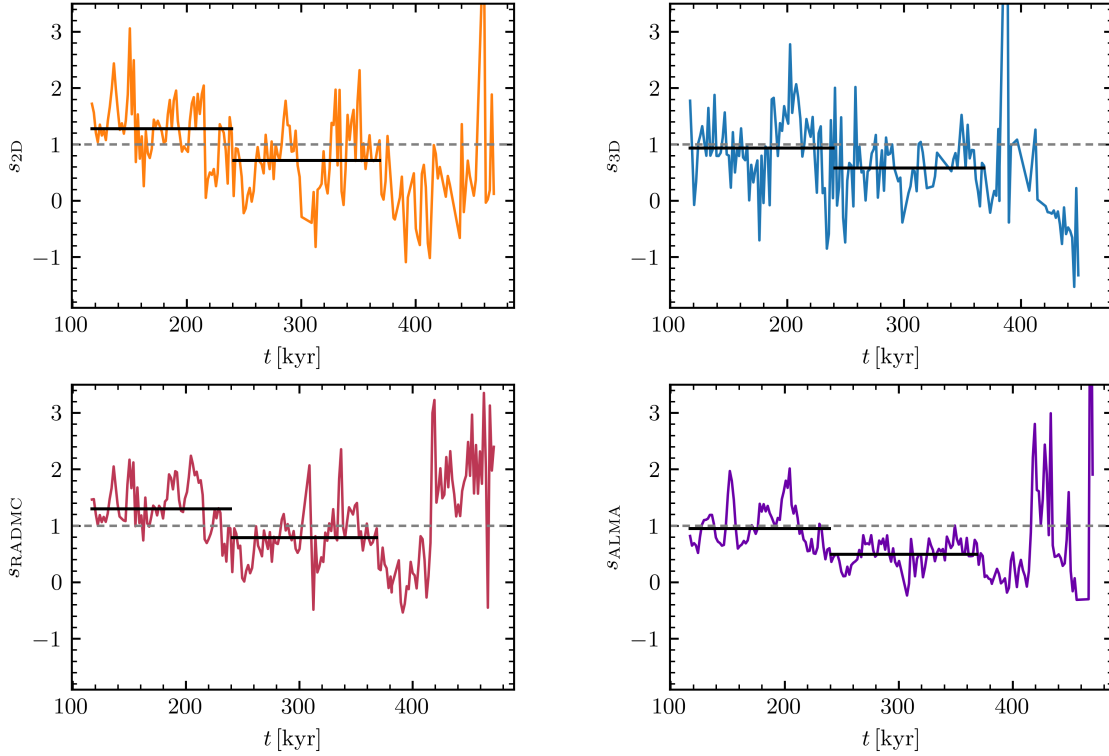


Fig. 4: Ratio of the inner-to-outer power-law slope around the most massive sink, shown for the projected column-density profile (top left), the median 3D density profile (top right), and the RADMC-3D and ALMA intensity profiles (bottom left/right). Dashed lines indicate $s = 1$. Median slope ratios are shown for two epochs: 0–220, kyr (pre-ionization) and 220–370, kyr (from the onset of ionization until the core is disrupted by the expanding H,II region). In 3D, the median ratio decreases from $s_{3D} \approx 1.0$ in the early phase to ≈ 0.6 in the later phase. The projected profile shows a similar shift, with $s_{2D} \approx 1.3$ at 0–220, kyr dropping to ≈ 0.7 at 220–370, kyr. The flux-based ratios follow the same qualitative trend, decreasing from ≈ 1.8 to ≈ 0.7 for RADMC-3D and from ≈ 1.0 to ≈ 0.5 for ALMA.

figuration disrupts the surrounding envelope, so that a simple power-law description is no longer appropriate and can therefore lead to unusually shallow or even negative fitted values of p_{3D} .

In contrast, the projected slopes p_{2D} (orange line) remain considerably smoother and do not show negative values. Moreover, p_{2D} increases with increasing accretion rate (from ~ 0.7 to ~ 1.2), and p_{RADMC} follows the same trend (from ~ 0.8 to ~ 1.5). The ALMA slopes also rise with M_{sink} , but more slowly (from ~ 0.5 to ~ 1.0).

4.1.1. Envelope slopes for massive sinks

To highlight the dependence on sink mass, Fig. 6 summarizes the distributions of the inferred slopes in two mass bins: $M_{\text{sink}} < 8 M_{\odot}$ for lower-mass sinks and $M_{\text{sink}} \geq 8 M_{\odot}$ for massive sinks. In each violin, the left half corresponds to the low-mass bin and the right half to the high-mass bin, enabling a direct comparison of the typical slope and the intrinsic scatter as a function of sink mass. We restrict the sample to slopes with $R_X^2 > 0.9$ and exclude sinks that are no longer accreting ($\dot{M}_{\text{sink}} > 0$) as we want to focus on the early stages that are not feedback dominated. The 3D density slopes cluster around a median of $p_{3D} \approx 2.4$ for lower-mass sinks. For high mass stars the median is shifted to slightly larger values ($p_{3D} \approx 2.5$) but also exhibit a broader distribution. For the

projected profiles, the medians increase from $p_{2D} \approx 0.8$ (lower mass sinks) to $p_{2D} \approx 1.0$ (high mass sinks), with comparatively narrow distributions. The slopes inferred from the synthetic flux maps show the same mass-dependent trend but with substantially larger scatter. p_{RADMC} increases from a median of ≈ 1.0 to ≈ 1.4 and p_{ALMA} from ≈ 0.6 to ≈ 0.8 between the low- and high-mass bins. The broader distributions reflect additional sources of variance introduced by radiative-transfer effects and observational filtering, while the systematic offsets relative to p_{2D} indicate that the flux-based diagnostics do not trace the column-density slope one-to-one.

The tendency for massive sinks to have somewhat steeper slopes may arise for different reasons. As a sink grows, its deeper gravitational potential can focus inflow and draw more material toward the centre. Although material that crosses the accretion radius is partly removed from the envelope and added to the sink, the enhanced inflow can maintain a higher density in the inner envelope. This can steepen the fitted envelope slope.

In addition, the increasing role of feedback from massive sinks may contribute to the slight steepening and the enhanced scatter at $M_{\text{sink}} \gtrsim 8 M_{\odot}$. For the sink luminosities, we also include an accretion-luminosity component. Heating by non-ionizing radiation can affect the inner region, while ionizing radiation and its associated radiation pressure may further influence the envelope. The impact of ionizing radiation depends on

