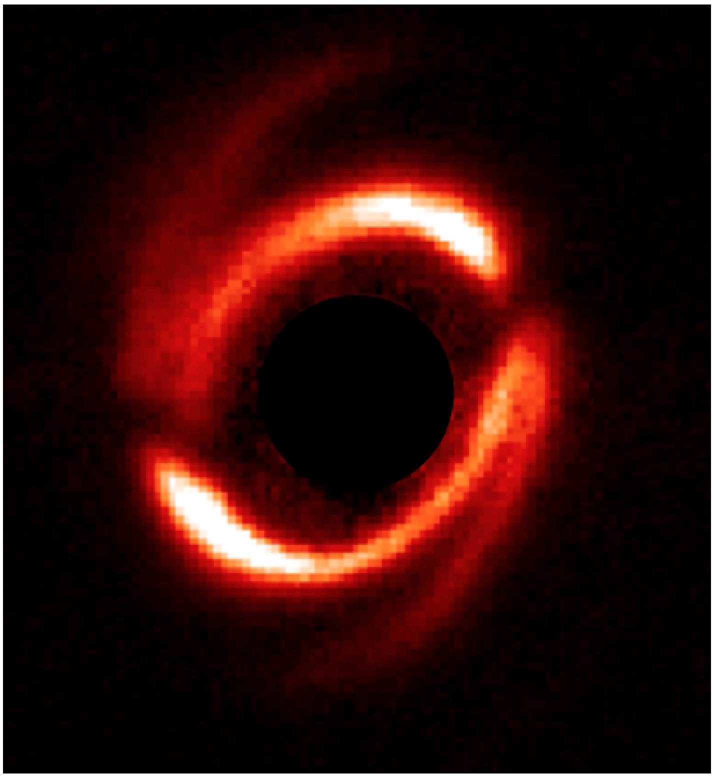
Planet Formation Witnesses and Probes: Transition Disks

Proposal for funding a DFG Research Unit



Speaker: Barbara Ercolano

Co-speaker: Cornelis Dullemond

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Cover image: The Transition disk HD 100453 as seen with the VLT-SPHERE instrument in scattered polarized light. From: Benisty et al. (2017).

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2. Summary

Recent surveys have shown an overwhelming diversity of extrasolar planetary systems, prompting the question of how did they form, and whether some may end up looking like our own and being able to sustain life. Hints to answer such fundamental questions may be hidden in the many trends that are slowly emerging from the data. An example are the deserts and peaks in the distribution of giant exoplanets, with clear implications for habitability of systems, given the role played by giants on the delivery of volatiles to terrestrial planets (e.g., Quintana & Lissauer 2014).

The environment in which planets form plays a major role in understanding both the variety of exoplanets and the emerging trends. Planets are born out of the dust and gas left over whenever a new star forms: the protoplanetary disk. The initial conditions for planet formation are thus determined by the protoplanetary disks, which evolve and disperse as they give birth to planets. Interestingly, the timescales of disk dispersal are comparable to those of planet formation, suggesting that the dispersal mechanism dominates disk evolution right at the time at which planets form. Conversely, the planet formation process also strongly affects the disk, making the combined problem of planet formation and disk evolution a strongly coupled and complex problem.

Disks on the verge of dispersal, so-called "Transition Disks" (TDs), are thus particularly important witnesses of the planet formation process, and they can be used as probes of the different mechanisms at play at this crucial time of disk evolution. Latest research has shown, however, that TDs, which are usually identified as disks showing evidence of an (at least partially) evacuated inner dust hole, are in reality a diverse class of objects. Some TDs have relatively small dust holes (a few AUs) and are weakly accreting, if at all. On the other hand an apparently distinct population of TDs show evidence for much larger inner dust cavities (several to many tens of AU) and vigorous accretion, signifying that a large amount of gas is present inside the dust cavity. Different physical processes may be at play for the formation of different TD types (e.g. photoevaporation, MHD processes, dust evolution, planet-disk interactions), each being a piece of the complex planet formation puzzle.

Until recently, observations of protoplanetary disks provided very few constraints on our understanding of disk evolution and planet formation. That was in part due to the lack of spatial resolution of telescope facilities at infrared and (sub-)millimetre wavelengths, but also in part because protoplanetary disks tend to be opaque, and therefore much of the planet formation process is hidden from view. Both these obstacles impede an unobstructed view of the physical processes happening inside these planetary nurseries. Both problems may now start to be overcome with the enormous recent advances in the observational facilities. At near infrared wavelengths and at millimetre wavelengths we now start to obtain extraordinarily detailed images of these disks. They turn out to feature complex (often non-axisymmetric) structures that challenge our theoretical understanding of these disks. In particular, many TDs show spectacular structures including lopsided blobs, rings, spirals etc. It is suspected that some of these complex structures may be caused by newly formed giant planets that gravitationally perturb the disk, but exciting new alternative explanations, which not always involve planets are also emerging.

In our proposed Research Unit we aim at studying various aspects of TDs, leading to a better understanding of the different formation mechanisms of this very diverse class of objects. TDs are only now really becoming spatially resolvable thanks to facilities like ALMA and VLT-SPHERE, making their study a timely and urgent task. Only understanding the disk evolution and the planet-disk interactions allow the large body of existing and planned observations to be exploited to answer more complex questions like the formation of planetary systems capable to host life. This requires a focussed effort from several communities to devise a multi-pronged strategy to approach to tackle the problem. Specifically, multiwavelength ob-

servations of disks at different stages of evolution together with exoplanet and disk statistics should be used to constrain a concerted theoretical modelling effort including the hydrodynamics of the dust and gas component of disks, with and without planets, joint to chemical and radiative transfer calculations, particularly of the surface layers and winds of disks in (or just before) the transition phase. This is the motivation for the proposed Research Unit.

3. Introduction and motivation

The question of whether the Earth may be a unique and special place for life in our Universe has been the prime motivation for exoplanet finding missions and continues to be the driving force behind many observational campaigns and theoretical investigations in the field. While this question may have partially been answered by the recent exoplanet surveys, which have shown that, statistically speaking, most stars in the Milky Way have planetary companions (Cassan et al. 2012), other surveys have also highlighted the diversity of exoplanetary systems (Mullally et al. 2015). The question however remains as to which initial conditions may lead to the formation of planets. To answer this question many more aspects of the planet formation process and of their subsequent evolution must be understood.

Planets form from the dust and gas contained in the circumstellar disks surrounding nearly all young low- to intermediate-mass stars. These planet-forming disks are a by-product of the star-formation process, meaning that all stars have the potential to host a planetary system. Circumstellar disks are observed to evolve and finally disperse over a timescale of a few Myr, which is comparable to the timescales for planet formation by the core accretion process and to migration timescales for giant planets (see Armitage 2011, for a review). This implies that the processes driving the evolution and dispersal of disks play a crucial role in shaping new planetary systems and likely contribute to the observed variety of exo-planets (Alexander & Pascucci 2012; Ercolano & Rosotti 2015, see e.g.,).

For the largest part of their lives, the evolution of the surface density of disks seems to be well described by simple viscous theory (e.g. Hartmann et al. 1998; Lynden-Bell & Pringle 1974). This predicts a slow, homogeneous dispersal of the disk. Observations, however, show that the dispersal is not a continuous process: after having evolved viscously for a few million years, disks regularly seem to disappear abruptly (e.g., Kenyon & Hartmann 1995; Luhman et al. 2010). Indeed studies have shown that the dispersal timescales are about 10 times faster than the global disk lifetimes, and that disks mostly disperse from the inside-out (e.g., Ercolano et al. 2011; Koepferl et al. 2013). 'Transition Disks' (TDs), i.e. disks that have an evacuated inner cavity in dust (or at least an inner region which is severely depleted in optical depth), may be objects caught on the last gasps of their lives and may thus provide key insights on the mechanism responsible for their evolution.

It is however becoming clear that transition disks, which are identified observationally as having reduced near- to mid-infrared emission, are in reality a diverse class of objects. Some of them may not actually be short-lived objects caught in the act of dispersing their disks, but rather produced by a different rarer and longer lived phenomenon (see e.g., Owen 2016; Dong & Dawson 2016). It is of prime importance to understand the physical processes leading to the formation of rings, gaps and holes in planet forming disks, if these are to be used as probes of disk dispersal and/or planet formation. This is the overarching goal of this Research Unit.

A number of theoretical models have been proposed for the origin of transition disks, some of which are true disk-dispersal processes (e.g. Photoevaporation: (Clarke et al. 2001); MRI-driven winds: (Suzuki & Inutsuka 2009); MHD winds: (Bai 2016)), while others rather lead to dust-(and sometimes also gas)-depleted regions yielding the observed infrared dip (e.g. Planet-disk interactions: (Calvet et al. 2005); dust grain growth: (Dullemond & Dominik

2005); binary stars interactions: (Marsh & Mahoney 1992)), without necessarily leading to the removal of the disk.

Photoevaporation by energetic radiation from the central star is currently accepted as one of the main players in the late evolution of disks and has seen several dedicated theoretical efforts (e.g., Clarke et al. 2001; Alexander et al. 2006; Ercolano et al. 2008, 2009; Owen et al. 2010, 2011, 2012; Gorti & Hollenbach 2009; Gorti et al. 2009, 2015). Photoevaporation sets a crucial boundary condition to planet formation, putting an upper time limit to the formation of Gas Giant Planets, and possibly affecting the dust-to-gas ratio of the disk. Photoevaporation is successful in reproducing the observed dispersal timescales, the inside-out mode of disk dispersal, and can reproduce a subset ($\sim$50%) of the TD demographics around T-Tauri stars.

However, disk dispersal by photoevaporation, while certainly an important piece of the puzzle, does not tell the whole story behind the formation of all TDs.

Amongst the TD zoology, at least two separate classes seem to have emerged, which we will refer to in this proposal as Type 1 and Type 2 TDs. Type 1 TDs have small (a few AU) inner dust holes and show weak or no accretion of gas onto the central star. Conversely, Type 2 TDs have much larger inner dust cavities (tens of AU) and show evidence of vigorous accretion ($\sim 10^{-8}$ $M_{\odot}$/yr), with rates not too dissimilar from those measured on primordial disks (e.g., Manara et al. 2014). Type 2 TDs also tend to have high mm flux levels, meaning that they still contain large amounts of material in their outer regions. Owen & Clarke (2012) showed that it is statistically unlikely that these two groups of objects may be drawn from the same underlying population. When talking about TD demographics it is then important to draw the distinction between the two types, as the dominant formation mechanism is probably different.

Figure 1 shows a collection of known accretion rates versus inner hole radii for known TDs (Ercolano & Pascucci, 2017, in prep.), represented by circles. These are compared to photoevaporation model tracks from Owen et al. (2011), grey squares, and the photoevaporation models plus giant planet of Rosotti et al. (2013, 2015), grey lines. If stars of spectral type G or earlier (distinguishable by a light blue circle in the figure) are excluded, about half of the global TD population consists of Type 1 disks. The formation of Type 1 TDs is generally well reproduced by photoevaporation models (e.g., Owen et al. 2010, 2011). The large accretion rates and large hole radii of Type 2 TDs, on the other hand, are problematic for all photoevaporation models (e.g., Rosotti et al. 2013, 2015) or grain growth models (Birnstiel et al. 2012) to date, and the classical explanation is that these objects may have instead been carved by dynamical interactions with forming giant planets (e.g., Zhu et al. 2011). However, since the current models based on the classic planet scenario also generally fail to reproduce the Type 2 TD observations and their demographics (see e.g., Dong & Dawson 2016), a number of alternatives have recently been proposed which include magnetohydrodynamics effects (e.e., Wang & Goodman 2016), dust evolution (Pinilla et al. 2016) and inner disk asymmetries (Montesinos et al. 2016). Figure 2 shows a gallery of scattered light images of Type 2 TD.

ALMA now allows in some cases to measure the bulk of the molecular gas *directly*, showing than many Type 2 TDs have residual gas inside the dust cavities (van der Marel et al. 2016), in agreement with the planet scenario (but see also Wang & Goodman 2016). Furthermore, spatially resolved observations of type 2 TDs have shown many bizarre features that are not generally seen in primordial disks. For instance, they often display a huge dust ring (e.g., Casassus et al. 2013) which is sometimes strongly lopsided (e.g., van der Marel et al. 2013). The currently favored interpretation is that we see a key process of planet formation in action here: the mechanism of dust trapping in pressure maxima. Another spectacular kind of features often seen in TDs is spiral waves similar to those seen in galaxies (e.g., Muto et al. 2012; Benisty et al. 2015; Wagner et al. 2015, see Fig. 2). Their origin is currently not

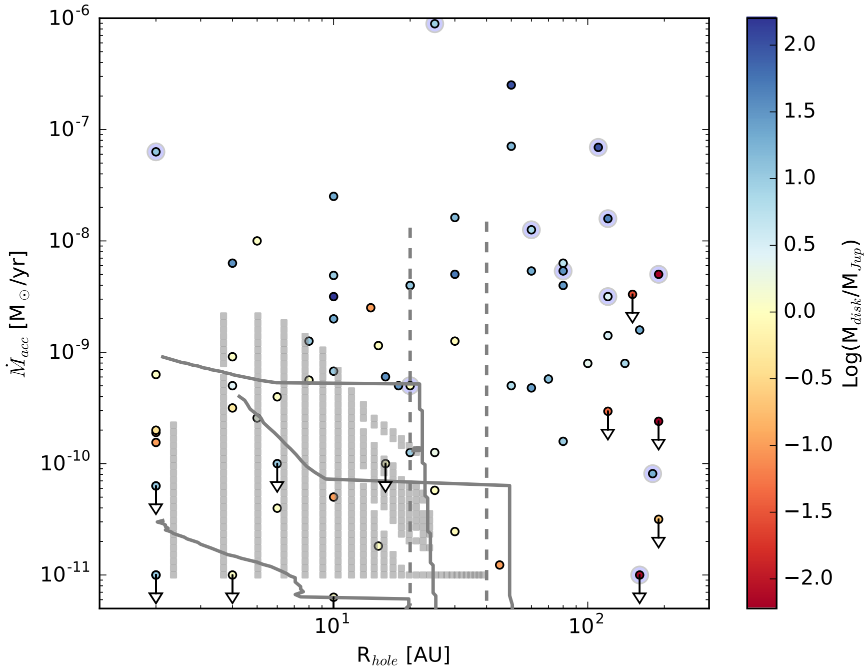


Figure 1: Mass accretion rate versus hole size for known transition disks (Ercolano & Pascucci 2017, in prep.). Circles are for observed star-disk systems. The color-coding shows total disk masses estimated from SED fitting. Sources surrounded by a light blue circle have spectral types G and earlier. Grey squares are snapshots of EUV-plus X-ray-driven photoevaporating disks from Owen et al. (2011) while grey lines are evolutionary tracks for the same photoevaporating disks with an embedded giant planet (Rosotti et al. 2013).

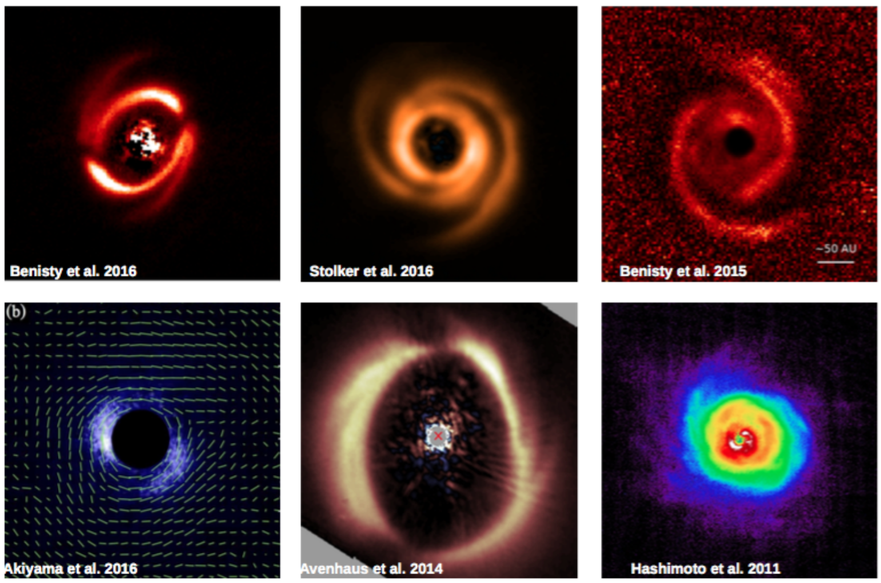


Figure 2: A gallery of scattered light images of Type 2 Transition Disks. **From left to right, top to bottom:** HD 100453 (Benisty et al. 2017), HD 135344b (Stolker et al. 2016), MWC 758 (Benisty et al. 2015), LkHα 330 (Akiyama et al. 2016), HD 142527 (Avenhaus et al. 2014), and AB Aurigae (Hashimoto et al. 2011).

understood, and trying to understand their physics may teach us about important processes taking place in these disks. One interesting new scenario, for example, was proposed to explain the bright ring of scattered light of HD 142527 which has two dark spots on roughly opposite sides (see Fig. 2). Marino et al. (2015) suggest that the shadows cast by an inclined small inner disk could explain the location of the spots, implying that HD 142527 is an "inclined disk inside a disk". In that case, Montesinos et al. (2016) claim that two shadows on opposite sides of the bright rim may cause a brief pressure loss and be at the origin of the m = 2 spiral waves. If confirmed this scenario opens a pandora of new physical questions as to how could the inner disk have a different rotation axis as the outer one?

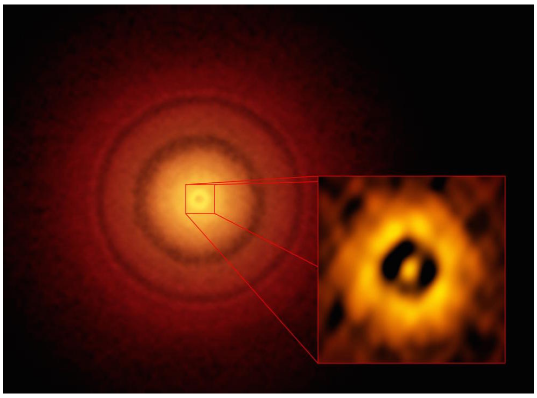
3.1 What can we learn about Planet Formation from TDs?

Both types of TDs can provide complementary information about the planet formation process, if the observations can be interpreted within a comprehensive theoretical framework. Type 1 TDs can inform us about the disk dispersal mechanism, which influences the physical conditions in the disk at the time of planet formation and migration. Type 2 TDs, if indeed formed by dynamical interactions with giant planets are direct witness of the planet formation process. Importantly, all disk-destruction mechanisms essentially 'open up' the disk, so that we can peek inside to see its inner workings, and see processes of planet formation in action. TDs therefore have the unique potential of unveiling key aspects of the planet formation process.

As mentioned above, as well as disk morphology, the interplay between disk evolution and dispersal and the planet formation process, of which both types of TDs are a by-product, is apparent on many other levels. For example the lifetimes of protoplanetary disks (a few Myrs) are comparable to the timescales for planet formation via the core accretion model. This highlights the relevance of studying disks at the end of their lives (i.e. TDs), and highlights the importance of the disk dispersal mechanism (e.g. photoevaporation) which sets the physical conditions in the disk at the time of planet formation, and also sets a time limit on the formation process of Gas Giant Planets. At the same time the similarity in the timescales for disk dispersal and planet formation may also hint at the possibility that the planet formation process plays a part in the final dispersal of the disks (e.g. Rosotti et al. 2013, 2015).

The recent ALMA image of the disk around the young solar-like star TW Hya is a prime example of a disk showing hints of planets orbiting at tens of AU, co-existing with a inner gap at 1 AU which could have been recently created by photoevaporation (Ercolano et al. 2017). The ALMA image is shown in the lef panel of Figure 3 and was obtained by a team including members of this Research Unit (Andrews et al. 2016). However both the existence of planets and the photoevaporated gap remain speculative at present. As shown in the right panel of Figure 3, current planet-disk interaction models fail to reproduce the shape of the gaps as obtained from scattered light observations taken with SPHERE (van Boekel et al. 2016). Furthermore, while several spectral line observations exist for TW Hya, the photoevaporation models do not yet have the predictive power to directly measure the mass loss rate in the wind from them. Until that becomes possible, even the nature of the gaps and rings in the nearest and best studied of all (pre-)Transition Disks, remain uncertain.

As a final example of the direct influence of the inside-out disk dispersal mechanism on the formation and evolution of planets, one should consider the final architecture of exoplanetary systems. While planet migration is necessary to explain (e.g.) the presence of large planets close to the central star, the so-called "hot Jupiters", this process alone cannot explain the pile-up and deserts in the semi-major axis distribution of exoplanets (see also Chatterjee & Tan 2014, 2015). An additional planet-parking mechanism is required, which may be provided by (e.g.) photoevaporation which opens a gap in the disk, forming a TD



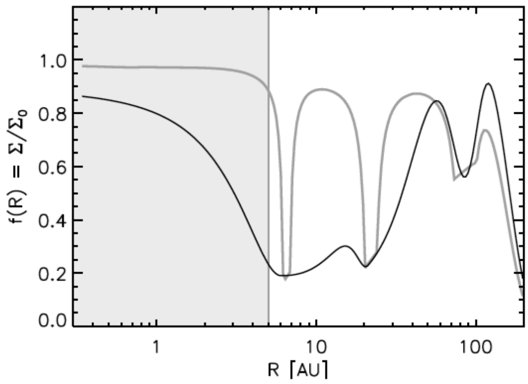


Figure 3: **Left:** ALMA image of the disk around the young, Sun-like star TW Hydrae. The inset image (upper right) zooms in on the gap at 1 AU . **Right:** Comparison between the derived radial surface density depletion factor (f(R), black curve) from van Boekel et al. (2016) and an implementation of the model of Duffell (2015) with three planets, approximately matching the depth of the gaps (grey curve). The innermost disk regions that are not well probed by the observations are masked.

and stopping further planet migration (e.g., Alexander & Pascucci 2012; Ercolano & Rosotti 2015).

3.1.1 Multi-Ringed Disks

The last few months, since the submission of the pre-proposal of this Research Unit, have seen an important observationally-driven development: it is becoming increasingly clear that multi-ringed structures may be ubiquitous in disks, regardless of their age and/or evolutionary stage classification (i.e. full disks or TDs). Obvious examples are the young (about 1 Myr) and massive HL Tau disk (ALMA Partnership et al. 2015) and the old (about 10 Myr) and evolved TW Hya disk (Andrews et al. 2016; van Boekel et al. 2016). Both object show bright rings alternated by darker areas, which could be a signature of planet formation (although note that the features in the two objects show some differences). The detection of ringed structures in very young disks is leading the community to abandon the classical concept of a 'proto-planetary' disk (i.e. a disk that exists before the planets form), but rather embrace the concept of 'planet-forming' disks, to highlight that the planet-formation process happens throughout a disk's lifetime.

Apart from nomenclature the ubiquity of ringed structures suggests a strong link with disk evolution. As an example, if the gaps at 22 AU and 37 AU in the disk of TW Hya, shown in Figure 3, have indeed been created by planets (but see also van Boekel et al. 2016), then one can expect the flow of gas into the inner disk to be reduced. A reduction of the accretion rate in the inner disk, favours the onset of photoevaporation (e.g. Rosotti et al. 2013, 2015), and indeed TW Hya also has a deep gap at 1 AU, which we have shown to be consistent with being photoevaporative in nature (Ercolano et al. 2017).

While the ringed HL Tau disk was already known before our pre-proposal and the rings in TW Hydra were just being published around the time of submission, only recently the ubiquity of such "Multi-Ringed Disks" has become evident. In addition to HL Tau and TW Hydra, multiple rings have since been found in ALMA data of HD 163296 (Isella et al. 2016) and Elias 24 (Carpenter et al. in prep). And in near-infrared scattered light images rings were very recently discovered in BP Piscium (de Boer et al. 2017), HR 97048 (Ginski et al. 2016) and PDS 66 (Wolff et al. 2016). Some Transition Disks also show such multi-ringed

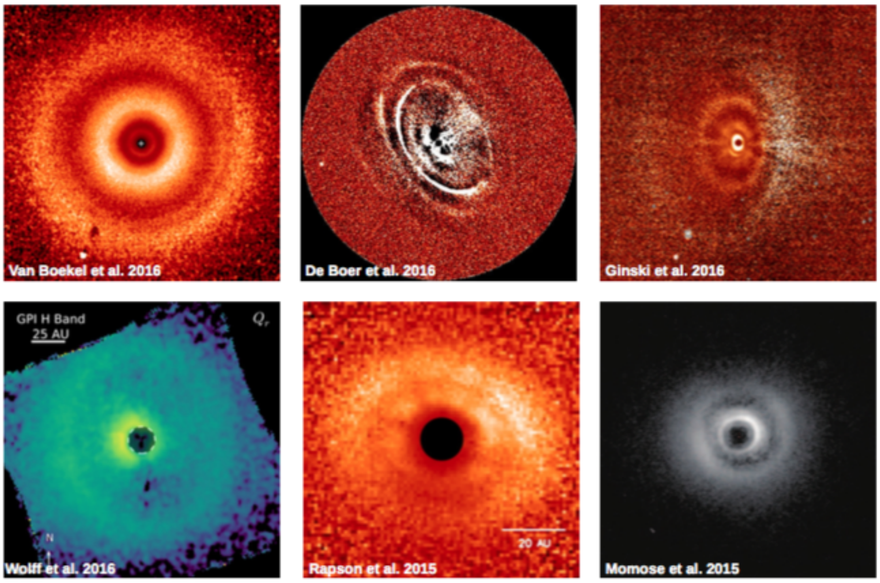


Figure 4: A gallery of scattered light images of Multi-Ringed Disks, which is a new class of protoplanetary disk objects, partly overlapping with, partly distinct from the class of TDs. See Section 3.1.1 for a discussion of their relevance to this Research Unit. **From left to right, top to bottom:** TW Hydra (van Boekel et al. 2016), BP Piscium (de Boer et al. 2017), HR 97048 (Ginski et al. 2016), PDS 66 (Wolff et al. 2016), V4046 Sgr (Rapson et al. 2015) and HD 169142 (Momose et al. 2015).

structures in their outer disk: TW Hydra (van Boekel et al. 2016), V4046 Sgr (Rapson et al. 2015) and HD 169142 (Momose et al. 2015), which suggests that TDs and Multi-Ringed Disks are somehow related, or at least have overlapping members.

It has therefore become clear that a study of the gaps and holes found in TDs would thus not be complete without an investigation of the possible nature of ringed structures in all disks. As well as through planet-disk interactions, bright and dark rings can also be created by dust traps, chemical effects, snowlines, radiative transfer effects and other mechanisms. It now appears to be increasingly evident that if we wish to study TDs to seek for indications of disk evolution and ongoing planet formation using our theoretical modelling strategy, it would be unwise to leave this new class of objects out of our scope. Many of the processes of dust radial drift, dust trapping, planet-disk interaction and gap formation, which we will numerically model in this RU, also readily apply to Multi-Ringed Disks. It is therefore straightforward to expand our methodology to this new class of objects, and it opens new possibilities for finding clues to disk evolution and evidence for planet formation processes at work in these disks.

The co-speaker of this RU is in fact one of the PIs of an ALMA Large Programme on Multi-Ringed Disks (Andrews, Perez, Dullemond & Isella, ALMA proposal ID 2016.1.00484.L), which was ranked A, so we expect a large flood of data starting around the summer of 2017.

Several projects in this Research Unit (in particular projects A1 and D1) have been expanded, compared to their pre-proposal version, to include multi-ringed structures more explicitly, as a response to these latest developments in spatially resolved observations.

3.2 Why is a Research Unit on TDs needed Now?

From the above argumentation it becomes clear that TDs and Multi-Ringed Disks are unique laboratory experiments created by Nature that allow us to test and update our understanding of disk structure and evolution as well as planet formation processes on the small scale (dust growth and dynamics) and large scale (planet assembly and planet-disk interaction).

New observational facilities including ALMA and VLT-SPHERE are revolutionising our view of these objects. We are now starting to obtain extraordinarily detailed images of these objects at infrared and millimetre wavelengths. The richness of patterns seen in TDs (rings, spirals, shadows, vortices, etc.) has made TDs popular as prime targets for new observational campaigns, whenever new modes of observation become available. They are thus among the best-observed galactic objects with these new facilities. Also the observational study of the disk dispersal mechanism is advancing. The tenuous gas inside the cavity and in the photoevaporation-driven wind can be studied with high resolution observations of emission line profiles. Surveys of such wind-sensitive lines in the optical are on-going on the VLT. And with the newly refurbished CRIRES+ to be commissioned in 2019, a wealth of new data in the near-infrared is expected.

A solid theoretical framework is now urgently needed in order to interpret these new observations and decode the message encrypted in the spectral and continuum emission of TDs and Multi-Ringed Disks.

The time is clearly ripe for a multi-pronged, yet concerted theoretical effort with the aim of finding out what these Transitional Disks can teach us about disk physics. The new models to be developed in this Research Unit are exactly what is needed at this stage.

With such an approach, TDs offer a unique chance to test and improve our understanding of the environment in which planets form. This, in turn, allows us to better estimate the boundary/environmental/initial conditions for models for the formation and evolution of planetary systems. This is particularly current with the newly installed DFG Schwerpunktprogramm SPP 1992 “Exploring the Diversity of Extrasolar Planets”. In that SPP the exoplanets and their formation processes are studied, but the structure, evolution and destruction of the protoplanetary disks in which these planet formation processes take place are explicitly excluded from the SPP. This Research Unit can therefore provide crucial new physical insights to several SPP project regarding the birth environments of planets.

To be able to understand the observed features and statistics of these fascinating Transitional Discs, we envision a concerted but broadly based theoretical/numerical modeling effort, combining the theory of disk structure, evolution and destruction with chemistry, dust growth and dynamics, as well as with planet-disk interaction and gas dynamics.

It can therefore not be done in a single or a set of DFG individual proposal, but requires a concerted, closely knit small network of projects involving several teams, covering the key observational and theoretical skills.

To make the link to the observations of these disks and their winds, which are typically done in scattered light (optical/IR), dust thermal emission (sub-millimetre), molecular rotational lines (sub-millimetre) and, for the winds, in atomic and molecular rovibrational lines (optical/near-infrared), our effort has to also include modeling of disk chemistry and radiative transfer. Finally, although this Research Unit puts strong emphasis on modeling, we also need projects that are dedicated to collecting and processing the latest data, and collaborate with the theoretical teams to link theory and observation.

4. Contribution of this team to the field

Our team is composed by theorists and observers, who have all contributed significantly to the state-of-the art of the field today. On the theory side our team includes dynamicists, experts in radiative transfer, dust evolution and astrochemistry, who are committed to exploit the synergies of the team to provide a holistic approach to understanding planet formation and disk evolution, via the study of TDs and their formation. On the observational side our team includes experts in protoplanetary disk observations (both ALMA and VLT), as well as observations of the host stars.

