PhD Thesis Proposal:
The Chemical and Physical Evolution of Protostellar Discs

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Star and planet formation are intimately entwined, and it is difficult to consider one without its implications for the other. In my PhD project I will simulate the formation of a protostellar disc and its associated chemical and physical evolution to investigate the implications this has for planet formation. Meteoritic evidence (such as high temperature inclusions) suggests certain temperature and density processing histories throughout the Sun's protostellar disc, however such environments are not typically found in observations or simulations of other discs. By simulating the collapse of a cloud into a star and disc, and tracing the path of gas throughout the disc, I hope to investigate the environments associated with the earliest stages of star and planet formation, and how these correspond to the processing of material found in meteorites. Comparing the results of my simulations to what is observed and found in meteoritic data will improve our understanding of how the early stages of star and planet formation are linked.

1 Background on Star and Planet Formation

In the past few decades over 3000 exoplanets have been discovered (Han et al., 2014). Some of these exoplanetary systems have vastly different architectures to that of our own solar system (e.g. hot Jupiters), and theories of planet formation must be capable of describing these differences. Planets are typically thought to form while stars are forming, and thus regions of active star formation are often observed with the aim of capturing planets at various stages of formation. Observations of planets at their earliest formation stages can give an indication of how, when and where they are forming.

Stars form in molecular clouds, which are cool clouds of dust and gas. When a region of the cloud is cool and dense enough, it may collapse to form a star, or cluster of stars (e.g. Krumholz, 2017). The first object to form when a cloud collapses is the first hydrostatic core, and is followed by the protostar phase (Larson, 1969; Dunham et al., 2014). Once the core accretes enough material, it collapses again to create the second hydrostatic core, known as a protostar (Dunham et al., 2014).

As a cloud collapses to form a star, a disc of dust and gas, called a protoplanetary disc will form around that star. As the name suggests, protoplanetary discs are where planets form, so young stars with discs are typically observed to better understand both star and planet formation.

There are two main theories for giant planet formation: core accretion and gravitational instability. Depending on where and when a planet forms in a disc, one of the processes is more likely. In the core accretion model, a rocky or icy planetary core forms and reaches a critical mass to start accreting gas (e.g. Pollack et al., 1996; Kley and Nelson, 2012). However, if a planet forms through disc fragmentation due to gravitational instability, regions of the disc break up and collapse to form planets (e.g. Boss, 1997; Kley and Nelson, 2012). Core accretion is more likely for planets in the inner regions of the disc (within $\sim 5\,\mathrm{AU}$) and gravitational instability is more likely for planets forming in the outer part of the disc ($R \gtrsim 50\,\mathrm{AU}$ Kley and Nelson, 2012). This is discussed in more detail below.

We have physical evidence from the formation of our own solar system in the form of meteorites and small grains of material. Using the chemical and petrological evidence provided by primitive meteorites and primitive dust grains, we can gain understanding of some of the physical and chemical environments that must have been experienced in the Sun's protoplanetary disc (e.g. Nittler and Ciesla, 2016). What this can tell us about the early stages of star and planet formation is discussed below.

1.1 Stages of Star Formation

As a cloud collapses into a star there are several distinct evolutionary stages which can be observed, and these are the Classes of star formation, as described by Lada (1987) and Barsony (1994). The observational Classes are linked to Stages, as the observations can be affected by reddening towards the star forming region (due to obscuration by dust), the inclination of the collapsing star, and other observational contaminants (Dunham et al., 2014). For this discussion, I assume that the Stages and Classes are aligned, so that the physical description of what occurs at each Stage is equivalent to what is observed in each Class.

An evolutionary sequence of a young stellar object (YSO), is shown in Figure 1, showing a schematic for the observed Class and evolutionary Stage . The left shows the spectral energy distribution (SED) of the objects for the Classes, and the right shows the inferred evolutionary Stage. A timeline is also included in Figure 1 to indicate the length of each evolutionary stage, and the ages these objects may be expected to have when they are observed.