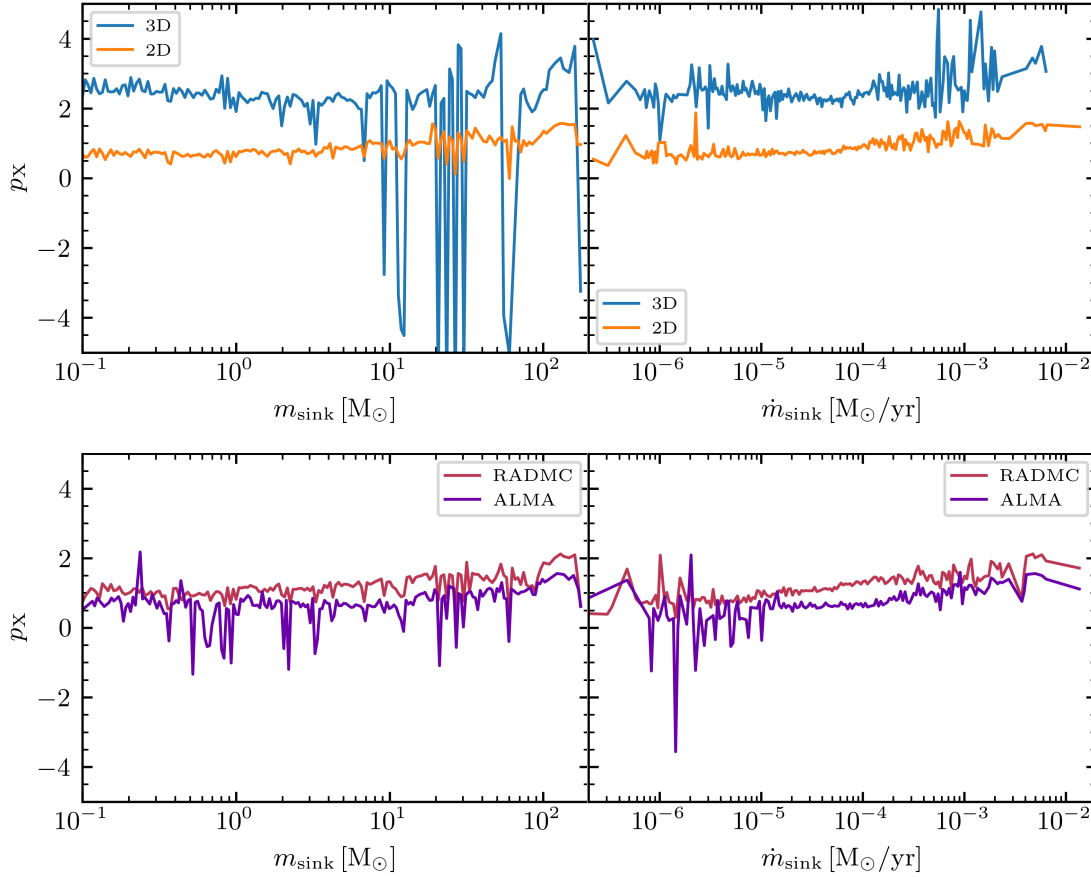


Fig. 5: Radial profile slopes as a function of sink properties. Top panels: intrinsic slopes from the 3D density profiles, p_{3D} , and the projected column-density profiles, p_{2D} . Bottom panels: slopes measured from the synthetic RADMC and ALMA maps, p_{RADMC} and p_{ALMA} . Only profiles with $R_X^2 > 0.9$ are included. Left panels show the dependence on sink mass, m_{sink} , and right panels the dependence on the sink mass-accretion rate, $\dot{m}_{\text{sink}}$. With increasing M_{sink} , p_{3D} decreases slightly (from ~ 2.6 to ~ 2.3) and becomes highly variable for massive sinks ($M_{\text{sink}} \gtrsim 8 M_\odot$), whereas p_{2D} increases weakly with mass (from ~ 0.7 to ~ 1.2). The RADMC slopes show a similar mild increase with M_{sink} (from ~ 0.9 to ~ 1.5), while the ALMA slopes remain approximately constant around ~ 0.5 with larger scatter and increase only for $M_{\text{sink}} \gtrsim 10 M_\odot$ to ~ 1.0 . As a function of $\dot{M}_{\text{sink}}$, p_{3D} shows some scatter but not such large negative slopes than as a function of m_{sink} . In 2D, the slope increases slightly with increasing accretion rate from ~ 0.7 to ~ 1.2 . The RADMC slopes increase accordingly (from ~ 0.8 to ~ 1.5), and the ALMA slopes also rise with $\dot{M}_{\text{sink}}$ but with a shallower trend (from ~ 0.5 to ~ 1.0).

whether the H II region remains trapped or is able to expand. Since we restrict the sample to accreting sinks ($\dot{M}_{\text{sink}} > 0$), we largely select phases in which ongoing inflow maintains high densities and ram pressure that confine the ionized gas and limit its expansion, so that the envelope is not rapidly dispersed. Even in this trapped or slowly expanding regime, ionizing radiation can heat the inner region and suppress accretion locally, while compressing neutral material into dense, shell-like structures. This non-spherical and time-variable restructuring naturally broadens the distribution of inferred slopes in both the 3D and 2D diagnostics and may also contribute to slightly steeper effective slopes if the fits preferentially trace the compressed inner-envelope component.

4.1.2. Inner-to-outer slope ratio for massive sinks

In Sect. 3.3, we quantified deviations from a single power law using the inner-to-outer slope ratio, s . We now examine whether

these deviations are present across the full sample and whether they depend on sink mass, i.e. whether profiles associated with massive sinks differ systematically from those around lower-mass sinks. We only include actively accreting sinks, but here we relax the goodness-of-fit threshold to $R_X^2 > 0.6$ (instead of 0.9) in order to also include profiles that deviate more strongly from a single power law.

For the spherical density profiles, the median ratio is $s_{3D} \approx 0.9$ for $M_{\text{sink}} < 8 M_\odot$, indicating that a single power-law fit provides a good description of the density structure in most cases (see Fig. 7, left panel). For massive sinks, the median s_{3D} decreases to ~ 0.6 and the distribution becomes significantly broader, suggesting that the relative steepness between the inner and outer envelope is more diverse at high mass. This increased spread is consistent with ionizing-radiation feedback beginning to influence and reshape the surrounding envelope structure.

For the projected profiles, s_{2D} drops slightly more than in 3D: the median decreases from ~ 1.2 for lower-mass sinks to

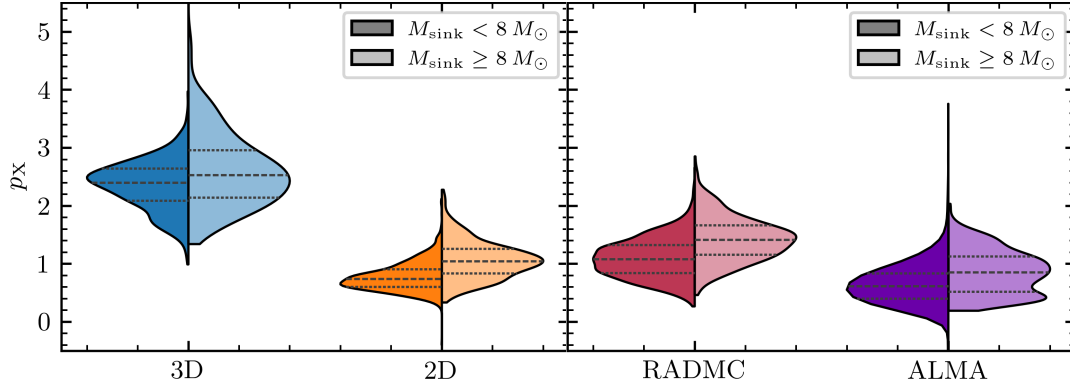


Fig. 6: Violin plots of the radial profile slopes for the spherical density profile, p_{3D} , and the projected column-density profile, p_{2D} (left panel), as well as for the flux-based slopes p_{RADMC} and p_{ALMA} (right panel). For each case, the left half shows the distribution for corresponding sink masses $M_{\text{sink}} < 8 M_{\odot}$, while the right half shows $M_{\text{sink}} \geq 8 M_{\odot}$. Only profiles with $R_X^2 > 0.9$ and for actively accreting sinks ($\dot{M}_{\text{sink}} > 0$) are included. The p_{3D} distribution has a median of ≈ 2.4 at low masses and shifts to slightly higher values ≈ 2.5 at high masses, accompanied by a broader spread. For p_{2D} , the median increases from ≈ 0.8 with a narrow distribution to ≈ 1.0 for higher masses. p_{RADMC} and p_{ALMA} distributions are broader but show similar mass-dependent trends with offsets relative to p_{2D} : p_{RADMC} has medians of ≈ 1.0 and ≈ 1.4 , and p_{ALMA} has medians of ≈ 0.6 and ≈ 0.8 for low- and high-mass sinks, respectively.

~ 0.7 for massive sinks (see Fig. 7, left panel). For lower-mass sinks, $s_{2D} \gtrsim 1$ indicates that the inner and outer fits are broadly similar, with at most a modest steepening toward smaller radii. For massive sinks, $s_{2D} < 1$ implies that the inner projected profile becomes systematically flatter relative to the outer part. This stronger decrease in 2D can naturally arise from projection, which integrates along the LOS and is therefore particularly sensitive to non-spherical structure. Partial clearing and low-density channels in the inner envelope efficiently reduce the central column density, while compressed material at larger radii can maintain (or steepen) the outer profile. As a result, the difference between the inner and outer slopes appears more pronounced in s_{2D} than in s_{3D} once feedback and dynamical asymmetries become important.

The flux-based ratios follow the same qualitative behaviour (see Fig. 7, right panel) but with the systematic offsets seen earlier. For RADMC, the median ratio decreases from $s_{RADMC} \approx 1.4$ at low mass to ≈ 0.8 at high mass, broadly tracking the evolution seen in s_{2D} but shifted to larger values. The higher s_{RADMC} at low masses indicates a more centrally peaked flux profile, with a comparatively steeper inner slope relative to the outer envelope. The ALMA ratios are systematically smaller, with medians of $s_{ALMA} \approx 0.6$ and ≈ 0.5 in the low- and high-mass bins, respectively. The coarser resolution leads to an overall flatter inner profile. The weak mass dependence further suggests that small-scale structure, including features produced in response to ionizing feedback, is increasingly smeared out and therefore difficult to detect.

Overall, the decrease of s_X toward massive sinks indicates that the relative inner-to-outer slope changes systematically with sink mass, while the increasing scatter in s_{3D} suggests that massive-sink envelopes exhibit increasingly heterogeneous and time-variable structures.

4.2. Relation to projected and spherical core mass

In observations, sink (or stellar) properties are typically not as readily accessible as they are in simulations. The quantity that

can be estimated from dust continuum observations is the (projected) core mass. Therefore, we relate the radial profile slopes to the core mass measured in the simulation, both intrinsically in 3D, m_{3D} , and in projection (2D), m_{2D} (see Fig. 8).

The core masses, m_{3D} and m_{2D} , are taken from Paper II. In 3D, the core mass is defined as the dust and gas mass enclosed within a sphere of radius 1500 au centered on the sink. In 2D, the core mass is defined from the corresponding LOS projection used to compute the radial profiles.