Speaker: **Prof. Barbara Ercolano (LMU)** has been studying the link between high energy radiation from the central star and disk evolution and dispersal (e.g., Ercolano et al. 2008, 2009; Owen et al. 2010, 2011, 2012). Before Ercolano et al. (2009), the importance of X-ray radiation from the central star on the dispersal of disks had not been recognised. This process is now accepted as one of the major player for disk dispersal, hence setting the timescale for planet formation. The models have been tested against observables (e.g. Ercolano & Owen 2010; Owen et al. 2013; Koepferl et al. 2013; Ercolano et al. 2015), producing several successes, but also opening new questions (e.g., Ercolano & Owen 2016), such as those to be approached as part of the projects proposed here. Prof. Ercolano and her team have also investigated the effects of X-ray irradiation on the final parking radius of exoplanets (Ercolano & Rosotti 2015), as well as on the intrinsic (Ercolano & Glassgold 2013; Mohanty et al. 2013) and observed accretion properties of protoplanetary disks (Ercolano et al. 2014). With the work of Rosotti et al. (2013, 2015) the interaction between planet formation and photoevaporation was first taken into account, in an attempt to match TDs statistics. Together with Dr. Testi, she recently published a Letter showing that the innermost gap in the closest planet-making disk to Earth, TW Hya, could be the first photoevaporative gap imaged. Prof. Ercolano is also the main author of the dust RT and photoionisation code MOCASSIN (Ercolano et al. 2003, 2005, 2008b), which is one of the main tools used for the subpojects in area B. This code includes X-ray processes and was recently ported to Voronoi grids (Hubber et al. 2016). For the development of MOCASSIN Prof. Ercolano received the Royal Astronomical Society Fowler Prize for early career achievements in 2010 (https://www.ras.org.uk/news-and-press/157-news2010/1713-ras-honours-outstanding-astronomers-and-geophysicists).

Co-Speaker: **Prof. Cornelis Dullemond (ZAH)** is an expert in modeling the radiative transfer in protoplanetary disks, to compute the (vertical) disk structure and the disk's appearance as seen by observational facilities. He is the author of the popular open source RADMC-3D radiative transfer modeling package, which he and his team employ to study protoplanetary disks, and linking models to observations at infrared and submillimetre wavelengths. He develops new methods for disk modeling, and has been involved in the development of new radiation hydrodynamics modules for the PLUTO code (Kuiper et al. 2010) and ZEUS (Ramsey & Dullemond 2015). His group has also played a leading role in global disk modeling with dust growth and drift (e.g., Brauer et al. 2008; Zsom & Dullemond 2008; Güttler et al. 2010; Zsom et al. 2010; Birnstiel et al. 2009, 2010a), the subsequent planetesimal formation (e.g., Ormel et al. 2010; Windmark et al. 2012; Drążkowska & Dullemond 2014), and the link between the disk/dust models and millimetre and infrared disk observations (e.g., Pinilla et al. 2012; van der Marel et al. 2013; Kataoka et al. 2016a,b). A key theme in the research of Dullemond's group is the study of physical processes and how we can constrain them with observations. The group often develops its own methods of computation and own codes to implement the new physics in existing models, and thereby opening new directions.

Applicant: **Prof. Wilhelm Kley (University of Tübingen**) is an expert in computational astrophysics with emphasis on the planet formation process, starting from the growth of small dust grains all the way to full grown planets. The numerical methods developed and used in his group range from molecular dynamics, smoothed particle hydrodynamics (SPH) and grid-based magneto-hydrodynamics (MHD) including radiative transport. These methods will be used in the theoretical modeling within the Research Group. One focus of his research has been on the important planet-disk interaction. Through multi-dimensional (2D and 3D) radiation hydrodynamical simulations his group demonstrated the possibility of strongly reduced or even outward migration (Kley & Crida 2008; Kley et al. 2009). Recently, models for the origin of the circumbinary planets have been presented (Kley & Haghighipour 2014). Here, longterm models of disks in the presence of a central binary have been simulated and the motion of an embedded planet has been followed. Concerning the main focus of this research group, Müller & Kley (2013) constructed time-dependent hydrodynamics models of transitional disks induced by the presence of a single planet. Specifically, the models investigated the amount of gas flow past the planet into the inner hole as a function of the planet mass, disk parameter and stellar irradiation. With Picogna & Kley (2015) significant advances were made in the understanding of the dust phase response to planet-disk interactions.

Applicant: **Prof. Paola Caselli (MPE)** is an expert on astrochemical modelling and observations of the earliest phases of star and planet formation. She has made important contributions on the chemical structure of pre-stellar cores (within which future stellar systems form.) She is now focusing on the link between molecular clouds and protoplanetary disks using high angular resolution observations, hydro- and magneto-hydrodynamical simulations, which incorporate various degrees of chemical complexity, and radiative transfer codes. She is interested in understanding the effects of different initial conditions in the physical and chemical evolution of protoplanetary disks. Already published work in this field include the chemical structure and ALMA observability of a self-gravitating disk orbiting around a protostar which will likely evolve into a future F-type main sequence star (Ilee et al. 2011; Douglas et al. 2013) as well as the chemical evolution of a self-gravitating disk surrounding a protosolar-type star (Evans et al. 2015). Using non-ideal MHD simulations of contracting dense cloud cores, she recently found that the disappearance of very small grains (VSGs), due to accretion onto larger grains, enables the formation of protoplanetary disks (Zhao et al. 2016). This is due to the fact that VSGs dominate the coupling of the bulk neutral matter with magnetic fields, thus allowing an efficient loss of angular momentum (via magnetic breaking) in regions where protoplanetary disks should form. Together with plasma physicists, she also started a detail study of dust grain charging and its effect on dust coagulation (Ivlev et al. 2015). Her expertise on basic astrochemical processes will be applied to the available and future dynamical models of transition disks.

Applicant: **Dr. Tilman Birnstiel (LMU starting in 02/2017)** has been studying the crucial early stages of planet formation by simulating growth, destruction, and global transport processes in disk (e.g. Birnstiel et al. 2010a). While some of the transport processes have been proposed in the 70s, they were often neglected as they seemed incompatible with observations of disks. Birnstiels models were the first to show, that these processes are not only consistent with many observations but are necessary to explain and understand the evolution of disks (Birnstiel et al. 2010b). His models successfully explained or even predicted observed signatures of growth and transport processes: the spectral index behavior predicted in Birnstiel et al. (2010b) was observed in Pérez et al. (2012), Tazzari et al. (2016) and others. Small scale pressure traps were needed to explain the integrated continuum emission properties of disks (Pinilla et al. 2012), which strikingly resemble the observations of ALMA Partnership et al. (2015) and Andrews et al. (2016). Sharp dust edges in protoplanetary disks as predicted in Birnstiel & Andrews (2014) are now seen in almost every observation that has high enough resolution and sensitivity (e.g. Andrews et al. 2016; de Gregorio-Monsalvo et al. 2013). Lately, for the first time, signatures of his predicted effect of dust accumulation inside the water snow line Birnstiel et al. (2010a) have been detected in Cieza et al. (2016). His models have substantial impact on the further evolution of planet formation via a range of effects: they provide the “pebbles” for pebble accretion, they predict how the planet forming material is redistributed within the disk, they determine the continuum opacity and therefore the temperature and observational appearance of disks, they feed the planetesimal formation factories and transport key volatile species along the way and finally they provide the surface area for chemical reactions that determine the chemical composition of the disk. To investigate these links to planet formation and to the disks chemical composition, he has been awarded an ERC starting grant that starts in March 2017, is hosted at the LMU, and perfectly complements the goals and work plan of this research group proposal.

On the observational side our group includes experts on the observations of young stellar objects, transition disks, initial stages of planet formation and planet disk interactions.Our observational team is experienced with state-of-the art observational facilities including: ALMA, IRAM-NOEMA and the VLA (continuum and spectroscopic interferometric observations) as well as optical/infrared high contrast imaging and spectroscopy using the LBT and the VLT instruments (in particular, but not limited to, XShooter and SPHERE).

Applicant: **Dr. Leonardo Testi (ESO)**, has accumulated years of expertise in the observation and analysis of young stars and their protoplanetary disks at infrared and millimetre wavelengths. He has investigated the initial stages of planet formation via extensive studies of properties and evolution of dust in disks (Testi et al. 2003, 2014). With his group at ESO has completed the first large observational surveys for dust growth in disks (Ricci et al. 2010b,a) and has developed the first self-consistent analysis tool to constrain dust properties as a function of radius in disks (Banzatti et al. 2011; Trotta et al. 2013; Tazzari et al. 2016). His group also developed the methodology to perform accurate measurements of the photospheric properties and accretion rates from broad-band XShooter spectra (Manara et al. 2013) and applied it to study the correlation between disk properties and mass accretion rates in young stars with disks (Manara et al. 2016). His current role as European ALMA Programme Scientist at ESO puts him in a very favourable position to lead an effort here in building a systematic catalogue of the available ALMA observations and help with the interpretation of these data in terms of the models. The new observational campaigns that we foresee for phase 2 of the Research Unit will also strongly benefit from his guidance.

Applicant: **Prof. Thomas Preibisch (LMU)** has many years of experience in the fields of stellar X-ray astronomy and infrared observations of young stellar clusters. He was deeply involved in the Chandra Orion Ultradeep Project (COUP, see Preibisch et al. 2005), the Chandra Carina Complex Project (CCCP, see Preibisch et al. 2011), and numerous other projects where the identification of the X-ray sources with optical and infrared counterparts was a crucial step for the studies of the relation between the X-ray properties and the stellar/circumstellar properties of the young stars. He has also performed several large-scale surveys of star forming regions in the near-infrared (e.g., Preibisch et al. 2011, 2014) and far-infrared regime (e.g., Preibisch et al. 2012) with the aim to identify protostars and study disk-bearing young stellar objects.

Co-Applicant: **Prof. Thomas Henning (MPIA)** is co-I on the VLT SPHERE disk programme and therefore has prime access to high-contrast high-resolution scattered light images of Transition Disks. He has been involved in many protoplanetary disk projects, both observationally and theoretically. He is co-author of the Klahr & Henning (1997) paper predicting the role of dust trapping in vortices in protoplanetary disks, something which has recently been observationally confirmed in transition disks. His involvement in this Research Unit will be through discussions/collaboration on the modeling and through comparison with the observations. He does not apply for funding from this Research Unit.

Co-Applicant: **Prof. Ewine van Dishoeck (MPE/Leiden)** is one of the founders of ALMA observatory. In recent years her group has focussed on studying Transition Disks with ALMA. In 2013 her team published the first strong evidence, based on ALMA data, for a dust-trapping vortex in the Transition disk Oph IRS 48 (van der Marel et al. 2013) and in 2016 her team found wide-spread evidence for dense molecular gas inside dust cavities (van der Marel et al. 2016). She has been involved in many protoplanetary disk studies, both observationally as well as from an astrochemical perspective. Her involvement in this Forschergruppe will be through discussions/collaboration on the modeling and through comparison with observations of the gas surface density structure. She does not apply for funding from this Research Unit.

5. Scientific Objectives

Planet formation and disk evolution feed back on each other. Indeed the formation and migration of planets in protoplanetary disks is clearly affected by the structure and the physical properties of the disk itself (e.g. Dürmann & Kley 2016; Ercolano & Rosotti 2015, to cite only a few of the works coming from our team). The structure and evolution of the disk, however, can be also deeply influenced by the planet formation process, as demonstrated by our recent calculations (e.g., Rosotti et al. 2013, 2015).

This has important consequences both in the interpretation of the observed exo-planet properties (eg. size and semi-major axis distributions) as well as in the interpretation of the disk structures, which are often used as tell-tale signs for planet formation, as in the case of the TDs. Our understanding of how the two processes influence each other is however still incomplete, but it can be improved by studying the physical process behind the formation of all different types of TDs . In this Research Unit we aim at achieving a more complete picture of planet formation and disk evolution by means of an interdisciplinary approach to tackle a number of important outstanding questions.

How can we use TDs as direct witnesses of the planet formation process?

- Which TDs are carved by planets and which are a result of disk evolution?
- What do the complex shapes of TDs (rings, blobs, spirals) teach us about the physical and dynamical processes taking place in protoplanetary disks?
- How does dust evolve and travel within disks to form planet(esimal)s?

How can we use TDs to learn about the disk dispersal mechanism?

- What are the mass loss rates of the disk wind and what parameter space in the TD demographics can thus be reproduced by photoevaporation?
- What are the dust and gas surface density distributions in TDs and how can they be explained?
- How does the high-energy emission from the central star regulate disk accretion and dispersal, leading to the formation of different types of TDs?
- Are Type 1 and Type 2 TDs really disjoint groups, caused by different physical processes?

To answer these questions we will use the following approach:

- *Investigate observationally the accretion properties and the distributions of dust and gas in the disks and winds of primordial compared to transition objects.* To this aim a systematic catalogue of observations will be built, which will provide the constraints to the modelling efforts described below.

- *Dust trapping and growth in TDs.* Dust and gas hydrodynamical models of disks with and without cavities will be produced to match the constraints from the observations. Dust motion and growth will be self-consistently modeled, linking both to observations and to planet formation.
- *Planet-disk interaction and envelope infall models.* These models will aim at reproducing observations of (mainly) Type 2 TDs and Multi-Ringed Discs, including their accretion properties, to pin down the formation mechanism of the observed huge inner cavities, ongoing accretion flows, rings, and asymmetric structures in these disks.
- *Modelling of photoevaporative winds.* By modelling the chemistry and dust entrainment of photoevaporative winds we will be able to predict observables of these winds, allowing a comparison to observations.
- *Determine the mass loss-rates of photoevaporative winds to pin down the mechanism producing Type 1 TDs.* Using the models of photoevaporative winds, appropriate wind diagnostics will be identified, comparing primordial to TDs. Existing archival observations will be used at first to compare with the models and a new observing campaign with ALMA will be devised, perhaps spilling into the second funding period of the Research Unit.
- *Determine the dominant dispersal mechanism.* We will use the archival observations and our newly developed models to analyse an initial sample of disks, the final statistics will be achieved however in the second funding period, where a population synthesis of TDs will be attempted.
- *Close the loop using mass loss rates, central star properties and accretion measurements to calibrate models.* At this point the models will have significantly less free parameters and can be used to extract the initial conditions for planet formation (e.g. mass, turbulence in evolved disks). This will make use of the new state-of-the art simulations and a homogeneous sample of accretion rates and central star properties including X-ray data.

6. Work plan

6.1 Overview over the Research Unit

The main goal of this Research Unit is to understand the morphology, spectroscopy and demographics of TDs, in order to answer basic questions about the planet formation process. We propose a four-pronged coordinated effort which includes (A) Observational studies; (B) disk dispersal models; (C) Dust physics; (D) Planet-disk interaction models. The division in subfields is not strict and is only given here in the aid of clarity. Subfields often overlap and/or feed back on each other, highlighting the need of strong collaborations as proposed here. The observations will provide the constraints to be simultaneously met by models developed in the other areas. Our team is supported by several external collaborators in particular Prof. T. Henning (MPIA) and Prof. E. van Dishoeck (MPE/Leiden) have agreed to take an active part in our project. The theoretical models in the three theory subfields require expertise in hydrodynamics, astrochemistry, dust evolution and radiative transfer, which is available in our team. The specific projects in each area, the support required and the respective key members of the team are summarised in Table 1.

A	**Observations**		
A1	“Solids and gas evolution in disks: observational constraints”	2 PhD	*Testi*
A2	“New constraints about disk-dissipation processes from the relation between accretion and X-ray activity”	1 PhD	*Preibisch*
B	**disk dissipation and chemistry**		
B1	“The radiation-hydrodynamics of photoevaporative winds with chemistry”	1 Postdoc	*Ercolano*
B2	“Astrochemistry in the atmospheres and winds of photoevaporating disks ”	1 Postdoc	*Caselli, Ercolano*
C	**Dust physics**		
C1	“Trapping the dust: planet formation ’hotspots’ in TDs”	1 PhD	*Birnstiel, Dullemond*
C2	“Gone with the wind: dust entrainment in photoevaporative winds"	1 PhD	*Ercolano*
D	**Planet-disk interactions**		
D1	“Transition disks and planetary systems”’	1 Postdoc	*Kley, Dullemond*
D2	“Origin of complex non-axisymmetric structures in Type 2 Transition Disks "	1 Postdoc	*Dullemond, Kley*

Table 1: Tabular overview of the Research Unit proposed here.

Details about some of the major links between projects are summarised in what follows.

Area A: Observations

The projects in area A both aim at obtaining observational constraints on the dust and gas properties of protoplanetary disks and their central stars. Project A1 focusses on collecting and analysing existing ALMA data and complementing those with additional ALMA, VLA and high-contrast infrared imaging observations. The aim is to characterize the content and properties of solids and gas in TDs and to compare with the demographical properties of evolving disk populations. Evidence for dust and gas evolution, including grain growth, and planet-disk interactions will be characterised in order to provide direct observational tests of planet formation and dispersal theories, necessary to interpret the observational appearance of Type 1 and 2 TDs. The focus of project A2 is on the central star properties and their relation to the accretion properties of the disk, which may be modulated by the disk dispersal mechanisms that lead to the formation of TDs. While both of these projects have self-contained aims, they will also provide the observational goalposts for the theoretical investigations of all projects in areas B, C and D, and indeed a legacy for future theoretical studies of this kind also by other groups.

Area B: disk dissipation and chemistry

The main objective of the projects in area B is to determine the mass loss rates in disk winds, and constrain once and for all the disk dissipation mechanisms, leading to the formation of Type 1 TDs. This is crucial to interpret the observed Type 1 demographics. We will perform quantitative spectroscopical modelling of disk winds, identifying and using new wind diagnostics, in particular comparing primordial and TDs. In project B1 we will develop the most comprehensive radiation-hydrodynamics models of photoevaporative disk winds to date. The physics beyond the X-ray heated layer will be accounted for for the first time. This will be achieved by coupling the (radiation-)hydrodynamics code PLUTO to an efficient chemical solver for a reduced network, developed in project B2. Project B2 aims at producing a detailed astrochemical model of the disk atmosphere and its wind. By means of radiative transfer calculations a synthetic spectrum will be obtained to be compared with state-of-the-art observation of spectrally resolved emission from disks, particularly those with known cavities (TDs). The intensity and profiles of emission lines tracing the base of the wind will allow us to put constraints on the wind-launching mechanism, responsible for the dispersal of the disks.

Both projects will use existing and new observational constraints coordinated in projects A1 and A2, and also provided by our external collaborators. The dust content of the wind which is of prime importance for the chemical modelling will be provided by project C2. Projects C1 and D1 will inform us on dust traps and planet-disk interactions which affect the underlying disk evolution and may help photoevaporation create gaps and holes at earlier times (see e.g. Rosotti et al 2013, 2015).

Area C: Dust Physics

The dynamics and evolution of dust grains in disks is the main subjects of area C. In project C1 we will study the growth and trapping of dust grains at hotspots in TDs that may lead to breaking through the meter-size barrier of radial drift, thus allowing the formation of planetesimals. We will use hydrodynamical modelling and dust coagulation models as well as 3D radiative transfer tools. Furthermore, we will be able to use the observational sample collected and analysed in project A1 to tackle fundamental open questions on the first stages of planet formation. This project will feedback and take inputs from the photoevaporation modelling performed in project B1 and it will eventually produce the underlying dust distributions for project C2, which aims at determining the dust content of photoevaporative winds. The latter will make use of state-of-the art models of photoevaporating primordial and TDs from project B1 as well as inputs for the dust distributions from project C1, in order to constrain dust entrainment in the wind, which is an important input to the chemical models in project B2. Finally, project C1 would highly benefit from the setups and methods developed in the more detailed models of Area D.

Area D: Planet-disk interactions

Projects in area D aim at constructing realistic simulations of planet-disk interactions and studying the dynamical processes leading to non-axisymmetric features in order to explain the wealth of new and intriguing observations of TDs. The overarching goal is to use these observation-constrained (from project A1) models to pin down the important details of the disk interaction processes. This is of fundamental importance to be able to disentangle the message about planet formation which is locked in TDs observations. In particular project D1 aims at significantly pushing forward the state-of-the art of (radiation)-hydrodynamical models of gap-forming giant planets embedded in disks including dust dynamics. This project will provide important inputs of gas and dust density distributions for project B1, particularly informing about the fate of dust grains at planet-gaps, which is also relevant to project C1. Project D2 aims at explaining the surprising non-axisymmetric structures recently observed with ALMA in a number of TDs, via detailed hydrodynamical and radiative transfer models, which will also account for realistic grain size distributions from project C1. Studying the

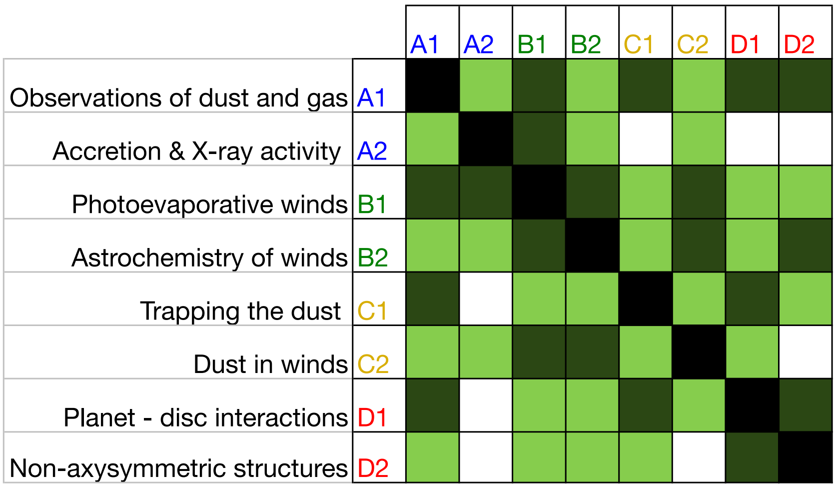


Figure 5: A matrix showing the links between the various projects. The connections are marked as light green - moderate - or dark green - strong connections. The most important individual links are summarised in Section6.1.1. A more detailed description of the connections within the Research Unit can be found in the description of the individual projects.

intriguing nature of these objects is likely to provide important insights on planet-disk interaction processes, thus enabling us to use these disks as proxies for planet formation.

6.1.1 The connection Matrix

Figure 5 summarises the connections visually in a colour matrix. The strong/moderate connections are marked with dark/light green. A brief summary of the project connections is included here, while a more detailed description can be found in the individual project descriptions. Note that the matrix is symmetric, XY connection = YX connection, thus only XY connections are described below.

A1-A2 The data-sets from projects A1 and A2 complement each other allowing a constraining comparison with synthetic disk populations obtained from the models developed in project B1 and B2, on the hydrodynamics and chemistry of photoevaporative winds, respectively.

A1-B1 & A1-B2 The demographical properties of gas in disks derived in this project in combination with the outcome of project A2, providing data on accretion and stellar properties, will be an essential asset for determining the initial conditions and constraints for the models developed as part of projects B1, on the radiation-hydrodynamics, and B2, on the chemistry of photoevaporative winds.

A1-C1 & A1-C2 The dust properties in disks from project A1 will provide key benchmarks for the models mainly developed in project C1, which focusses on dust evolution in pressure traps. The data will also help constrain the initial conditions in the underlying dust disks for models developed in project C2, which focusses on dust grain entrainment in photoevaporative winds.

A1-D1 One of the tasks in project A1 is to study observationally the evolution of the detailed physical properties of disks with embedded planets. The data will provide important constraints to models of planet-disk interactions carried out in project D1. Specifically, the data will constrain the model predictions for the development of rings, gaps and holes in (dust and gas) disks.

A2-B1 & A2-B2 & A2-C2 This project will collect and (re-)derive X-ray and accretion properties from a large number of sources. These will be used as inputs for the models developed in projects B1, B2 and C2, treating, respectively, radiation-hydrodynamics, astrochemistry and dust entrainment in photoevaporation models of disks. The statistical analysis of the data from this project, together with the gas and dust demographics obtained from project A2, will allow a direct comparison with synthetic disk populations obtained from the models developed in project B1, which will provide the latter with important constraints.

B1-B2 & B1-C2 This project will provide the radiation-hydrodynamic models of the wind which are needed by project B2 for the chemical calculations and by project C2 for the dust entrainment in the photoevaporative wind. Project BI depends on input from project B2 for the reduced network and on project A2 for observational input.

B1-C1 Project B1 connects to project C1, which is concerned with dust traps, by providing gas density structures to investigate possible pressure bumps at the edge of the cavity.

B1-D1 & B1-D2 Project B1 will connect with projects D1 (planet-disk interactions) and D2 (non-axissymmetric features) at the end of the first or in the second funding period of the Research Unit. At this stage the results from projects D1 and D2 will be available to combine photoevaporation to planet-disk interaction and non-axissymmetric disk calculations, to provide a unified picture of TDs.

B2-C1 & B2-C2 Astrochemistry is extremely sensitive to the dust abundances and size distribution. The team from project C1 will provide important inputs for the underlying dust disk model, while project C2 will provide the model for the dust grains entrained in the photoevaporative wind.

B2-D1 & B2-D2 An efficient astrochemical model for disks will be important for models of planet-disk interaction and those with non-axissymmetric structures developed in projects D1 and D2, respectively, in order to provide a possible observable chemical signature of the theoretically modelled structures. We expect this connection to become active toward the end of the first funding period or in the second funding period of the Research Unit.

C1-C2 The effects of dust traps studied in project C1 are relevant to the grains entrained in a photovaporative wind (C2), since these depend on the underlying dust distribution. Project C1 & C2 can thus tackle some common questions: "What is the effect of dust traps in the underlying disk on the grain entrainment? Can one expect signatures of this process to be observed either in the continuum emission in the wind or in the molecular lines observations?". The reverse question is also interesting:"What is the effect of photoevaporation on the evolution of the underlying dust grains?". If the wind removes the gas, but the dust has grown to large enough sizes that they are not dragged along (because they have settled below the base of the wind) then the dust-to-gas ratio in the disk will be increased, possibly triggering the streaming instability, and thus possible planet formation, albeit in a somewhat later stage of disk evolution (e.g. Throop & Bally 2005).

C1-D1 & C1-D2 The C1 project will also benefit from frequent exchange with projects D1 (planet-disk interactions) and D2 (non-axissymmetric features in disks) particularly the planet-disk interaction models and the Lagrangian particle modules for the PLUTO code. Vice-versa, D1 in particular will benefit from the dust and collision models created in this project.

C2-D1 & C2-D2 At the end of the first funding period, if time allows, or in the second funding period, the dust entrainment models developed in project C2 will be expanded to investigate the effects of non-axisymmetric underlying disks, for which the models developed in projects D1 (planet-disk interactions) and D2 (non-axissymmetric features in disks) will provide the initial conditions.

D1-D2 A strong technical collaboration within this Forschergruppe will be carried out between the postdocs of projects D1 and D2, mainly because they employ (in spite of their different goals) to a substantial extent similar modelling techniques and codes. This collaboration with be more than the sum of the two, because it will allow both postdocs to more easily overcome the unavoidable technical difficulties of 3-D hydrodynamic modelling of protoplanetary disks.

6.2 Future perspectives

While all projects presented here are self-contained and will provide specific intermediate science products, the major strength of this program is the collaborative work to produce a holistic picture of protoplanetary disk evolution and dispersal, which through the study of TDs and Multi-Ringed Discs can be used to inform us on the planet formation process. At the end of Phase 1 of the Research Unit all theoretical models will have been significantly improved to allow a much more realistic approach to match the observational constraints. At the same time the systematic analysis of the existing observations and the collection of new data will have also provided a much clearer picture of disk structures, as possible planet formation signatures. At the end of Phase 1 our team will be then perfectly posed to perform the most advanced simulations of individual objects, but also and perhaps more importantly, we will be able to tackle the issue of demographics of TDs and Multi-Ringed Discs. Via population synthesis models of these discs including disc dispersal, planet formation, dust evolution, some simplified chemistry and radiative transfer, we will be able for the first time to use disks to make predictive models of planet formation and evolution to match existing exo-planet statistics.

We thus foresee two interesting and connected lines of research in Phase 2:

i) Detailed modelling of individual objects.

This will follow mainly from the joint work of all areas and will target both Type 1 and 2 TDs as well as Multi-Ringed Disks. The insights gained in Phase 1 of the Research Unit will allow us to construct tailored models of planet-disk interactions to explain specific observations of Type 2 TDs (not necessarily obtained by our group). It will also be interesting to perform case-specific studies of photoevaporating warped or misaligned disks in 3D, which may lead to some of the asymmetric structures observed. The tailored models will allow us to decode the message in the many interesting new features highlighted already by spatially resolved observation, which, by the beginning of the second funding period, will have surely delivered more surprises.

ii) Statistical distributions/demographics of Type 1 TDs.

The work carried out in Phase 1 in areas A, B and C will have resulted in the most advanced disk dispersal models, which would have also been calibrated for important quantities with direct observations. We will use these models to construct population synthesis of Type 1 TD demographics (e.g. inner hole radius vs accretion rate), to compare with available surveys in individual clusters. This will be a very strict, direct test of our disk models, and will allow us to predict realistic initial conditions in a disk population at the time of planet formation and migration, which are fundamental inputs for planet formation models (the latter are however beyond the scope of this proposal).

It is inappropriate at this stage to design a more detailed program for a potential Phase 2 of the Research Unit. As well as depending on the outcome of our Phase 1 projects, the exact focus of a potential extension would depend on the developments of the field as a whole. Some general ideas go in the direction of providing the basis for more detailed chemical and physical evolution of Solar-Nebula-type disks, needed to gain a better understanding of the Solar System origin and composition, including the large variety of minerals and organics found in comets and meteorites.

6.3 Research Environment of the Research Unit

The new Research Unit members will be welcomed in a stimulating environment, where complementary research programs and activities are being carried out at all of the institutions involved.

Universitäts-Sternwarte München, Ludwig-Maximilians-Universität (LMU), Munich
At the LMU, Dr. Birnstiel's group (funded by an ERC starting grant) will focus on several aspects of dust evolution in planet-forming disks, with the aim of pushing the state-of-the-art of what is possible with current codes. Prof. Preibisch's group can provide support on observational aspects of high energy radiation from young stars. Prof. Ercolano's group comprises experts who are expert dynamicists and together with other Computational Astrophysics Group members (led by Prof. Burkert) will be able to provide extensive support for the numerical aspects of the projects. Prof. Ercolano is also a research area leader (Star and Planet Formation) at the Excellence Cluster "Universe", which hosts the C2PAP computing centre, which, as well as computing facilities, provides a team of professional code developers to be booked on a project basis. The coding support positions have been guaranteed by the LMU to be continued after the end of the Universe Cluster, independent of an eventual award for a new Cluster, which is in any case being applied for.