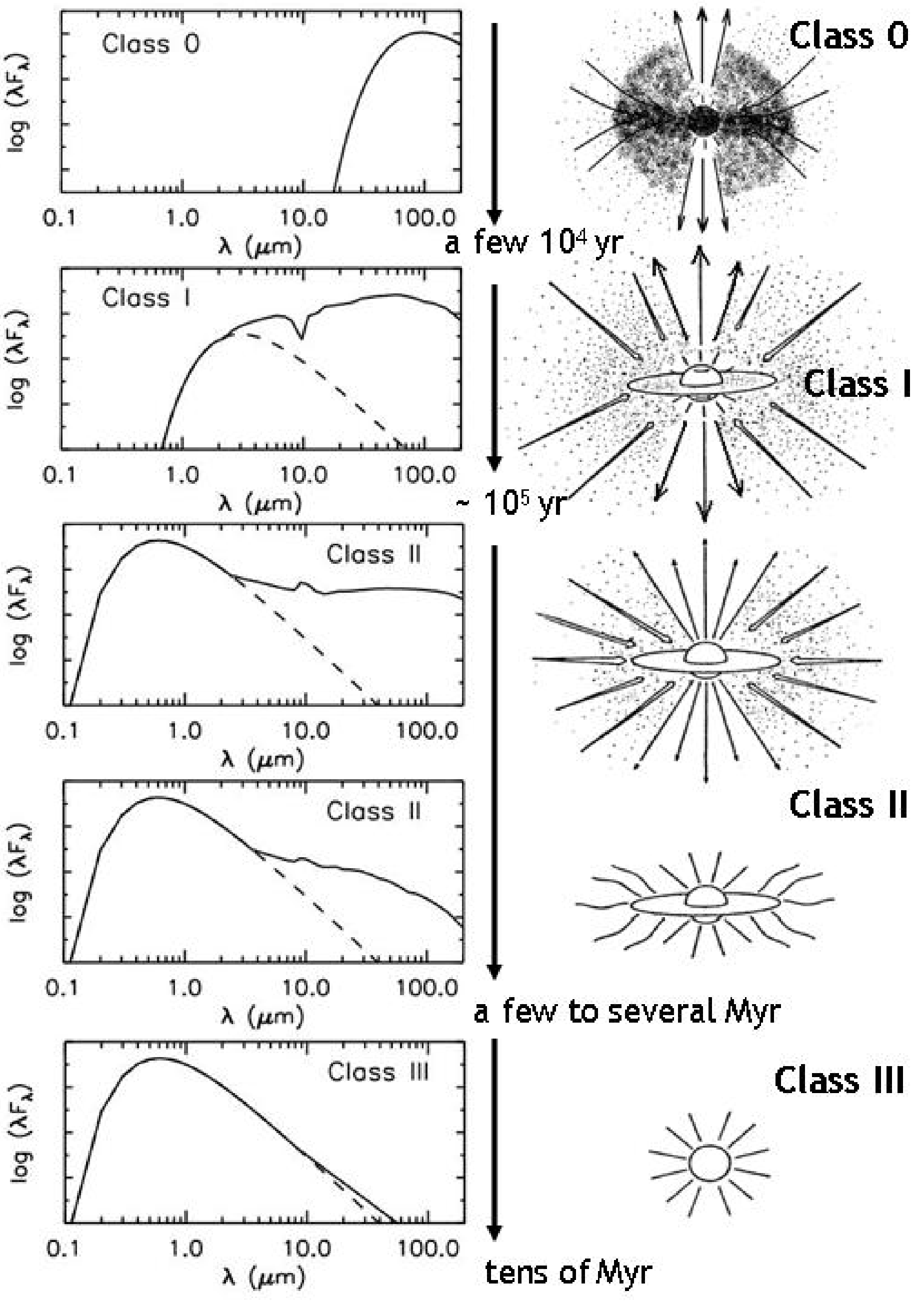
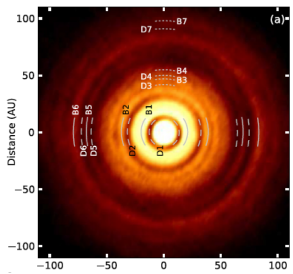


Figure 1: Evolution of protostars and their SEDs through the Lada (1987) classes. Image credit Furlan (2013), where it was adapted from Wilking (1989) and Shu et al. (1987).

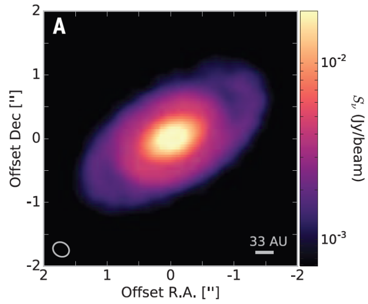
At Class 0, a cloud is still collapsing and the protostar has not yet formed and is still heavily embedded in the protostellar envelope. This corresponds to the first hydrostatic core as the cloud collapses (Dunham et al., 2014). The SED of a Class 0 object is simply black body spectrum peaking at cooler sub-mm wavelengths (Barsony, 1994; Dunham et al., 2014). There are a small number of these objects that have been observed, for example a recent paper found that the isolated dark cloud BHR7 has a heavily embedded Class 0 protostar, which was found using multiwavelength observations (Tobin et al., 2018).

In a Class I object, the protostar is still heavily embedded in the envelope and material is still falling onto it, but might have jets, and a disc may be observed. A Stage I object has a protostar, as the second hydrostatic collapse has occurred (Dunham et al., 2014). Class I objects have a rising mid infrared (IR) excess, meaning there is much more flux in the mid infrared than would be expected from the blackbody of the star (Lada, 1987; Dunham et al., 2014). This is the stage upon which much of this work will focus.

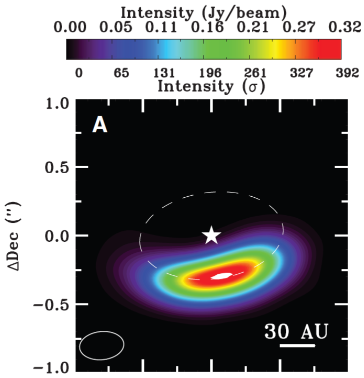
Class II objects have a flat to declining mid IR excess, and have discs that are observable. At this point the Stages easily match up to the Classes, so a Stage II object is one with a prominent disc (Dunham et al., 2014). The star may be heavily embedded in the disc, but the object is typically no longer embedded in the protostellar envelope. These objects are generally the target for planet formation studies, as they can have structures in their dust and gas distributions that could be indications of planet formation (e.g. van der Marel et al., 2013; ALMA Partnership et al., 2015; Pérez et al., 2016). These structures include gaps, rings, asymmetries and spiral arms, all of which are shown in Figure 2.



(a) Ringed structure of HL Tau. Image credit ALMA Partnership et al. (2015).



(b) Sprial structure of Elia 2-27. Image credit Pérez et al. (2016).



(c) Asymmetric dust distribution of Oph IRS 48. The mm sized dust grains are concentrated on one side of the disc, causing an asymmetry in the distribution of this dust at 60 AU. Image credit van der Marel et al. (2013).

Figure 2: Various disc structures discovered recently with ALMA. All features may be signs of planet formation.