The p_{3D} slopes show substantial scatter and remain somewhat variable overall. The mean trend is nearly constant as a function of m_{2D} (left panel) and increases only slightly with m_{3D} (right panel). In contrast, p_{2D} show less variation and increases with both m_{2D} and m_{3D} with fitted slopes of 0.50 and 0.59, respectively. This suggests that both m_{2D} and m_{3D} can be related to p_{2D} via

$$\log_{10} m_{2D} = 2.00 p_{2D} - 1.64, \quad (5)$$

$$\log_{10} m_{3D} = 1.69 p_{2D} - 1.76. \quad (6)$$

The flux-based slopes, p_{RADMC} and p_{ALMA} , follow the same qualitative trend. The increase with both m_{2D} and m_{3D} is similar, but with a different offset. This suggests that, within our simulation, both the projected and spherical core masses are related to the flux-based slopes. The corresponding relations are

$$\log_{10} m_{2D} = 1.41 p_{RADMC} - 1.54, \quad (7)$$

$$\log_{10} m_{3D} = 1.25 p_{RADMC} - 1.76, \quad (8)$$

and

$$\log_{10} m_{2D} = 1.41 p_{ALMA} - 0.80, \quad (9)$$

$$\log_{10} m_{3D} = 1.22 p_{ALMA} - 1.06. \quad (10)$$

Note that at low m_{2D} and m_{3D} , the ALMA-derived slopes become unreliable due to a limited flux-to-noise ratio. In Paper I, we derived a minimum reliably detectable core mass of $\gtrsim 0.3 M_{\odot}$.

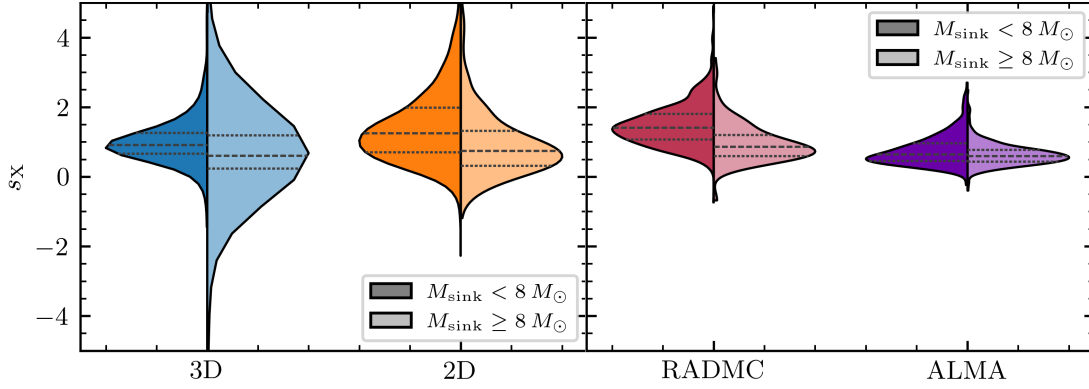


Fig. 7: Violin plots of the inner-to-outer slope ratio, s_X , for the spherical density profile (p_{3D}), the projected column-density profile (p_{2D}), and the flux-based slopes (p_{RADMC} and p_{ALMA}). Only profiles with $R_X^2 > 0.6$ are included, and the corresponding sink is actively accreting ($\dot{M}_{\text{sink}} > 0$). For each violin, the left half shows profiles with $M_{\text{sink}} < 8 M_\odot$, while the right half shows $M_{\text{sink}} \geq 8 M_\odot$. The median ratios are $s_{3D} \approx 0.9$ for $M_{\text{sink}} < 8 M_\odot$, decreasing to ≈ 0.6 for massive sinks, where the scatter becomes substantially broader. For s_{2D} , the median decreases from ≈ 1.2 to ≈ 0.7 between the low- and high-mass stars. The flux-based ratios show a similar shift. s_{RADMC} decreases from ≈ 1.4 to ≈ 0.8 , while s_{ALMA} changes from ≈ 0.6 to ≈ 0.5 . Values of $s_X < 1$ indicate that the inner profile is flatter than the outer and decreasing s_X implies a flatter inner slope, a steeper outer slope, or both.

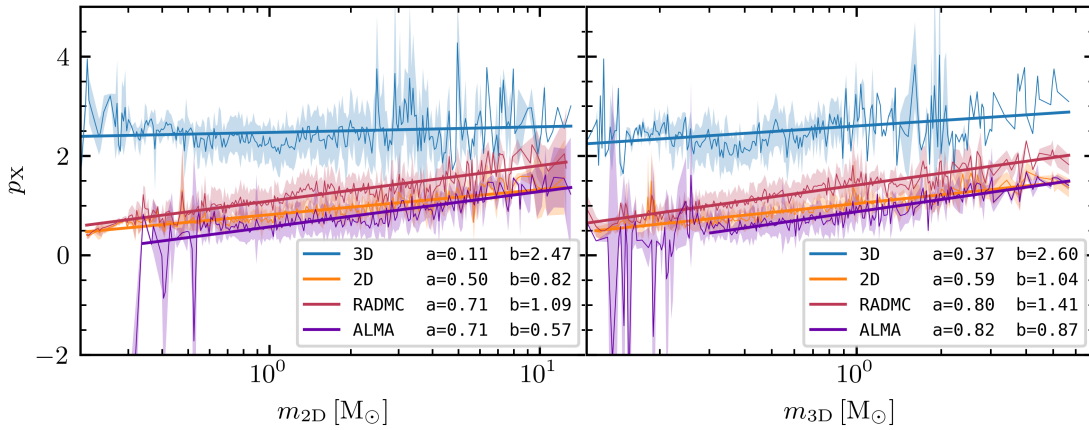


Fig. 8: Radial profile slopes as a function of the projected core mass, m_{2D} (left), and the spherical core mass, m_{3D} (right). Shown are slopes from the 3D density profiles (p_{3D}), the projected column-density profiles (p_{2D}), and the intensity profiles measured from the synthetic RADMC-3D and ALMA maps (p_{RADMC} and p_{ALMA}). The thin lines show the median values with the standard deviation indicated by the shaded region. The thick lines show linear fits of the form $p_X = a \log_{10}\left(\frac{m_X}{M_\odot}\right) + b$ where m_X denotes m_{2D} or m_{3D} ; the corresponding fit coefficients a and b are listed in the legend. Only profiles with $R_X^2 > 0.9$ are included, and the corresponding sink is actively accreting ($\dot{M}_{\text{sink}} > 0$). The p_{3D} slopes show substantial scatter, with little dependence on m_{2D} and only a weak increase with m_{3D} . In contrast, p_{2D} increases with both m_{2D} and m_{3D} . The flux-based slopes, p_{RADMC} and p_{ALMA} , follow the same qualitative trend. At low m_{2D} and m_{3D} , the ALMA-derived slopes become unreliable owing to the limited flux-to-noise ratio.

Figure 9 shows the ratio of the inferred masses (from Eqs. 5–10) to the simulation masses as a function of simulation mass. The distribution clusters around unity but also reveals substantial scatter. However, because the relation between the power law index, p_X , and the mass is not very steep, estimating m_{2D} and m_{3D} from it alone might be not reliable. Nevertheless, the slope may still serve as a useful additional feature for core-mass estimation, for example in machine-learning approaches, as explored in Paper II. Including this information could improve the mass estimates derived from observational data.

4.3. Linking projected and intrinsic slopes

Across the full sink/core population, we compare the evolution of the core-envelope power-law slopes inferred from p_{3D} and p_{2D} (see Fig. 10). Thick lines show profiles restricted to $R_{3D}^2 > 0.9$ and $R_{2D}^2 > 0.9$ for which the corresponding sink particle is still accreting ($\dot{M}_{\text{sink}} > 0$), while dotted lines show the full sample without restriction. The restricted sample of p_{3D} (thick line) remains nearly constant until ~ 300 kyr and slightly increases afterward (see Fig. 10, left panel). The unrestricted sample (dotted line) shows a clear response to the dynamical feedback of ion-