Max-Planck-Institut für Extraterrestrische Physik (MPE), Garching
The Max Planck Society (MPG) is Germany's research organization for basic research and covers a broad range of scientific disciplines. MPE is composed of four scientific divisions and currently hosts around 280 scientific staff. The division lead by Prof. Paola Caselli is the Center for Astrochemical Studies (CAS), where observational, theoretical and laboratory studies are carried out. CAS is composed by 25 members, including Postdoctoral Fellows, PhD students and research scientists. The main objectives in the CAS group are chemical and physical processes in star and planet forming regions. Prof. Paola Caselli is an expert on star formation, astrochemistry, molecular spectroscopy, magneto-hydrodynamic shocks, single dish/interferometric observations and simulations. CAS has available office space and computer facilities for visiting scientists and students. CAS is building 3 laboratories (operations have started in 2016): 1. A conventional long pathlength cell for the study of transient and stable molecules of interstellar interest; 2. A chirpd-pulse spectrometer and supersonic jets for the study of complex organic molecules and transient molecules at very low temperatures; 3. Ice experiment. The MPE also hosts part of the research group of Prof. Ewine van Dishoeck. Her group is specialized in ALMA observations of protoplanetary disks, in particular transition disks. This involves both dust and gas diagnostics, and employs astrochemical and radiative transfer models for their interpretation.

European Southern Observatory (ESO), Garching
ESO, the European Southern Observatory (or formally the European Organisation for Astronomical Research in the Southern Hemisphere), is the leading intergovernmental astronomy organisation in Europe, supported by 16 Member States, along with the host state of Chile. Its approximately 110 staff astronomers, 40 fellows and 40 PhD students conduct frontline research in fields ranging from exoplanets to cosmology. ESO's Star and Planet Formation group currently has a total of 19 staff members, 9 post-doctoral fellows, and 4 PhD students, producing over 300 publications since 2015. One of Leonardo Testi main areas of expertise is in infrared and submillimetre observations of protoplanetary disks. He is currently supervising the work of 4 postdoctoral fellows and one student in this scientific area. Young researchers and students at ESO enjoy full access to the Garching campus scientific life and infrastructure, including a rich portfolio of seminar series, direct access to state of the art computing facilities and expertise for the data reduction of millimetre and infrared obser-

vations. Leonardo Testi's group at ESO meets weekly on Thursday to discuss progress on internal projects and on Fridays, jointly with Paola Caselli's group at MPE, to review literature and discuss common interest projects.

Institute for Theoretical Astrophysics (ITA), Zentrum für Astronomie der Universität Heidelberg (ZAH), Heidelberg

The Institute for Theoretical Astrophysics (ITA) is one of the three sub-institutes of the Zentrum für Astronomie der Universität Heidelberg (ZAH). The ZAH is the largest university institute of astronomy in Germany with a wide range of astronomical fields of study. It has 46 PhD students, 40 postdocs, 2 prize research group leaders, 35 permanent research staff and 10 full Professors. It hosts the SFB "The Milky Way System", and has numerous activities including various seminars and colloquia. On average the ZAH supervises around 40 Bachelor and Master projects. PhD students are usually part of the IMPRS programme of the MPIA, and thus get a broad education. The Planet Formation group of Prof. Dullemond at ITA is specialized in numerical modelling of protoplanetary disks, dust evolution and planet formation. The development of new algorithms and codes is one of the driving elements. The open source 3-D radiative transfer code RADMC-3D was developed partly at ITA, partly at the MPIA. The group has a lively discussion culture, and has weekly informal meetings, in which group members discuss their work and/or recent papers.

Max-Planck-Institut für Astronomie (MPIA), Heidelberg

The Max-Planck-Institut für Astronomie (MPIA) is an institute consisting of two large departments. The Planet and Star Formation (PSF) department consists of approximately 80 scientists and is headed by Prof. Henning. Apart from studying star formation, this department puts also a strong focus on the study of planet formation and protoplanetary disks, both from an observational perspective as well as through theoretical modeling. The MPIA is strongly involved in instrument-development, and has thus privileged access to instruments such as VLT-SPHERE. It is actively involved in the interpretation of SPHERE observations with radiative transfer modeling. The MPIA hosts the IMPRS-HD programme and has a thriving scientific culture.

Eberhard Karls Universität, Tübingen

The prime research focus of the Computational Physics group in Tübingen, led by Prof. Kley, is the formation of stars and planets. This includes an understanding of the physics of accretion disks, the origin of the turbulence, dynamics and growth processes of small embedded dust particles, planetesimal formation, planet migration, circumbinary disks. Additionally the groups interest lie in the field of computational astrophysics where new numerical methods are being developed and implemented which includes particle-based and grid-based approaches. The group presently hosts a Emmy-Noether research group on 'Massive star formation' with group leader Rolf Kuiper, who is an expert in implementing radiation transport algorithms in hydrodynamical codes. In total the group consists on average of about 15-20 young people providing an inspiring scientific environment.

Relevant past and current activities of these institutes

– The LMU hosted in 2012 the "Planet Formation and Evolution" conference (organised by Prof. Ercolano and Prof. Preibisch), the 8th in a series of conferences held regularly in Germany.

– The ZAH and the MPIA organized the 6th edition of the "Protostars and Planets" conference series (held in 2013 in Heidelberg), and published the corresponding review volume (eds. Beuther, Klessen, Dullemond & Henning, 2014, UAP).

– In 2017 Prof. Kley, Prof. Ercolano and Dr. Testi are organising a 4-week long workshop on disk evolution and Planet Formation at the Munich Institute for Astronomy and Particle Physics (MIAPP), in Garching bei München, which will bring together scientists from various theoretical, observational and experimental fields, with the aim to stimulate interdisciplinary discussion between astronomy, planetary science, mineralogy, laboratory work, and other adjacent fields. The proposed Research Unit will obtain high visibility through the workshop, which will also help find the best candidates for the available positions.

6.4 Interactions between projects and institutions

The projects planned are not only collaborative amongst institutions, but also have strong dependencies on each other, which is the motivation for setting up a Research Unit. Several members of the network already work regularly together, so we foresee that this compact network will benefit from close-knit collaboration amongst its members. As well as links between the projects we have also links between various institutions within one project, which are led by people from different institutions. Furthermore, we foresee strong links between our groups and those of our external collaborators, in particular Prof. T. Henning (MPIA) and Prof. E. van Dishoeck (MPE/Leiden). Each group will reserve a workplace especially for such exchanges, both within Munich/Garching as well as across the nodes.

Furthermore, we plan to keep communications between and within teams in projects as lively as possible. This requires regular travel. We plan the following meetings and working visits:

- A kickoff and wrap up events at the start and end of Phase 1 of the Research Unit. These events will also be open to non-members, who may provide external support and collaborate on some of the projects.
- Twice a year a two-day face to face meeting with all members at rotating locations amongst the institutes in the Research Unit (The first and last of these meetings will be replaced by the kick-off and wrap-up meeting described above).
- Connected to these meetings we will occasionally (in particular in the first year) organize special-purpose tutorials and lectures for the PhD students and Postdocs of this RU. This is done by adding one or two extra days to the above mentioned meetings. The tutorials are aimed at learning each-other's methods (e.g. the use of a particular hydrodynamics or radiative transfer code, or standard software such as CASA or Python libraries) and will be given by volunteers among the PhD students and postdocs themselves. The lectures will be given by volunteers among the PIs of this RU, and are aimed to bring the PhD students and Postdocs of this RU up to the same knowledge level on the topics of this RU. Both tutorials and lectures will be RU-member-only, so as to have small groups and thus excellent interactivity.
- Once a month a video conference amongst members of a given area, where the young researchers will present status reports of the various projects. A concise summary of the meeting will then be compiled on a rotation basis by the students/postdocs in the area and then distributed to all members.
- Collaboration meetings between individual projects, which can be organized in an ad-hoc fashion.
- We request a substantial budget for longer working visits so that students/postdocs will not work in just one institute, but effectively work in multiple.

6.5 Promotion of Early career researchers

We have requested a mix of PhD and Postdoc positions, the latter because of the complex computational aspects of some of the projects in this building phase of the Research Unit. We are very committed to the training and the promotion of young researchers, and indeed most of the Postdocs are planned to be junior positions (within three years of PhD). The nature of the projects themselves is favourable to the promotion of early career researchers by providing them with definite and clear science products as well as training them in highly sought-after skills, which will propel them in today's challenging academic world. The planned tutorial/lecture sessions discussed in Section 6.4, with the emphasis on small interactive groups and "for-student-by-student" tutorials on often-used techniques, will contribute to this. The Research Unit with the thriving interactions and the team work towards a common goal also provide a perfect environment to develop a broad view of interrelated, but fundamentally different research areas, which will especially benefit PhD students and academically young postdocs. The postdocs will be encouraged and supported to develop independence, which will set them up on a career path to individual fellowships.

6.6 Gender Equality Measures

Our PI team is already relatively balanced in terms of gender. We will continue to work towards creating a still more balanced team of female and male PhDs and Postdocs in this Research Unit. We will also particularly stimulate women to apply for the theoretical research positions of our Forschergruppe, to amend the relative paucity of women in theoretical areas of (astro)physics.

6.7 Family Support Measures

Family support is of prime importance in our Research Unit, and we are aware of the complicated issues of work/family balance. In particular care will be taken in the scheduling of the biannual Research Unit meetings, which will necessarily involve traveling, in order to minimise disruption to family life. When possible we will use video-conferencing (e.g. for the regular monthly meetings), and will provide financial support to members who wish to travel with a caretaker for their small children for the face-to-face meetings, which we foresee to be at least twice a year (on top of the Phase 1 kick-off and wrap-up meetings), and for the longer collaboration visits. Details are given in Project Z.

7. Financial Overview

The total funds requested in all categories for all 8 projects are summarized in the following (all amounts in €).

Personnel

We request funding for 5 PhD students at 75% E13 and 4 Postdocs at E13 level.

Project	Positions	Year 1	Year 2	Year 3
A1	2 PhD	94.950	94.950	94.950
A2	1 PhD	47.475	47.475	47.475
B1	1 Postdoc	68.400	68.400	68.400
B2	1 Postdoc	68.400	68.400	68.400
C1	1 PhD	47.475	47.475	47.475
C2	1 PhD	47.475	47.475	47.475
D1	1 Postdoc	68.400	68.400	68.400
D2	1 Postdoc	68.400	68.400	68.400
Total: (€)		510.975	510.975	510.975

Consumables

The costs listed here is to cover computing needs that are beyond the standard base equipment (Grundausstattung) as detailed in the individual projects

Project	Year 1	Year 2	Year 3
A1	10.000	0	0
A2	0	0	0
B1	3.000	0	0
B2	3.000	0	0
C1	3.000	0	0
C2	3.000	0	0
D1	6.000	0	0
D2	3.000	0	0
Total: (€)	31.000	0	0

Publications

Project	Year 1	Year 2	Year 3
A1	750	750	750
A2	750	750	750
B1	750	750	750
B2	750	750	750
C1	750	750	750
C2	750	750	750
D1	750	750	750
D2	750	750	750
Total: (€)	6.000	6.000	6.000

Travel

The amounts for travel refers to money allocated directly to the individual projects, to support visits to and from external collaborators, and to support expenditures related to attendance to national and international meetings. This money is in addition to that in project Z.

Project	Year 1	Year 2	Year 3
A1	9.834	9.834	9.834
A2	5.000	5.000	5.000
B1	5.400	5.400	5.400
B2	5.800	5.800	5.800
C1	5.000	5.000	5.000
C2	5.400	5.400	5.400
D1	6.333	6.333	6.333
D2	6.333	6.333	6.333
Total: (€)	49.100	49.100	49.100

Central Budget (Project Z)

The total funds requested for Project Z are summarized in the following table.

	Year 1	Year 2	Year 3	Total
Management	24.550	24.550	24.550	73.650
Travel and meetings	49.300	54.900	74.900	179.100
Computing Facility	30.000	0	0	30.000
Total: (EUR)	103.850	79.450	99.450	282.750

Grand Total for project Z: *282.750 €*

Total Budget

Listing of total costs

Item	Year 1	Year 2	Year 3
Research Personnel	510.975	510.975	510.975
Travel (projects)	49.100	49.100	49.100
Consumables	31.000	0	0
Publications	6.000	6.000	6.000
Project Z	103.850	79.450	99.450
Total: (€)	700.925	645.525	665.525

The total cost for three years of the Research Unit is of 2.011.970 €.

8. Signatures

The project leaders have agreed to be responsible for the scientific work of their projects.

The Speaker and co-Speakers of the Forschergruppe: Planet Formation Witnesses and Probes: Transition Disks

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Munich, January 11th, 2017

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Project A1:

Solids and gas evolution in disks: observational constraints

Authors:
Applicants: L. Testi (ESO)
Co-Applicants: B. Ercolano (LMU), T. Preibisch (LMU), T. Henning (MPIA), E. van Dishoeck (Leiden, MPE)
Cooperation Partners: H. Baobab Liu (ESO), J.M. Carpenter (ALMA), A. Miotello (Leiden), I. Pascucci (Arizona), M. Tazzari (IoA), J.P. Williams (Hawaii)

Requested positions: 2 PhD students

Abstract:
This project aims at obtaining observational constraints on the dust and gas properties of protoplanetary disks as a function of evolutionary stage (e.g. primordial to transition) and the physical properties of the central star. We will analyse systematically the ALMA observations of young stars with disks in nearby star forming regions already collected as part of a series of programmes and we will complement these with additional ALMA and VLA observations. We will firmly characterize the level of grain growth and the gas content as traced by CO and isotopologues in disks as a function of stellar mass, evolutionary stage and morphology of the disk, and we will search for evidence of disk-planet interaction in the disks structure and kinematics of transitions disks. We will provide direct observational tests of different planetesimal formation theories and how/if they apply in different environments.

1. State of the art and preliminary work

The aim of this project is to provide an observational characterization of the dust and molecular gas (as traced by CO and its isotopologues) in transition disks as part of the global population of protoplanetary disks in nearby star forming regions.

Transition Disks (TDs) are generally observationally defined based on the observed Spectral Energy Distribution (SED) and disk sub-mm morphology, which are characteristic of disks with an inner region with low dust opacity. There is still uncertainty on their relation to disk evolution and planet formation, but are generally thought to be a transition phase that primordial full disks undergo as they are dissipated (see e.g. Williams & Cieza 2011). In recent years the brightest disks with the largest holes have started to be characterized with high angular resolution submm continuum and spectral line observations. Pre-ALMA observations have been used to quantify the dust surface density drop required to explain the observed inner cavities (e.g. Andrews et al. 2011), and ALMA is now allowing a more detailed study of the molecular gas content (e.g. van der Marel et al. 2015). The relationship between TDs and dust evolution and planet formation has also started to be investigated, but with very limited studies so far (e.g. Pinilla et al. 2014; Sallum et al. 2015). These initial studies have provided fundamental insights on the properties of TDs, but a systematic comparative study with the properties of the global population of disks in different star forming regions is lacking. With this project we propose to make full use of the ALMA and VLA capabilities complemented by high contrast infrared observations at the LBT and VLT. These facilities are now providing us the possibility to perform comparative demographical studies of full samples of young evolving populations as well as detailed

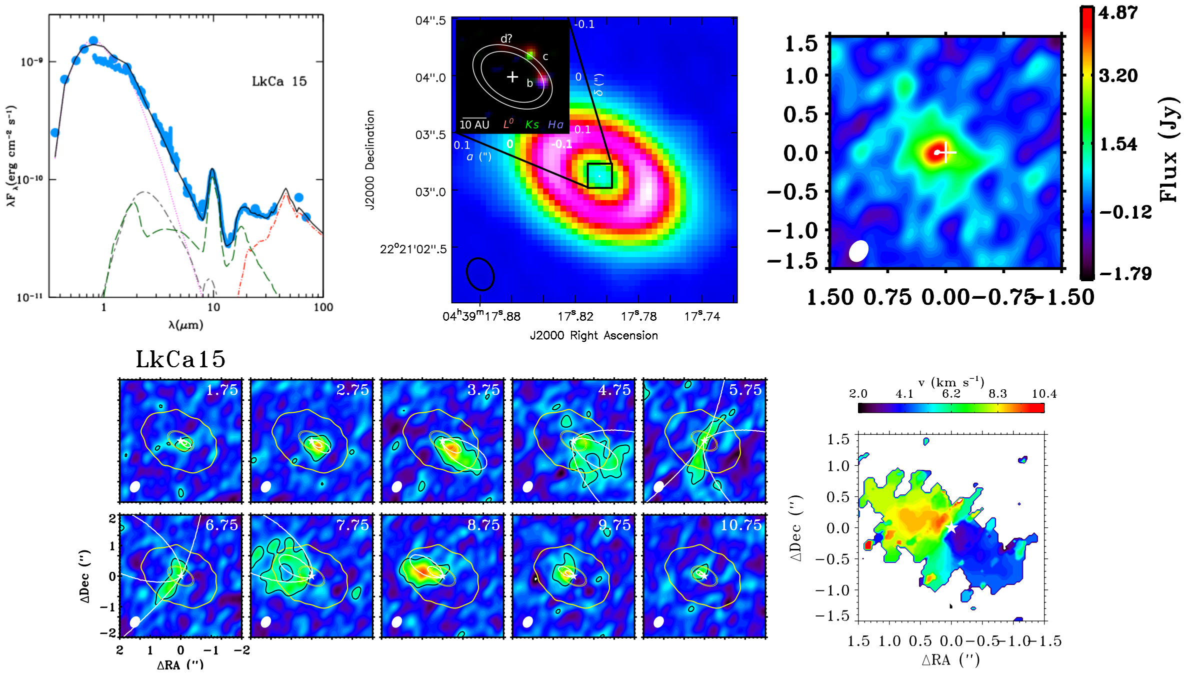

Figure 1: The LkCa15 Transition Disk. **From left to right and top to bottom:** SED of the LkCa15 system showing the characteristic dip of TDs in the mid-infrared, followed by a rise at far-infrared wavelengths (Espaillat et al. 2011); ALMA dust continuum image, showing the inner hole (in this case the cavity outer radius is $\sim$45 AU), the inset shows the location of the young planets detected in this system (Sallum et al. 2015); the ALMA observations of ^{12}CO(6-5) observations show the presence of warm gas inside the cavity (van der Marel et al. 2015).

analysis of planet forming disks in different evolutionary stages.

A systematic assessment of the properties and evolution of dust and gas in TDs as compared with the rest of the disk population is required to constrain the nature of TDs and their relation to the global disk evolution and planet formation process. Four main properties need to be studied and can now be constrained observationally: the dust properties and distribution, the gas properties and distribution, the wind and accretion properties, and the presence and properties of planets. These properties are related to the evolution of disks and the formation of planets: dust grains are expected to grow to pebbles and planetesimals and eventually form the cores of planets; the disk gas content is the reservoire out of which planetary atmospheres are formed, its evolution is linked to the interplay between planet formation and disk dispersal; accretion onto the central star and the wind properties are key observables to compare with disk dissipation models; the effects of planets on the disk, once they are formed, can profoundly influence the future ability of the disk to form more planets and its dissipation.

Detailed studies of a few TDs exist on all the aspects above (see Fig. 1 for the case of LkCa15, one of the very few TDs with directly imaged planets inside the inner cavity), but it is now possible to explore the properties of TDs in the broader context of the demographics of planet forming disks as a function of age and as a function of the properties of the central star.

In the following four subsections, we summarize the state-of-the-art of our observational constraints on the four main properties outlined above and point out one key question in each area that we will address as part of this project and in collaboration with the rest of the RU teams.

1.1 Dust properties and distribution

The properties of the dust distribution is the main observable quantity that sets the TDs class apart form the rest of the disk population. The presence of a hole in the dust distribution can be inferred from the SED, and the hole size roughly constrained through modeling, but only direct, high-angular resolution imaging at (sub-)millimetre wavelengths can provide an accurate measure of the inner hole size and dust depletion factor. Grain growth is a stage of planet formation that can be directly observed due to the effects on particle emissivity. Planetesimals and early planetary cores formation are difficult to probe observationally, while growing planetary bodies can be studied through their influence on the disk structure or directly imaged in the outer disk, when sufficiently young and large.

Submillimetre and centimetre wave observations over the last decade have established that grain growth occurs very early in the protoplanetary disks lifetime, large grains and pebbles are present in disks throughout their lifetime. This is at odds with simple grain evolution theories in gaseous disks, and several ideas have been put forward to explain this fact. Modern theoretical models require large grains confinement in specific regions of the disk associated with local pressure maxima in the gas phase transitions of abundant molecules (snowlines), or regions with very low gas to dust ratio. The new ALMA high angular resolution observations of the protoplanetary disks suggest that small rocky proto-planets may form early and help trapping millimetre and centimetre-size grains in disks (HL Tau, ALMA Partnership et al. 2015), in other cases there is compelling evidence for more massive planets affecting the disk dust and gas distribution (Isella et al. 2016; Pérez et al. 2016).

As of today, relatively few and bright (massive) disks have direct measurements of the inner hole from sub-mm imaging and even fewer constraints on the dust properties in the disk. The most comprehensive catalog of candidate TDs, based on SED modeling, is that of van der Marel et al. (2016c), which includes over 130 high probability TDs in nearby star forming regions. However, for the small fraction of disks with inner cavity measurements from mm interferometry the correlation between the inferred hole sizes from the SED and the sizes from direct imaging shows a large dispersion (see Figure 2). Using the limited quality data available so far, Pinilla et al. (2014) showed a potential correlation between the average dust properties in TDs and the size of the inner cavity. This result is consistent with a scenario in which inside-out planet formation consumes the large grains in the inner regions of the disk to form planets, and, as the disk is progressively evacuated by planets and photoevaporation, the average dust properties are dominated by smaller grains in the outer regions of the system. These result seem to be in qualitative agreement with the expectations that the global evolution of dust in disks produces a radial stratification with the larger grains contained in the inner regions of the system (Birnstiel et al. 2011, 2010), which is then removed in the TDs formation process. Our group has developed a detailed analysis technique of multi-wavelength millimetre and radio observations of disks, and we have confirmed the expectation of the radial stratification of dust properties in a small sample of full disks (Pérez et al. 2012, 2015; Guidi et al. 2016; Tazzari et al. 2016). Nevertheless, the current radially resolved measurements are mostly limited to full disks and pre-ALMA data: there are still large uncertainties and biases on the measurements of TDs hole sizes and on the dust properties. In addition, there is marginal evidence for the dust properties to vary in different star forming regions (see Figure 2, bottom panels), hence to properly understand TDs evolution it is necessary to compare with the dust properties of the full disk populations in the same star forming regions.

Q1: *Can we trace the evolution of the grain size distribution in full disks and TDs as disk dissipation and planet formation progress?*

1.2 Gas properties

Most of the primordial disk mass is in the form of molecular gas. As cold H_2 is not directly observable due to the lack of a permanent dipole moment, the gaseous component of the disks can only be traced by the much less abundant molecules. CO is the prime tracer of molecular gas in planet forming disks. The few TDs with detailed gas observations from ALMA show that in many cases the inner cavities are

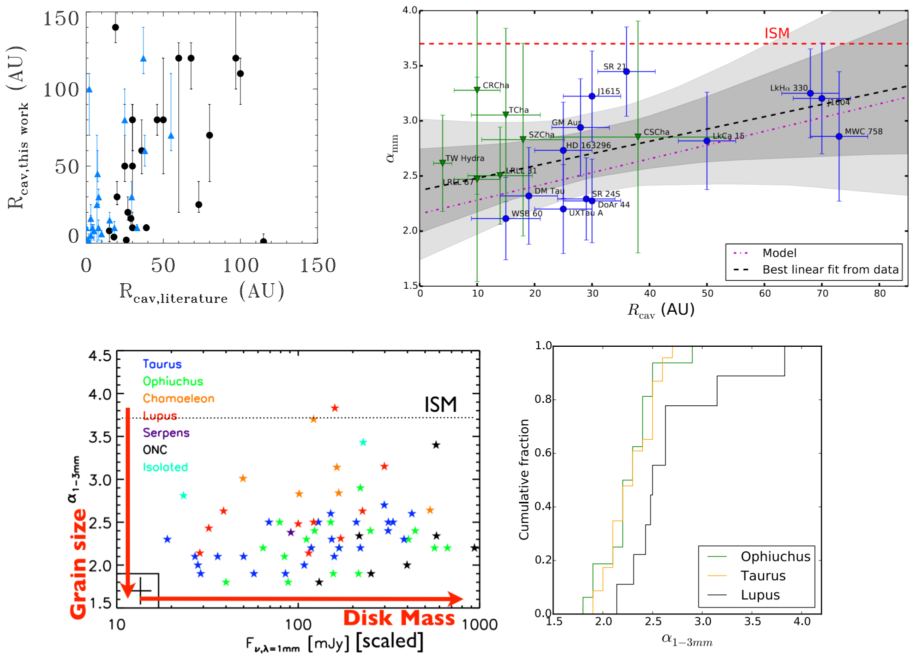

Figure 2: **Top left:** TDs hole sizes as derived from SED fitting and direct imaging (black points only; adapted from van der Marel et al. 2016c). **Top right:** relationship between TDs hole radius and mm spectral index (as a proxy of grain growth in disks, large grains correspond to small values of α; adapted from Pinilla et al. 2014). **Bottom left:** compilation of pre-ALMA photometric estimates of grain growth in disks from millimetre spectral indices (adapted from Testi et al. 2014). **Bottom right:** distributions of the mm spectral indices for objects in the young Taurus/Ophiuchus regions (yellow/green lines, data from Ricci et al. 2010a,b), and the slightly more evolved Lupus region (black line, data from Lommen et al. 2007; Ubach et al. 2012).

not empty, but contain warm gas, while the outer disk is rich in cold molecular gas, as primordial disks (van der Marel et al. 2015). Nevertheless, our current understanding is not yet clear-cut: quantifying the amount of gas inside the inner hole and in the outer disk is essential to provide constraints on the ability of disks to form and interact with planets and for the disk dissipation models.

The characterization of the gas contents of disks during their evolution is an area that is being profoundly transformed by ALMA: for the first time we have the sensitivity to study large samples. Our group made a key contribution in this area in 2016 with the results of the Lupus ALMA Disks Survey (LADS, Ansdell et at. 2016): for the first time an almost complete and unbiased sample of planet forming disks in continuum and gas was used to estimate the demographics of disk gas properties in an entire star forming region for TDs and full disks. The picture that we derive from an accurate analysis combining dust and $^{13}CO/C^{18}O(3\text{-}2)$ emission and detailed modelling of the gas (including selective photodissociation and freezing out) is intriguing in many respects: the gas-to-dust ratios that we derive from modeling the CO are lower by one or two orders of magnitudes as compared to expectations; there is no significant difference in this result between TDs and normal disks (see Fig. 3; Ansdell et al. 2016; Miotello et al. 2016b). There are cases in which full disks show an apparent hole in the CO isotopologues (e.g. see the example in Fig. 3), most likely this is the effect of continuum optical depth suppressing the line emission (see also Isella et al. 2016), which emphasizes the importance of a detailed modeling of the disk emission to extract the gas properties.

The LADS results are tanatalizing, but they need to be followed up to understand the cause of the apparent low gas-to-dust ratio as measured from the CO isotopologues.

Two other surveys of disks in nearby star forming regions have been completed: Upper Sco (Barenfeld et al. 2016), and Chamaeleon I (Pascucci et al. 2016). These surveys have not yet been fully analysed

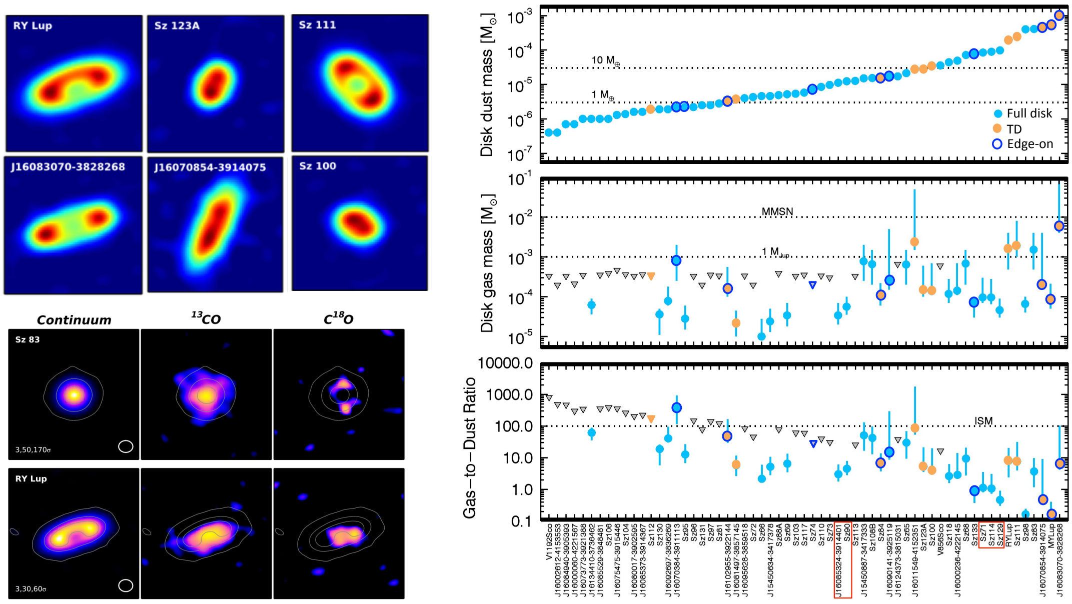

Figure 3: **Top left 6 panels:** ALMA 890 μm continuum images of six of the TDs in Lupus (LADS survey; adapted from Ansdell et al. 2016). **Bottom left panels:** Comparison of the LADS continuum (left colormap and contours in all panels) and ^{13}CO (center colormaps) and C^{18}O (right colormaps) for a full disk (top) and a TD (bottom), note the C^{18}O emission in the inner hole in the TD (adapted from Ansdell et al. 2016). **Right panels:** From top to bottom: dust disk mass, gas disk mass (from CO modeling), gas to dust ratio; TDs are shown as orange circles, while full disks are blue symbols, grey triangles are upper limits (adapted from Miotello et al. 2016b).

for the molecular gas content. ALMA data for two additional surveys of RCrA and σOri have been obtained by our group, the data is expected to be delivered to us in Winter 2016-2017. A complete survey of the Ophiuchus disk population is being carried out by another group, we expect the data to become publicly available in mid-2018.

Q2: *can we trace the evolution of molecular gas as a function of disk evolution and in TDs as disks are dissipated and planet formation is occurring?*

1.3 The disk-wind-accretion connection

Three mechanisms are considered to be the possible main drivers of disk evolution: viscosity, magnetically driven disk winds, and photoevaporation. Each one modifies the disk structure with time in a different fashion. Viscous theory (e.g. Lynden-Bell & Pringle 1974) describes how turbulence redistributes the disk material and the angular momentum. This results in an inward flow of disk material, which eventually accretes onto the star. The initial intense accretion rate ($M_{acc} > 10^{-6}$ M$_{\odot}$/yr) slows down on timescales of $\sim$ 1 Myr to $M_{acc} \leq 10^{-8}$ M$_{\odot}$/yr, and the circumstellar disk then slowly evolves until it becomes optically thin on timescales $\geq$10 Myr (e.g. Hartmann 1998; Ercolano et al. 2011). Viscous evolution is able to explain the general evolution of disks, and we have recently found observational evidence confirming a basic prediction of this theory (e.g. Dullemond et al. 2006): the existence of a correlation between M_{acc} and the disk mass (Manara et al. 2016), as measured through the *dust* emission. This finding supports the idea that viscous evolution may be the main ingredient of early disk evolution. Nevertheless, there are still some major caveats that need to be understood: the correlation between M$_{dust}$ vs. M_{acc} is *not* the expected one, as it is the gas, not the dust, that is supposed to be viscously evolving, in addition the timescale for the disk dispersal predicted from this theory is much too long to be in agreement with observations, and the origin of the turbulence in disks is still unclear (e.g. Turner et al. 2014). In addition, resolved disk observations with ALMA or near-infrared high-resolution imaging (e.g., SPHERE) show structures, such as holes and spirals, as well as inhomogeneities in the gas and dust distribution that cannot be explained by viscous evolution alone (e.g. Benisty et al. 2015).