A notable protostar which is between Class I and II is HL Tau. The disc of HL Tau, as observed with ALMA, has rings in its dust distribution which have possibly been carved by planets or the interaction of a planet with the disc (ALMA Partnership et al., 2015; Dipierro et al., 2015; Testi et al., 2015). HL Tau is still somewhat embedded in its infalling envelope, making it difficult to observe at optical wavelengths, and leading to its classification as still being partially a Class I object (ALMA Partnership et al., 2015). The deprojected image of the rings in the HL Tau disc are shown in Figure 2a.

Class III objects have a mostly cleared disc, and as such have very little mid IR excess. A Stage III object is still a pre-main-sequence star, but is close to being evolved (Dunham et al., 2014). Structure in these discs can be an indication of planets that have already formed and are shepherding the remaining material into rings (e.g. Thilliez and Maddison, 2016). It is thought that most planets will be formed by this stage, and that the disc is mostly evolved.

1.2 Planet Formation

Planets form in the discs of dust and gas around young stars known as protoplanetary discs. Specifically they grow from dust grains to pebbles, boulders, planetesimals, protoplanets and eventually planets. For terrestrial planets the story can stop there, but for giant planets there are other formation stages and scenarios that are important, such as whether they continue to grow by core accretion or through disc fragmentation due to gravitational instability.

Growth from dust grains to planets runs into several barriers, which need to be overcome for the continued growth of the planet. At first the grains grow by sticking to each other with van der Waals forces or through collisional impacts. However once they reach a certain size (mm-cm), they are more likely to bounce off each other than they are to collide and grow. This is known as the bouncing barrier (Güttler et al., 2010; Blum, 2018). There are several ideas for how to overcome this barrier, and it is still a very active field of study (e.g. Booth et al., 2017). One is that the dust grains have icy mantles, or are at least partially icy, as this can increase adhesion (Blum, 2018). Another is that they collapse together due to self gravity, because of the streaming instability (Blum, 2018).

The next barrier on the road to planet formation is known as the metre-barrier. This occurs when an object is too large ($\sim 1\,\mathrm{m}$, depending on distance from star) to remain easily coupled to the gas, which is moving at a Keplerian velocity, and so becomes sub-Keplerian and has radial drift towards the star (Testi et al., 2014). Objects this size are also likely to fragment if they collide, rather than continuing to grow (Zsom et al., 2010). If the objects survive long enough to sweep up smaller dust grains, or to become concentrated in a dust trap, they may grow to larger sizes (Zsom et al., 2010; van der Marel et al., 2013).

Once the planetesimals are large enough ($\sim 1\,\mathrm{km}$), pebbles and boulders will preferentially stick to them because the gravitational field of the larger body attracts the smaller particles. Growth will continue and eventually they will become spherical under their own gravity, and then possibly become geologically differentiated (this means that the silicates will float to the surface with iron and other dense metals sinking into the core).

Once a planetesimal reaches a certain mass, it is able to accrete gas, and become a giant planet. This is the core accretion model for giant planet formation (Pollack et al., 1996; Kley and Nelson, 2012). In this scenario, a protoplanet, which is a rocky or icy core, will accrete gas from the disc and evolve into a planet. The gas flows onto the planet, and may form a circumplanetary disc as it accretes that may be observable in near-infrared wavelengths (Zhu, 2015). The planet undergoes similar gravitational collapse as a star, and eventually accretes or ejects its envelope (Pollack et al., 1996).

Another mechanism for the formation of giant planets is when gravitational instability causes the disc to fragment. For disc models, the gravitational instability occurs in the outer regions of the disc (10s of AU), but there is also instability of dust in the disc, which can become concentrated and collapse (Boss, 1997; Kley and Nelson, 2012). As the disc fragments, it creates clumps of dust and gas that undergo gravitational collapse into planets (Boss, 1997; Blum, 2018). This method of planet formation can occur on shorter timescales than the core accretion model (Boss, 1997).

1.3 Solar System

When it comes to the formation of our own solar system, we rely on materials left behind from these early stages to piece together the timeline and environment of formation. These samples are in the form of meteorites, interplanetary dust grains, and pre-solar grains, either found where they have fallen to Earth or from sample return missions (e.g. reviews by Davis et al., 2014; Nittler and Ciesla, 2016).

The meteoritic record contains snapshots of the various stages of planet formation and grain growth. Pre-solar grains, are identified by vastly different isotopic ratios than those found in the solar system, implying that they are from outside it, or before it (Nittler and Ciesla, 2016). The alteration, or lack thereof of these presolar grains gives an indication of the heating and cooling history of the solar system (Davis et al., 2014).

Chondrites are a family of meteorites that are considered primitive, and are inferred to have formed on a body too small to have undergone differentiation. Chondrites have four main components, refractory inclusions (calcium-aluminium inclusions - CAIs, and amoeboid olivine aggregates - AOAs), chondrules and matrix (see reviews by e.g. Davis et al., 2014; Nittler and Ciesla, 2016). CAIs are high-temperature minerals with compositions indicating they are likely the first solids to condense from the solar nebula. Chondrules are spherical aggregates of crystals (and glass), typically made of olivine or other iron- or magnesium-rich silicates. Chondrules form from molten or partially molten droplets in low gravity environments and form a sphere with low surface area/volume. The last part of a chondrite is the matrix, this is the fine grained phyllosilicate, oxide/sulfide (and possibly carbonate) material that holds the CAIs and chondrules together.