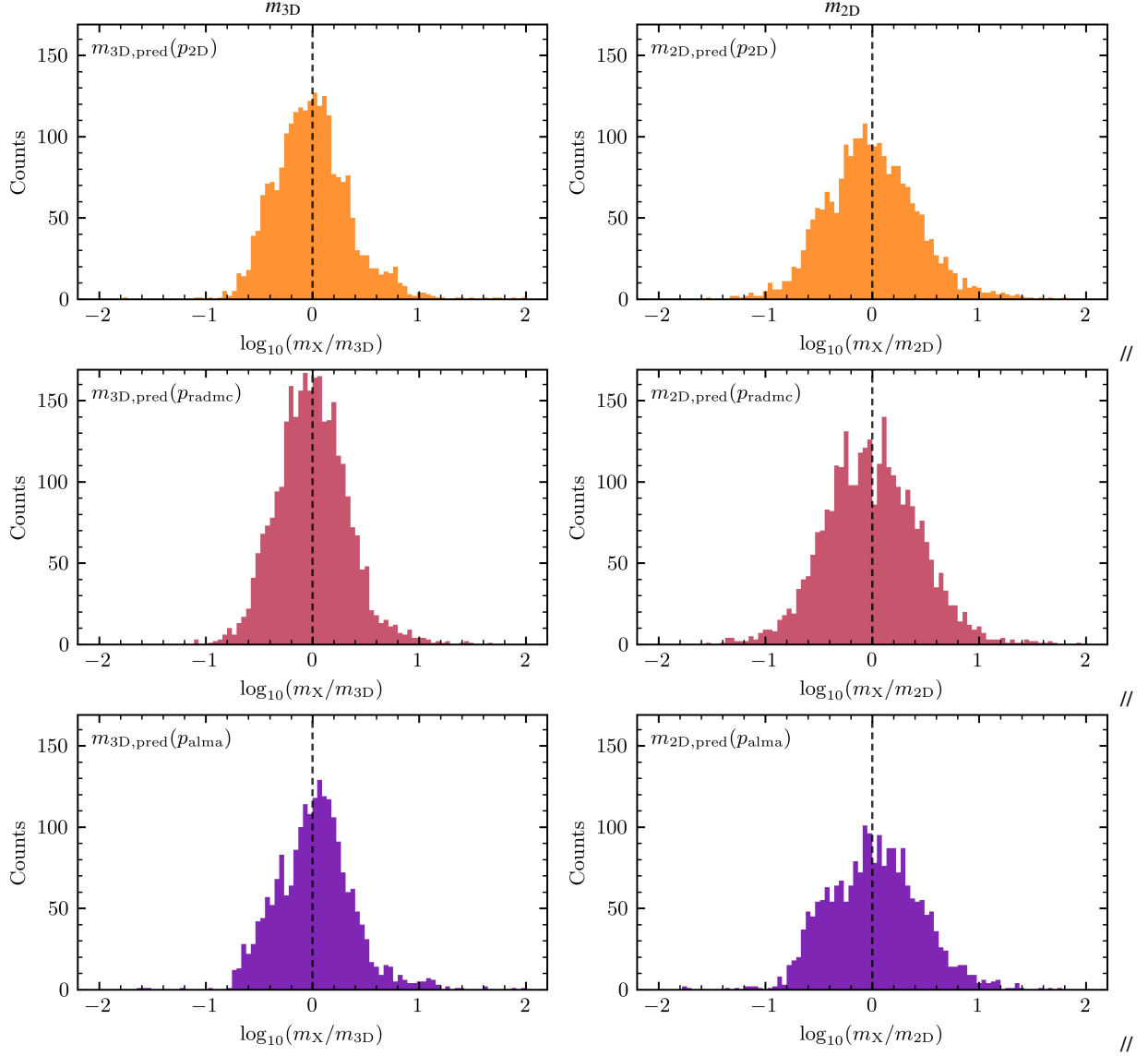


Fig. 9: Histograms of the logarithmic mass-prediction ratio, $\log_{10}(m_{\text{pred}}/m_{\text{true}})$, for m_{3D} (left) and m_{2D} (right). From top to bottom, m_X is inferred from p_{2D} , p_{radmc} , and p_{alma} . The dashed vertical line marks unity. Predicted masses m_{pred} are obtained by inverting Eqs. 5 - 10. The predicted masses cluster around unity, but show noticeable scatter.

izing radiation after ~ 240 kyr, and the slopes decrease and become highly variable. The restricted projected slopes p_{2D} stay close to constant, while the full sample shows a decrease as soon as ionizing radiation affects the dynamics of the clump. The global trend is consistent with the MMS analysis, indicating that for most core-envelope profiles, a single power-law approximation no longer provides a robust description of the radial density structure during feedback-dominated phases.

Furthermore, for the restricted sample, the ratio p_{3D}/p_{2D} follows an approximately linear trend during the early evolution (100–300 kyr) (see Fig. 10, right panel). Based on our simulation data, the intrinsic 3D slope, p_{3D} , can be estimated from the projected 2D slope, p_{2D} , via the time-dependent relation:

$$p_{3D} = (-6.4 \times 10^{-3} t + 4.4) \cdot p_{2D},$$

where t is measured in kyr.

Figure 11 investigates the extent to which the power-law slopes derived from the RADMC maps, p_{RADMC} , and the ALMA maps, p_{ALMA} , reproduce p_{2D} (left panel) and how they relate to the p_{3D} (right panel). We use the same sub-sample as in Fig. 10, requiring $R_{3D}^2 > 0.9$, $R_{2D}^2 > 0.9$, and $\dot{M}_{\text{sink}} > 0$ to enable a one-to-one comparison. The left panel shows p_X/p_{2D} (with $X \in \{\text{RADMC}, \text{ALMA}\}$). During the early evolution, p_{RADMC} is steeper than p_{2D} , but becomes flatter at later times. p_{ALMA} is systematically flatter than p_{2D} . Both ratios decrease with time. From the simulation, we fit the following relations between p_{2D} and p_{RADMC} and p_{ALMA} :

$$p_{2D} = \frac{p_{\text{RADMC}}}{-4.3 \cdot 10^{-3} t + 2.04}, \quad (11)$$

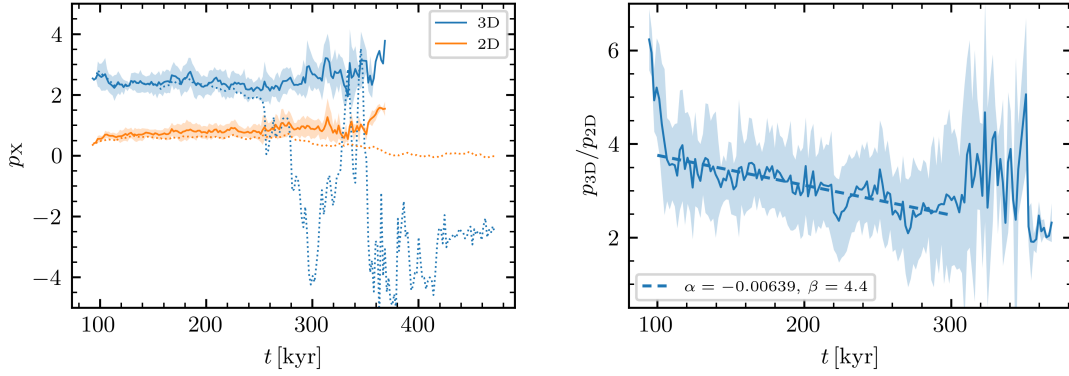


Fig. 10: Time evolution of the core-envelope power-law slopes of the spherical density profile, p_{3D} , and the projected column-density profile, p_{2D} (left), and of their ratio p_{3D}/p_{2D} (right). Thick curves show the restricted sample, requiring $R_{3D}^2 > 0.9$, $R_{2D}^2 > 0.9$, and ongoing accretion ($\dot{M}_{\text{sink}} > 0$); the dotted line in the left panel shows the unrestricted sample. In the right panel, the shaded region indicates the standard deviation about the median ratio, and the dashed line shows a linear fit to the median over 100 – 300 kyr, $p_{3D}/p_{2D} = \alpha t + \beta$. In the restricted sample, p_{3D} and p_{2D} remain nearly constant (with a slight rise in p_{3D} after ~ 300 kyr), while in the unrestricted sample p_{3D} becomes highly variable and p_{2D} declines slightly from ~ 240 kyr onward; the restricted ratio p_{3D}/p_{2D} stays roughly constant to ~ 300 kyr.

and

$$p_{2D} = \frac{p_{\text{ALMA}}}{-2.6 \cdot 10^{-3} t + 1.08}, \quad (12)$$

where t is given in kyr.

However, the ratios p_{RADMC}/p_{3D} and p_{ALMA}/p_{3D} remain almost constant, with only a slight decrease. (see Fig. 11, right panel). While p_{3D}/p_{2D} decreases with time, p_{RADMC}/p_{2D} and p_{ALMA}/p_{2D} decrease in a similar manner, so that these trends largely cancel in p_{RADMC}/p_{3D} and p_{ALMA}/p_{3D} , implying a nearly time-invariant offset between the intrinsic 3D slope and the RADMC-3D and ALMA estimates over this phase. However, p_{3D}/p_{RADMC} and especially p_{3D}/p_{ALMA} remain small, suggesting that p_{RADMC} and, in particular, p_{ALMA} cannot be robustly related to the intrinsic three-dimensional density structure, p_{3D} .

The time dependence in the estimation of p_{3D} poses a challenge because, observationally, the exact evolutionary time of a system is usually not known. However, Fig. 12 also shows that a direct comparison between p_{3D} and p_{2D} exhibits substantial scatter. This indicates that there is no simple one-to-one mapping between the intrinsic 3D density slope and the slope inferred from the projected column density, and that even in simulations, converting from 2D profile slopes to intrinsic 3D slopes is not following a simple rule. This is expected, since mass flow onto protostars is often highly non-spherical and time-dependent. Accretion can proceed along filaments and asymmetric streamers that feed the envelope and disk from preferred directions. For example, Pineda et al. (2020) report a $\sim 10,500$ au streamer feeding a young protostellar system. More generally, recent surveys indicate that streamer-like accretion may be common rather than exceptional (e.g. Valdivia-Mena et al. 2024). In addition, the larger-scale environment can be organized into networks of filaments and fibers that naturally guide gas toward star-forming clumps and cores and can imprint strong asymmetries on envelope structure (Hacar et al. 2018).

4.4. Summary of slope offsets

To summarize how the flux-based profile slopes relate to the numerical simulation profile slopes, we compare the distributions

of slope ratios for all profiles with $R^2 > 0.9$, $\dot{M}_{\text{sink}} > 0$, and $m_{3D} > 0.1 M_{\odot}$ (see Fig. 13).

In particular, we assess how well the flux-profile slopes inferred from the synthetic RADMC and ALMA maps recover the projected column-density slope by considering the ratio p_X/p_{2D} (see Fig. 13, left panel). The distributions show some scatter but only modest systematic offsets. p_{RADMC} is typically steeper than p_{2D} , with a median ratio of ≈ 1.4 , whereas p_{ALMA} is slightly flatter, with a median ratio of ≈ 0.8 .