Observations of disks show that they eject large amounts of material in the form of wide-angle, slow winds, collimated jets, and molecular outflows (e.g. Frank et al. 2014). These ejections are driven by the magnetic field in the disk, which gives rise to magnetically driven winds and jets, remove angular momentum from the disk and thus drive accretion in the disk and onto the central star (Pudritz et al. 2007). These disk winds have been suggested recently as fundamental ingredients for the disk evolution (Armitage et al. 2013; Bai et al. 2016). Indeed, they can accomodate the main features of disk accretion and the timescales of disk dispersal. Moreover, theoretical work is showing that disk winds have a strong impact on planet formation, since they can inhibit the drift of grains and type-I migration of planets (Suzuki et al. 2016). However, quantitative constraints on this theory are still lacking because MHD simulations are local and not global, and the large number of free parameters makes these predictions still qualitative. In addition, photoevaporative winds accelerated from the disk surface by high energy X-ray and UV photons coming from the central star are dominant at late stages when accretion has decreased. Migration of planets may be stopped at $\sim$1-2 au from the central star in disks affected by photoevaporation, thus explaining the observed peak in the exoplanet semi- major axis distributions (Alexander & Pascucci 2012; Ercolano & Rosotti 2015). Photoevaporation explains the rapid final disk dispersal and formation of holes in TDs (Alexander et al. 2014), but falls short in explaining accretion in objects with large cavities (Owen & Clarke 2012).

On the observational side, in (Manara et al. 2016) we showed that stellar photospheric parameters and mass accretion rates can now be derived from optical/infrared spectroscopy with sufficient accuracy to test predictive theories. As part of our ongoing efforts, our group has been acquiring optical/infrared spectroscopy for large samples of star-disk systems in nearby star forming regions. These data will be available to complement the ALMA data on the gas and dust properties of full disks and TDs. We will be able to address the potential correlation between disk properties and mass accretion rate and to search for an evolution or deviation from the naive expectation of viscous evolution theories connected to the effects of disk winds and photoevaporation, and the formation of TDs.

Q3: *can we trace the transition from viscous dominated to disk wind and photoevaporation dominated evolutionary phase in disk and TDs?*

1.4 Presence and properties of planets

Observational studies and simulations of TDs suggest that the presence of planetary-mass companions within the inner hole may be common, and indeed, in a few cases of TDs there are clear observational evidences (e.g. Reggiani et al. 2014; Sallum et al. 2015; van der Marel et al. 2016a, see also Fig. 1). Nevertheless, as outlined above, ALMA is now revolutionizing our view of the evolution from full disks to TDs as it allows for the first time to resolve in exquisite detail the solids and distribution and reveal the process of planet formation as it unfolds.

High angular resolution continuum observations of protoplanetary full disks with ALMA reveal a variety of small scale structures. The most famous and dramatic example is the ring system around the young star HL Tau (ALMA Partnership et al. 2015), but many more are being published by various groups from the PI-science observations of dust distributions in disks at 1.3mm and/or 890μm at 0.05-0.1 arcsec angular scales (e.g. TW Hya, HD 163296, Elias 2–27, Andrews et al. 2016; Isella et al. 2016; Pérez et al. 2016, among others). The variety of single wavelength millimetre continuum morphologies observed so far is very broad: dark rings, with variable depth and location, spiral structures with different contrasts and threads, with and without inner rings, as well as TDs with fully developed holes. Particularly relevant in this context are the observations of Isella et al. (2016), who showed that the gaps observed in the dust distribution are also associated with depressions in the gas surface density, indicating the presence of relatively large planets.

A key feature, first suggested by the observations of HL Tau, seems to be that planet formation in the outer disk (R$\geq$10-20 AU) can occur very early in the disk life, much earlier than the typical 2-3 Myr lifetime. This could be the result of planet formation via gravitational instabilities in massive young disks. Massive planets (M$\geq 1-5$ M_{Jup}) formed by gravitational instabilities in the outer disk should be able to quickly open gaps in the disk leading to some of the observed features. More specifically, recent simulations on embedded planets in dusty disks, suggest that the minimum planetary mass needed to carve a gap in both dust and gas is as low as 1 to a few M_{Jup}, depending on the parameters of the system (Dipierro et al. 2016). An alternative scenario could imply a slower development of planets, where Earth-mass rocky cores are responsible for confining the dusty rings observed in the younger disks, followed by a phase in which Saturn-Jupiter mass planets open well developed dust and gas gaps, to a final TD phase where large holes are opened before the final disk dissipation. These scenarios can now be tested observationally, combining data from ALMA and the LBT and VLT. Young planets down to $\sim$1 M_{Jup} should then be observable through the gaps they open in the disk using state-of-the-art thermal and near infrared high contrast imaging instruments at large telescopes. We have initiated a survey program using LBT/LBTI and VLT/SPHERE to survey for planetary mass companions in planet forming disks that show dust and gas gaps and holes with ALMA high angular resolution observations. The initial results demonstrate the possibility to achieve the goal of detecting Jupiter-mass companions in the outer disk.

Q4: *are $\geq$1 M_{Jup} planets common in planet forming disks and which is their relationship with the observed distribution of dust and gas in full disks and TDs?*

1.5 Project-related publications

Ercolano, B., Rosotti, G.P., Picogna, G. & **Testi, L.**, *A photoevaporative gap in the closest planet-forming disc*, 2017, MNRAS, 464, 95. This paper testifies the collaboration between modellers and observers on the topic of TDs, which is a model for the kind of collaboration planned in this Research Unit.

Ansdell, M., Williams, J.P., van der Marel, N., Carpenter, J.M., Guidi, G., Hogerheijde, M., Mathews, G.S., Manara, C.F., Miotello, A., Natta, A., Oliveira, I., Tazzari, M., **Testi, L.**, van Dishoeck, E.F. & van Terwisga, S.E., *ALMA Survey of Lupus Protoplanetary Disks. I. Dust and Gas Masses*, 2016, ApJ, 828, 15. This paper shows how simultaneous dust and gas observations with ALMA can be employed to study the dust-to-gas ratio in these disks, which is a crucial parameter for planet formation models. See also Fig. 3.

Manara, C.F., Rosotti, G., **Testi, L.**, Natta, A., Alcalá, J.M., Williams, J.P., Ansdell, M., Miotello, A., van der Marel, N., Tazzari, M., Carpenter, J., Guidi, G., Mathews, G.S., Oliveira, I., Prusti, T. & van Dishoeck, E.F., *Evidence for a correlation between mass accretion rates onto young stars and the mass of their protoplanetary disks*, 2016, A&A, 591, 3. This work shows how ALMA observations can be correlated with observations at optical wavelengths to correlate disk properties with accretion properties. The results show that the disk mass correlates with accretion rate, as predicted from viscous accretion disk theory, but that this correlation is only seen in the dust, not in the CO-derived gas masses. This puts interesting constraints on the dynamics and growth of dust, as well as the correlation between CO and gas mass.

Guidi, G., Tazzari, M., **Testi, L.**, de Gregorio-Monsalvo, I., Chandler, C.J., Pérez, L., Isella, A., Natta, A., Ortolani, S., Henning, Th., Corder, S., Linz, H., Andrews, S., Wilner, D., Ricci, L., Carpenter, J., Sargent, A., Mundy, L., Storm, S., Calvet, N.; Dullemond, C., Greaves, J., Lazio, J., Deller, A. & Kwon, W., *Dust properties across the CO snowline in the HD 163296 disk from ALMA and VLA observations*, 2016, A&A, 588, 12. This is another example of the power of combining CO and continuum ALMA/VLA observations, this time showing how the dust reacts to CO sublimation across the CO snow line.

Tazzari, M., **Testi, L.**, Ercolano, B., Natta, A., Isella, A., Chandler, C.J., Pérez, L.M., Andrews, S., Wilner, D.J., Ricci, L., Henning, T., Linz, H., Kwon, W., Corder, S.A., Dullemond, C.P., Carpenter, J.M., Sargent, A.I., Mundy, L., Storm, S., Calvet, N., Greaves, J.A., Lazio, J. & Deller, A.T., *Multiwavelength analysis for interferometric (sub-)mm observations of protoplanetary disks. Radial constraints on the dust properties and the disk structure*, 2016, A&A, 588, 19. This paper describes how to self-consistently constrain the disk structure and the radial variation of the dust properties from high angular resolution observations at several (sub-)mm wavelengths, one of the key tools that will be used and further developed as part of the proposed project.

Dipierro, G., Pinilla, P., Lodato, G. & **Testi, L.**, *Dust trapping by spiral arms in gravitationally unstable protostellar disks*, 2015, MNRAS, 451, 974. This paper shows an example of the modeling of dust motion and trapping in protoplanetary disks, and how this may relate to observed features with ALMA and in scattered light observations.

Testi, L., Birnstiel, T., Ricci, L., Andrews, S., Blum, J., Carpenter, J., Dominik, C., Isella, A., Natta, A., Williams, J.P. & Wilner, D.J., *Dust Evolution in Protoplanetary Disks*, 2014, in Protostars and Planets VI, eds. Beuther, Klessen, Dullemond & Henning. This work discusses the methods and results to constrain the dust properties in planet forming disks. This is a review chapter in the "Protostars and Planets" book series, considered to be the "state of the art" review series of the field.

Isella, A., Guidi, G., **Testi, L.**, Liu, S., Li, H., Li, S., Weaver, E., Boehler, Y., Carperter, J.M., De Gregorio-Monsalvo, I., Manara, C.F., Natta, A., Pérez, L.M., Ricci, L., Sargent, A.I., Tazzari, M., and Turner, N., *Ringed Structures of the HD 163296 Protoplanetary Disk Revealed by ALMA*, 2016, Phys. Rev. Lett. 117, 251101. This paper shows detailed methods to derive dust and gas surface density profiles from ALMA observations and how to use them to constraint the presence of embedded young planets.

Mathews, G.S., Klaassen, P.D., Juhász, A., Harsono, D., Chapillon, E., van Dishoeck, E.F., Espada, D., de Gregorio-Monsalvo, I., Hales, A., Hogerheijde, M.R., Mottram, J.C., Rawlings, M.G., Takahashi, S., **Testi, L.**, *ALMA imaging of the CO snowline of the HD 163296 disk with DCO+*, 2013, A&A, 557, 10. This paper shows how measurements of gas lines of CO and its isotopologues can be used to infer properties of ices as a function of radius in the disk. Note that this is part of a strong collaboration with the team of

Prof. van Dishoeck, which will continue in this Research Unit.
Birnstiel, T., Ricci, L., Trotta, F., Dullemond, C.P., Natta, A., **Testi, L.**, Dominik, C., Henning, T., Ormel, C.W. & Zsom, A., *Testing the theory of grain growth and fragmentation by millimeter observations of protoplanetary disks*, 2010, A&A, 516, 14. This shows how a model of grain growth can be tested against with millimeter wave observations of protoplanetary disks. This is also an example of the strong collaboration between observational and theoretical groups that are part of this RU

2. Objectives and work programme

2.1 Anticipated total duration of the project

3 years

2.2 Objectives

To address the four questions **Q1**–**Q4** outlined in Section 1., it is essential to characterize observationally the dust and gas properties of TDs in the context of the evolving populations of planet forming disks. For this purpose, we will carry out a comparative study of the observational properties of TDs and full disks in evolving young stellar populations. The results of the observations will provide the data to develop and benchmark the theoretical studies and numerical simulations in all other areas of this Research Unit and in the wider community[1]. To this end, the final aim of this project is to provide the observational constraints on the dust and gas properties in disks based on ALMA observations, and making use of the complementary high contrast infrared imaging observations at the LBT and the VLT carried out within the project team (especially the group of Prof. Dr. Th. Henning).

The immediate objectives (O1 to O6) for this project can be outlined as follows:

O1 an homogeneous analysis of the ALMA surveys for the dust mass and surface density properties of disks in star forming regions in the Solar neighborhood. We aim in particular at determining the timeline for the evolution of the total solid mass and distribution as disks evolve during the planet formation phase (1-5 Myr), comparing the properties of full disks with TDs;

O2 an analysis of the overall level of grain growth and of the radial and vertical stratification of grain properties in disks. We will provide constraints on the dust evolution and transport models as a function of age and mass of the central star and morphology (full vs. TD) of the disks;

O3 an homogeneous analysis of the CO-gas content in disks in nearby star forming regions. The key goal will be to understand whether the apparent CO-emission deficit observed in disks at $\sim$3 Myr is due to an evolution of the gas-to-mass ratio or due to other (e.g. chemical) effects, comparing the properties of full disks with TDs;

O4 a detailed analysis of a selected sub-sample of protoplanetary disks observed by ALMA and the VLA at high angular resolution to characterize the dust properties as a function of the location in the disk and in relationship with key features related to disk evolution and disk-planet interaction, especially the development of the inner holes (TDs);

O5 a detailed analysis of a selected sub-sample of protoplanetary disks observed by ALMA at high angular resolution to characterize the properties of gaps (in full disks) and holes (in TDs) in the dust and gas surface densities, in relation to the possible presence of planetary mass companions;

O6 a detailed analysis of the gas kinematical properties in disks observed at high angular resolution, to derive constraints on the non thermal line broadening as a function of radius and height and to investigate the presence of kinematical evidence for disk-planet interaction.

[1] The text highlighted in green refers to the connection of this project to other projects of this Research Unit.

Table 1: Relationship between the six objectives of this project **O1**–**O6**, in combination of the outcome of other projects in the Research Unit, and the four outstanding questions outlined in Sect. 1..

	Objectives of this project						Other RU Projects						
Question	**O1**	**O2**	**O3**	**O4**	**O5**	**O6**	**A2**	**B1**	**B2**	**C1**	**C2**	**D1**	**D2**
Q1: Dust evolution	✓	✓		✓						✓	✓	✓	
Q2: Gas evolution			✓		✓		✓	✓	✓	✓			✓
Q3: Disk-wind-accretion			✓		✓	✓	✓	✓	✓		✓		
Q4: Disk-planet interaction				✓	✓	✓						✓	✓

These objectives, in combination with the outcome of other projects in the Research Unit,will provide the necessary observational constraints to address the four outstanding questions **Q1**–**Q4** outlined in section 1.. In Table 1 we show which of the six objectives, in combination with the outcome of other projects of the proposed Research Unit, will address each of the four questions.

The six objectives **O1**–**O6** are ambitious, but achievable with the available or planned observations, expertise and tools available to our group, as we detail in the sections below. The high angular resolution analysis for **O4**, **O5** and **O6** will initially focus on a subset of disks for which ALMA and high contrast infrared imaging are both already available or are being collected as part of approved programmes.

2.3 Datasets for the proposed project

To achieve the objectives **O1**-**O6** listed in paragraph 2.2 it is necessary to analyse a diverse set of ALMA observations. The ALMA data that we intend to use for this project comes either from (completed or scheduled) projects for which one of the team members is Principal Investigator, or from high-priority scheduled projects that will be completely observed in 2017 and for which the data will be publicly available in the course of 2018 through the ALMA Archive.

ALMA Data for objectives O1, O2, and O3.

In Table 2 we summarize the datasets already available for this projects and those that will be observed in the first half of 2017 (as part of ALMA Cycle 4), and will become public in the ALMA Archive by the end of 2018. The listed datasets will be sufficient for fully achieving **O1** and **O3**. The approved programmes and data will also allow us to obtain an initial set of results for **O2**, also including a comparison with previously published surveys (see Ricci et al. 2010ab and Testi et al. 2014). The available datasets are also shown in graphical form in Fig. 4, where we also mark with light symbols the objects for which XShooter spectra are available (which will be exploited in connection with project A2).

Additional observations may be requested as part of ALMA Cycle 5 (2017/2018) or Cycle 6 (2018/2019) to expand the ALMA 2-3 mm surveys. We see little risk in obtaining additional data at these wavelengths given the limited amount of time required, the strong science case, also based on the results of the complete ALMA surveys at 1.3 and 0.89 mm, and the fact that our team has a proven track record in obtaining ALMA data for this type of projects.

ALMA Data for objective O4, O5 and O6.

Objective O4 requires a combination of high angular resolution and high sensitivity data, to be able to resolve the gaps and holes and to detect at sufficient signal to noise ratio. There are several datasets either in the ALMA archive or scheduled to be observed that can be used. We will initially focus on three objects, in different evolutionary stages, for which detailed ALMA and VLA observations are available and for which we have acquired, or are in the process of acquiring, complementary high-contrast infrared observations: the young disk in HL Tau, the full disk HD163296, and the TD around

Table 2: ALMA disk surveys that will be used to address objectives **O1**, **O2**, and **O3**. For each star forming region we list the age, number of disks, range of stellar masses, objective for which they will be used, principal investigator (in bold face if collaborator to this project), status of the observations and expected data availability. All surveys have angular resolution in the range 0.2-0.5 arcseconds. The surveys useful for objectives **O1** and **O3** cover 1.3 or 0.89 mm continuum and CO and/or isotopes. The follow-up surveys useful for **O2** target the detection of the 3 mm continuum emission.

Region	age (Myr)	number of disks	star mass range ($M_\odot$)	Objectives O1	O2	O3	PI	status and availability
ρ-Ophiuchi	$\sim$ 1	$\sim$ 100	$\sim$0.1-2	✓		✓	L. Cieza	Schedued: Spring 2017
Corona Australis	$\sim$ 1	43	$\sim$0.2-2	✓		✓	**H. Baobab Liu**	Available, end 2016
Lupus	$\sim$ 2	89	$\sim$0.1-2	✓		✓	**J. Williams**	Available
		98	$\sim$0.1-2		✓	✓	**J. Williams**	Observed, exp. Jan 2017
		36	$\sim$0.1-2		✓		**M. Tazzari**	Available, end 2016
Chamaeleon I	$\sim$ 3	93	$\sim$0.05-2	✓		✓	**I. Pascucci**	Available
σ-Orionis	$\sim$ 4	34	$\sim$0.5-2	✓		✓	**J. Williams**	Observed, exp. Jan 2017
Upper Scorpius	$\sim$ 5	106	$\sim$0.15-1.7	✓		✓	**J. Carpenter**	Available
		24	$\sim$0.15-1.7		✓		L. Ricci	Observed; exp. mid 2017

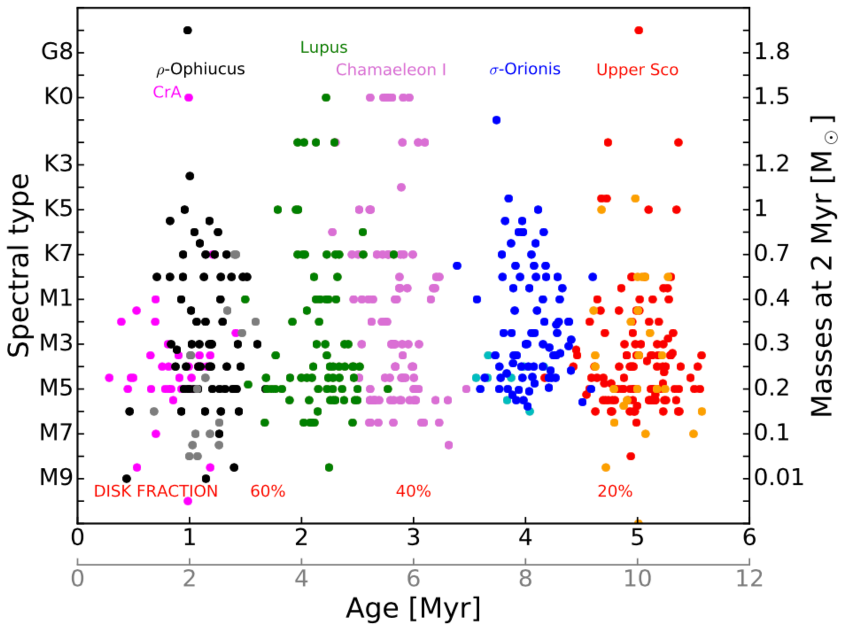

Figure 4: Samples for which ALMA observations of disks will be available for this project. The spectral types are actual measurements; the ages are assigned randomly to each point using the mean age and age dispersion in each region.

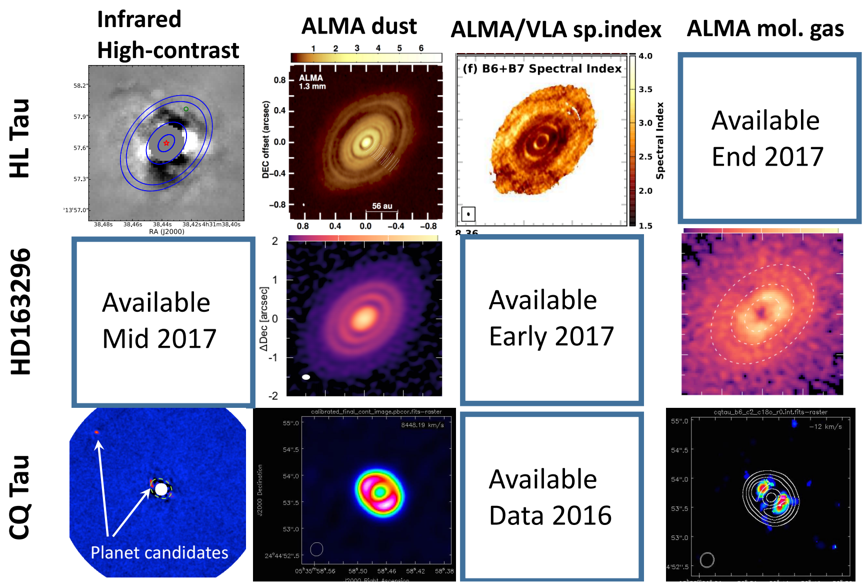

Figure 5: **From Top to Bottom:** available data for HL Tau, HD163296 and CQTau. In **each column** we show: the complementary high-contrast infrared data to search for planetary mass companions, the ALMA continuum image, the ALMA spectral index image, the molecular line integrated image. On the high contrast images we show the position of the gaps in HL Tau (Testi et al. 2015), and the position of the outer edge of the disk cavity in CQ Tau (Testi et al., in preparation); HD163296 will be observed at the Keck telescope with the high-contrast imager in Jun 2017. The ALMA continuum images are at 1.3 or 0.89 mm (ALMA Partnership et al. 2015; Isella et al. 2016, Perez et al. in preparation). New high sensitivity data from the VLA and ALMA will be used to construct the spectral index maps for HD163296 and CQ Tau (data being acquired); several ALMA programs aiming at observing the gas distribution in HL Tau, HD163296, and CQ Tau are in progress.

CQ Tau.

All three objects already have, or we expect to receive in early 2017 from ALMA and the VLA, multi-wavelength continuum observations that allow us to trace the dust properties at different disk locations. Our own and archival datasets will also provide observations of the molecular gas in the three objects. The initial modeling results that we aim to verify is that these three disks are in different stages of the planet formation process: HL Tau contains rocky cores of planets that can effectively create gaps in the dust, but not in the gas surface density; HD163296 has sub-jupiter planets able to open gaps of varying depth in the dust and gas distributions; CQ Tau contains large planets and is in an advanced phase of disk dissipation.

A summary of the available data on these three disks is shown in Figure 5, including the complementary high-contrast imaging data that our team is acquiring to complement this project. In addition to these three disks, for which our team has direct access to available or planned multi-wavelength ALMA and VLA observations, we are in the process of securing additional high-contrast NIR imaging and high-resolution ALMA observations for an extended sample of five additional disks (2 TDs and 3 full disks), for which ALMA data exist or observations are planned.

2.4 Tools for data analysis

In the last few years, our group has been developing and testing new tools to analyse planet forming disk observations and derive the properties of the dust and gas components. The two main tools that we expect to use and improve as part of this project are described below. The tools have been developed as part of two PhD Thesis at LMU and Leiden University.

Dust properties and surface density as a function of radius

As part of the PhD thesis of M. Tazzari at LMU (completed at the end of 2016), under the supervision of the project Applicant Dr. L. Testi and the Co-I Prof.Dr. B. Ercolano, we developed an effective analysis tool that can be used to derive the dust properties and surface density as a function of radius. The novel modeling toolkit, allows to efficiently model multi-wavelength continuum observations of disks at millimetre and radio wavelengths to self-consistently derive the disk physical parameters (including the dust surface density distribution) and the level of grain growth as a function of radius in the disk. This tool has been verified and successfully applied to observations of planet forming disks, allowing for a direct comparison with global dust evolution models in disks (Tazzari et al. 2016, Tazzari et al. in prep.).

The tool has three basic modules: a disk model, with parameters that describe the physical structure of the disk and of the dust population; an likelyhood calculator, which computes proper interferometric model visibilities and compares them with the data; and a highly efficient Markov Chain Monte Carlo sampler. We already tested the code modular approach by using different disk models (e.g. Guidi et al. 2016; Tazzari et al. 2016; Tazzari 2016), and we have made a considerable effort (in collaboration with the Excellence Cluster 'Universe' C2PAP in Munich and with the support of NVIDIA) to structure the likelyhood calculation and the MCMC sampler to fully use a multi-CPU/multi-GPU architecture (developed on our data analysis server at ESO and fully tested on the HYDRA cluster as part of the collaboration with Prof. Dr. P. Caselli group at MPE). This effort allows to run effective multi-wavelength analysis on large samples (typical full analysis time is currently 24hrs/disk with observations at four wavelengths), and opens the possibility of expanding the analysis to the fit of multiple velocity channels for simple line emission models.

Disk gas masses from ALMA observations

As part of her PhD thesis at the University of Leiden (to be completed in 2017) and under the supervision of project collaborator Prof. Dr. E. van Dishoeck, A. Miotello is developing an accurate method to measure the amount of molecular gas protoplanetary disks from CO and isotopologues millimetre observations. To overcome some of the difficulties in in deriving reliable gas surface densities from observations of line intensities, the method relies on a detailed chemical-physical computation of the disk dust and gas structure based on the infrastructure provided by the DALI code (Bruderer et al. 2012), including selective effects on the CO isotopologues. Miotello et al. (2016a) have used this method to derive measurements of the molecular gas content in disks using a combination of line luminosities in different CO isotopologues, improving on the method of Williams & Best (2014).

The application of this method to the Lupus ALMA disks survey Miotello et al. (2016b, see also Fig. 3) has shown a significant inconsistency between the disk masses measured using dust or CO as tracers. This inconsistency could be related to a real deficit of the gas content in the Lupus disks, or to unexpected chemical depletion of CO and isotopologues. In collaboration with the Lupus team, and as part of the last part of A. Miotello PhD, we are exploring which of these two possibilities is correct using multi-transition CO and isotopologues data coming from approved ALMA programmes. This new analysis will be used to improve the method in the course of 2017. In collaboration with the group of J. Williams in Hawaii, we also plan to expand the method to derive gas surface densities for spatially resolved observations of gaseous disks.

2.5 Work programme including proposed research methods

We request funding for two PhD students for three years to work on this project. Each student will be responsible for one of the two main sub-topics: evolution of the demographics of disk properties and evolution of the detailed physical properties of disks with embedded planets. The workplan for the two sub-topics is detailed below.

2.5.1 Evolution of the demographics of disk properties

Months 1-12

We will start with the detailed analysis of the continuum properties of the Lupus disks from the combination of the ALMA surveys at 0.89, 1.3 and 3 mm. Dust emissivity, surface density and temperature distributions are key uncertainties when deriving disk dust masses from sub-mm observations. The combination of the multi-wavelength observations of the Lupus disks will allow to greatly reduce the uncertainties. Using the modeling tool described in Sect. 2.4) we have already investigated the possibility of refining the dust mass estimates by applying a correction that depends not only on the stellar luminosity (see the attempts by Andrews et al. 2013; van der Plas et al. 2016), but also on other parameters like the radial extent of the millimetre wave emission (Tazzari et al. 2017). These initial results need to be validated using the multi-wavelength sample, in order to check for potential systematic effects introduced by the varying dust properties (see e.g. Banzatti et al. 2011; Trotta et al. 2013; Tazzari et al. 2016). All the data for this analysis is available, as the data has been delivered at the end of 2016. We also expect that at the beginning of the project all Lupus datasets will be already calibrated and ready for analysis.

The modeling procedure is already fully developed and tested on the single wavelength Lupus data, the key result that we will obtain for each modeled disk, once we add the multi-wavelength observations, will be: the total disk mass, the average dust properties (and possibly an indication of the dust properties as a function of radius), and the radial extent of the disk containing the bulk of the dust mass. The collaboration with M. Tazzari, will be crucial in this phase of the project and the student may spend some time (4-6 weeks) visiting the Institute of Astronomy in Cambridge (UK), where Tazzari is a postdoc. From our initial results on the Lupus 0.89 mm survey, we estimate that we will be able to carry out this analysis to almost half of the Lupus sample ($\sim$ 35 disks). This sample contains 7-10 TDs (seven previously known, plus three that we have preliminarily reclassified as TDs), so we will also be in the position of addressing a first systematic assessment of the comparison of dust properties of TDs versus full disks. The results will be an important initial benchmark for the models developed in projects C1 and C2.

During this period the student will also learn how to prepare the data from the other surveys available for this analysis. We will collect and re-process the ALMA data in a uniform way and, for all regions, we will use the optical/infrared spectroscopic data and methodology of Pascucci et al. (2016) to recompute the stellar parameters, as this is a more robust technique than the one used in the initial studies of Ansdell et al. (2016) and Barenfeld et al. (2016).

Single wavelength data for the dust continuum emission and stellar parameters will be available at the end of this period for the following star forming regions (on top of Lupus): Corona Australis, Chamaeleon I, σ-Orionis, Upper Scorpius. The line data will also be calibrated, but not analysed yet, at this stage. Proposals will be submitted to ALMA to expand the multi-wavelength samples, and additional data may become available, but it will not be critical for the success of the project.

Products:

- One publication on the dust properties and continuum masses in the Lupus cloud, including a comparison between full disks and TDs.
- ALMA proposal to extend the studies of the multi-wavelength dust properties to other regions beyond Lupus and Upper Sco
- Datasets and methods ready for the comparative analysis of different star forming regions

Months 13-24

We will develop the statistical tools to compare the dust measurements in the different regions. Different regions have different properties in terms of the stellar populations, fractions of stars with disks and completeness of the surveys. These limitations have not been taken fully into account in previous comparisons between the properties of disks in different star forming regions (e.g. Ansdell et al. 2016; Pascucci et al. 2016). To take into account the sampling and completeness biases, we will compare observational data to Monte Carlo simulations, building on and extending the methodology developed by Andrews et al. (2013).