The environments indicated from meteoritic data (chondrites), are more extreme than what is expected from observations of protoplanetary discs. The temperatures, pressures and densities required to form the components of chondrites (CAIs, chondrules and matrix), provide evidence for a diverse range of temperatures existing throughout the Sun's protoplanetary disc. CAIs are highly refractory and their cores require temperatures of $< 650\,\mathrm{K}$, but then the rest of the CAI requires temperatures of over $1000\,\mathrm{K}$ with specific conditions under which to cool to form in the way that they do, likely in the midplane of the disc close to the star (Davis et al., 2014; Nittler and Ciesla, 2016). Similarly chondrules show evidence of rapid melting and cooling, suggesting localised heating events in dense regions (Davis et al., 2014; Nittler and Ciesla, 2016). However, there must also be good mixing of these heated components throughout the disc, as they are found in multiple meteorite families, thus it is likely that material in chondrites has experienced a range of temperatures over time. The focus of this work will be to understand where and how these temperatures are experienced throughout the disc.

2 Earliest Stages of Star Formation

The early stages of planet formation and how they follow those of star formation are still somewhat mysterious. In our own solar system we trace timescales from when CAIs formed, as we can use radiometric dating to accurately find these ages (e.g. Davis et al., 2014). From astronomical observations and models we know that the Class 0 and I phases of star formation are relatively short, with Class II and III being longer (e.g. Dunham et al., 2014). Thus exactly how the CAI ages line up with these early stages still warrants investigation.

In a recent review Nittler and Ciesla (2016) consider the timescales of star and planet formation and how the stages of star formation align with the formation and evolution of chondrite components. Figure 3 shows the resultant timeline comparison of Nittler and Ciesla (2016). The timelines here suggest that CAIs formed during the first (0th) Stage of star formation, and that chondrule formation extends into the Stage/Class II of star formation. This works under the assumption that t_0 (the start of the solar system) occurs at the same time as the first hydrostatic core is formed. With further investigation into the environments of discs at these earlier stages, I aim to more clearly determine when the overlap between them occurs.

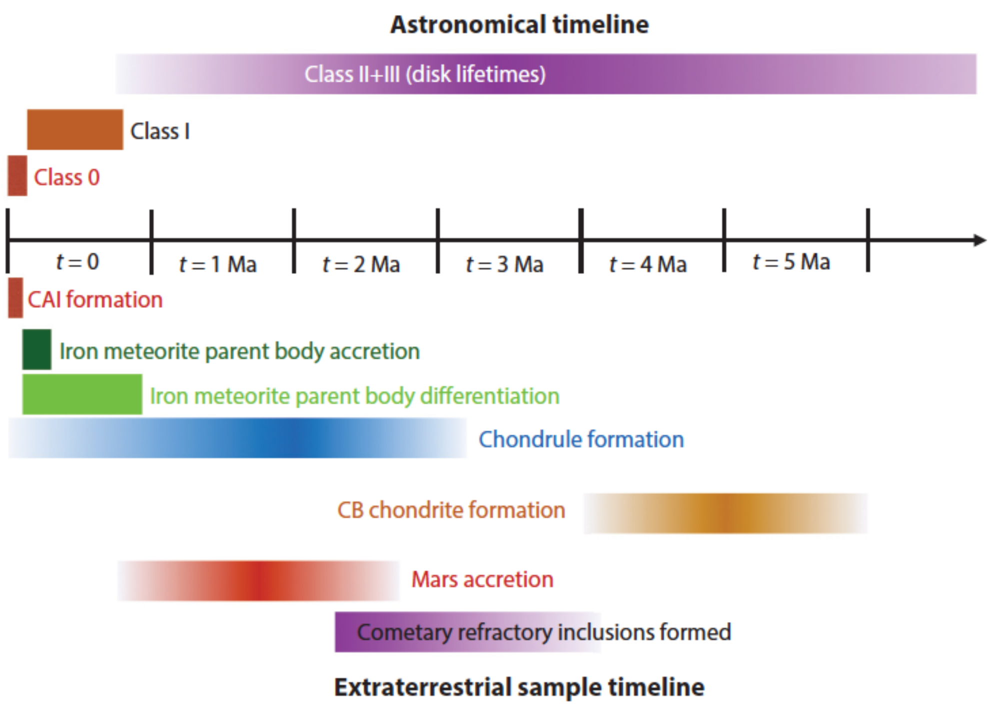


Figure 3: Timelines of astronomy and geology. From astronomy there are the observed classes of star formation. From the rock record there are the times for components to coalesce measured from CAI formation. (CB chondrites are the Bencubbin-type carbonaceous chondrite subclass known to have formed later than chondrules in the evolution of the Solar System.) Image credit Nittler and Ciesla (2016).

In discussions of the earliest stages of planet formation, it is important to consider all the evidence available to us, so that we can better understand how, when and where planets form. For example simulations of protoplanetary discs are often compared to observations (both imaging and spectra). However, simulations and observations are less often compared with the meteoritic data, which tells us about the formation of our own solar system. Understanding the comparisons of astronomical simulations (which are informed by observations) and meteoritic data are at the core of this thesis.

2.1 Using Astronomical Observations to Examine Early Star Formation

Observations of the earliest stages of star and planet formation are challenging, as these objects are typically still heavily embedded in their protostellar envelope. Imaging of the protostellar envelope and the discs of these objects is possible with space telescopes such as Herschel, Spitzer and Hubble (see Dunham et al., 2014, for review), and with state-of-the-art ground-based observatories such as Keck and ALMA. Observations at different wavelengths can reveal different information about YSOs and their discs. For example a region of a disc which is cleared of dust may not be cleared of gas, or dust of different grain sizes or compositions may be distributed differently throughout the disc (e.g. Geers et al., 2007; Brown et al., 2012; van der Marel et al., 2013, 2016a).

Heavily embedded, dusty objects often need to be imaged in infrared or longer wavelengths, both to see dust and then also see through it. For example, using long wavelength observations such as those in the mm, the disc around young stars can be imaged and the dust can be seen to have structure (e.g. HL Tau as observed by ALMA Partnership et al., 2015).