Comparing the projected slopes to the underlying 3D density slope shows that p_{3D} is generally significantly larger than the corresponding 2D-based slopes (see Fig. 13, right panel). The median ratio in the numerical simulation is $p_{3D}/p_{2D} \approx 3.0$. For the flux-based profiles, the median offsets are $p_{3D}/p_{\text{RADMC}} \approx 2.1$ and $p_{3D}/p_{\text{ALMA}} \approx 3.4$, consistent with p_{RADMC} being systematically steeper and p_{ALMA} systematically flatter than p_{2D} . The p_{3D}/p_{ALMA} ratio, however, exhibits a particularly broad scatter about its median, suggesting that p_{ALMA} is a noisier proxy for the underlying 3D slope on a profile-by-profile basis. Part of this broadening may be driven by the comparatively flat ALMA slopes: when p_{ALMA} becomes small, the ratio p_{3D}/p_{ALMA} is amplified and can develop a high-value tail.

4.5. Different initial clump density profiles

It is not obvious whether core-envelope profiles are directly linked to the initial parent-clump density profile. Therefore, we compare the power-law slopes of the gas density profiles for two simulation runs, RFL9 and FLAT (see Fig. 14). The run RFL9 is initialized with a centrally concentrated clump, following a steep density profile of $\rho \propto r^{-2}$, whereas FLAT starts from an initially uniform-density clump. For each run, we measure the core density slopes p_X from both the spherical (3D) density profiles and the projected (2D) profiles. Even with the different initial clump density profiles, the resulting slope distributions and their median values are very similar for runs RFL9 and FLAT: in 3D the medians are 2.42 and 2.48, and in 2D they are 0.77 and 0.80. This indicates that once the global and local collapse proceeds and cores are formed, the local density structure in the core envi-

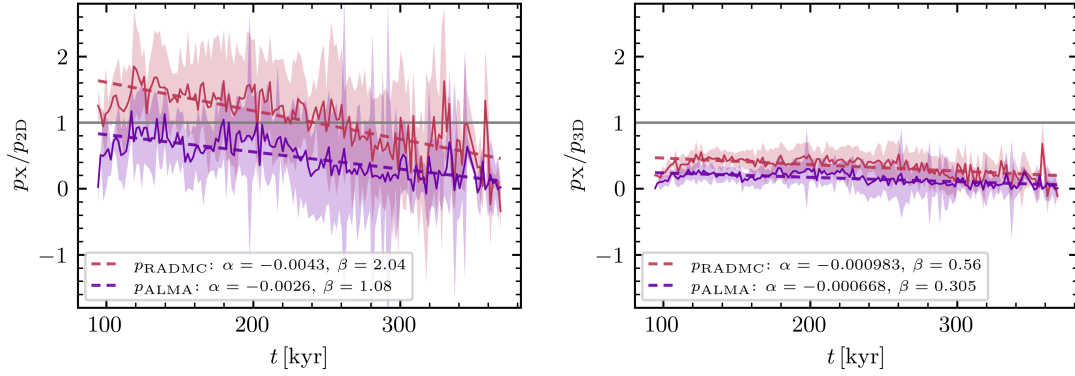


Fig. 11: Ratio of the RADMC-3D and ALMA slopes to p_{2D} (left) and to p_{3D} (right). All quantities are restricted to the same subset as in Fig. 10, requiring $R_{3D}^2 > 0.9$, $R_{2D}^2 > 0.9$, and ongoing accretion ($\dot{M}_{\text{sink}} > 0$). Dashed lines show a linear fit $p_X/p_{2D/3D} = \alpha t + \beta$. The horizontal line marks a ratio of unity. At early times the RADMC slopes are steeper than p_{2D} , but become flatter at later times, while the ALMA slopes are systematically flatter than p_{2D} . Both ratios show a decreasing trend with time. The ratio p_{RADMC}/p_{3D} and p_{ALMA}/p_{3D} are approximately constant.

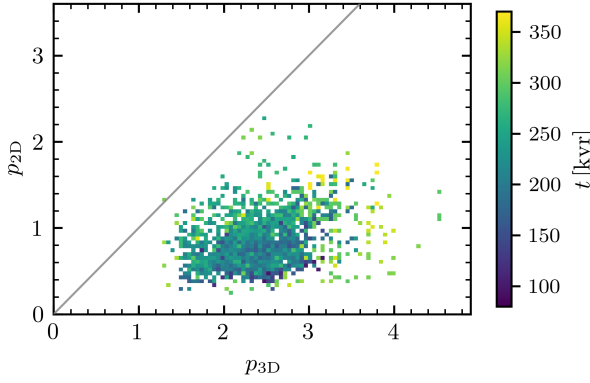


Fig. 12: Relation between the core-envelope power-law slope of the spherical density profile, p_{3D} , and the projected column-density slope, p_{2D} . Profiles are restricted to those with $R_{3D}^2 > 0.9$ and $R_{2D}^2 > 0.9$ and for which the corresponding sink is still accreting ($\dot{M}_{\text{sink}} > 0$). The gray line shows the unity relation. The broad scatter indicates that no simple one-to-one mapping between p_{3D} and p_{2D} can be established.

ronment becomes largely insensitive to the global initial density profile of the parent clump. Instead, the density profiles around cores are primarily regulated by fragmentation, the ongoing core collapse and accretion dynamics. Notably, we also do not find a strong imprint of the overall clump density profile in p_{2D} , even though the projection could, in principle, include additional LOS material from the surrounding clump and thus be more sensitive to the mass distribution in the parental clump than the 3D profiles.

4.6. Radial Profiles of the Dust Temperature

The time evolution of the dust temperature slopes shows much less variation than the corresponding density profile slopes (see Fig. 15). The relative stability of the temperature slope is expected because the temperature profile is primarily set by the central heating source. The dust temperature at a given radius is

mainly controlled by how the source luminosity is deposited and re-radiated through the envelope.

The spherical (3D) slope, q_{3D} , varies only moderately over time, remaining in the range $\sim 0.3 - 0.5$. Variations within this range likely reflect changes in the balance between internal heating (dominated by accretion luminosity onto the sink, which can vary rapidly) and the amount of material available to absorb and re-emit that radiation (i.e. optical depth and envelope geometry). During the early evolution ($t \lesssim 240$ kyr), the density-weighted projected (2D) slope, q_{2D} , is typically lower than q_{3D} , but the two become comparable at later times (Fig. 15, left).

Both slopes show a weak increase with sink mass, consistent with stronger internal heating for more massive, actively accreting objects; the trend is more pronounced in 2D because the density weighting and LOS integration emphasize the warm, dense central regions (Fig. 15, right).

Considering all cores in our restricted sample, the median slopes are $p_{3D} = 0.40$ and $p_{2D} = 0.34$ (Fig. 16). The small systematic offset between 3D and 2D is therefore consistent with projection effects, while the substantial overlap and similar scatter indicate that these effects do not qualitatively alter the inferred range of temperature slopes. The remaining dispersion likely reflects genuine core-to-core differences in evolutionary stage and accretion state.

4.7. Connecting intensity, temperature and density profile slopes

From observations, it is difficult to infer the three-dimensional structure of cores and their envelopes directly. What can be measured is the projected two-dimensional continuum emission. A common approach is therefore to relate the 3D density slope p_{3D} to the observed radial intensity slope m and an assumed or estimated temperature slope q (e.g. Adams 1991; Motte & André 2001). For optically thin dust emission and power-law profiles, one obtains

$$p_{X,3D} = m + 1 - q. \quad (13)$$

In our notation, m denotes the slope inferred from the synthetic observations, i.e. $m \in \{p_{\text{RADMC}}, p_{\text{ALMA}}\}$. This allows us to compute $p_{\text{RADMC},3D}$ and $p_{\text{ALMA},3D}$ and to compare them to the simulation value p_{3D} (Fig. 17).

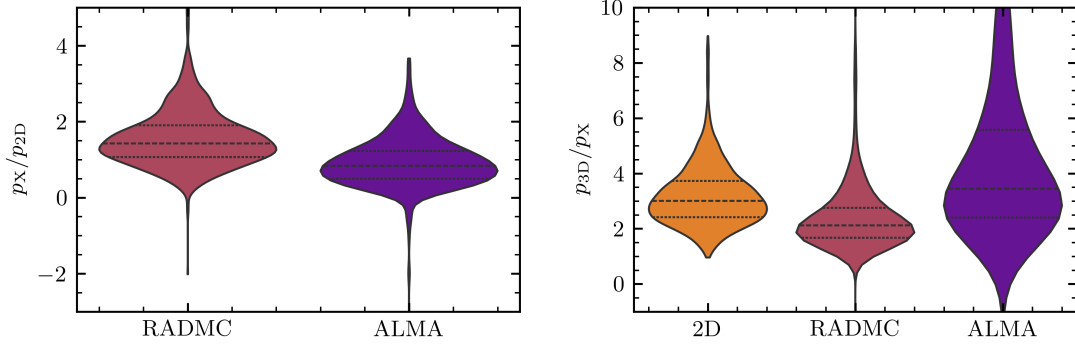


Fig. 13: Violin plots of slope ratios. Left: ratios of the flux-profile slopes to the projected column-density slope, p_X/p_{2D} , for RADMC and ALMA. Right: ratios of the 3D density slope to the projected slopes, p_{3D}/p_X , for p_{2D} , p_{RADMC} , and p_{ALMA} . The RADMC slopes are typically steeper than p_{2D} , with a median ratio $p_{RADMC}/p_{2D} \approx 1.4$, whereas the ALMA slopes are flatter, with $p_{ALMA}/p_{2D} \approx 0.8$. The median p_{3D}/p_X ratios are ≈ 3.0 for p_{2D} , ≈ 2.1 for p_{RADMC} , and ≈ 3.4 for p_{ALMA} , with the latter showing a particularly broad scatter.