The comparative study of the properties of the continuum emission of all star forming regions planned in this study will be completed in this phase. This will include the disks in ρ-Oph if the ALMA data will be available in time. This analysis will be made possible combining the dataset and expertise of the project collaborators (see Table 2), especially the groups of Prof.Dr. Th. Henning and Prof.Dr. Ewine van Dishoeck. The comparative study of dust properties in evolving populations of disks will provide the key benchmarks for the models developed by projects C1 and C2.

The database will be extended to include the molecular line maps of the disks.

Products:

- One publication on the comparative properties of dusty disks in star forming regions as a function of age, including a comparison between full disks and TDs (achieving objectives **O1** and **O2**).
- Statistical methods ready to be applied to the analysis of the gas properties

Months 25-36

The demographical analysis of the gas properties will be carried out during the third year. This analysis will be carried out as part of the collaboration with A. Miotello, J. Williams and the group of Prof.Dr. Ewine van Dishoeck, using the methods that are currently being refined and are described in Sect. 2.4. For this analysis we will use the simplified fitting functions, rather than performing a full chemical modeling of each disk, which would be a prohibitively time consuming activity if applied to all the disks in our surveys. The fitting functions provided by Miotello et al. (2016a) will be improved following the ongoing studies (as described in Sect. 2.4), in addition, as part of our collaborations, we are planning to extend the model grids for a range of the stellar photospheric parameters. These new grids will be applied to derive more accurate measurements of the gas content to be compared with the solids content in disks as a function of the evolutionary status. As part of the outcome of this analysis we will also compare the results of the analysis of the gas in disks with the measurements of the M_{acc} as derived from our optical spectroscopy database.

Our results on the demographical properties of gas in disks will be an essential asset, in combination with the outcome of project A2, for the benchmarks of the assumptions and results of the models developed as part of projects B1 and B2, but will also be important constraint for project C1.

Products:

- One publication on the comparative properties of the gas content in disks in star forming regions as a function of age, including a comparison between full disks and TDs (achieving objective **O3**).
- Investigation of the possible evolution of the overall gas-to-dust ratio in disks as a function of age, evolutionary stage and stellar parameters; with particular emphasis on determining possible population differences between full disks and TDs

2.5.2 Evolution of the detailed physical properties of disks with embedded planets

Months 1-12

In this first phase we will collect and reprocess the ALMA and VLA high angular resolution observations of CQ Tauri and HD163296 (the HL Tau continuum data are already available). The expert postdoctoral Fellow at ESO and collaborator on this project (Baobab Liu) will support this data calibration effort.

As the reprocessing will be completed, we will perform the multi-wavelength continuum analysis of one of the disks HD163296 or CQTauri, for both the data is available, or in the process of being delivered to us. The analysis method that we plan to apply will be similar to the one that we already adopted with HL Tau (Carrasco-González et al. 2016), as part of a collaboration between the ESO group and the group of Prof.Dr. Th. Henning in Heidelberg. The results will be compared against the models of dust growth, confinement and migration developed as part of project C1, D1 and D2.

The most significant part of the time for this first year will be used to modify the model part of the multi-wavelength analysis tool to incorporate a fast (parametric) computation of the line emission. We have already developed a parametric model to describe line emission for our recent work on HD163296 (Isella et al. 2016), and we plan to incorporate an optimized version of this model in the analysis tool. We will develop this as part of the multi-CPU/multi-GPU version of the analysis code. The main modifications that we will implement in the model are a parametric description of the position of gaps and holes in the disk and the associated gas and dust depletion factors; a version that allows for an analysis of gaps and rings in the dust emission is already working (e.g. Guidi et al. 2016), but we need to add the modifications required for the analysis of the gas.

In this phase we also plan to submit additional proposals to extend the ALMA observations to more disks. These additional data are not essential for the success of the project, but will be incorporated in the program if the proposals are successful.

Products:
- One publication with the application of the continuum analysis tool to one of the disks observed at high angular resolution with ALMA
- New version of the analysis code with incorporated the model required to perform a parametric analysis of the dust and gas emission in disks with gaps and holes

Months 13-24

The second year will be dedicated to the extensive use of the molecular line analysis tool to the line observations of the disks. We will start by benchmarking the tool against the results of previous lower resolution observations of disks or disks that we have already been analysed with less sophisticated techniques (e.g. Isella et al. 2016). This approach was successfully used to develop and test the continuum analysis tool by Tazzari et al. (2016), and we will extend it to the line analysis.

One key additional aspect for the line analysis tool will be to benchmark its results against the results of the more computationally intensive detailed chemical models for the molecular abundance and excitation in disks. Hence one key benchmark of our analysis tool will be against the results obtained by the detailed modeling using the DALI code of transition disks with holes (van der Marel et al. 2016b). For this purpose the collaboration with the group of Prof.Dr. Ewine van Dishoeck and A. Miotello will be essential.

During the course of the second year, we do expect to complete the benckmarking of the analysis code against previous observational results and against detailed model simulations with DALI. We will also complete the analysis of the continuum data of the disk that was not completed in the first year and start to apply the line analysis tool.

If the ALMA proposals submitted in the first year will be successful, the ALMA data will be collected and delivered during the second year. In this case, one of the collaborators in the project will support checking and calibration of the data and the preparation for the subsequent analysis.

Products:
- One publication with the benchmarking of the line analysis tool
- One publication on the analysis of the continuum data for the remaining disk in the original sample and comparative analysis: completion of objective **O4**
- Inital application of the analysis tool to the high resolution line data for one of the disks in the original sample

Months 25-36

The analysis of the disks observed at high angular resolution and high sensitivity multi-wavelength ALMA observations and complementary high-contrast near infrared imaging will be completed in this final year, applying the modeling tool modified in the first phase of the project. Including the results of the analysis methods for the gas to derive a reliable measurement of the gas surface density in these disks. The data will be compared with models developed as part of other projects in the RU to understand if the different dust and gas properties and the potential detection of planetary mass companions are consistent with an evolutionary scenario. In particular this will be relevant for projects C2, D1 and D2 of the RU. The data will constrain the model predictions for the development of gaps (in dust and gas) in the two full disks, and the hole and dust/gas properties in the TD.

In particular we aim at a full comparative analysis between (at least) the three disks of: dust distribution and grain properties and the gas surface densities. We will also focus on the characterization of the mm-size dust and molecular gas depletion factors in rings and holes, and the comparison with constraints form the complementary NIR high-contrast observations on the potential planetary mass companions. This challenging work will be possible by combining the strengths and expertises of the observational/analysis groups of Testi, Henning and van Dishoeck. The theoretical/modeling groups in the RU will provide the essential link with the theoretical disk-planet interaction expertise.

Products:

- One summary pubblication with the comparative high angular resolution analysis of gas in disks in different evolutionary stages (objective **O5**)
- One publication on the detailed comparison of the gas kinematics with models (objective **O6**)

2.6 Data handling

ESO is acquiring a dedicated computing cluster for the processing of science data from ALMA (and other observatories/instruments). The computing cluster architecture is copied from the ALMA Regional Centre Cluster architecture, this ensures that all ALMA data processing applications can be used and will work at peak efficiency. We expect to have direct access to this system once will be installed and open to the ESO astronomers (expected by February 2017).

Our group at ESO has direct access to a high-end server that we used for the analysis of the Lupus disks presented in Tazzari et al. (2017, in prep.). This server has an hybrid multi-CPU (2 CPUs with 14 compute cores, each capable of double threading), multi-GPU (2 NVIDIA Tesla-K40) architecture that we used to develop and test the advanced data analysis software developed in Tazzari (2016).

We have access to, and we will continue to use, the computing facilities in the Garching campus offered by the Excellence Cluster (the C2PAP cluster) and the Max Planck Institutes (the Hydra cluster). We have already been using these facilities to successfully and effectively model the dust properties and distribution in protoplanetary disks (Guidi et al. 2016; Tazzari et al. 2016; Tazzari 2016).

Given the large amount of data analysis for this project, we will need to upgrade the fast-io storage of the server in our group, which is required for effective ALMA data processing in CASA. In addition we require a high-end desktop computer with a large data storage external drive for post processing and analysis of the data. To share data and analysis results with the rest of the team, we plan to use one of the commercially available cloud storage services (e.g. Dropbox, GoogleDrive, OneDrive, etc).

As part of this project, we will make available the re-processed ALMA data via a dedicated website. The data will be released in progressively together with the publication of the research papers.

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4. Requested modules/funds

4.1 Basic Module

4.1.1 Funding for Staff

As part of this project we plan to employ two PhD students (75% E13) that will be enrolled at the Ludwig Maximillian Universitaet in Munich and will carry out their work on the project at the ESO headquarters in Garching bei Muenchen.

4.1.2 Direct Project Costs

4.1.2.1 Equipment up to EUR 10,000, Software and Consumables

- **desktop:** high-end desktop for ALMA data analysis (4k€)
- **storage:** upgrade of the ESO data reduction server fast-io storage (3k€)
- **storage:** external slow (e.g. USB disk) large storage (30Tb class) for project data (1.5k€)
- **storage:** cloud storage service for collaboration data sharing (1.5k€)

Total equipment cost: 10k€

4.1.2.2 Travel Expenses

Travel within the Research Unit is handled in project Z. In addition we request funding for conference travel for the personnel and one Applicant. This includes one national (1.000 €) and one international (1.500 €) conference trip per year, totalling 2.500 € per person per year.

For this project this totals 7.500 € per year for the two PhD students and one Applicant, which is in total 22.500 €.

4.1.2.3 Visiting Researchers (excluding Mercator Fellows)

Given the distributed nature of the collaboration, including collaborators in USA and Chile, we expect to host 2 1-week visits per year. Typically, we expect each visit to cost 0.5-1k€, depending on the trip details and assuming that these visits will be connected to other trips to Europe for the overseas visitors (which would then require just an intra-european trip extension). We thus estimate a total expense of 5.000 € for the visits.

4.1.2.4 Other Costs

Given the distributed nature of the collaboration, we expect to organize one team meeting in Munich for this project. We thus require funding to cover the general expenses of the organization of the meeting (2k€).

Total other expenses: 2k€

4.1.2.5 Project-related publication expenses

We request 750€ per year (a total of 2 250€) for publication expenses, mainly to support open access options or whenever necessary, publication in non-free journals.

5. Project requirements

5.1 Employment status information

Leonardo Testi, Full Astronomer at ESO (permanent)
Barbara Ercolano, Professor at the Ludwig-Maximilians-Universität München (permanent)
Thomas Preibish, Professor at the Ludwig-Maximilians-Universität München (permanent)

5.2 Composition of the project group

Dr. H. Baobab Liu, Postdoctoral Fellow at ESO, he is an expert in ALMA data calibration and PI of one of the major surveys that will be used in this project
Dr. J.M. Carpenter, ALMA Observatory Scientist at the Joint ALMA Observatory in Santiago de Chile (permanent NRAO staff member), he is an expert of ALMA observations in general and of millimetre continuum observations of disks in particular, he is PI and Co-I of some of the ALMA surveys that will be used for this project
Prof. Dr. Th. Henning, Director of MPIA (permanent), he is an expert of disk, dust and gas physics, his department at MPIA is heavily involved in disk surveys with high-contrast imagers at LBT and VLT and also with ALMA and VLA observations of planet forming disks, he is Co-I of ALMA and VLA surveys as well as key complementary data used for this project
A. Miotello, currently student at Leiden University, has been offered a 3-yr ESO postdoctoral Fellowship starting Fall 2017, she has been developing the analysis tool to derive the disk gas content from CO and isotopologues ALMA measurements that will be refined and used for this project
Dr. M. Tazzari, postdoc at the Institute of Astronomy in Cambridge (UK), he has been developing the analysis tool to derive the dust properties from multi-wavelength observations of disks, this tool will be further developed and used for this project
Prof. I. Pascucci, University of Arizona (permanent), she is an expert of disk physics and planet formation, she is PI of ALMA surveys used for this project
Prof. Dr. E. van Dishoeck, University of Leiden and MPE (permanent), she is an expert of astrochemistry and disk physics, her expertise is critical for the measurements of the gas properties in disks and she is Co-I of many of the ALMA surveys used in this project
Prof. J.P. Williams, University of Hawaii (permanent), he is an expert of continuum and gas emission from planet forming disks and is PI of some of the ALMA surveys that will be used for this project.

5.3 Cooperation with other researchers

5.3.1 Planned cooperation on this project

5.3.1.1 Collaborating researchers for this project within the Research Unit

Within the RU, this project focuses on deriving the observational constraints on the cold dust and gas components of the disks. Using mainly ALMA and VLA observations, complemented by high-contrast near infrared observations, we will constrain the demographical properties of evolving disk populations and the detailed properties of a small sample of disks in different evolutionary stages. Our project will thus provide observational results that will be combined with those of project A2. The combined results of A1 and A2 together will be essential to assemble a consistent dataset to describe the demographical evolution of young star-disk-wind systems. The collaborations with the groups of Prof.Dr. Ewine van Dishoeck and Prof.Dr. Thomas Henning will also be key to achieve our goals, given the complementary datasets and analysis tools they will enable us to access.

The dust properties, evolution and detailed analysis in a subset of disks that we plan to complete will be used in the context of projects C1, C2, and D1. The modeling tools developed as part of those projects will be used to interpret correctly our observational results.

The accurate measurements of the molecular gas properties of disks that we will obtain, will be an essential benchmark for the models developed as part of projects B1, B2, and C2. The combination of the models in B1, B2, and C2 with the observations of the dust/gas components of the disk and the wind/accretion properties derived combining with the results of A2, will all be necessary to derive a consistent picture of the effects of winds on disk evolution and dissipation.

The high angular resolution studies of the dust and gas properties in disks in different evolutionary stages, combined with the complementary high-contrast nir observations, will be used in collaboration with projects C1, D1, and D2

The connections between our project and the other RU projects is also summarized in Table 1.

5.3.1.2 Collaborating researchers for this project outside of the Research Unit

For this project, we will strongly collaborate with the groups of Dr. John Carpenter (JAO/NRAO), Prof. Ilaria Pascucci (Univ. of Arizona), and Prof. Jonathan Williams (Univ. of Hawaii), as they are part of a collaboration, which include other members of the RU, to obtain ALMA surveys of the evolving disk populations in star forming regions in the Solar neighbourhood (see Table 2).

Collaborations with Dr. Claire Chandler (NRAO), Prof. Andrea Isella (Rice Univ.), Dr. Laura Perez (MPIfR, Univ de Chile) are well developed and will continue on the high angular resolution observations with ALMA and VLA of individual disks.

Collaborations with Dr. Juan Alcala (INAF), Dr. Carlo Manara (ESA) and Brunella Nisini (INAF) will enable us to access the the optical and near infrared determination of the photospheric properties of young stars, their mass accretion rate and winds, in synergy with project A2 within our RU.

On top of the strong connections with the modeling expertise of the other groups within the RU, mentioned above, we also have strong connections, which will continue in the coming years, with the groups of Prof. Cathie Clarke (IfA, Cambridge) and Prof. Lodato (Univ. of Milano) for the interpretation of our observations.

5.3.2 Researchers with whom you have collaborated scientifically within the past three years

J.M. Alcalá (INAF), S. Andrews (CfA), R. Cesaroni (INAF), C. Chandler (NRAO), C. Codella (INAF), A. Ginsburg (NRAO), I. de Gregorio-Monsalvo (JAO, ESO), G. Guidi (INAF), G. Herczeg (Kavli-Beijing), A. Isella (Rice University), I. Jimenez-Serra (QMUL), A. Maury (CEA Saclay), C. Manara (ESA), S. Molinari (INAF), A. Natta (DIAS, INAF), L. Perez (MPIfR, UChile), L. Ricci (Rice University), G. Rosotti (IoA), A. Sargent (Caltech), A. Scholz (St. Andrews), M. Walmsley (DIAS, INAF)

5.4 Scientific equipment

Our group at ESO has direct access to a data reduction server equipped with 2 Intel E5-2683 v3 CPUs, each with 14 cores with multi-thread capability, two NVIDIA Tesla K40 GPUs, 512Gb RAM, 12 Tb of conventional HDD capacity and 2Tb of fast-io SSD capacity. The server is used to reduce ALMA data and to develop the disk analysis tool.

For running intensive computing applications we have access to the C2PAP infrastructure and to the multi-CPU/multi-GPU Hydra cluster at the local Max Planck (through the collaboration with Paola Caselli group).

ESO is in the process of expanding the ALMA data reduction capabilities for the science staff by cloning the ALMA Regional Center processing cluster architecture. The new cluster will initially be composed by a Lustre file system and three computing nodes each with $\geq$512Gb RAM and 24-48 cores. The new cluster is expected to be installed in the first quarter of 2017 and will be available for the analysis of the ALMA data for this project.

Project A2:

New constraints on disk-dissipation processes from the relation between accretion and X-ray activity

Authors:
Applicant: Thomas Preibisch (LMU)
Co-Applicant: Barbara Ercolano (LMU), Leonardo Testi (ESO)

Requested positions: 1 PhD student

Abstract:
As discussed in the general introduction, Type I transition disks (TDs), which present small inner cavities and a depleted accretion signature, are thought to be objects caught in the act of dispersal. Photoevaporation from X-ray radiation from the central star is thought to be the main driver in the dispersal of disks around solar and later-type stars.

We want to test models of X-ray driven disk photoevaporation leading to the formation of transition disks by using new observational data to study the relation between accretion rates of young stars and their X-ray emission. The aim is to combine the numerous available high-quality X-ray data of young stars in different regions with new and highly reliable accretion rates that can be derived from the new spectroscopic data on these stars. In this way, we will be able to study the relation between X-ray emission and accretion with much larger samples (hundreds of stars rather than just a few dozen) and for different regions spanning a range of ages, and to test the predictions of theoretical models of X-ray driven disk photoevaporation and the corresponding effects on the disk accretion rate. This is of fundamental importance to understand the formation and residual accretion rate distribution of transition disks.

1. State of the art and preliminary work

a) Scientific Context: the evolution of circumstellar accretion disks

In this project we want to study the connection between the X-ray radiation of young stellar objects and the properties and temporal evolution of their accretion disks. In order to define the scientific context, we start here with a very brief description of the evolution of young stellar objects (YSOs), which proceeds through a sequence of stages with different characteristics. In order to keep the text concise, it is written with a minimal amount of references; for a much more comprehensive and detailed description and references to the literature we refer to the monograph of Hartmann (2008) and the recent reviews of Alexander et al. (2014) and Hartmann et al. (2016).

When a cloud core collapses, angular momentum conservation naturally leads to the formation of a circumstellar accretion disk around the protostar. After a few 100 000 years, most of the material in the original envelope around the YSO has either collapsed onto this disk or was blown away by the outflows typically driven from protostars. The photosphere of the YSO becomes directly visible at infrared and optical wavelengths for the first time, and the YSO enters the *"T Tauri star"* (TTS) phase. The photospheric emission allows to determine the luminosity and effective temperature of the TTS. The spectral energy distribution of TTS shows an infrared excess that is caused by the warm dust in

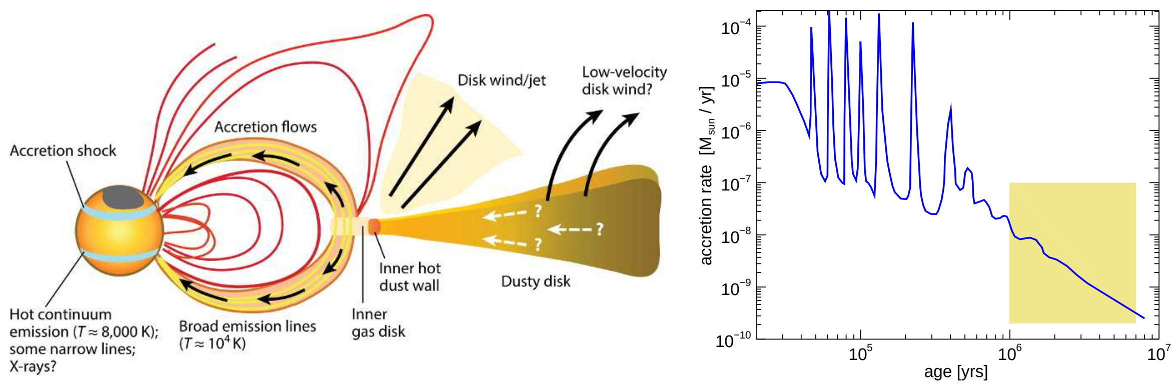

Figure 1: **Left:** Reproduction of Fig. 1 from Hartmann et al. (2016), illustrating the main features of disk accretion in YSOs. **Right:** Schematic illustration of the temporal evolution of the accretion rate (adapted from Hartmann 2008). The light-brown shaded area marks the age range we address in this project.

the disk and allows to estimate the masses of the circumstellar disks, typically a few percent of the stellar mass.

Objects in the evolutionary phase of *"classical T Tauri stars"* (CTTS) are observationally characterized by strong optical emission lines ($W(\mathrm{H}\alpha) \geq 10\,\text{Å}$), which are caused by accretion of circumstellar material onto the young star. Typical accretion rates in the CTTS phase are of order $\dot{\mathrm{M}} \sim 10^{-8}\,\mathrm{M}_\odot/\mathrm{yr}$. The accretion of matter from the circumstellar disk onto the central star is thought to be magnetically controlled. Stellar magnetic field lines connect the stellar surface to the surrounding disk (see illustration in Fig. 1) and lead to a truncation of the disk at or near the co-rotation radius, i.e. the radius where the Keplerian angular velocity of the disk matches the stellar angular velocity, typically a few stellar radii. The magnetic field lines connecting the disk to the star produce a complex 3D system of "accretion funnels" that channel the accretion flow to the stellar surface. The gas in the accretion funnels reaches free-fall velocities of several 100 km s^{-1} and finally generates shocks at the (proto-)stellar surface. This hot shocked gas produces the UV and optical excess emission and the strong optical emission lines of CTTS.

During the following few Myrs, the disk mass decreases, as some part of the circumstellar matter is accreted onto the star and another fraction is removed by a disk wind. As a consequence, the accretion rate also drops and the spectroscopic signatures of disk accretion get weaker; the object evolves into a so-called *"weak-line T Tauri star"* (WTTS). During this evolution, the structure of the accretion disk also changes. Observational evidence shows that many of these older disks seem to evolve an inner hole in the disk, i.e. the dust in the inner few AUs of the circumstellar environment is somehow cleared (e.g., Alexander et al. 2014; Koepferl et al. 2013). This typically happens at an age of roughly 2 ... 5 Myr, and the result is a so-called *"transition disk"* (TD) (see Owen 2016).

In the subsequent evolution, the remaining material in the outer disk is dispersed by a strong disk wind. This final disk dispersal process is very rapid ($\sim 10^5$ years) and proceeds from inside-out (Ercolano 2014). As described below in more detail, the irradiation with ionizing radiation from the central star seems to be the most important driving mechanism for this disk wind.

In the course of this evolution, the accretion rate generally decreases with time. During the very young, protostellar stages, the accretion process shows strong variability on a wide range of timescales, including rare (see Hillenbrand & Findeisen 2015), but very strong bursts of very rapid accretion (FU Ori bursts), during which the accretion rates can be enhanced by one or more orders of magnitudes for timescales from months to decades (see Hartmann et al. 2016, and the illustration in Fig. 1). With increasing age (and correspondingly lower average accretion rates), however, the frequency as well as the amplitude of the accretion rate bursts is strongly decreasing, and at ages of ≥ 1 Myr (i.e. in the

TTS stage) the accretion variability is typically less than a factor $\sim 2 - 3$ (see Venuti et al. 2014).

Although this description is mainly based on theoretical arguments and numerical simulations (Ercolano et al. 2011; Alexander et al. 2014), it is well supported and confirmed by an increasing body of new observational data that were collected during the last several years. In particular, numerous observations have clearly established that the fraction of YSO with optically thick disks decreases very quickly with age. The inferred (e-folding) lifetime of these disks is only about 2–3 Myr, and the fraction of disks in clusters with ages of > 5 Myr is very low (e.g., Hernández et al. 2007). This yields a clearly established upper limit to the lifetime of protoplanetary disks of less than 10 Myr, which provides a very important constraint for theories of planet formation (especially the formation of gas-giants).

While the general picture of the accretion process on YSOs is now quite well established, several observational facets of the accretion and disk evolution processes are still not well understood. One of these open questions concerns the explanation of the rather wide distribution of individual disk lifetimes around the median lifetime of about 2.5 Myr. The observational data show that some 15% of the stars disperse their disks very quickly, within just about 1 Myr. On the other hand, a similar fraction of stars manage to keep their disks even at ages of more than $5 - 6$ Myr. The exact reason for this considerable differences in disk lifetimes is not yet well known. This is important as the lifetime of a disk determines the timescale over which (giant) planet formation must occur. Hence the success of a given system in producing a planetary system containing gas giants strongly depends on this.

A second important question concerns the explanation of the observed wide range of individual stellar accretion rates. Observations of young clusters, where all the stars have a very similar age, indicate that for any given stellar mass, the accretion rates show a scatter of at least two orders of magnitude (see, e.g., Fig. 16 of Venuti et al. 2014). The reason why stars with the same age and mass display such a wide range of accretion rates is also not yet clear and may be related to the disk dispersal process (Owen, Ercolano & Clarke 2011; Ercolano 2014).

An aspect of fundamental importance in this context is that the disk is not just a passive “road” for the accreted material, but there is a close interconnection and interaction between the TTS and its disk. The properties of the disk determine the global accretion rate (e.g., via the viscosity) as well as the details of how the disk material is finally deposited onto the stellar surface. This determines not only how fast the star can gain mass via accretion, but also influences the temporal evolution of the internal stellar structure (and thus influences the luminosity of the protostar) as well as the evolution of its rotation rate (which is important for magnetic dynamo activity). Recent studies also suggest that the early accretion history impacts the stellar properties even after several Myr, i.e. long after the accretion process has ceased (see Baraffe et al. 2016).

On the other hand, the luminosity of the central star (which results partly from the release of gravitational energy in the accretion shock at the stellar surface) determines the irradiation of the disk, which is a major heating source for the disk and strongly influences its temperature structure. This also affects the accretion rate in the disk, which depends strongly on the temperature and the microphysical properties on the disk (e.g., via the viscosity).

As will be described below in more detail, recent results clearly suggest that the high-energy radiation of the young star, and in particular the X-ray emission, plays a very central role in the evolution and final dispersal of the circumstellar disk (Ercolano et al. 2008a,b, 2009; Owen et al. 2010; Owen, Ercolano & Clarke 2011; Owen et al. 2012).

This intricate interconnection and interaction between the evolution of the star (mass growth rate, rotational evolution, magnetic dynamo activity, level of high-energy radiation) and the evolution of the disk (time dependence of the accretion rate and the disk mass-loss rate) constitutes several feedback loops and is thus of fundamental importance for the understanding of the evolution of YSOs.

In recent years, circumstellar disks evolved into an extremely prominent research topic because they are the sites where planets form. The properties of the disk around TTS determine the conditions under which the planets form and the observational upper limit on the disk lifetime places very severe constraints for planet formation theories. This highlights the fact that a good understanding of the properties and the evolution of circumstellar disks is also highly relevant for our theories about planet formation and early evolution.

Since the above mentioned (mostly theoretical and numerical) studies of the star-disk interaction suggest that stellar X-ray emission is of enormous importance for the structure and the evolution of disks, it also has far-reaching consequences for the planet formation process (Ercolano & Rosotti 2015; Rosotti et al. 2013, 2015). It is therefore very important to test these models for disk evolution and disk dispersal against observations. For this, a solid understanding of the X-ray emission properties from YSOs is a basic requirement.

b) X-ray emission from YSOs

Numerous X-ray observations obtained during the last decades have clearly established that YSOs in all evolutionary stages from protostars to ZAMS stars show highly elevated levels of X-ray activity (Feigelson & Montmerle 1999; Preibisch, Zinnecker, & Herbig 1996; Preibisch & Zinnecker 2002; Preibisch et al. 2005, 2011, 2014). Typical X-ray luminosities of $\sim$ solar mass YSOs are about 10^{30} erg/s, i.e. are up to $\sim 10^4$ times higher than seen in our current Sun. The temperatures of the X-ray emitting plasma on young stars are typically 10 to 20 MK, i.e. about ten times higher than in the solar corona. The X-ray emission of the young stars is therefore considerably harder than the solar X-ray spectrum, and contains substantial fluxes in the energy range above 3 keV.

Although the relations between the X-ray activity of young stars and their stellar / circumstellar parameters were investigated in many star forming regions, nearly all of these studies suffered from limited sensitivities and corresponding incomplete X-ray detections. These problems were finally solved with the *Chandra* Orion Ultradeep Project (COUP), a uniquely deep (10-day long) observation of the Orion Nebula Cluster (ONC) with *Chandra*/ACIS (for details of the observation and data analysis see Getman et al. 2005). It is still the deepest and longest X-ray observation ever made of a young stellar cluster and produced the most comprehensive dataset ever acquired on the X-ray emission of young stars (Preibisch et al. 2005). Nearly all of the 1616 detected X-ray sources could be unambiguously identified with optical or near-infrared counterparts. With a detection limit of $L_{X,\mathrm{min}} \sim 10^{27.3}$ erg/sec for lightly absorbed sources, X-ray emission from more than 97% of the $\sim$ 600 optically visible and well characterized late-type (spectral types F to M) cluster stars was detected (Preibisch et al. 2005). Since the COUP TTS sample is *complete*, the COUP data do not suffer from the selection effects that plague the less sensitive X-ray studies of other young clusters, where a considerable fraction of the lowest mass stars remained undetected.

Two results of fundamental importance for the proposed project derived from the COUP data are, that

1. X-ray luminosity scales to stellar mass as $L_X \propto M^{1.4}$ (Preibisch et al. 2005), and
2. the X-ray luminosity of TTS is approximately constant for $\geq$ 10 Myr (Preibisch & Feigelson 2005) i.e., during the full period of time for which disks usually exist.

The COUP data also confirmed that the strong X-ray emission from YSOs is predominantly originating from a hot, magnetically confined plasma in the stellar corona, which is the result of magnetic dynamo activity (Preibisch et al. 2005). The high X-ray activity levels are thus thought to be ultimately a consequence of the very fast rotation of the young stars (e.g., Alexander & Preibisch 2012).

Theoretical arguments suggest that the strong X-ray emission of young stars has far-reaching implications for the physical structure and processes in their circumstellar environment (e.g., Glassgold et al. 2005; Wolk et al. 2005; Ercolano & Glassgold 2013), the evolution of the disk (e.g., Ercolano 2014), the formation of planetary systems (e.g. Ercolano & Rosotti 2015), and the evolution of the atmospheres of young planets (e.g., Johnstone et al. 2015). However, detailed observational diagnostics for these suggested influences have been hard to come by, so far. One of these topics is the question we want to address in this project: How does the X-ray emission affect the evolution of the protoplanetary accretion disks?

c) Previous observational results on the relation between X-ray emission and accretion disks

About 15 years ago, X-ray observations of young stellar clusters provided the first indications that the X-ray luminosities of young stars seem to depend on the presence and the properties of accretion disks (e.g. Stelzer & Neuhäuser 2001). However, no strong conclusions could initially be drawn due to problems related to small sample sizes, incompleteness of the X-ray detected samples, and ambiguities about the disk properties. A fundamental clarification of the tentative relations between X-ray emission and the properties of accretion disks was finally provided by the COUP data. COUP showed unambiguously and in a statistically significant way that the absolute as well as the fractional X-ray luminosities of accreting young stars are systematically *lower* by a factor of $\sim 2-3$ than the corresponding values for non-accreting stars.