Another reason YSOs are observed at a wide variety of wavelengths is so that an SED can be created for them, which can provide information on their evolutionary stage, and the structure and composition of the disc. Information about the disc and thus the environment for planet formation can be deduced using combinations of observations at multiple wavelengths, hyperspectral data and photometry.

2.2 Using Astrophysical Simulations to Examine Early Star Formation

In this work I plan to investigate the physical and chemical evolution of a protostellar disc by tracking parameters such as the temperature, density, pressure, magnetic field and radiation field as they evolve with time throughout the disc. These parameters can be considered all together in a magnetohydrodynamical (MHD) model that evolves with time, or could be investigated separately, using static phenomenological models. Static modelling can also be done as a post-processing step on dynamical models, for example to determine the chemistry or radiation field.

Simulations of a star collapsing from its parent cloud typically include solving the MHD equations. One approximation that can be made for solving the MHD equations is to assume ideal MHD, meaning that the gas is perfectly coupled to the magnetic field. These assumptions can be relaxed to add another layer of complexity to a model.

One can simulate the stages of star formation that are more difficult to image, i.e., the heavily embedded stages of star formation, at the earliest phase. Here we have some observational and physical constraints, but the goal is understanding how the stars and discs are forming and evolving rather than developing a model to explain a particular observation. This type of simulation models the formation of a star from the collapse of its parent cloud and includes varying levels of physical complexity, (such as magnetic fields, jets/outflows from the star, radiation transport, feedback - both stellar and radiation, non-ideal MHD, chemistry, turbulence; e.g., Federrath (2015)).

Modelling of the early stages of star formation can occur at many scales, depending on whether the models are of stars forming in a cluster or individual stars. In this work I will be modelling the formation of a single star, meaning spatial scales less than a parsec, and timescales less than a million years. Detail can be added to the model in a number of ways, including chemical analysis or radiative transfer that occurs on-the-go, meaning that it is completed at each timestep (Buntemeyer et al., 2016).

Depending on the evolutionary stage of the YSO, a static model may be appropriate. This would be for replicating structure seen in observations, or matching to an SED, and could be completed with a radiative transfer model of a disc (e.g. van der Marel et al., 2016b). This is often completed for Stage II YSOs, as they have lifetimes on the scale of Myr, and a simpler model setup than a collapsing cloud. One could also model the dynamical stability of the disc to check whether the features observed are transient, and how they may be caused.

The focus of this work will be on the earliest stages of star formation and the evolution throughout a protostellar disc. The environment of the simulated protostellar disc will be investigated through the use of Lagrangian tracer particles. Tracers are particles that move on Lagrangian trajectories (i.e., following the gas flow in and around the disc and star) throughout the simulation and record information without having any back-reaction on the gas flow in the simulation. In this work I will use a similar approach to Federrath et al. (2008), where tracers were introduced to investigate the effects of turbulence in the interstellar medium. Here the particles will trace the gas as it moves throughout the disc and record information about parameters such as the density, temperature and pressure in particular regions of the disc.

2.3 Using Meteorites to Examine Early Star Formation

Evidence for the early stages of planet formation come from chondritic meteorites, which are thought to have undergone the least processing as part of a larger body. The reason they are thought to be the least processed is that they are made up of very old material, and show little evidence of reprocessing and heating (e.g. reviews by Davis et al., 2014; Nittler and Ciesla, 2016). These components are the CAIs and chondrules, both of which require very specific conditions to be formed, and maintained. However, the environments needed to form these components are not often simulated, as obtaining the resolution and scales required can be difficult and computationally expensive.

The formation and survival of CAIs give an indication of the temperatures that can be expected in some parts of the disc. The composition of CAIs indicates that they are formed at temperatures of $1300-1500$ K (Ebel, 2006; Nittler and Ciesla, 2016). Given that CAIs are typically the oldest components of meteorites, they are considered to have formed at the earliest stages of the disc (Nittler and Ciesla, 2016, and references therein).

Chondrules also suggest the presence of high temperatures in the disc. The texture of chondrules along with their spherical shape implies that they were formed from droplets of molten rock (Davis et al., 2014; Nittler and Ciesla, 2016). The temperatures required to melt the components of chondrules are $1700 - 2400$ K (Connolly and Desch, 2004; Desch et al., 2012; Nittler and Ciesla, 2016), which is higher than what is expected for CAIs to condense. The dust grains that formed chondrules are modelled to have formed at temperatures of < 650 K (as iron-sulfides are found in chondrules). Chondrule formation occurs when material is heated to ~ 2000 K in a very short time ($\sim$minutes), followed by slow cooling ($10 - 1000$ K/h) (Desch et al., 2012; Davis et al., 2014; Nittler and Ciesla, 2016). It is not yet known what is responsible for this rapid heating, but there are indications that it may be caused by shocks in the disc (Nittler and Ciesla, 2016).

The final piece of the chondrite puzzle is the matrix, which holds it all together. Pre-solar grains are sometimes found in the matrix of chondritic meteorites, but if they were subjected to the same temperatures required for chondrule formation they would be destroyed (Nittler and Ciesla, 2016). The inclusion of material more sensitive to high temperatures in the matrix implies that there must be mixing occurring in the disc (Nittler and Ciesla, 2016).