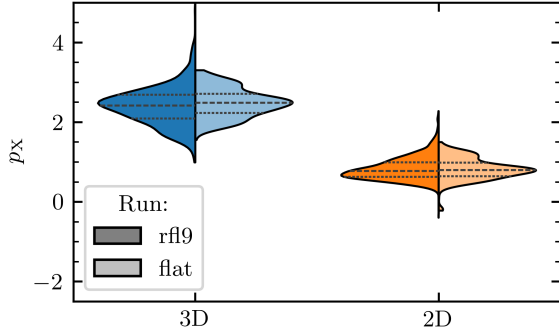


Fig. 14: Violin distributions of the fitted power-law slope p_X for the FLASH density profiles in runs RFL9, which has an initially clump density profile of $\rho \sim r^{-2}$ (dark shading), and FLAT, which has an initially flat clump density profile (light shading), shown for the spherical (3D) and projected (2D) profiles. Only fits with $R_X^2 \geq 0.9$ and $\dot{m}_{\text{sink}} > 0$ are included. The slopes in both runs are similar in 3D and 2D, suggesting that p_X is set primarily by internal collapse rather than by the global initial clump density profile.

We find that $p_{RADMC,3D}$ systematically underestimates p_{3D} , with a median ratio $p_{RADMC,3D}/p_{3D} = 0.73$. The bias is stronger for $p_{ALMA,3D}$, for which the median ratio is $p_{ALMA,3D}/p_{3D} = 0.48$.

5. Discussion

In the following, we discuss radial profiles and continue the convention that positive slope values correspond to quantities (e.g. p_{3D} and q_{3D}) that decrease with radius, while negative values correspond to quantities that increase with radius. Radial profiles have been investigated both in idealised models and in observational approaches. Two widely used idealised collapse solutions predict power-law density structures but differ in their collapse dynamics. In the inside-out collapse model of Shu (1977), an expansion wave propagates outward from the center. Inside the

expansion wave, the gas is collapsing with $\rho \propto r^{-3/2}$, whereas outside the wave the envelope remains close to the initial hydrostatic profile, $\rho \propto r^{-2}$. In contrast, the solution of Larson (1969) and Penston (1969) likewise yields $\rho \propto r^{-2}$ on large scales, but corresponds to a more dynamical, outside-in collapse with significantly higher infall velocities ($v \sim -3.3 c_s$). Both solutions assume idealized, spherically symmetric cores (typical for low-mass star formation).

A pressure-confined isothermal (starless) sphere (e.g. Bonnor-Ebert sphere) initially exhibits a flat inner region and approaches $\rho \propto r^{-2}$ only at larger radii. In the rigidly rotating Bonnor-Ebert models of Walch et al. (2009, 2010), a collapse wave propagates from the outside in, while the central density rises until protostar formation after approximately one free-fall time. In this picture, the outer envelope starts moving first, the infall region grows inward, and the flat inner region is compressed to progressively smaller radii as the central density increases, while the large-scale density profile remains close to $\rho \propto r^{-2}$.

Ward-Thompson et al. (1994) present 800 μm dust-continuum maps of starless cores showing centrally flattened profiles, with a shallower inner region and a steeper outer envelope. Similarly, Bacmann et al. (2000) (7 μm ISOCAM absorption) and Alves et al. (2001) (near-IR extinction of Barnard 68) derived centrally flattened column-density profiles consistent with pressure-confined Bonnor-Ebert-type structures. For the prestellar core IRAS16293E (Oph 464), Spezzano et al. (2025) used azimuthally averaged Herschel continuum profiles and a spherically symmetric radiative-transfer model to infer 3D radial profiles. Beyond a flat inner region of ~ 3000 au and out to $\sim 5 \times 10^4$ au, they find a volume-density profile $p_{3D} \approx 2.45$, which agrees to our findings of $p_{3D} \approx 2.4$. Note, however, that our fits are restricted to smaller radii (~ 5000 au). However, they also find a slightly increasing temperature with radius with a slope of $q_{3D} \approx -0.12$, possibly due to environmental feedback.

In the low-mass regime, Motte & André (2001) compared radial (sub-)mm continuum profiles of protostellar envelopes in isolated and clustered environments and found intensity profiles of $m \approx 0.4 - 1.8$, which are broadly consistent with our derived RADMC slopes with a median $p_{RADMC} = 1.1$. They convert to density gradients (in 3D) of $p_{3D} \approx 1.5 - 2.5$, (using Eq. 13 $q_{3D} = 0.4$) which overlaps with the distribution of our slope values. Shirley et al. (2000) presented SCUBA 450 and 850 μm maps of

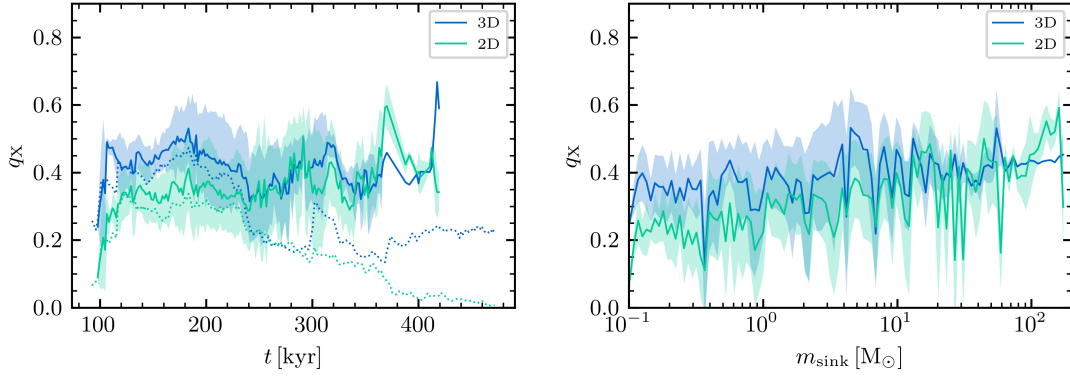


Fig. 15: Evolution of the dust-temperature profile slopes for the spherical (3D) and density-weighted projected (2D) profiles as a function of time (left) and sink mass (right). Profiles with $R^2 \geq 0.9$ and $\dot{m}_{\text{sink}} > 0$ are shown with thick lines, while dotted lines indicate the full, unrestricted sample. The 3D slope q_{3D} varies over time, typically spanning $\sim 0.3 - 0.5$, whereas the 2D slope q_{2D} shows a modest increase with time. Both slopes increase slightly with sink mass, with the trend being somewhat steeper for q_{2D} than for q_{3D} .

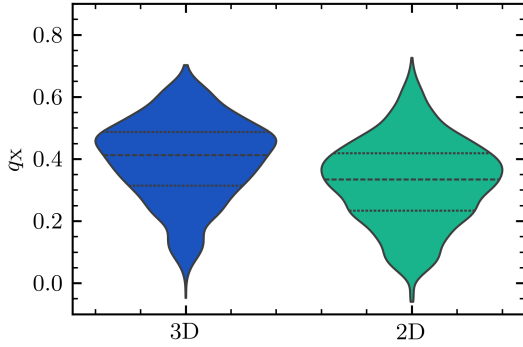


Fig. 16: Violin plots of the dust temperature profile slopes for the spherical (3D) and density-weighted projected (2D) profiles. Only profiles with $R^2 \geq 0.9$ and $\dot{m}_{\text{sink}} > 0$ are included. The median slopes are $q_{3D} \approx 0.40$ and $q_{2D} \approx 0.34$.

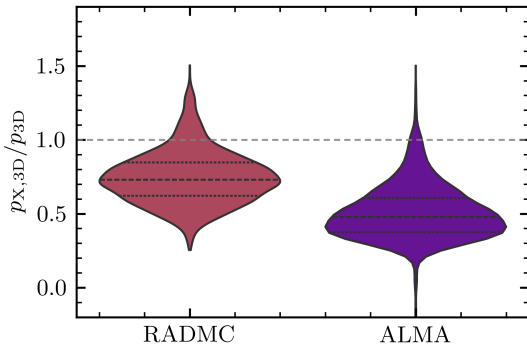


Fig. 17: Violin plot of the normalized 3D density slopes inferred from synthetic observations using Eq. 13. The underlying 3D simulation slope p_{3D} is underestimated, with median ratios $p_{\text{RADMC},3D}/p_{3D} = 0.73$ and $p_{\text{ALMA},3D}/p_{3D} = 0.48$.