In order to find possible explanations for this surprising result, a more detailed analysis of the relation between X-ray emission and disk accretion is required. The best data on accretion rates and accretion luminosities available at the time of the COUP project were those from the study of Robberto et al. (2004), who had determined accretion rates and accretion luminosities for 30 young stars in the Trapezium cluster from Hubble Space Telescope *U*- and *B*-band photometry. The COUP data showed a weak anti-correlation of the fractional X-ray luminosity with accretion rate (and also with accretion luminosity). However, the statistical significance of this result was low, because the number of stars for which estimates of the accretion rate were available at that time was too small. Nevertheless, these results were supported by similar findings from a deep X-ray survey of the Taurus star forming region, which also showed that the X-ray activity of accreting young stars appears to be somehow suppressed (Briggs et al. 2007).

Several possible explanations for this anti-correlation between X-ray activity and mass accretion rate were suggested. One model assumed that changes in the coronal magnetic field structure by the accretion process could lead to lower X-ray emission (Romanova et al. 2004). This idea was based on the fact that the pressure of the accreting material may distort the large-scale stellar magnetic field and the magnetospheric transfer of material to the star can give rise to instabilities of the magnetic fields around the inner disk edge. The presence of accreting material should also lead to higher densities in (parts of) the magnetosphere; these high densities could inhibit magnetic heating of the accreting material to X-ray emitting temperatures.

Another suggestion was that the accreting material would cool the corona when it penetrates into active regions and mixes with hot plasma. If the plasma would be cooled below a few MK, its very soft X-ray emission would be essentially undetectable for the CCD X-ray detectors of *Chandra* and XMM-Newton, and thus the observed X-ray luminosity of the accreting stars would be lower than that of non-accretors (see also Telleschi et al. 2007).

Yet another theory suggested that the stripping of the coronal magnetic field by the interaction with the disk might reduce the coronal volume and thus the X-ray emission (Jardine et al. 2006). In stars without a circumstellar disk, the coronae extend outwards to the radius where the pressure of the hot coronal gas overcomes the magnetic field, explaining the observed increase in the X-ray emission measure with increasing stellar mass. In stars that are surrounded by a circumstellar accretion disk, the outer parts of the coronal magnetic field could be stripped by the interaction with the disk, and this might explain the observed lower X-ray luminosities of accreting stars.

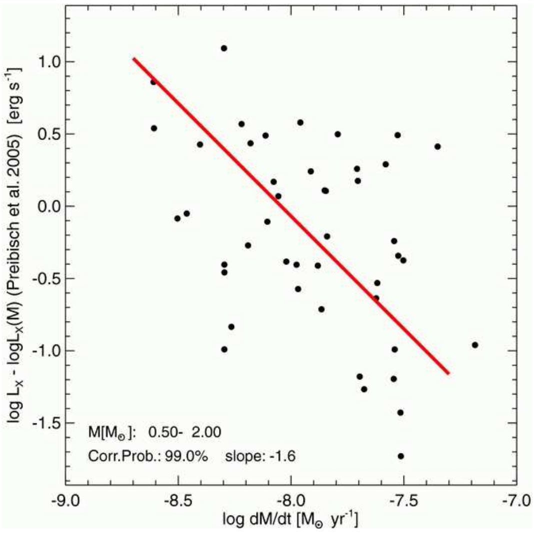

Figure 2: Reproduction of Fig. 3 from Drake, Ercolano, et al. (2009), showing the anti-correlation between X-ray luminosity and accretion rate.

d) The new model of photoevaporation-starved accretion

While the previous models were based on the idea that accretion somehow suppresses, disrupts or obscures coronal X-ray activity, Drake et al. (2009) developed an alternative model by suggesting that the X-rays may instead modulate the accretion flow. They explained this effect with the X-ray heated accretion disk models of Ercolano et al. (2008a,b, 2009) and showed that photoevaporative mass-loss rates of disks are strongly dependent on stellar X-ray luminosity and sufficiently high to be competitive with accretion rates. As described in more detail below, the strength of the coronal X-ray emission determines the accretion rate, and stars with strong X-ray emission should accrete at lower rates because their disks suffer from higher photo-evaporative mass-loss rates. This implies that the stellar X-ray activity controls the evolution of the disk, and thus should have far-reaching consequences, e.g. on the process of planet formation and on the disk dissipation timescale.

As a first test of this new theory, Drake et al. (2009) compared X-ray luminosities and accretion rates for stars in the Orion Nebula Cluster and found an anti-correlation between these two quantities (see Fig. 2). However, these conclusions remained tentative, because they were based on a rather small sample of just 44 stars, for which accretion rate estimates were available at that time. Because of the fundamental importance of this theory, the relation between X-ray activity and disk accretion should be tested in much more detail.

e) Disk Dispersal by Photoevaporation

Theoretical arguments clearly suggest that photoevaporation driven by the ionizing radiation from the central young star is the most important mean for the dispersal of disks (see Alexander et al. 2014, for a recent overview). A simple outline of the physical mechanism is as follows: The high-energy radiation from the star ionizes the H atoms in the surface layer of the disk and thereby heats this gas to temperatures of typically 10 000 K. At radii where the corresponding sound speed of the heated gas ($\sim$ 10 km/s) is similar or larger than the escape speed from the gravitational well (typically a few AU), the hot gas is then essentially unbound; it can stream away and escape from the disk in the form of a thermally driven wind.

This mass loss from the outer disk interrupts the supply of material into the inner parts of the disk,

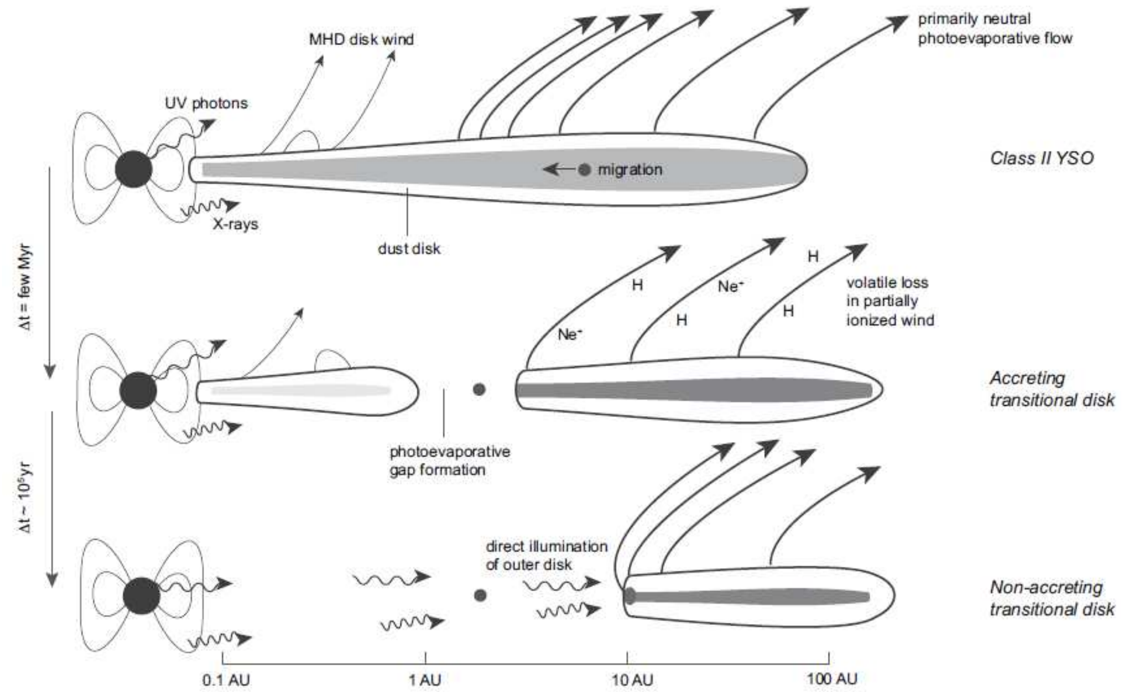

Figure 3: Illustration of major steps in the evolution of a circumstellar accretion disk from the CTTS phase to the formation of an inner hole and up to the complete dispersal of the disk (from Alexander et al. 2014).

which is still viscously accreting onto the star. As illustrated in Fig. 3, this leads to the formation of a hole in the inner regions of the disk. In the following phases, the outer disk (which is now fully exposed to the stellar irradiation, because the shielding from the inner disk does no longer exist) is finally fully dispersed on rather short timescales. This sequence of evolutionary steps is illustrated in Fig. 3.

Until a few years ago, it was generally assumed that the stellar EUV radiation (similar to the chromospheric emission from our Sun) is the dominant agent of disk dispersal (Alexander et al. 2006). For the typical EUV fluxes of roughly solar-mass young stars ($\sim 10^{41}$ photons per second), mass-loss rates of $\dot{\mathrm{M}} \sim 3 \times 10^{-10}\,\mathrm{M}_\odot/\mathrm{yr}$ have been estimated in numerical simulations. These mass-loss rates are limited by the fact that the stellar EUV photons can penetrate only to very small values of the gas column density ($N_\mathrm{H} \sim 10^{18}\,\mathrm{cm}^{-2}$), because the photo-absorption coefficient for EUV radiation is very high. Therefore, the EUV radiation can ionize only a thin surface layer of the disk, where the gas density is quite low.

Only recently it became clear that stellar X-ray photons are considerably more efficient in producing disk winds (Ercolano et al. 2008a,b, 2009). The fact that the typical fluxes of X-ray photons (roughly 10^{39} photons per second) are considerably lower than the EUV photon fluxes, is offset by the much larger penetration depth of X-ray photons compared to EUV photons. As the photo-absorption coefficient for keV photons is 4 to 5 orders of magnitude lower than for EUV photons, the X-rays can reach much further down into the deeper layers of the disk (up to $N_\mathrm{H} \sim 10^{24}\,\mathrm{cm}^{-2}$), where the disk densities are much higher. Therefore, the X-ray driven disk wind starting from these denser regions closer to the disk midplane can produce much higher mass-loss rates, around $\dot{\mathrm{M}} \sim 3 \times 10^{-8}\,\mathrm{M}_\odot/\mathrm{yr}$ for the typical X-ray fluxes of young stars.

The temporal evolution according to this model depends sensitively on the flux and the spectrum of the X-ray photons and the resulting strength of the driven disk wind.

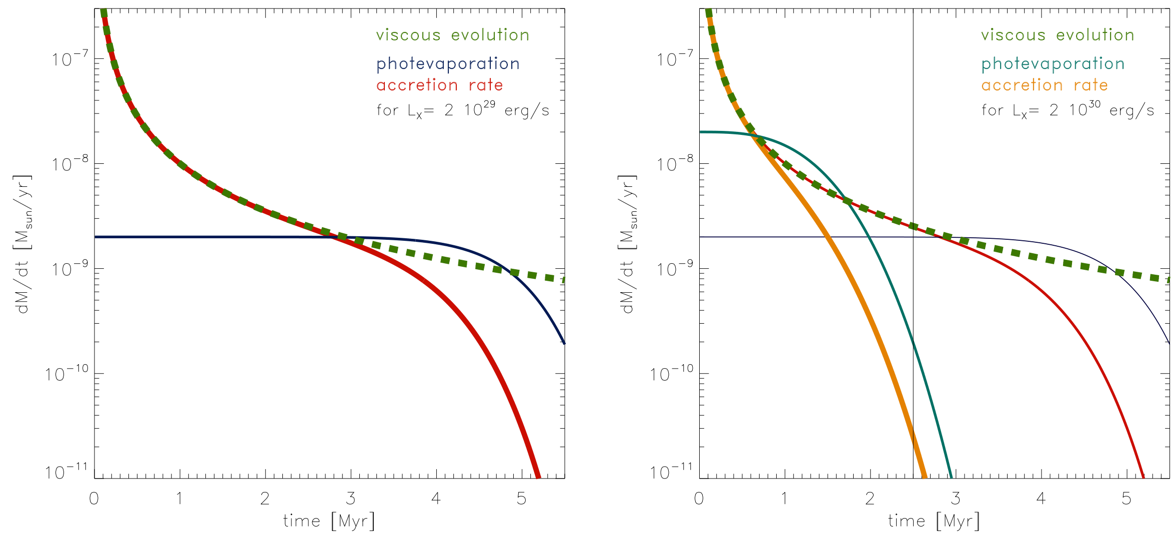

Figure 4: Illustration of the temporal evolution of photoevaporative wind mass loss rate and accretion rate according to the scenario of X-ray photoevaporation-starved accretion. The **left plot** shows the case of a TTS with moderate X-ray luminosity of 2×10^{29} erg/s. The thick dashed green line shows the purely viscous accretion rate that would result if there were no photoevaporation. The dark blue line shows the mass loss rate resulting from X-ray photoevaporation, and the thick red line the actual accretion rate.
In the **right plot**, model curves for the case of a 10 times higher X-ray luminosity are added. Comparison of the curves for the accretion rate in both cases (dark red and orange lines) at the age of 2.5 Myr (solid vertical line) illustrates the much lower accretion rate of the high X-ray luminosity case compared to the low X-ray luminosity case.

1.1 Project-related publications

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Th. Preibisch, S. Hodgkin, M. Irwin, J.R. Lewis, R.R. King, M.J. McCaughrean, H. Zinnecker, L. Townsley, P. Broos, 2011, *Near-Infrared properties of the X-ray emitting young stellar objects in the Carina Nebula*, Astrophys. Journal Supplement, 194, 10

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2. Objectives and work programme

2.1 Anticipated total duration of the project

3 years

2.2 Objectives

The main objective of this project is to establish the role played by stellar X-ray radiation in shaping the accretion rate distributions of Type I transition disks. The model of photoevaporation-starved accretion makes quite specific predictions on the temporal evolution of the disk accretion rate as a function of the strength of the X-ray irradiation (Drake et al. 2009; Owen, Ercolano & Clarke 2011). As illustrated in Fig. 4, the model predicts that as soon as the viscous accretion rate drops to values comparable to the wind mass-loss rate due to photoevaporation, an inner disk gap and then a hole forms (i.e. the disk becomes a Type 1 TD) and the accretion rate onto the star will drop strongly within a short period of time. This predicts that a higher X-ray luminosity should lead to an earlier formation of the inner disk hole. At a given time, stars with higher levels of X-ray activity should therefore display lower accretion rates.

The immediate objective of this project is to test these model predictions with more, and especially more reliable, observational data. The observational tests proposed here will provide a stringent constraint to the models developed in projects B1 (PI Ercolano)[1].

This is very timely now, because during the last few years, the availability of data required for reliable accretion rate determinations has improved very substantially. This is to a large degree related to the recent advent of new powerful spectrographs like X-SHOOTER at the VLT, that combine high spectral resolution with a very wide wavelength coverage (the entire optical and near-infrared range, in the case of X-SHOOTER). Several spectroscopic surveys of young stars in different regions have been performed in the last few years or are ongoing and provide a wealth of new, high-quality data, which can be exploited now (see Manara & Testi 2014).

2.3 Work programme including proposed research methods

In this project, we aim at combining the numerous available deep X-ray observations of star forming regions in the *Chandra* and XMM data archives with new and reliable measurements of the accretion rates of young stars in these regions. We want to build up a large sample of young stars of different mass and age, for which we then can perform a detailed statistical analysis of the relation between X-ray activity and accretion in mass- and age-stratified stellar sub-samples.

This was not possible in the past, because accretion rates determinations were only available for few stars, and even when available, the results were often plagued by large uncertainties. The main problem with most previous accretion rate estimates was that they were usually based on color excesses or equivalent-width determinations of single tracer lines (such as Hα). The other important parameters, i.e. the stellar effective temperature and the extinction, which are needed to convert color excesses or equivalent-widths to accretion rates, had to be derived from separate observations, or (more usually) collected from the literature. This combination of different observational data can easily lead to substantial uncertainties in the derived accretion rate estimates and the stellar parameters. A good example of this is the study of Orion Nebula Cluster stars by Robberto et al. (2004), who determined accretion rates for a sample of 40 young stars in the Trapezium cluster from Hubble Space Telescope *U*- and *B*-band photometry. As the computation of the accretion parameters from the UV excess involves numerous assumptions, their values had considerable uncertainties; for 25% of their stars, they found even negative (i.e. unphysical) values for the accretion luminosities.

The most important advantage of the new high-resolution wide-wavelength range spectra is that they allow a self-consistent and simultaneous determination of all the important parameters, i.e. the stellar effective temperature, the extinction, and the accretion rate, at the same time and from one coherent data set. This results in a far more reliable determination of accretion rates (see Manara & Testi 2014).

The recent study of Manara et al. (2013) provides a very good illustration of this fundamental aspect: They investigated two stars in the Orion Nebula Cluster for which previous data suggested a very strange combination of quite old ages ($>$ 10 Myr) and rather high accretion rates (as estimated from the equivalent width of the Hα line). Manara et al. used VLT/X-SHOOTER spectra combined with an

[1] The text highlighted in green refers to the connection of this project to other projects of this Research Unit.

accurate method to re-determine the stellar parameters and the ages of the targets in a self-consistent way. The results of their analysis showed that the earlier studies had strongly underestimated the extinctions and thus the luminosities of these two stars. With the new extinction, luminosity, and accretion rate values derived from X-SHOOTER, these two stars could be shown to be in fact rather typical accreting young stars, and not mysterious “old accretors” as claimed before.

As described below in more detail, a brief scan through the available X-ray archive data and matching recent reliable accretion-rate determinations from the literature suggests that it will be possible to construct a sample consisting of several hundred young stars. This number is already much larger than the sample-size of 44 objects, on which the above described previous statistical study was based, which yielded strong hints, but no really statistically significant proof for an anti-correlation between X-ray luminosity and accretion rate.

We also plan to actively enlarge the sample of stars with reliable accretion rate measurements by 1) re-analyzing existing X-SHOOTER spectra in the ESO archive in order to derive accretion rates in a consistent way, and 2) performing new X-SHOOTER spectroscopic observations of young stars in selected clusters.

In this way we will assemble a large, comprehensive, and consistent database on accretion and X-ray data for YSOs with a wide range of stellar masses and ages. With an expected final sample of several hundred objects we can then perform a detailed statistical analysis of the relation between X-ray activity and accretion in mass- and age-stratified sub-samples of young stars. The results will provide crucial new constraints for theoretical models of the X-ray-disk interaction by photoevaporation, including those developed in project B1, and allow us to draw conclusions on the expected accretion rate distributions of young stars.

2.3.1 Work programme including proposed research methods

The work programme consists of three blocks in which high-quality data on the accretion rates and X-ray luminosities of young stars are collected, and a final block for the statistical analysis and comparison to the theoretical models.

In the first block, we want to perform a detailed study of the $\sim$ 700 young stars in the Orion Nebula Cluster, for which new and reliable accretion rate data are now available (part 1a). In this analysis, we will also investigate the possible effects of variability of the accretion rates as well as the X-ray luminosities on the correlation between these two parameters (part 1b). Furthermore, using new optical spectroscopic data from recent X-SHOOTER and MUSE observations of Orion Nebula Cluster stars, we want to increase the sample of stars with accretion rate determinations (part 1c).

In the second part of the project we will use the existing X-SHOOTER spectra for numerous young stars in various star forming regions to derive new and self-consistent measurements of the stellar parameters and the accretion rates. We will determine X-ray luminosities of these stars and then use these new data, as well as published results, for a statistical analysis. This will allow us to extend the investigation to stars that are younger or older than the stars in the Orion Nebula Cluster.

In the third part of the project, we plan to obtain new X-SHOOTER spectra for selected stars in order to increase the sample and to optimize the coverage of the parameter space with respect to stellar age and mass.

In the final part of the project, all these data will be statistically analyzed and used to test the theoretical models.

Project Part 1: Orion Nebula Cluster

The first target for this study will be the Orion Nebula Cluster, for which the COUP data provide the most sensitive and complete X-ray data set on a sample of about 1000 young stars.

Part 1a: Correlation analysis of the existing X-ray and accretion data

The first step in the work will be to use the new accretion rates that have been determined for $\sim$ 700 young stars in the Orion Nebula Cluster from Manara et al. (2012) and correlate them with the available X-ray data from the COUP project. Manara et al. (2012) derived accretion rates from both the U-band excess and the Hα luminosity, after determining empirically both the shape of the typical accretion spectrum across the Balmer jump and the relation between the accretion luminosity and the Hα luminosity. Their tables also report fundamental stellar parameters such as the effective temperature, extinction, luminosity, radius, and the age. This is particularly important, since it makes sure that the data on accretion rates are consistent with the stellar parameters.

This stellar sample will be cross-correlated with the COUP source table, that lists the X-ray properties of the 1616 X-ray detected objects in the Orion Nebula Cluster. Due to the large sample size, this will allow already a much more detailed statistical analysis of the relation between X-ray activity and accretion properties in mass- and age-stratified samples than possible before.

Part 1b: Investigating the effects of variability

The known variability of the X-ray emission as well as the temporal variability of the accretion rates is a potential complication for the investigation of the relation between X-ray emission and accretion, given the fact the X-ray and accretion rate measurements are usually not obtained simultaneously. For the case of the ONC, the COUP X-ray observations were performed in January 2003, whereas the HST observations, from which the accretion rates have been determined, were carried out between October 2004 and April 2005. We therefore have to take into account the typical amplitudes of variations on timescales of a few years, and consider the corresponding possible effects on the correlation analysis.

X-ray luminosities of young stars show typical variations of about a factor of 2 on timescales of months to years (e.g. Wolk et al. 2004). Stronger variations can, of course, occur if the star happens to show a particularly strong X-ray flare during the observation. However, these flares can easily be recognized by inspection of the X-ray lightcurve. In the case of the COUP data set, the derived X-ray luminosities provide an average over more than 10 days, i.e. more than one rotation period for almost all of these stars. Since lightcurves have been analyzed and objects with strong flares during the observation are known, this information can be used in the statistical analysis.

As described in the introduction and illustrated in Fig. 1, the variability of the accretion rates in YSOs is strongly dependent on the age and evolutionary state of the objects. Very strong variability is expected during the very young, protostellar stages. At the typical ages of our target stars (about 1 to 5 Myr), accretion rate variability is much more moderate than during the very young phases. An important quantification of the typical accretion variability of T Tauri stars was recently provided by the detailed monitoring study of Venuti et al. (2014) and Venuti et al. (2015). They found that the variability of the accretion luminosity, as traced by UV excesses, typically amounts to a factor of $\sim 2-3$ on timescales from weeks to several years. This amplitude of accretion variability is thus clearly much smaller than the large scatter (two to three orders of magnitude) seen in the distribution of the accretion rates of the cluster stars. This result shows that the observed wide range of accretions rates in a young cluster is **not** primarily due to accretion variability, but rather reflects the large range of individual accretion rates of the individual stars. This supports the model we want to test in this project, i.e. that the accretion rate of individual YSOs depends sensitively on the high-energy emission of the central star.

The results from Venuti et al. (2014) are consistent with numerous monitoring studies of YSOs, which also trace the accretion variability as one part of the total photometric variability of a YSO. These studies generally found that the typical amplitudes of photometric variability of YSOs in the TTS stage are not more than a few tenths of a magnitude (i.e. about a factor of two) on timescales from days to several years. For the case of the Orion Nebula Cluster, several studies of optical variability on timescales between a few hours and several years have been performed during the last years (Herbst et al. 2002; Stassun et al. 2006, 2007; Parihar et al. 2009; Rice et al. 2015) and confirmed the generally quite moderate levels of variability. For the large majority of the monitored stars, the observed brightness variations were well below about 0.5 magnitudes.

The recent determination of the frequency of strong accretion rate outbursts for YSOs by Hillenbrand & Findeisen (2015) also fits into this picture: while the accretion outburst frequency may be as high as $10^{-3}\,\mathrm{yr}^{-1}\,\mathrm{star}^{-1}$ for very young (≤ 0.25 Myr old) protostars, it drops to just about $3 \times 10^{-6}\,\mathrm{yr}^{-1}\,\mathrm{star}^{-1}$ for ≥ 1 Myr old TTS (which are the targets in our project). This suggests that in a sample of ~ 1000 TTS, the likelihood to catch a significant accretion outburst on at least one star in a 10 year period (i.e. the upper limit for the time difference between the X-ray and accretion rate observations) is just a few percent.

To summarize, these results are consistent with the assumption that the time difference between the X-ray and accretion rate observations should lead to uncertainties that are not much larger than about a factor of $\sim 2-3$ in the accretion rate values for most stars. While this will increase the scatter in the relations between X-ray emission and accretion rate, it does not constitute a fundamental problem for a statistical analysis. The few stars that showed stronger variability in the available monitoring studies can be excluded or treated separately in our correlation study.

Nevertheless, it cannot be excluded that some objects have perhaps undergone a larger variation of the accretion luminosity since the time of the X-ray observation. In order to identify such possible cases in the Orion sample, we have recently started a multi-year and multi-color photometric monitoring project. The aim of this project is to identify stars that show significant brightness variations indicative of strong accretion rate variability on timescales from months to years. These observations are performed with our own (LMU) 2m Fraunhofer Telescope on Mount Wendelstein. The new wide-angle camera WWFI (providing a 0.5° field-of-view) is ideally suited for this monitoring project, since it allows to cover the entire cluster, including the full field of the COUP X-ray observation ($17' \times 17'$), in one exposure. Figure 5 shows a first test image of the ONC obtained with WWFI with an overlay of the COUP field. A first and preliminary analysis of these test images shows that more than 450 of the X-ray detected young stars are bright enough (in comparison to the surrounding nebulosity) to allow a photometric monitoring with these data.

We plan to obtain optical images in up to three bands about every second week during the season of observability. Over the 3-year period of the proposed project, this will yield a comprehensive dataset for a photometric analysis of long-term variability. This will thus allow us to identify objects that show a strong variation of their brightness on a multi-month to multi-year timescale. Stars with strong variability on even longer timescales can also be identified by comparing the photometry from our Wendelstein observations with older literature data. If any such highly variable objects are identified, they can be excluded (or treated separately) in the statistical correlation analysis between X-ray emission and accretion.

Part 1c: New accretion rates for ONC

Nineteen young stars in the Orion Nebula cluster have already been observed with X-SHOOTER. We will use these data to derive accretion rates for these stars. This will allow a detailed comparison with the above mentioned accretion rate determinations and increase the size of the sample, for which we can correlate accretion and X-ray data.

Another very interesting spectroscopic dataset was recently obtained with the ESO Multi Unit Spectroscopic Explorer (MUSE), an integral-field spectrograph operating in the visible wavelength range at the ESO 8m Very Large Telescope. The MUSE consortium has released data cubes and maps of the Huygens region of the Orion Nebula published by (Weilbacher et al. 2015). These data provide a spatial sampling of $0.2''$ per pixel, a spectral resolution of 0.85 Å per pixel, and cover the wavelength range 4595 Å to 9366 Å. We have retrieved and inspected these data, and found that useful optical

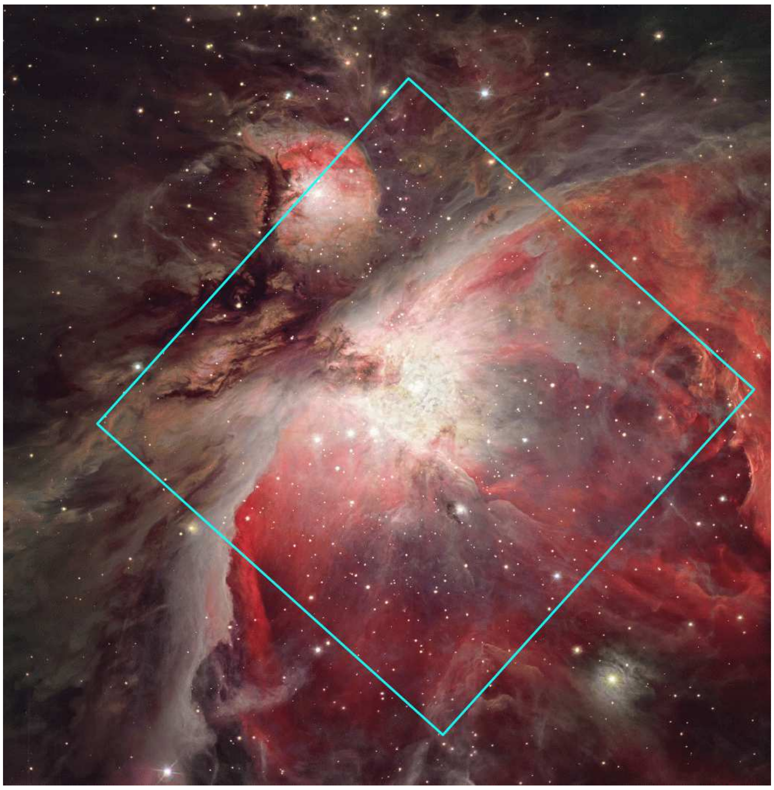

Figure 5: Optical image of the ONC obtained with the WWFI camera at our 2m Fraunhofer Telescope on Mount Wendelstein [image processing by M. Kluge, USM]. The image is a three-color composite of *u*-band (blue), *g*-band (green), and *r*-band (red) exposures. The cyan rectangle shows the 17′ × 17′ field of the COUP X-ray observation.

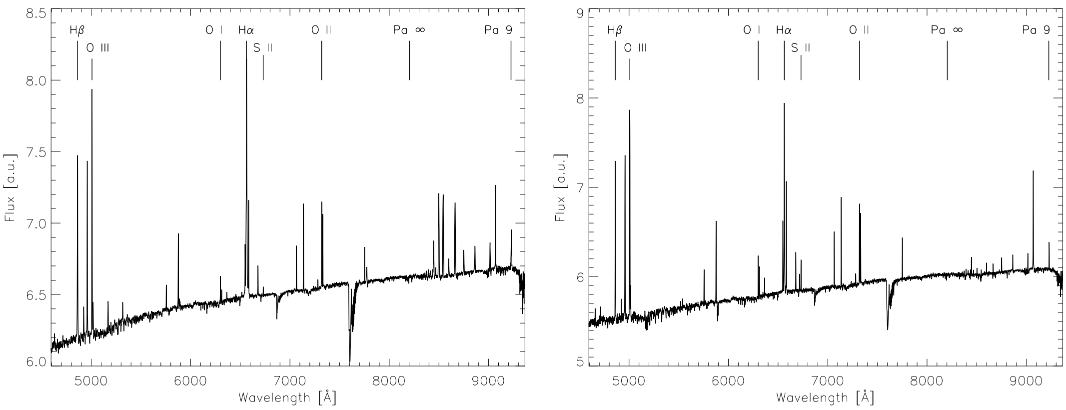

Figure 6: Spectra of two stars (COUP 758 and COUP 855) extracted during our preliminary analysis of the MUSE data cube of the Orion Nebula.

spectra can be extracted for at least 359 of the COUP X-ray sources. Two examples of objects with strong emission lines, indicative of high accretion rates, are shown in Fig. 6

These MUSE spectra can complement the X-SHOOTER data and thus increase the number of stars with spectroscopic accretion rate determinations. Finally, a comparison of MUSE and X-SHOOTER spectra for stars observed with both instruments can also provide important information on time variability of the accretion rates.