2.4 Combining the Simulations, Observations and Meteoritic Evidence

The temperatures indicated by inclusions in primitive meteorites are not found extensively throughout the disc, but there are regions where they may occur. Temperatures in the very inner part of the disc can greatly exceed 1000 K, but in the outer regions of the disc (~ 100 AU) the disc can be as cold as 10 K (Dullemond and Monnier, 2010). The typical dust sublimation temperature (where the disc ends as close to the star as it can survive) is ~ 1500 K (Dullemond and Monnier, 2010), which is similar to the temperature of CAI formation, and chondrule formation, but possibly does not allow for the same cooling history. Thus by investigating different paths through the disc, we may be able to get an indication about where these environments are and how these interactions occur.

3 Project Proposal

This project will investigate the early stages of star and planet formation by simulating the formation of a Sun-like star, at high spatial and temporal resolution. The results of these simulations will be compared with the physical evidence from our own solar system to gain a better understanding of the physical and chemical environments of planet formation. The method and development of this project are outlined below.

3.1 Potential projects and papers

Here I will outline a path that the research for this project may take, discussing how the components link together and can be separated into three initial papers.

3.1.1 Investigation of Disc with Tracer Particles

First I will investigate the early stages of a protostellar disc with the grid-based, adaptive mesh refinement (AMR) MHD code FLASH (Fryxell et al., 2000; Dubey et al., 2008), using tracer particles, and using radiative transfer. This will provide an indication of the physical environments of the early stages of star and planet formation. This part of the project may involve adjusting the current radiative transfer module (Buntemeyer et al., 2016) of FLASH to make it less computationally expensive, as radiative transfer will be a crucial component in understanding the temperatures throughout the disc. I will also require a high temporal and spatial resolution (i.e. I would like to resolve $< 0.1\,\mathrm{AU}$, and would likely need timesteps on the order of minutes to do this), because the results of the simulations will be compared to meteoritic components which form quickly on small spatial scales, and would need to make this computationally viable.

This project will use the FLASH to model the formation of a single star and protoplanetary disc, with the inclusion of Lagrangian tracer particles. FLASH solves the MHD equations and uses a grid to do so, the grid can be refined, with more refinement (finer detail) in the denser regions of the simulation. Levels of refinement are added to the grid as shown by the schematic in Figure 4, each new cell is half the size of the old one, in two dimensions as shown in the figure, each cell is split into four at the new refinement, and in 3 dimensions, it would become eight cells. The condition for refinement that will be used here is that the Jeans length must be resolved on at least 4 grid cells, as has been used in Federrath et al. (2010), and is based on the Truelove criterion (Truelove et al., 1997).

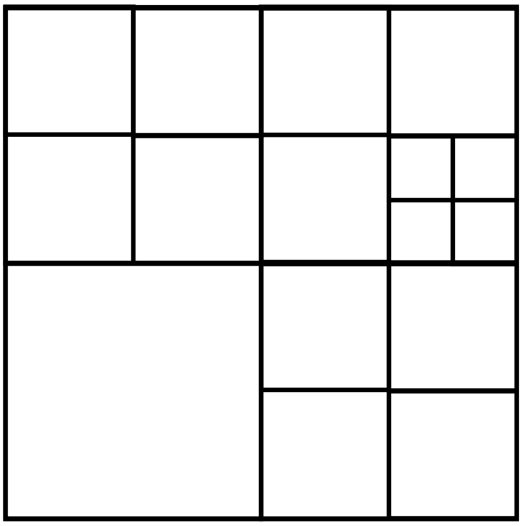


Figure 4: Schematic of adaptive mesh refinement, each new cell is half the size of the old cell.

The ideal MHD equations to be solved are typically the conservation of mass, energy and momentum, Equations 1, 2 and 3 respectively, along with Equations 4 and 5 for the magnetic field.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{1}$$

$$\rho\Big(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla\Big)\mathbf{v} = \frac{(\mathbf{B} \cdot \nabla)\mathbf{B}}{4\pi} - \nabla P_{\mathrm{tot}} + \rho \mathbf{g} \tag{2}$$

$$\frac{\partial E}{\partial t} + \nabla \cdot \Big((E + P_{\mathrm{tot}})\mathbf{v} - \frac{(\mathbf{B} \cdot \mathbf{v})\mathbf{B}}{4\pi}\Big) = \rho \mathbf{v} \cdot \mathbf{g} \tag{3}$$

$$\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{v} \times \mathbf{B}) = 0 \tag{4}$$

$$\nabla \cdot \mathbf{B} = 0 \quad (5)$$

In the above equations (1-5) ρ is the gas density, $\mathbf{v}$ is the velocity, $\mathbf{B}$ is the magnetic field strength, P_{tot} is the total pressure (thermal and magnetic), $\mathbf{g}$ is the graviational acceleration of the gas and E is the total energy density.

To simulate the formation of a star, we will use the sink particle implementation described in Federrath et al. (2010). The sink particles represent the formation of a star, and when the density in a cell is above a threshold value, a sink particle may be formed, assuming these six criteria are met:

1. the cell is on the highest level of refinement
2. the gas converges to that cell
3. the cell is a central gravitational minimum
4. the material in the cell is Jeans unstable
5. the material is bound
6. the forming sink is not within the accretion radius of another sink particle.

The sink particles can then accrete gas from the grid, based on how much material is above the density threshold within the sink's accretion radius, and the mass of the sink particle will be increased. The graviational interactions of the gas with the rest of the gas, the sinks on the gas, the gas on the sinks and the sinks with other sinks are also computed.

Most of the capabilities are already available in FLASH, and would not require an extensive reworking or addition to the code. The capability of having tracer particles with sink particles was mostly possible in the code and has only required minor adjustments. Tracer particles are points distributed throughout the simulation that follow the movement of the gas, and track the properties of the gas, but without interacting with the simulation. The particles interpolate the properties of the gas using the cloud-in-cell method, where they take information a region the size of one cell around them and weight the quantity based on this region. They then trace the quantities as the particle moves throughout the disc. The tracers will initially be dispersed in a lattice throughout the simulation, but will soon move along with the gas. By having particles that move with the gas, and trace different paths through the disc, I will be able to better understand the chemical and physical evolution throughout the disc.