Class 0/I protostellar cores and estimate intensity profiles of $m \approx 1.44$ and 1.52 , assuming a temperature profile slope of $q_{3D} \approx 0.4$ which results in density power-law slopes of $p_{3D} \sim 2.1$. Their intensity slopes lie in the upper range of our p_{RADMC} distribution while the density slope is slightly lower than our median value of $p_{3D} \approx 2.4$. Chandler & Richer (2000) used high dynamic-range SCUBA continuum imaging of Taurus and Perseus protostars and found density exponents of $q_{3D} \approx 1.5 - 2$ (using Eq. 13 and assuming $q_{3D} \approx 0.33 - 0.4$). This lies again the lower end of our distribution.

In the high-mass regime, sub-mm studies of envelopes around ultracompact H II regions and hot cores found comparatively shallow density gradients, with $p_{3D} \approx 1.0 - 1.5$, which is the other direction we found. van der Tak et al. (2000) modeled 14 massive YSO envelopes using (sub-)mm continuum and line data, and obtained density profile slopes of $p_{3D} \approx 1.0 - 1.5$ assuming $q_{3D} = 0.4$. They also discuss two hot cores, which indicates that feedback is already present, with a density slope of $p_{3D} \approx 2$. Although the main profile slopes are generally lower, this still support our results that feedback-driven density profiles may be steeper.

Hatchell et al. (2000) analyzed SCUBA 450/850 μm profiles of five ultracompact H II regions and found that the envelopes are best reproduced by $p_{3D} \approx 1.5$. On the other hand, Gieser et al. (2021) inferred an average density power-law index of $p_{3D} \approx 2.0 \pm 0.2$ from the 1.37 mm dust-continuum visibilities, and an average temperature power-law index of $q_{3D} \approx 0.4 \pm 0.1$ by fitting line emissions.

Beuther et al. (2002) reports 1.2 mm dust-continuum observations of 69 massive star-forming regions in very early evolutionary stages, before the development of an UCH II region. They found a mean inner intensity slope of $m \approx 1.2$, which they translate (with Eq. 13 with correction terms and $q = 0.4$) into a volume-density index $p_{3D} \approx 1.6 + 0.5$. They claim that the inferred density structure is broadly comparable to that of low-mass protostellar envelopes.

Observers commonly use Eq. 13 to convert the measured radial intensity slope into an estimate of the 3D density slope. For the temperature term, it is often assumed that the dust temperature follows a power law with slope $q_{3D} \approx 0.4$, which perfectly matches the 3D median temperature-profile slopes in our sample.

The median value of our 3D power-law slopes is $p_{3D} \approx 2.4$. Therefore, our profiles are somewhat steeper than the idealised analytic cases and are on the steep end of the range reported observationally. However, we also saw that using Eq. 13 might underestimate the profile slopes by a factor between ~ 0.5 – 0.75 . We also find a flattened inner region similar to observations. However, because the inner ~ 1000 au around a sink corresponds to the accretion region, this feature should be interpreted with caution. Interestingly, we find the steepest slopes in cores hosting the most massive sinks, whereas observations often suggest that more evolved, feedback-processed envelopes tend to exhibit shallower profiles. At the same time, we find that the inner region flattens while the outer envelope steepens, suggesting that the inferred slope depends on the radial range over which the profile is measured. This indicates that a single power-law index may not capture all features of the radial structure and should therefore be interpreted with care.

6. Conclusions

We have quantified sink-centred radial density and dust-temperature profiles in a radiation-hydrodynamic simulation of massive star formation and the corresponding synthetic RADMC-3D and ALMA-like observations. We have connected the intrinsic three-dimensional envelope structure to projected, continuum-based diagnostics inferred from the synthetic observations. Using a consistent profile-extraction and fitting procedure, we characterised profiles with power-law slopes, fit quality (R^2), and deviations from a single power law via an inner-to-outer slope ratio.

We find that the usefulness of a single power-law description depends on the evolutionary state of the core. For actively accreting sinks with good fits, the inferred slopes are relatively stable around $p_{3D} \approx 2.4$ and provide a compact summary of the envelope structure. As accretion declines and feedback reshapes the envelope, the slopes become more variable, fit quality decreases, and a single power law often fits poorly. Nevertheless, a single exponent cannot capture all profile features, but it remains a useful summary statistic.

Across the core population, intrinsic spherical density slopes, p_{3D} , are typically ~ 3 times steeper than projected column-density slopes, p_{2D} , and their relation shows broad scatter, indicating real object-to-object variation due to projection and non-spherical substructure. Slopes inferred from synthetic continuum profiles are systematically offset from p_{2D} : RADMC-3D intensity profiles are typically steeper, whereas ALMA-like slopes are systematically flatter and show the largest scatter, consistent with beam convolution and interferometric filtering.

In our simulation, we derive empirical relations linking fitted slopes from projected column-density profiles and synthetic RADMC-3D and ALMA-like maps to both projected and spherical core masses, m_{2D} and m_{3D} . Although these relations exhibit intrinsic scatter, they indicate that the radial shape of projected and continuum profiles carries statistical information about a cores' mass.

We find systematic differences between massive ($> 8 M_{\odot}$) and lower-mass sinks. Massive sinks tend to exhibit broader distributions of both, the profile slopes and the inner-to-outer slope ratios, indicating more heterogeneous envelope structures in the high-mass regime. On average, fitted slopes are steeper for massive sinks (with a median value of ≈ 2.5), while the inner-to-outer slope ratio decreases, suggesting a relative flattening of the inner profile together with a steeper outer decline. This signature is more pronounced in the projected diagnostics than in

the intrinsic 3D profiles, consistent with projection amplifying the impact of non-spherical structure, nearby companions, and feedback-shaped cavities.

Comparisons between simulations with different initial clump density profiles (flat and $\rho \propto r^{-2}$) show that the local density structure in the core environment is primarily determined by local conditions and is largely insensitive to the global initial density profile of the parent clump.

The dust temperature around cores exhibits a stable, non-isothermal radial gradient with a median slope of $q_{3D} = 0.40$, primarily set by local core evolution and heating, while projection effects introduce only a small systematic flattening ($q_{2D} = 0.34$).

Overall, radial profile slopes provide compact descriptors of envelope structure, but their interpretation depends on projection and observational response. Also, the slopes become less robust in feedback-dominated phases. The controlled comparison between intrinsic profiles, projected profiles, and synthetic continuum diagnostics presented here provides a basis for interpreting observed radial slopes statistically and for assessing the biases and scatter introduced by radiative transfer and interferometric imaging.

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CONCLUSIONS AND OUTLOOK

10.1

SUMMARY

This work investigates the signatures of high-mass star-forming regions using simulations and synthetic observations, exploring how different conditions affect the collapse of a high-mass star-forming clump and how well the resulting signatures can be recovered from synthetic ALMA-like (sub-)mm continuum maps.

Paper I In the first paper we follow the collapse of an isolated, turbulent massive star-forming clump with mass $M = 1000 M_{\odot}$ and radius $R = 1$ pc. We include a novel scheme for radiative transfer of ionizing radiation, including radiation pressure from ionizing photons, as well as heating by non-ionizing radiation. The gas, dust, and radiation temperatures are calculated self-consistently. We investigate the early evolution of the collapse until star formation is mostly completed and (ultracompact) H II regions are established. We focus on the effects of ionizing radiation and its radiation pressure on fragmentation and the star-formation efficiency (SFE) of the clump. We find that ionizing feedback limits further growth of forming stars by shutting off accretion, while radiation pressure from ionizing photons supports the expansion of H II regions. We also find that the outcome depends on numerical resolution. Higher resolution forms more sinks in denser gas, which traps ionizing radiation for longer and can lead to a higher SFE. Finally, we investigate the impact of the clump's initial conditions by varying the density profile from steep to flat (with power-law index of 2, 1.5, and a flat profile), the metallicity from solar to $0.5 Z_{\odot}$ and $2 Z_{\odot}$, and the virial parameter ($\alpha_{\text{vir}} = 0.2, 0.6$, and 1.2), and we discuss the resulting differences in fragmentation and SFE, which span roughly $\sim 35\%$ – 57% across the explored parameter space.

Paper II We post-process the simulations from Paper I with radiative transfer (RADMC-3D) and interferometric imaging (CASA), adopting observing and imaging conditions consistent with the ALMAGAL studies, to generate synthetic 1.36 mm dust continuum maps. We define cores around sink particles using a fixed physical radius of 1500 au, enabling a direct one-to-one comparison between intrinsic 3D simulation properties, idealised dust emission, and synthetic ALMA-like observations. With this setup, we quantify how reliably dense-core masses and dust temperatures can be inferred from (sub-)mm continuum observations of high-mass star-forming clumps. We find that the intrinsic simulation resolution (e.g. 400 au versus 50 au) still affects how sharp and well separated structures appear, despite the coarser effective ALMA beam (~ 1200 au). We derive an empirical scaling that predicts sink (stellar) mass from the projected core mass, although the inferred stellar masses remain uncertain. Foreground and background material cause projected (2D) core masses to exceed spherically enclosed (3D) masses by factors of ~ 2 – 3 . We test three dust-temperature estimators: a clump-scale L/M prescription, an improved $L/M + \text{flux}$

model, and a supervised machine-learning approach, which progressively improve the reconstruction of the true core dust temperatures and thereby reduce the associated mass-estimation biases, especially for higher-mass cores. Interferometric flux reconstruction in the synthetic ALMA images can deviate from the idealised RADMC-3D case and bias the mass estimate. Temperature and flux-reconstruction uncertainties together yields typical ALMA continuum core-mass uncertainties of a factor ~ 3 –5. We found a minimum reliable core mass of $\gtrsim 0.3 M_{\odot}$. Finally, we provide simulation-calibrated quantitative “observer guidelines” for interpreting ALMA-like core catalogues.