Part 2: New accretion rates for other star forming regions

In the second part of the project, we will extend the analysis to young stars in other star forming regions, for which either reliable accretion rate determinations or X-SHOOTER spectra are available. Correlating these data with *Chandra* and XMM X-ray observations will provide further samples of young stars, in which we can investigate the relation between X-ray luminosity and accretion. This will allow us to extend the parameter space, e.g. by observations of clusters that are somewhat younger or older than the Orion Nebula Cluster.

Reliable accretion rate determinations are available for the following regions:

1) NGC 2264:
Venuti et al. (2014) determined stellar parameters and accretion rates for about 750 YSOs in this cluster. Accretion rates were determined from *U*-band excess emission as well as emission lines.

This cluster was also extensively studied with *Chandra*: eight deep ACIS-I observations of the different parts of this region are available in the *Chandra* data archive.

2) IC 348:
Dahm (2008) performed a spectroscopic investigation of accretion diagnostics for 40 near solar mass members of IC 348 and derived accretion luminosities and rates for these stars.

The X-ray properties of these stars are very well known, since IC 348 has been very well observed in X-rays: initially with ROSAT (Preibisch, Zinnecker, & Herbig 1996), with several deep *Chandra* observations (Preibisch & Zinnecker 2002; Stelzer, Preibisch. et al. 2012) and also with XMM-NEWTON (Preibisch & Zinnecker 2004).

Reliable accretion rate determinations and/or X-SHOOTER spectra are also available for:

3) the sigma Ori cluster (accretion rates from U-band photometry from Rigliaco et al. (2011); X-SHOOTER spectra for 10 stars)

4) the ρ Ophiuchi region (accretion rates for 104 stars from Natta et al. (2006); X-SHOOTER spectra for 17 YSOs from Manara et al. (2015))

5) the Lupus region (accretion rates for 36 YSOs from X-SHOOTER spectra by Alcalá et al. (2014))

6) the Chamaeleon I region (accretion rates from X-SHOOTER spectra by Manara et al. (2016))

7) the Upper Scorpius association (X-SHOOTER spectra for 25 stars)

8) the TW Hya association (X-SHOOTER spectra for 15 stars)

9) the Taurus region (X-SHOOTER spectra for $\sim$ 15 stars).

Deep X-ray observations of all these clusters and associations are available in the Chandra and XMM data archives. We will retrieve these X-ray data and analyze them in a homogeneous way using the most recent analysis tools (like ACIS-Extract for the Chandra data) to detect and characterize X-ray sources. The determination of the X-ray luminosities will be based on a model fitting analysis of the X-ray spectra with CIAO and XSPEC for sources with a sufficient number of source counts. For weaker X-ray sources, the X-ray luminosities can be determined from the observed number and energy of the detected X-ray photons with the `srcflux` tool in the Chandra analysis software. Cross-correlating the resulting X-ray source lists with the catalogs of spectroscopically observed stars will yield the samples for which we can investigate the relations between X-ray activity and accretion.

In order to extend our database to higher stellar masses, we also plan to analyze the available X-ray data for the 91 Herbig AeBe stars (YSOs in the mass range from $\approx 2 - 8\,M_{\odot}$) for which accretion rates were determined from X-Shooter spectra in the recent study of Fairlamb et al. (2017).

Part 3: New X-SHOOTER observations

In the course of the project, we also plan to perform new observations with X-SHOOTER in order to extend the spectroscopic sample and to optimize the overlap with the X-ray observations. We note however that the achievement of many of the goals of this project is also possible with the current observations, which would also be sufficient to successfully complete a PhD Thesis.

Part 4: Statistical analysis

The final aim of the observational part of this project is to get as many and as reliable as possible data points to perform detailed statistical analysis of the relation between X-ray activity and accretion in mass- and age-stratified samples of young stars in different young clusters. This will provide crucial new constraints for theoretical models of the X-ray-disk interaction. At this point we will work closely with the project B1 team to create synthetic disk populations from the 2D models to compare with the observational dataset from this project and the gas and dust demographics from project A2. The theoretical wind profiles will be used in conjunction with a one-dimensional viscous model to follow the evolution of disks into the transition phase (see e.g. Owen, Ercolano & Clarke, 2011). This is a unique and crucial test which will allow us for the first time us to directly constrain and calibrate the models.

The earlier theories (described in Sect. 1c) that tried to explain how accretion somehow may reduce the X-ray emission, could not make testable predictions. The proposed effects (like changes in the coronal magnetic field structure by the accreted material, stripping of the coronal magnetic field by the interaction with the disk, or a reduced differential rotation in the star due to magnetospheric coupling) would depend very sensitively on the details of the interaction. The resulting reduction of the X-ray luminosities could be quite strong, but also rather weak, and should thus essentially introduce scatter in the relations between the X-ray properties and accretion properties.

The Drake, Ercolano, et al. (2009) model, however, makes a rather clear prediction that the observed accretion rate for stars at a given age should scale inversely proportional to the X-ray luminosity. This direct relation between accretion and X-ray luminosity for stars of a given age can be tested with the observational data in different stellar mass and age regimes.

2.4 Data handling

All required tools for analyzing the X-ray and optical data are available.

2.5 Other information

none

2.6 Information on scientific and financial involvement of international cooperation partners

none

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4. Requested modules/funds

4.1 Basic Module

4.1.1 Funding for Staff

We ask for one PhD position (75% E13) for three years to work at the LMU under the supervision of Prof. Preibisch.

4.1.2 Direct Project Costs

none

4.1.2.1 Equipment up to EUR 10,000, Software and Consumables

Will be provided by the host institution.

4.1.2.2 Travel Expenses

Travel within the Research Unit is handled in project Z. In addition we request funding for conference travel for the personnel and one Applicant. This includes one national (1.000 €) and one international (1.500 €) conference trip per year, totalling 2.500 € per person per year.
For this project this totals 5.000 € per year for the PhD student and one Applicant, which is in total 15.000 €.

4.1.2.3 Project-related publication expenses

We request 750 € per year (a total of 2 250 €) for publication expenses, mainly to support open access options or whenever necessary, publication in non-free journals.

5. Project requirements

5.1 Employment status information

Thomas Preibisch, Professor at the Ludwig-Maximilians-Universität München (permanent)
Barbara Ercolano, Professor at the Ludwig-Maximilians-Universität München (permanent)
Leonardo Testi, Faculty Member at the European Southern Observatory (permanent)

5.2 First-time proposal data

not applicable

5.3 Composition of the project group

Prof. Preibisch (PI) and Prof. Ercolano (co-I) at the LMU, Dr. Testi co-I at ESO.

5.4 Cooperation with other researchers

5.4.1 Planned cooperation on this project

5.4.1.1 Collaborating researchers for this project within the Research Unit

This project will collect and re-derive X-ray and accretion properties from a large number of sources. These will be used as inputs for the models developed in projects B1, B2 and C2, treating, respectively, radiation-hydrodynamics, astrochemistry and dust entrainment in photoevaporation models of disks. These projects are lead by Prof. Ercolano and Prof. Caselli. The statistical analysis of the data from this project, together with the gas and dust demographics obtained from project A2, will allow a direct comparison with synthetic disk populations obtained from the models developed in project B1, which will provide the latter with important constraints.

5.4.1.2 Collaborating researchers for this project outside of the Research Unit

5.4.2 Researchers with whom you have collaborated scientifically within the past three years

F. Niederhofer (STSci, USA); M. Hilker (ESO, Garching); N. Bastian (U. Liverpool, UK); M. Guarcello (U. Palermo, Italy); M. Tazzari (U. Cambridge, UK); A. Natta (Florence, Italy); R. Alexander (U. Leicester); D. Hubber (LMU); J. Dale (U. Hertfordshire, UK); C. Koepferl (LMU); I. Bonnell (U. St. Andrews, UK); A. McLeod (ESO, Garching); D. Boneberg (U. Cambridge, UK); R. Parker (U. Liverpool, UK); R. Wesson (UCL, London, UK); M. Barlow (UCL, London, UK); A. Glassgold (u. Berkeley, USA); C. Manara (ESA, Noordwjik, Netherlands); A. Danekhar (CfA, Harward, USA); Q. Parker (Sidney, Australia); S. Casassus (U. de Chile, Santiago, Chile); I. Pascucci (U. Arizona, USA); A. Bevan (UCL, London, UK). J.M. Alcalá (INAF), S. Andrews (CfA), R. Cesaroni (INAF), C. Chandler (NRAO), C. Codella (INAF), A. Ginsburg (NRAO), I. de Gregorio-Monsalvo (JAO, ESO), G. Guidi (Univ. di Firenze, INAF), G. Herczeg (Kavli-Beijing), A. Isella (Rice University), I. Jimenez-Serra (QMUL), A. Maury (CEA Saclay), C. Manara (ESA), S. Molinari (INAF), A. Natta (DIAS, INAF), L. Perez (MPIfR, UChile), L. Ricci (Rice University), G. Rosotti (IoA), A. Sargent (Caltech), A. Scholz (St. Andrews), M. Walmsley (DIAS, INAF)

5.5 Scientific equipment

Large computer facilities are not required for this project. The University already provides sufficient computational support.

5.6 Project-relevant interests in commercial enterprises

None

5.7 Additional information

None

Project B1:

The radiation-hydrodynamics of photoevaporative winds with chemistry

Authors:
Applicant: B. Ercolano (LMU)
Co-Applicant: P. Caselli (MPE)
Cooperation Partners: J. Owen (Princeton, USA), T. Grassi (STARPLAN, Copenhagen)

Requested positions: 1 Postdoc

Abstract:
Type 1 Transition disks (TDs) are thought to be disks in an advanced stage of dispersal (see introduction to the Research Unit). The modality of disk dispersal has been shown to be of fundamental importance to planet formation, yet the responsible mechanism is still largely unconstrained. Photoevaporation from the central star is currently a promising avenue to investigate, but the models developed to date do not yet have enough predictive power for a piecewise comparison with the observations. In this project we aim at building the most comprehensive radiation-hydrodynamical calculations of irradiated disks, coupled to photoionisation, chemistry and radiative transfer calculations for a large parameter space, covering stars of different masses and X-ray properties. This will constitute the backbone for the work carried out in several projects of this proposal (e.g. B2, C2), which together aim at performing quantitative spectroscopy of disk winds. Comparison with existing and upcoming observations will allow us to constrain the mass loss rates and the launching regions of the wind and thus pin down the underlying driving disk dispersal mechanism. The models developed in this project will also the able to tackle several important outstanding questions about the formation and evolution of Type I TDs, as disussed in more detail below.

1. State of the art and preliminary work

1.1 Scientific Background

Understanding disk dispersal is a key piece in the puzzle of planet formation. Type 1 TDs, which are considered to be objects caught in the act of dispersal, provide a tight constraints on the underlaying dispersal mechanism. For example, their (low) frequency, in relation to the global disk population in a given cluster, implies dispersal timescales of order 10% of the global disk timescale, and their evolution on the colour-colour plane (e.g. K-[8] versus K-[24]) points to an inside-out mode of dispersal (e.g., Ercolano et al. 2011; Koepferl et al. 2013; Ercolano et al. 2015).

The most successful of the various disk dispersal mechanisms proposed to date is considered to be photoevaporation by radiation from the central star (e.g., Clarke et al. 2001). Indeed, when combined with viscous theory for the accreting disk, this model can reproduced the observed dispersal timescales. As described in more details below, in this framework the disk is dispersed because the mass loss rate due to a photoevaporative wind eventually exceeds the mass accretion rate through disk, allowing the disk to quickly be eroded from the inside-out.

Recent work suggests that magnetohydrodynamic (MHD) effects may also drive disk winds (e.g., Bai & Stone 2013) which may lead to disk dispersal and at the same time remove angular momentum from the system, thus allowing the inward flow of material, i.e. accretion. Some preliminary estimates suggest that MHD winds may be comparable to photoevaporative winds in their strength, and that non-ideal MHD effects may also dominate over magneto-rotational-instability (Balbus & Hawley 1991, MRI,) in the transport of angular momentum (i.e. accretion) through the disk. While these models are still in their infancy and the mass loss and accretion rates from MHD winds are at present highly uncertain, they still raise important questions about the validity of the majority of disk models which rely on α prescriptions. However a number of important uncertainties need to be resolved before the relevance of non-ideal MHD effects to disk evolution can be assessed. These include include the strong dependence of the wind and accretion rates on the completely unknown magnetic flux distribution through the disk and, most importantly, magnetic flux evolution as a function of surface density of the disk (e.g. discussion in Armitage et al. 2013) Another key ingredient is the level of ionisation in the atmosphere of disks, which determines the nature of the gas coupling to the magnetic field. While details of the magnetic field structure and evolution are difficult to determine at present, the joint efforts of projects B1, B2 and C2 can deliver the most detailed case-specific assessment to date of the ionisation structure in disk atmospheres. This is indeed one of the aims, which is described in project B2 (PIs Caselli & Ercolano)[1].

In this project we focus solely on photoevaporative winds, where the underlying physics is better understood and the observations can be used to constrain a number of important parameters, thus reducing the degrees of freedom involved.

In the following two sections the state-of-the art for photoevaporation models, to which the Applicant and collaborators have made significant contributions, will be discussed.

1.1.1 Photoevaporation models

All models of photoevaporation show that radiation from the central star heats the disk atmosphere, setting off a thermal wind. The wind is centrifugally launched from the location where the thermal energy of the heated gas exceeds the local gravitational binding energy. Disk dispersal then sets in as a consequence of this wind when the mass loss rate exceeds the accretion rates in the disk. According to viscous theory, young disks accrete at a vigorous rate, which naturally decreases as time goes by (e.g., Hartmann 2008), until, after a few million years, accretion rates fall to values smaller than the wind rates, allowing photoevaporation to take over the further evolution of the disk. Once the dispersal sets in the disk is then quickly eroded from the inside out going through the transition disk phase, before disappearing completely (see e.g., Alexander et al. 2014; Armitage 2011, for recent reviews of this process).

While the community now agrees on this broad brush picture, quantitatively speaking, the dispersal mechanism is still largely unconstrained. There is currently a hot debate in the literature as to what type of radiation may be the main driver of the wind: Extreme-, Far-UV or X-ray. This is a fundamental question as the mass-loss-rates implied by the different models can differ by orders of magnitudes. The mass loss rates determine the timescales of dispersal for given initial disk conditions. The wind profile, i.e. the region of the disk that is most affected by photoevaporation, is also very different in each scenario (e.g. Alexander et al. 2014; Armitage 2011). Figure 1 shows the mass loss profile for the X-ray+EUV (Owen et al. 2010), EUV-only (Font et al. 2004) and FUV (Gorti et al. 2009) profiles. The X-ray profile is much more extended than the EUV profile, which predicts mass loss only from a vary narrow range of disk radii. The FUV model is again very different, showing mass loss from the outer regions of the disk, hence predicting in some cases an outside-in mode of dispersal. These differences have important implications for the planet formation and the migration process. For example, the total mass loss rates in the disk sets the timescales for the formation of gas giants, and together with the wind profiles it sculpts the disk density distributions, profoundly affecting the evolution of all planetary systems, by putting a stop to migration via the formation of gaps in the gas. As

[1] The text highlighted in green refers to the connection of this project to other projects of this Research Unit.

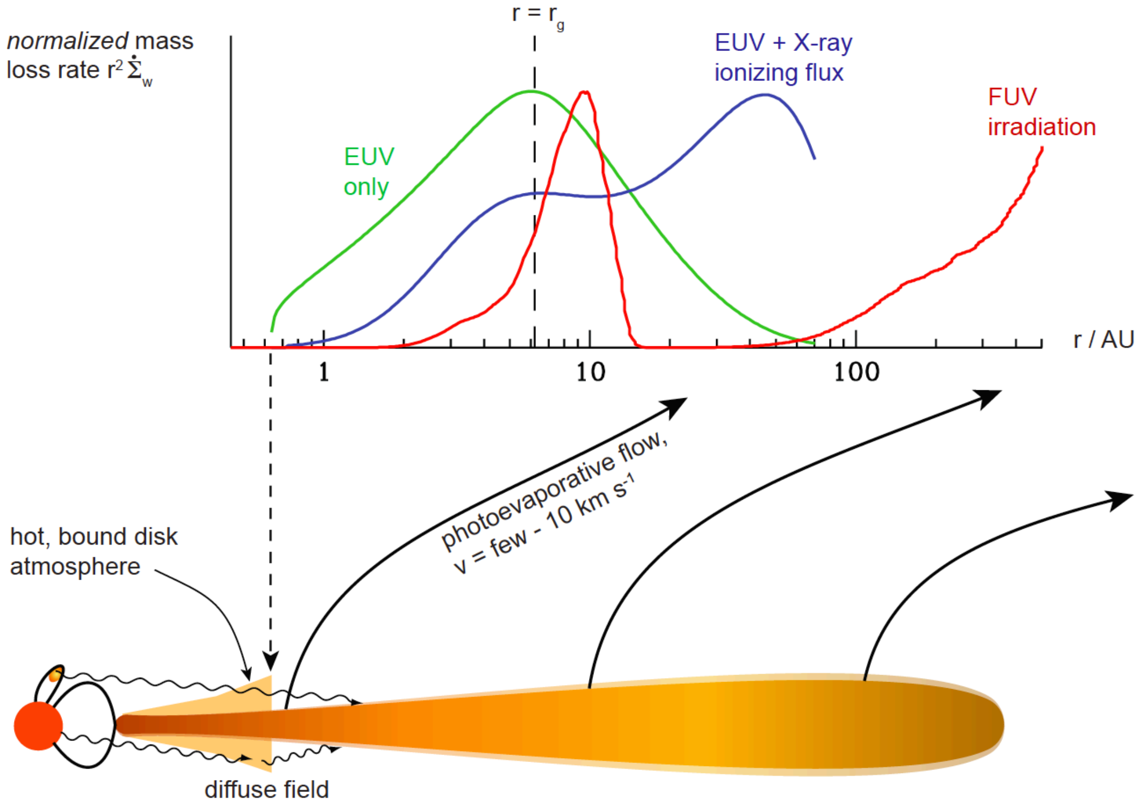

Figure 1: From Armitage (2011). Different photoevaporation profiles corresponding to the EUV-only model of Alexander et al. (2006a,b), the EUV+X-ray of Owen et al. (2010) and FUV model estimates of Gorti et al. (2009). The profiles have been normalised, where the total mass loss rates can differ by over two orders of magnitude.

an example, we have shown that the photoevaporation profile strongly influences the final semi-major axis distribution of exo-planets (Ercolano & Rosotti 2015).

While the importance of the final stages of disk evolution to understand planet formation and explain the diversity of exoplanets is largely recognised, a quantitative model describing this phase is still lacking. The reason for that is that all current models are somewhat incomplete. Some models focus on hydrodynamics and assume isothermal gas (e.g. the EUV-only model of Font et al. 2004) others focus on chemistry but do not perform hydrodynamical calculations (e.g. the FUV model of Gorti et al. 2009). None of the existing models take into account dust evolution in the underlying disk and entrainment of grains in the wind. Together with James Owen, a former PhD student I co-supervised at the Institute of Astronomy in Cambridge, I performed the only existing radiation hydrodynamic calculations of X-ray + EUV driven winds to date (Owen et al. 2010, 2011, 2012). For this calculation we used realistic gas temperatures obtained from X-ray photoionisation calculations (Ercolano et al. 2008a, 2009). This led to a fundamental re-think to the whole problem, as previous isothermal calculations had yielded much lower mass loss rates (by two orders of magnitude). However, our models, which still represents the state-of-the-art, also have important limitations, since, most importantly, they do not include chemistry and ignore the dust phase. Furthermore the resolution at which the simulations were performed is insufficient to study lines with emission regions extending close to the disk inner edge. The parameter space covered by these models is also rather small. These limitations make the application of current models to observations impossible.

As well as the uncertainties on mass loss rates and wind profiles, which directly affect planet formation, there are also a number of open questions regarding photoevaporation and the formation of the observed TDs. A recent review by Owen (2016) provides a discussion of the current successes and problems of theoretical models in explaining the origin and evolution of TDs. Here we will just list a few issues that we believe should have priority in the development of a quantitative theory which can be used to interpret observations.

1. The observations of TDs have yet to reveal objects with large holes that do not accrete. Photoevaporation, however, predicts that a significant population of them should exist, unless the final removal is dominated by a fast run-away phase called "thermal sweeping". (Owen et al. 2012). The efficiency of "thermal sweeping" has however recently been called into question (Haworth et al. 2016), however as will be discussed in more details below, a detailed calculation of thermal sweeping is still lacking.

2. The role played by FUV heating in the removal of the outer disk is unclear, due to the lack of hydrodynamical calculations that include this heating channel. FUV heating may provide a solution to the previous item, at least in some cases.

3. Current estimates of the TD demographics as predicted by the X-ray model are based on extrapolations of the results with stellar mass and stellar emission properties. The validity of these extrapolations has yet to be proved.

1.1.1.1 Contribution of this team to the current state-of-the-art

The first photoevaporation models developed were based on EUV irradiation only. This was mainly due to the need of simplifying the hydrodynamics by assuming an isothermal gas (Alexander et al. 2006a,b). An EUV heated gas, where hydrogen is almost fully ionised, is indeed roughly isothermal ($\sim 10^4$K), while the temperatures of a quasi-neutral X-ray heated gas generally vary from a few hundred to a few thousand Kelvin. Here the hydrogen gas cannot directly be ionised by the X-ray photons, thus it achieves only a very low level of ionisation, with the exact ionisation level influencing the efficiency of the X-ray heating. While the EUV-photoionisation process occurs of via the removal of a single valence electron, X-rays generally remove an inner-shell electron from a metal (e.g. C, N, O). The ejected supra-thermal electron produces then secondary ionisations (of mostly H and He). A further complication is that multiple electrons may be ejected as a consequence of inner shell ionisations, linking together non-adjacent ionisation levels.

The host of microphysics regulating X-ray ionisation and heating is self-consistently included in the three-dimensional photoionisation code MOCASSIN (Ercolano et al. 2003, 2005, 2008b) and has been applied to the X-ray photoionisation and photoevaporation problem of protoplanetary disks (Ercolano et al. 2008a, 2009; Ercolano & Owen 2010, 2016; Owen et al. 2010, 2011, 2012)

In Ercolano et al. (2008a, 2009) the relevance of the X-ray photoevaporation process to the dispersal of disks was proven for the first time. Indeed the mass loss rates calculated were approximately two order of magnitude larger than those previously obtained by the EUV-only model, able to compete with observed accretion rates from T-Tauri stars. These early results were based on hydrostatic calculations, which were later improved by our 2D radiation-hydrodynamic calculations (Owen et al. 2010, 2011, 2012), which still represent the state-of-the-art in this field. This work also provided detailed mass-loss radial profiles that have been used by us and others to study the photoevaporation process in combination with planet formation in 1D and 2D (e.g., Rosotti et al. 2013, 2015; Ercolano & Rosotti 2015).

Over the last few years we explored several possibilities to test and refine our models against observations. In Ercolano & Owen (2010, 2016) and in Schisano et al. (2010) we produced synthetic line profiles of forbidden transitions of heavy metals observed in the optical and in the mid-infrared. We came to the conclusion, however, that the strong temperature dependance of these lines makes them unsuitable for use as wind diagnostics.

In Ercolano & Clarke (2010) we explored the metallicity dependance of the mass loss rates, hoping for hints from disk statistics in several regions. While available data support our predictions (Yasui et al. 2009, 2010), these observations are challenging and have remained sparse. The importance of the effects we noted in this work for planet formation has however been widely recognised (e.g., Lopez 2016).

In Owen et al. (2013) we tested the models using predictions at radio wavelengths. We were able to show in that work that our observations of the famous transition disk around GM Aur were consistent with our models, but could not really distinguish between a EUV-only or an X-ray driven scenario. This line of work was however used again by Pascucci et al. (2014) to show that the EUV flux impinging on protoplanetary disks is generally low, hence arguing against a EUV-only model for dispersal.

The work described in this section has provided the basis for many theoretical and observational investigations, which cannot all be described here. We will only finally mention our most recent application where we were able to use our model to argue that the inner-most gap imaged with ALMA by Andrews et al. (2016) in the disk around TW Hya, is likely photoevaporative in origin (Ercolano et al. 2017).

1.2 Project-related publications

Ercolano, B., Drake, J.; Raymond, J., Clarke, C. *X-Ray-Irradiated Protoplanetary Disk Atmospheres. I. Predicted Emission-Line Spectrum and Photoevaporation*, 2008, ApJ 688, 398. In this paper we use the MOCASSIN code to present a first estimate of the magnitude of the X-ray photoevaporation process in protoplanetary disks. We obtain mass loss rates that are significantly higher than previous estimates, showing the relevance of this process to the dispersal of disks. Before this work the importance of X-ray photoevaporation had not been recognised.

Ercolano, B., Clarke, C., Drake, J. *X-Ray Irradiated Protoplanetary Disk Atmospheres. II. Predictions from Models in Hydrostatic Equilibrium*, 2009, ApJ 699, 1639. We further develop our models to include the feedback of X-ray heating on the disk-structure in hydrostatic equilibrium, and obtain more accurate estimates of the photoevaporation rates, which confirm our previous conclusions that the X-ray photoevaporation process is a main player in the dispersal of disks. These calculations provide the starting conditions for the full hydrodynamical investigations to Owen et al. (2010).

Owen J., **Ercolano B.**, Clarke, C. *Radiation-hydrodynamic models of X-ray and EUV photoevaporating protoplanetary disks*, 2010, MNRAS, 401, 1415. We perform the first radiation-hydrodynamic calculations of an X-ray and EUV irradiated disk in 2D. For that we modified a standard hydrodynamics code (ZEUS-2D) to include the X-ray heating rates calculated in the previous papers (Ercolano et al. 2008, 2009). The rates obtained here for the standard model still represent the state of the art and are widely used in the community.

Ercolano B., Owen J. *Theoretical spectra of photoevaporating protoplanetary disks: an atlas of atomic and low-ionization emission lines*, 2010, MNRAS 406,1553. We postprocess the models of Owen et al. (2010) and obtain synthetic observations of atomic and low-ionisation emission lines to be compared with the observations. We show that our models compare favourably with the observations available at the time.

Owen J., **Ercolano B.**, Clarke C. *Protoplanetary disk evolution and dispersal: the implications of X-ray photoevaporation*, 2011, MNRAS, 412, 13. We explore the role of X-ray photoevaporation in the evolution and dispersal of viscously evolving T Tauri disks. Our models confirm that X-rays play a dominant role in the evolution and dispersal of protoplanetary disks giving rise to the observed diverse population of transition disks, including those with massive outer disks and with residual gas in their inner holes, which provides detectable accretion signatures.

Owen J., Clarke & **Ercolano B.** *On the theory of disk photoevaporation* 2012, MNRAS, 422, 1880. We derive analytical scaling relations and derive estimates for the total mass-loss rates, as well as discussing the existence of similarity solutions for flows from primordial and transition disks. In this paper we catch a first glimpse at a new process for the clearing of the very last stages, which we name "thermal sweeping".

Ercolano B.,Rosotti G. *The link between disk dispersal by photoevaporation and the semimajor axis distribution of exoplanets*, 2015, MNRAS 450, 3008. We show here that details of the photoevaporation models (rates and profiles), strongly affect the planetary system configurations emerging from those disks. We suggest that the deserts and peaks seen in the distributions are a result of photoevaporation parking the giant planets at specific radii.

Ercolano B., Owen J. *Blueshifted [O I] lines from protoplanetary disks: the smoking gun of X-ray photoevaporation*, 2016, MNRAS 460. 3472 We produce new synthetic observations of a particularly promising diagnostic, [OI] 6300 and demonstrate that the observations available at the time (before Simon et al. 2016) are consistent with the photoevaporation model. We show however that this line cannot be used to measure mass-loss-rates and suggest that a thermochemical model of the wind launching region is necessary.

Ercolano B., Rosotti G., Picogna G., Testi L. *A photoevaporative gap in the closest planet-forming disk*, 2017, MNRAS 464L, 95 In this letter we show that the innermost gap in the disk around TW Hya, recently imaged by Andrews et al. (2016) with ALMA, is very likely due to X-ray photoevaporation. We demonstrate how all current observational data fit the predictions of the model and provide new estimates for the timescales of dust-draining from the inner disk.

Keto E. and **Caselli P.** *The Different Structures of the Two Classes of Starless Cores*, 2008, ApJ 683, 238. We construct a reduced chemical network for oxygen chemistry (including water and carbon monoxyde), include it into a hydrodynamical code of the evolution of Bonnor-Ebert (BE) spheres and compare the results with observations. For the first time, we demonstrate that dense cloud cores contract as unstable quasi-equilibrium BE spheres, while the singular isothermal sphere and Larson-Penston solutions for dense core contraction do not reproduce the observed line profiles. This was only computationally possible because the number of reactions was reduced to the core. A similar approach will be used in B1 and B2.

2. Objectives and work programme

2.1 Anticipated total duration of the project

36 months

2.2 Objectives

The overarching aim of this project, in common with projects B2 (PI Caselli & Ercolano) and C2 (PI Ercolano), is to identify new wind tracers and use them to constrain mass loss rates and hence disk dispersal models, leading to the formation and evolution of Type 1 transition disks.

The new comprehensive radiation-hydrodynamics photoevaporation models developed in this project will enable a quantitative spectroscopic evaluation of new diagnostics of disk winds, via detailed astrochemical models developed together with project B2, using the dust model for the wind and atmosphere from project C2.

We will perform a comparison between TDs and primordial disk to provide important constraints on the wind architecture and the mechanism driving the dispersal. Type 1 TDs, are particularly interesting as the streamline architecture of their winds and the profiles of the lines that are produced in the wind differ from those of primordial disks. (e.g. Ercolano & Owen 2010, Ercolano & Pascucci, 2017, in prep.). Indeed the lines are expected to be broader and brighter for e.g. inner cavities of a few to 10 AUs.

The immediate objective of project B1 is to produce a new set of X-ray+UV photoevaporation models which goes well beyond the current state-of-the-art, described in the previous section.

The new models will constitute the backbone for the joint investigation to be carried out in projects B2 and C2, as well as allowing us to address the following important unsolved questions in the formation of Type 1 transition disks and their further evolution:

1. How fast do Type 1 TDs evolve/disappear after the inner disk has drained?
2. How does the formation & evolution of Type 1 TDs scale with stellar mass and stellar emission properties?
3. What is the role of FUV heating in the late evolution of Type 1 transition disks?

2.3 Work programme including proposed research methods

In this project we will construct a library of high resolution X-ray+EUV wind solutions for an extended grid of X-ray luminosities and stellar masses, covering all observed values. Our new calculations will make use of a new temperature scheme (Ercolano, Picogna & Owen, 2017, in prep.), derived from new more extensive X-ray + EUV photoionisation models. The new temperature scheme significantly reduces the error at low ionisation parameter values, allowing us to make solid predictions of the late evolution of transition disks.