An example of paths that may be of interest in the disc are shown by the pink arrows in Figure 5. Here the disc is represented by the brown cone, with the darker region indicating the midplane of the disc. The outflows from the inner disc (due to the star formation) are shown as yellow and red cones. Paths of interest are through the midplane of the disc, at the surface of the disc, inside the outflow, and a trajectory that follows gas that is launched in the outflow but falls back onto the disc. A comparison of the environment experienced in the midplane, as opposed to the surface of the disc will give an indication of the importance of density to the disc and dust grain evolution. Also whether material launched in a jet falls back to the disc to be re-processed, and how this process occurs is of interest for various chondrule formation scenarios.

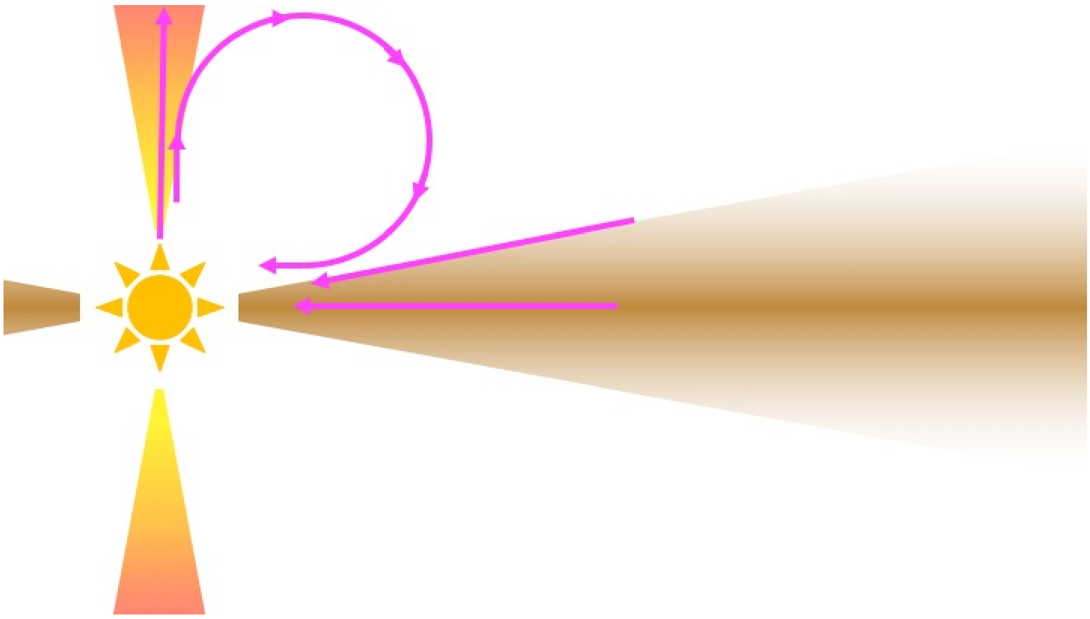


Figure 5: Schematic of disc model (brown), with outflows (yellow and red). Pink arrows indicate possible paths that may be of interest to trace.

The simulation setup that we will utilise will be the single star case that has been studied by Kuruwita et al. (2017). This simulation begins with a spherical cloud of gas that has a mass of $1\mathrm{M}_\odot$, and a radius of 3300 AU, with initial angular momentum $1.85 \times 10^{51}\,\mathrm{g\,cm^2\,s^{-1}}$, and a uniform density of $3.82 \times 10^{-18}\,\mathrm{g\,cm^{-3}}$ (Kuruwita et al., 2017). In this setup the highest resolution cells were ~ 1.95 AU across, however, I plan to use a higher spatial and temporal resolution, to further capture the small scale detail within the disc. The Kuruwita et al. (2017) simulation does not yet include radiative transfer, but this is something that those authors are considering, and that I will consider for this work at a higher resolution. The radiative transfer extension is available within FLASH (Buntemeyer et al., 2016), however, it is computationally expensive, and may require adjustments to be used effectively for our purposes. Thus this work will complement the work done previously in our group using FLASH.

The computational modelling will predominately be done on the Raijin high performance computer system managed by the National Computational Infrastructure. This project will use part of the time allocated to the Federrath research group under the project EK9.

3.1.2 Studying Chemical Evolution Throughout the Disc

The next step in this thesis will be to compare the output of the computational results to meteoritic data and to results from gas-solid reaction experiments. This is where we will explore the chemical environments of the disc, and how the physical environment informs the chemistry. Here we would compare the results of our simulation with the experimental results found by Penny King's research group (such as interactions between the surfaces of chondrules and various gases - e.g. CO, CO_2, O_2), as well as to data from the literature indicating the environments that chondrules and CAIs require in order to form.

Once the simulations of the star formation are complete, the tracer particles can be analysed. Using the information obtained from the tracers about how the temperature, pressure and density evolve in the disc with time and position I will investigate how these align with processing history of meteoritic material. An example of a pressure temperature path and the minerals and mineral phases that may be created along that path are shown in Figure 6, where the line marked 'P, T Profile' shows a potential path of pressure and temperature and the mineral lines show the upper limit of where that mineral is stable. Thermodynamic modelling such as this can be computed on the pressures, temperatures and densities from the tracer particles and then the minerals that would be potentially formed and processed can be compared to those found in meteorites and gas-solid reactions.