Paper III We use the simulations and synthetic RADMC-3D and ALMA maps from Paper II to derive sink-centred radial profiles of the gas density and dust temperature from the simulation, as well as continuum-intensity profiles from the synthetic observation maps. For each core we extract median profiles in a radial range of $r = 800$ –5000 au (for three lines of sight in 2D) and fit power laws, $y(r) \propto r^{-p}$, in log–log space. We characterise the resulting slopes, the goodness-of-fit (R^2), and deviations from a single power law via a broken inner/outer fit and the inner-to-outer slope ratio $s = p_{\text{inner}}/p_{\text{outer}}$. We find that a single power law describes the radial profiles mainly during phases of active accretion (high R^2), while slopes become time-variable and R^2 decreases during accretion halts and feedback-dominated phases. Intrinsic spherical density slopes are systematically steeper than projected column-density slopes, with a typical ratio $p_{3D}/p_{2D} \simeq 3$. Slopes inferred from synthetic continuum profiles show systematic offsets: p_{RADMC} is typically steeper than p_{2D} , whereas p_{ALMA} is flatter and exhibits the largest scatter. Massive sinks ($\gtrsim 8 M_{\odot}$) tend to show steeper slopes but lower inner-to-outer slope ratios s than lower-mass sinks. The slope distributions are similar for simulations with different initial clump density profiles. Dust-temperature profiles are comparatively stable, with a median slope of ~ 0.4 .

10.2

CONCLUSIONS

In our simulations, turbulent clump collapse forms a cluster of sinks but is typically dominated by the most massive sink (MMS). The MMS can remain deeply embedded such that its ionising photons are initially trapped while accretion continues, whereas massive sinks in lower-density gas launch the first expanding H II regions. Once MMS feedback breaks out, it rapidly disperses the parent cloud. Ionising radiation is the primary mechanism terminating accretion and setting final stellar masses, while radiation pressure enhances H II region expansion. Early non-ionising heating suppresses fragmentation and sets the sink multiplicity.

Fragmentation remains resolution-dependent until the isothermal-to-adiabatic transition density is resolved. Higher resolution produces more low-mass sinks, reaches higher densities (and hence higher dust temperatures), and thus prolongs the MMS trapped-feedback phase, which allows additional accretion, increasing the total SFE. Clump initial conditions further affect the fragmentation and SFE.

Varying the initial density profile, virial parameter, and metallicity changes the collapse speed and fragmentation outcome. Flatter profiles collapse more slowly yet produce more sinks and higher SFE; low virial parameters yield fewer, more massive sinks with stronger ionising output that lowers the SFE; high virial parameters delay collapse, enhance substructure, and slightly increase the SFE. Metallicity regulates

dust cooling and fragmentation: lower metallicity suppresses fragmentation and, once feedback is included, decreases the SFE. Overall, the SFE is highly sensitive to how long massive stars remain deeply embedded and whether compact H II regions are delayed; faster collapse does not necessarily imply higher SFE once radiative feedback becomes dynamically dominant.

We construct ALMA-like synthetic dust-continuum maps and compare the resulting dense-core properties with those in the simulations. Even without instrumental effects, projection introduces a substantial and largely resolution-independent bias: projected core masses exceed intrinsic spherical masses by factors of ~ 2 – 3 due to line-of-sight contamination and non-spherical structure. The main observational uncertainties arise from both the dust-temperature estimate and interferometric imaging. The clump-scale L/M temperature prescriptions reproduce global trends but fail to capture the large core-to-core scatter, leading to mass errors of several. Including local continuum information improves temperature estimates, and supervised machine-learning models trained on the simulations perform best among the tested approaches, making them the most promising avenue for future work. Interferometric flux loss and spatial filtering add comparable uncertainty, with mass errors up to factors of ~ 3 . Combined, these effects imply typical uncertainties of ~ 3 – 5 in individual ALMA continuum core masses (and up to ~ 10 in extreme cases). The synthetic observations capture the global evolution of the clump and its cores, although individual core masses can still be uncertain by factors of a few.

Finally, radial-profile power-law indices are useful for statistical studies of core envelopes, even though a single number cannot capture the full complexity. Slopes are most informative during active accretion, but become less robust in feedback-dominated phases as envelopes develop complex structures. Intrinsic 3D density slopes are systematically steeper (by a factor of ~ 3) than projected slopes. Cores hosting massive stars tend to show flatter inner profiles and steeper outer slopes. Overall, radial envelope profiles are set primarily by local conditions rather than the initial clump structure. The inferred 3D density slopes (~ 2.4) are somewhat steeper than typically reported in the literature and observations. However, converting observed intensity profiles into 3D density slopes typically relies on simplifying assumptions and can introduce biases of ~ 0.5 – 0.75 , bringing our values into closer agreement. However, the dust-temperature slope (~ 0.4) is consistent with literature values and with the values commonly adopted in observational analyses.

10.3

OUTLOOK

The data produced within this thesis opens up a wide range of follow-up possibilities, and the simulations are already being used in several ongoing projects by other scientists. A sub-grid model for sink particles is under development to include binaries and higher-order multiplicity, with the goal of capturing the relevant small-scale physics and reduce the limitations due to finite numerical resolution. In parallel, tracer particles are being analysed to quantify mass flow, identify dominant accretion channels, and characterise the role of filamentary structures in feeding forming stars. Building on this, a complementary chemistry project combines tracer-particle histories with astrochemical modelling to follow the evolving composition of accreted gas and translate it into synthetic molecular signatures that can be compared directly to observations.

In the future, several natural extensions of this work are possible. On the

catalogue level, dendrogram-based source extraction, and algorithms such as CuTex used in [Coletta et al. \(2025\)](#), can be applied to the synthetic maps to compare observationally identified cores to sink-centred cores in the simulations, and to assess which structures in ALMAGAL-like observations are classified as cores. In addition, machine-learning approaches can be developed further for improved dust-temperature estimation and thus more accurate continuum-based core masses.

Beyond dust continuum, the synthetic-observation framework can be extended to radio continuum emission to trace H II regions and to radiative transfer of spectral lines to add molecular and kinematic constraints. Such kinematic information is particularly promising for constraining core structure and could help reconstruct three-dimensional core properties from two-dimensional observational data using simulation-calibrated machine-learning models.

Finally, we can explore image-reconstruction approaches that connect simulations and synthetic observations in both directions using methods similar to [Ho et al. \(2020\)](#). As a first step, we will use simple Gaussian beam matching to bring simulation and synthetic maps to a common angular resolution for controlled comparisons. As a next step, we will test a learning-based reconstruction that is trained to invert progressive spatial filtering and to recover plausible small-scale structure beyond the interferometric beam. We will then move to full CASA-based forward modelling and inverse reconstruction. The goal is to recover higher-resolution physical information that is otherwise lost in interferometric imaging.

Future work should not be limited to the current simulation setup and resolution. A natural next step is to pursue improvements along two complementary directions: (i) adding missing physical processes that may shape massive-star formation, and (ii) increasing numerical efficiency and effective resolution where it matters most.

On the physics side, including protostellar outflows would be particularly valuable, as they can regulate accretion and clear the inner envelope. For more evolved massive objects, stellar winds should also be added and studied together with ionizing radiation to capture their combined impact on the surrounding gas. Finally, magnetic fields should be included. Even in ideal MHD, magnetic support and magnetic braking can change the fragmentation behaviour and the global star-formation efficiency. These processes are already implemented in FLASH. Instead of relying on a simple dust-opacity prescription, one could train a model to predict a small set of dust-population parameters (or a discrete “dust state”, e.g. bare grains, ice mantles, or grain growth). The simulation would then obtain the frequency-dependent opacity from a precomputed table, $\kappa_\nu(T, \rho, \text{state})$. This hybrid approach could keep the simulation numerically stable while ensuring that the opacities remain physically plausible.

On the numerical and technical side, porting computationally expensive parts of the workflow from CPU, as we use it for FLASH, to GPU could substantially reduce runtime. Adaptive time stepping with for example independently evolving mesh patches (as implemented, for example, in the DISPATCH code ([Nordlund et al., 2018](#))) could further improve efficiency by matching the time step to the local dynamical state. Finally, the effective resolution near sinks could be improved by combining different grid structures: while Cartesian AMR is well suited for the global cloud, spherical or nested grids are often advantageous for discs and inner envelopes as used in e.g. [Oliva & Kuiper \(2020\)](#). Implementing such multi-geometry gridding would allow smaller physical scales to be resolved and would improve the modelling of disc and accretion physics around forming stars. However, these improvements are not feasible within FLASH and would require moving to a new

code base.

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DATA AVAILABILITY

The data underlying this thesis will be shared on reasonable request to the author.

USE OF AI TOOLS

An AI-based tool (ChatGPT 5) was used in the preparation of this dissertation only for limited, supportive purposes (e.g. language polishing). All scientific content, including the analysis, interpretation, conclusions, and the selection and verification of sources, was produced and checked by the author.