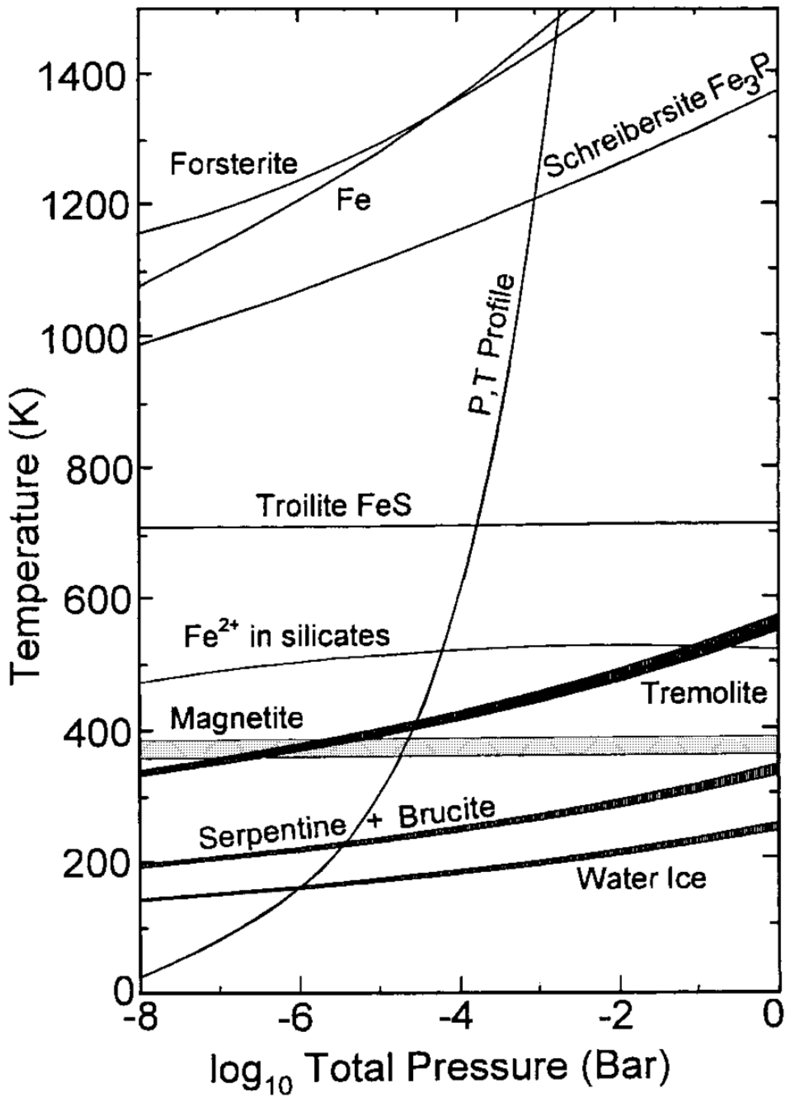


Figure 6: Pressure-temperature diagram showing the stability of certain minerals and a potential pressure-temperature path. The mineral lines can be considered upper limits of where the mineral is stable. The line marked 'P, T Profile' is a potential path through pressure and temperature that material in the disc may take. Image credit Fegley (2000)

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3.1.3 Extending upon the Simulations

The third project depends on the results of the second. If we find that there is a discrepancy between the results of the theoretical astrophysical model and the experiments, we can explore what needs to be changed in our model and what physics need to be added to the model. Adjustments and extensions may include better on-the-go radiative transfer, more MHD effects (e.g. ambi-polar diffusion, Hall effect, Ohmic resistivity), different chemistry of the gas, or addition of dust chemistry (e.g., via KROME, Grassi et al., 2014) to the simulation. Even if there is no discrepancy between the theoretical and experimental results, the effects of adding this extra detail to the model can still be explored.

3.2 Supervisory Panel

The supervisory panel for this project and their expertise are summarised in table 1.

Table 1: Supervisors for PhD

Position	Name	Relevant Expertise
Primary Supervisor/Chair of Panel	Christoph Federrath	Star Formation and Computational/Theoretical Modelling
Advisor	Penny King	Gas-Solid Interactions and Planet Formation
Advisor	Mike Ireland	Exoplanet Detection and Planet Formation

3.3 Timeline

A timeline for the PhD research is included in Table 2.

Table 2: Timeline for PhD

Date	Task
2017	
September	Start PhD
	Understanding FLASH
December	Attend and Present at FAABExo
2018	
	Tests with tracers and sink particles
February	Attend and present at ANITA
March	Submit and Present Thesis Proposal
May	Complete initial modelling
Ongoing	Analysis of tracer paths and results
June	Attend and Present at ASA (and possibly attend Harley Wood School)
July	Submit and Present Annual review
August	Feed tracer particle data into detailed chemical evolution code
September	Draft of first paper
September	Attend and present at EF White conference on gas solid reactions at ANU
October	Attend and present at Take a Closer Look Conference (Germany)
Ongoing	Comparison of tracers to meteoritic and lab evidence
December	Attend and present at Australian Exoplanet workshop
2019	
February	Attend and present at ANITA
Ongoing	Extend model and chemistry comparisons
June	Attend and Present at ASA (and attend Harley Wood School)
July	Submit and Present Annual review
September	Draft of second paper
December	Attend and present at Australian Exoplanet workshop
2020	
Ongoing	Extend model and comparisons
February	Attend and present at ANITA
June	Attend and Present at ASA (and attend Harley Wood School)
July	Submit and Present Annual review
September	Draft of third paper
September	3 years
	Write up thesis
December	Attend and present at Australian Exoplanet workshop
2021	
	Writing up
February	Attend and present at ANITA
March	Submit Thesis

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