Furthermore, our previous calculations (Owen et al. 2010, 2011, 2012), could only account for heating in the ionised phase of the wind, ignoring that the region beyond the layer heated by the soft X-ray ($< 1keV$) which could be heated by FUV radiation with typical PDR or XDR characteristics. While we show in Owen et al. (2012), that this should not affect the mass loss rates at around 1-10 AU, the effect of FUV heating at larger radii may be important. This is particularly relevant to the late evolution of transition disks, when the cavity becomes larger than approximately 30 AU. Indeed one of the problems with current photoevaporation models is the prediction of a large number of non-accreting transition disks with large holes (e.g., Owen 2016). In this project we will be able to test the suggestion that FUV heating may take over the late-stage evolution of transition disks, speeding up their final complete erosion.

2.3.1 Research Tools

For this project we will need the following tools:

1. A hydrodynamical code modified to include the effects of X-ray + EUV irradiation as we did in Owen et al. (2010). For that we use the Pluto code, for which extensive expertise exists in our team and in other teams of this Research Unit (e.g. D1 & D2 – Applicants Kley & Dullemond).

2. An efficient astrochemistry package to include a reduced chemical network into PLUTO. For that we will use KROME (Grassi et al. 2014) and link it with PLUTO. Dr Grassi will take active part in helping with the implementation of the algorithm.

3. An efficient radiative transfer algorithm to model the region just beyond the X-ray dominated region. We can use initially the implementation of radiative transfer and stellar irradiation for the PLUTO code (Kolb et al. 2013), developed by the group of Kley (PI of project D2). If this is proved not to be sufficient for our aims, the Applicant also has experience in the development of hybrid algorithms (Owen et al. 2014).

2.3.2 Research Plan

2.3.2.1 Preparatory work

In this section we will describe preparatory work that is currently being carried out by Dr Picogna. Dr Picogna is currently employed in the group of Prof. Ercolano via an Excellent Initiative grant from the LMU, awarded to the Applicant to carry out preparatory work for this Research Unit proposal. The grant, which was extended using funds from the faculty will end in November 2017.

The determination of gas temperatures in a photoionised gas, in a photodissociation region (PDR) or in an X-ray dissociated region (XDR) is computationally expensive. It requires, first of all performing a radiative transfer (RT) calculation in order to determine the radiation field at each point of the region. Then matrices of thermal and ionisation balance and/or rate equations have to be solved. The RT and the balance/rate equation are often coupled through the temperature-dependent gas opacities, and one needs to iterate to obtain a solution. There is a host of microphysics that needs to be taken into account, last but not least the thermal coupling of the gas and the dust phase. Even an extremely

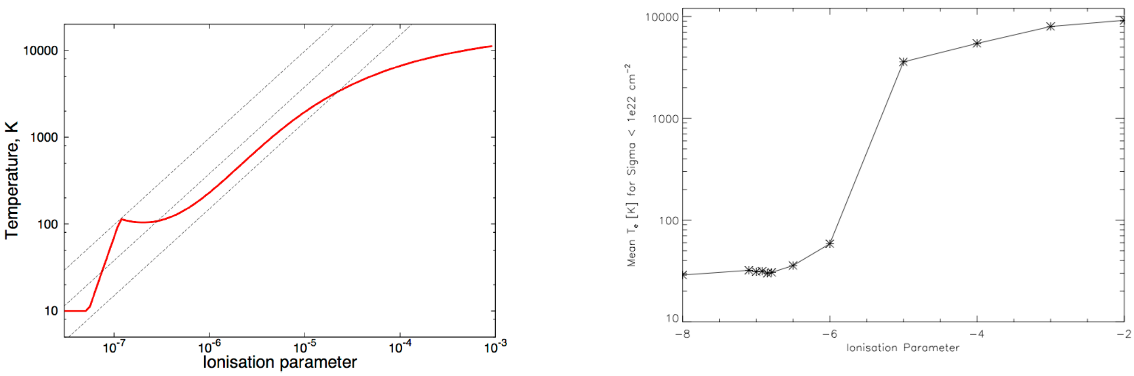

Figure 2: The electron temperature versus ionisation parameter relation in the calculations of Haworth et al. (2016), **left panel**, compared to our most recent calculations Ercolano, Picogna & Owen, (in preparation), **right panel**.

simplified version of the above has large computational costs, if it needs to be performed at every time-step of a hydrodynamical calculation.

In such cases it is convenient to look for parameterisations of the gas temperature in terms of quantities that are easy to determine on the fly during the hydrodynamical run (e.g. gas properties and/or column density). Indeed the radiation-hydrodynamical calculations of X-ray + EUV driven photoevaporative winds of Owen et al. (2010, 2011, 2012), described in the previous section, were performed using such a temperature paremeterisation. The parameterisation was determined via detailed X-ray photoevaporation models using the MOCASSIN code (Ercolano et al. 2008a, 2009) The models were run with a version of the ZEUS2D code which was modified by us to include a temperature scheme based on the ionisation parameter at each cell in the calculation. This was based on our previous work (Ercolano et al. 2008a, 2009). where it was shown that, within the penetration depth of ∼1keV X-rays ($\sim 10^{22} cm^{-2}$), the temperature of a parcel of gas with hydrogen number density, n_H, at distance r from the central star, could be roughly approximated by a function of the ionisation parameter, defined as $L_X/(r^2 n_H)$, whereL_X is the stellar X-ray luminosity. The error on the temperature was found to be small for high ionisation parameter values, but it becomes systematically larger at the low end.

As the gas temperature enters the hydrodynamics via the square root dependance in the sound speed, the small error at high values of the ionisation parameter, typical for the regions where the bulk of the wind is driven from in primordial disks, is unlikely to produce large uncertainties in the mass loss rates. For more evolved objects, like transition disks in the phase of final dispersal, however, the ionisation parameter decreases dramatically as the cavity becomes larger. The evolution of transition disks depends thus sensitively on the temperature of the gas at low ionisation parameters, which is currently poorly represented by the parameterisation of Ercolano et al. (2008a, 2009). Note that the recent work of Haworth et al. (2016), presents a form of the temperature ionisation parameter relation which is incorrect at low values of the ionisation parameter. The kink at ionisation parameters just above 10^{-7} (left panel of Figure 2) is an artefact of their implementation of the photoionisation models. We have recently performed new detailed photoionisation calculations and obtained the curve shown in the right panel of Figure 2 (Ercolano, Picogna & Owen, 2017, in prep.). Figure 2 shows no kink in the temperature parameterisation at low ionisation parameter, which is important as some of the conclusions reached by Haworth et al. (2016) are a consequence of this kink. Our collaborators J. Owen and C. Clarke, as well as the first author, Dr Haworth, have been informed of the problem and agree with our more recent calculations. Furthermore we have now found a more accurate scheme that allows us to reduce the error on the temperature by taking into account the gas column density as an additional parameter.

As well as the major shortcoming highlighted above, the Owen et al. (2010) calculations which were

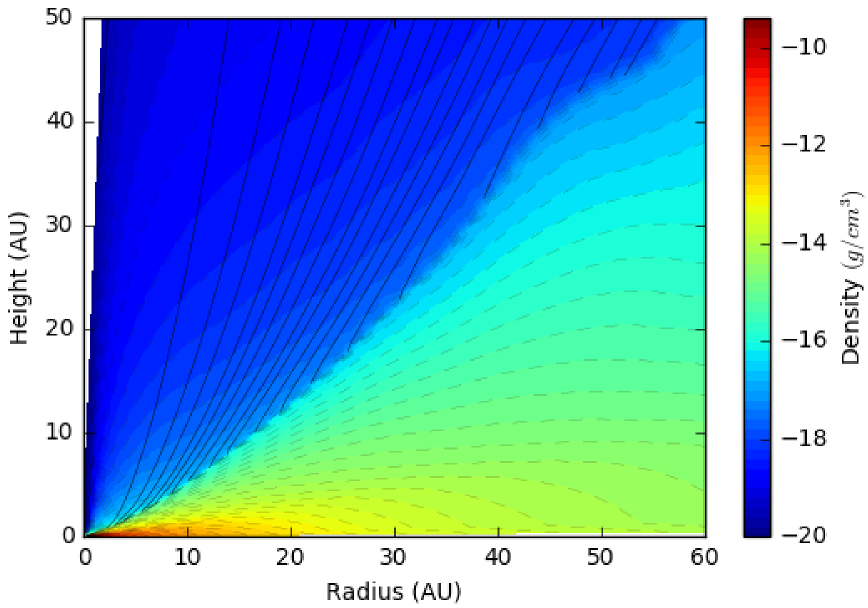

Figure 3: Column density map of our PLUTO simulation of the standard model from Owen et al. (2010), i.e. a 0.7 $M_\odot$ star with X-ray luminosity of $2{\times}10^{30}\,erg/sec$. The figure is in polar coordinate, where the colour scale indicates column density and the overlain black lines are the streamlines tracing the outflow.

used to make predictions on the ionised phase of the wind spectra (Ercolano & Owen 2010, 2016), suffered from low spatial resolution, precluding us from being able to model the inner region of the bound disk, which may be relevant to interpret the broad wings of some of the wind-tracing emission lines presented in the recent work of Simon et al. (2016). Furthermore, a very limited parameter space was investigated, which included only two values for stellar mass, 3 values of X-ray luminosity for primordial disks and a single stellar mass and X-ray luminosity value for transition disks with 3 values for the cavity radius. This is not enough to draw significant conclusions about trends in possible wind diagnostics.

In this project we aim at constructing new photoionisation models to remedy the shortcoming of the current models highlighted above. To that aim we have modified the hydrodynamical code PLUTO (Mignone et al. 2007, 2012) to include the effects of X-ray and EUV irradiation using the temperature-ionisation parameter from Ercolano et al. (2008a, 2009) also employed by Owen et al. (2010) for the ZEUS2D calculations. We have implemented the standard scheme in order to be able to compare our wind solutions to those available for a 0.7 and 0.1 $M_\odot$ central stars (Owen et al. 2010, 2011, 2012), for similar spatial resolution. This will ensure that we have implemented the algorithm correctly in PLUTO, before we move on with project B1 and implement the improved temperature scheme.

Figure3 shows a snapshot from our most recent simulation with our modified version of PLUTO aiming at reproducing the standard model of Owen et al. (2010). This is for 0.7 $M_\odot$ star with X-ray luminosity of $2{\times}10^{30}\,erg/sec$. For further details on the simulation set-up we refer to Owen et al. (2010). The figure shows column densities in a quarter of the disk in two-dimensional polar coordinates. Overplotted black lines are streamlines showing the outflowing gas. As mentioned above, in order to test that our implementation of the temperature scheme works correctly we have used the same parameterisation used by Owen et al. (2010).

We match the global mass-loss-rate to within 15% (we obtain a value of $1.2{\times}10^{-8} M_\odot/yr$ and we can reproduce the approximate wind profile, shown in Figure 4. This plot shows the cumulative mass-

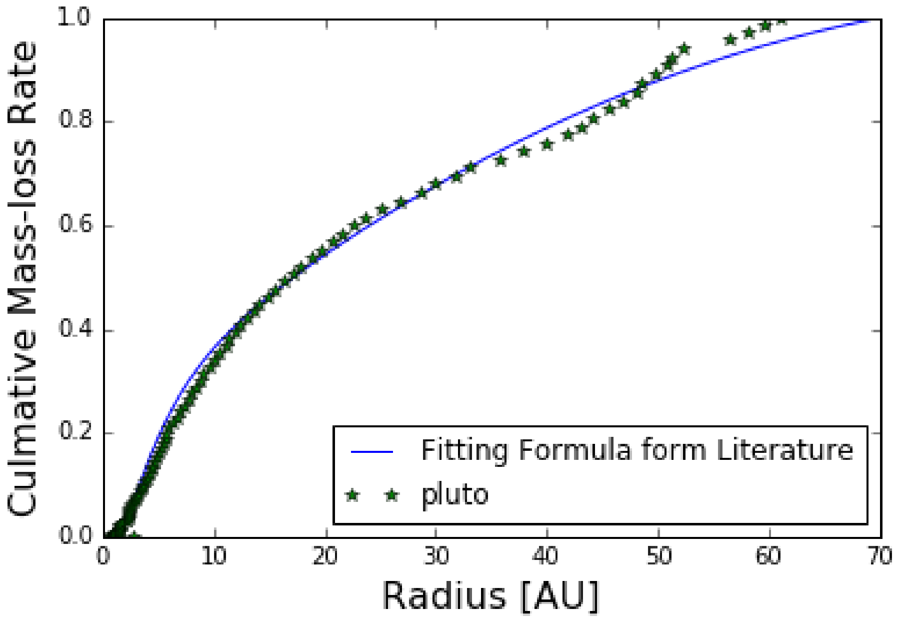

Figure 4: The cumulative mass-loss-rate as a function of disk radius from the PLUTO calculation (green stars) is compared to the fitting formula (solid blue line) obtained from the literature (Owen et al. 2010). The integrated value (to 100 AU) of the mass loss rate is approximately $1.2\times10^{-8} M_{\odot}/yr$.

loss-rate as a function of disk radius from the PLUTO calculation (green stars), compared to the fitting formula (solid blue line) obtained from the literature (Owen et al. 2010).

2.3.3 Months 1-12

In the preparatory work described in the previous section we have implemented the standard temperature scheme from Ercolano et al. (2008a, 2009) into PLUTO and have benchmarked the results against the work of Owen et al. (2010). In the first 12 months of the Research Unit we will then proceed with the implementation of the new, more accurate temperature scheme described in the previous Section (Ercolano, Picogna & Owen, 2017, in prep.). We will compare the resulting wind rates and profiles for the primordial and transition disk case presented by Owen et al. (2010). While we do not foresee large changes in the rates for primordial disks, as described in the previous section the evolution of transition disks will be most likely affected.

In particular we will test the late evolution of transition disks to estimate whether there is a radius for the inner cavity at which photoevaporation stalls. In that case one would expect to be able to observe a population of transition disks with large cavity and no accretion signature (relic disks), which to date remains elusive. A solution to this problem, form the theoretical stand-point, would be the triggering of a fast final clearing phase, as the proposed final thermal sweeping (Owen et al. 2011). Our models will be able to test this hypothesis in detail for the first time, as previous works have all been limited by the uncertainties in the temperature parameterisation of the X-rays at low ionisation parameters (e.g. Haworth et al 2016). We will then create synthetic transition disk population to check the occurrence of relic disks and compare it with the limits shown by current observational surveys from which we will be informed by the A1 team.

Furthermore, the new models will have much higher spatial resolution extending much closer into the star, in order to allow tracking the profile components of emission line which may be produced from the inner bound atmosphere of the disk (see discussion in Ercolano & Owen 2016 and in the Introductory section of this proposal).

This first set of models for ∼solar mass stars at a typical X-ray luminosity (∼ 10^{30}erg/sec) will be then passed on to projects C2 and B2 for the dust and detailed chemistry calculations.

2.3.4 Months 13-24

Once our machinery is complete and well-tested we will be able to switch to production-mode and extend significantly the parameter space of the calculations. Specifically, we will vary the mass of the central star and its X-ray luminosity as well as the accretion properties of the disk. Furthermore models of transitions disks at several stages of evolution, as tracked by the radius of their inner cavity, will be performed.

As new models become available and we populate the parameter space, we will make the grids available immediately to projects C2 and B2 for the dust and detailed chemistry calculations. At this stage we will already start to regularly check our model predictions against observations, with the help of experts from projects A1 and A2.

The new models will also allow us to investigate how the photoevaporation process scales with stellar mass and stellar emission properties. We will test the theoretical relations for X-ray photoevaporation predicted by means of semi-analytical models and ab-initio arguments by Owen et al. (2012). These relations are already being widely used in the literature and they are a crucial ingredient for population synthesis models of planet formation, where photoevaporation is included in the disk evolution and affects the timescales and location for the formation of giant planets, as well as their successive migration.

The larger parameter space will also allow us to improve on our initial calculations to construct more accurate synthetic populations of evolved disks to match the observed demographics of Type 1 TDs. Note that project A1 will keep an up-to-date record of the transition disk demographics throughout the duration of the Research Unit.

2.3.5 Months 25-36

The role of FUV heating in supporting or competing with the X-rays in the removal of the disk is still uncertain. As we discussed in the previous sections, the work of Gorti, Dullemond & Hollenbach (2009), based on 1+1D thermochemical calculations in hydrostatic equilibrium, suggest that a vigorous thermal wind may be driven as a result of FUV-heating. For some disk parameters (in particular in the presence of PAHs), the FUV is shown to reach mass-loss-rates comparable to those driven by X-rays. An hydrodynamical calculation of an FUV driven wind is however still lacking and it is urgently needed in order to assess the importance of this process, in particular at large disk radii, which is relevant to the problem of disk relics, amongst other things.

At this stage of the Research Unit a robust and well tested reduced chemical network should be available from project B2 (PI Caselli, Ercolano). We will now couple our modified version of the PLUTO code to the KROME package to solve the chemistry using the reduced network from B2 and obtain the temperatures of the gas on the fly in the regions beyond the X-ray dominated regions. For that we will receive help from our collaborator Dr. Grassi, who is the main developer of the KROME code. Dr. Picogna has already attended the KROME school this year (`http://kromepackage.org/bootcamp/`) and a simple feasibility test has shown that this is a realistic task. As an example, KROME is already implemented in a number of hydrodynamics codes (e.g. RAMSES, ENZO, FLASH, GASOLINE, GIZMO). A number of publications performed with these codes are listed on the KROME webpage (`http://www.kromepackage.org/`).

A streamlined form of radiative transfer will be needed in PLUTO at this point, meaning that these calculations will probably be expensive to run. This is however necessary in order to estimate the value of the FUV field reaching different regions of the disk atmosphere, where the optical depth are not high enough to justify the use of a (grey) flux limited diffusion method. Implementation of an efficient radiative transfer algorithm in PLUTO will be carried out together with the Applicant who has experience in the development of hybrid algorythms (e.g., Owen et al. 2014). A simple RT scheme is already available for PLUTO (Kolb et al. 2013), which was developed in the group of our Prof. Kley (PI from project D1). Hence there is a substantial body of experience within our Research Unit team to successfully perform this task.

Note that we do not plan to run a full parameter space grid including the effects of the FUV heating. Our simulations will be limited to a selected number of cases aimed at specifically testing how strongly, and for what initial conditions, FUV heating may affect the evolution of the outer regions of disks, in particular of those in transition.

2.3.6 Future Outlook

A natural further step of this work is to perform a small set of 3D simulations to explore the effects of asymmetries in the inner disk and/or the presence of giant planets in the disk. We expect to see dramatic effects in the photoevaporation profile and in the wind architecture, which may lead to the formation of large hole TDs. This avenue has never been explored before and, while these models come at severe computational costs, they are likely to provide us with important insights on the structure and origin of TDs.

In particular in the second funding period of the Research Unit, the results from projects D1 and D2 will be available to us, and the natural further step will be to combine photoevaporation to planet-disk interaction calculations.

2.4 Data handling

A library of the hydrodynamical solutions in steady state (gas density and velocity) will be shared initially amongst the Research Unit members only and will be made available online on the public partition of the Research Unit server at the end of the first funding period.

2.5 Other information

Not Relevant

2.6 Information on scientific and financial involvement of international cooperation partners

Not Relevant

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4. Requested modules/funds

4.1 Basic Module

4.1.1 Funding for Staff

We require funding for one Postdoc to work at the LMU in the group of Prof. Ercolano. In case of an award Dr Picogna has expressed interest in taking on the post. Dr Picogna is currently employed in the group of the PI and is performing preparatory work for the project. Dr Picogna's expertise in astrophysical fluid dynamics and his familiarity with the subject is of great advantage for the achievement of the aims of this project. Dr Picogna's contract ends in November 2017.

4.1.2 Direct Project Costs

4.1.2.1 Equipment up to EUR 10,000, Software and Consumables

Theoretical numerical research can only be done when sufficient and appropriate computational facilities are available. While production runs will be done on supercomputer facilities, a substantial part of the work in this project is code development. Testing these codes on realistic problems requires a workstation for the postdoc – which is beyond the standard base equipment (Grundausstattung). We therefore request a workstation-grade desktop computer for the postdoc position for 3 000 €.

4.1.2.2 Travel Expenses

Travel within the Research Unit is handled in project Z. In addition we request funding for conference travel for the personnel and one Applicant. This includes one national (1.000 €) and one international (1.500 €) conference trip per year, totalling 2.500 € per person per year.

For this project this totals 5.000 € per year for the postdoc and one Applicant, which is in total 15.000 €.

4.1.2.3 Visiting Researchers (excluding Mercator Fellows)

During the course of the project a one week long visits to our main international collaborator, Dr J. Owen (currently at Princeton University, will move to Imperial College London in 2017). This includes airfare and 6 overnight stay 1200 €

4.1.2.4 Other Costs

None

4.1.2.5 Project-related publication expenses

We request 750 € per year (a total of 2 250 €) for publication expenses, mainly to support open access options or whenever necessary, publication in non-free journals.

4.1.3 Instrumentation

None

4.1.3.1 Equipment exceeding EUR 10,000

None

4.1.3.2 Major Instrumentation exceeding EUR 100,000

None

5. Project requirements

5.1 Employment status information

Barbara Ercolano, Professor at the Ludwig-Maximilians-Universität München (permanent)

5.2 First-time proposal data

Not Relevant

5.3 Composition of the project group

Paola Caselli, Director of MPE and of the Centre of Astrochemical Studies at the MPE (permanent). Prof. Caselli will provide guidance in treating the heating and cooling channels due to chemistry at the base of the flow into our hydynamics calculations.

Dr. Wing-Fi Thi, postdoc (current contract ends in 2009), works in the CAS group of Prof. Caselli and is an expert in chemical models of protoplanetary disks.

Dr Alexei Ivlev, researcher (permanent), works in the CAS group of Prof. Caselli and is an expert in grain charging and X-ray transport.

5.4 Cooperation with other researchers

5.4.1 Planned cooperation on this project

5.4.1.1 Collaborating researchers for this project within the Research Unit

This project will provide the radiation-hydrodynamic models of the wind which are needed by project B2 (PI: Prof. Caselli & Prof. Ercolano) for the chemical calculations and by project C2 (PI: Ercolano) for the dust entrainment. Project BI depends on input from project B2 (PI: Prof. Caselli & Prof. Ercolano) for the reduced network and on project A2 (PI Prof. Preibisch) for observational input. Specifically project A2 (Prof. Preibisch) can provide insights on the emission properties of the irradiating stars. We already have made used extensively of the results coming from the group of Prof. Preibisch in terms of realistic X-ray luminosity functions for the construction of population synthesis of disks and of the individual X-ray spectra, when considering the ionisation and heating of individual sources. At the end of the first funding period and particularly in the second funding period of the Research Unit, the results from projects D1 (PI Kley) and D2 (PI Dullemond) will be available to us, and the natural further step will be to combine photoevaporation to planet-disk interaction calculations. Project B1 will provide project C1 team (PIs Dr. Birnstiel, Prof. Dullemond) with the hydrodynamical models for photoevaporating disks, to allow them to investigate dust growth in pressure bumps formed at the inner edge of the outer disk.

5.4.1.2 Collaborating researchers for this project outside of the Research Unit

Dr. James Owen (Princeton) will be heavily involved in the project. Dr. Owen developed the original phoionisation models during his PhD project at the Institute of Astronomy in Cambridge, which was co-supervised by Prof. Ercolano. It is envisioned that Dr. Owen will pay regular visit to our group to help with the development of the new models.

Dr. Tommaso Grassi (STARplan Copenhagen, Denmark) is an expert of chemistry and the microphysics of the ISM coupled with hydrodynamical simulations of (e.g.) star-forming regions. He leads the development of the KROME package (http://www.kromepackage.org/).

5.4.2 Researchers with whom you have collaborated scientifically within the past three years

Maite Bertran (INAF-Osservatorio Astrofisico di Arcetri), Aaron Boley (University of British Columbia), Sandra Brünken (University of Cologne), Stephanie Cazaux (University of Groningen), Cecilia Ceccarelli (Univ. Grenoble Alpes), Francesco Fontani (INAF-Osservatorio Astrofisico di Arcetri), Thomas Hartquist (University of Leeds), Izaskun Jimenez-Serra (Queen Mary University London), Eric Keto (Harvard-Smithsonian Center for Astrophysics), Marco Spaans (University of Groningen), Jonathan Tan (University of Florida), Stephan Schlemmer (University of Cologne), Charlotte Vastel (Université de Tulouse), Malcolm Walmsley (INAF-Osservatorio Astrofisico di Arcetri); F. Niederhofer (STSci, USA); M. Hilker (ESO, Garching); N. Bastian (U. Liverpool, UK); M. Guarcello (U. Palermo, Italy); M. Tazzari (U. Cambridge, UK); A. Natta (Florence, Italy); R. Alexander (U. Leicester); D. Hubber (LMU); J. Dale (U. Hertfordshire, UK); C. Koepferl (LMU); I. Bonnell (U. St. Andrews, UK); A. McLeod (ESO, Garching); D. Boneberg (U. Cambridge, UK); R. Parker (U. Liverpool, UK); R. Wesson (UCL, London, UK); M. Barlow (UCL, London, UK); A. Glassgold (u. Berkeley, USA); C. Manara (ESA, Noordwjik, Netherlands); A. Danekhar (CfA, Harward, USA); Q. Parker (Sidney, Australia); S. Casassus (U. de Chile, Santiago, Chile); I. Pascucci (U. Arizona, USA); A. Bevan (UCL, London, UK).

5.5 Scientific equipment

The group of Prof. Ercolano has two own computer clusters comprising

- 2 CPU Intel Xeon X5650 (Westmere, beginning 2010, 2.66 GHz) 6 cores each 12 cores total (24 virtual) 74 GB ram.
- 4 CPU Intel Xeon E7-4850 (Ivy Bridge, beginning 2014, 2.30 GHz) 12 cores each 48 cores total (96 virtual) 660 GB ram.

Further computational power is provided through the C2PAP facility of the Excellence Cluster to which the group has guaranteed time. This comprises 126 nodes, each node with 2 CPU Intel Xeon E5-2680 (Sandy Bridge, beginning 2012, 2.7 GHz) 8 cores each 16 cores total (32 virtual) 64 GB ram. Note that while the future of the Excellence Cluster Universe is uncertain, the C2PAP facilities will be in any case supported by the LMU.

The CAS group of Prof. Caselli has also its own cluster: an HPC cluster comprising of 25 nodes with 20 cores and 128 GB memory each; 4 nodes with 20 cores and 256 GB memory each (Infiniband, 50 TB storage, Login-Node, Batch-System; 2 Compute nodes, i.e. 2 nodes with 20 cores and 512 GB (10 TB storage).

The HPC facilities at the Leibniz Rechenzentrum (LRZ) are also available to us. These include iDataPlex HPC System HYDRA with Intel Ivy Bridge processors (3500 nodes with 20 cores at 2.8 GHz each).

Furthermore the CAS centre led by Prof. Caselli has available computer facilities for visiting scientists and students. CAS has its own cluster: an HPC cluster comprising of 25 nodes with 20 cores and 128 GB memory each; 4 nodes with 20 cores and 256 GB memory each (Infiniband, 50 TB storage, Login-Node, Batch-System; 2 Compute nodes, i.e. 2 nodes with 20 cores and 512 GB (10 TB storage).

Project B2:

Astrochemistry in the atmospheres and winds of photoevaporating disks

Authors:

Applicants:	Paola Caselli (MPE), Barbara Ercolano (LMU)
Co-Applicant:	Ewine van Dishoeck (MPE/Leiden))
Cooperation partners:	Wing-Fai Thi (MPE), Alexei Ivlev (MPE), T. Grassi (STARPLAN, Copenhagen)

Requested positions: 1 Postdoc

Abstract:
Protoplanetary disks lose mass via a slow disk wind, probably driven by photoevaporation from the central star, which eventually creates a cavity, leading to the formation of a Type 1 TD (see discussion in the Introduction to the Research Unit). The strength and profile of these winds remains, however, unconstrained from the models, as no suitable diagnostic to directly determine the wind properties from observations is known. This is due to the fact that a thermochemical study of this important component of evolved disks does not exist to date. The study of the chemistry in disk winds however relies on a knowledge of the opacities, which are largely dominated by small dust grains which are entrained in the wind from the underlying disk at the launch point. In this project we plan to develop a reduced chemical network appropriate for photoevaporative wind conditions and couple our chemical codes to space and time-varying dust distribution obtained in project C2. Using state-of-the-art radiation-hydrodynamic models of photoevaporating primordial and TDs obtained from project B1, we will for the first time be able to draw detailed chemical profiles of these winds and provide predictions by using radiative transfer codes[1]. This is of fundamental importance to identify and interpret new spectral line diagnostics in existing and upcoming observations.

1. State of the art and preliminary work

1.1 Models of disk Dispersal

Disk dispersal models, like photoevaporation, have been motivated by the observation that the dispersal of protoplanetary disks is not a continuous process. In particular the detection of transition disks i.e. disks with an evacuated inner dust and/or gas gap/cavity, and their frequency with respect to full disks has encouraged models which could match dispersal timescales about 10 times faster than the global disk lifetimes, and inside-out dispersal (e.g. Ercolano, Clarke & Hall 2011; Koepferl, Ercolano et al. 2013).

Recent reviews (e.g. Alexander et al. 2014, Armitage 2011) describe the available photoevaporation models in detail, and they point out that the predictions from these differ, sometimes by order of magnitudes in critical wind properties like mass loss rates and profiles (see Introduction to the Research Unit and project B1). Current photoevaporation models differ substantially in the approach to the complex problem of driving a thermal wind from the surface of a disk.

The different models can be grouped, depending on the type of stellar radiation supposed to be driving the wind. They include basically 3 categories':

[1] The text highlighted in green refers to the connection of this project to other projects of this Research Unit.

1. FUV-driven models (e.g. Gorti, Dullemond & Hollenbach 2009). Photons just below 13.6 eV, mass loss rates vary strongly with input, but up to $10^{-8} M_\odot/yr$, mass loss profile extending from $\sim$1 AU to $>\sim$100 AU for a solar mass star. Main model limitations: no hydrodynamics.
2. EUV-driven models (e.g. Alexander et al. 2006). Photons at roughly 13.6 eV, mass loss rate approx $10^{-10} M_\odot/yr$, mass loss concentrated at the gravitational radius (around 1AU for a solar mass star). Main model limitations: isothermal calculation, input flux unknown.
3. X-ray-driven models (e.g. Owen, Ercolano et al. 2010). Photons with $13.6 < E <$ a few 100 eV, mass loss rate approx $10^{-8} M_\odot/yr$, mass loss profile broader extending from $\sim$1 AU to $\sim$70 AU for a solar mass star. Main model limitations: no chemistry.

The consequences of these large differences in the dispersal model on the formation and evolution of planets have been often demonstrated (e.g. Ercolano & Clarke 2009; Ercolano & Rosotti, 2015; Alexander & Pascucci 2012), but still no quantitative dispersal model exists. The fundamental reason why the theoretical models still wildly disagree with each other is because until now they could not be directly tested with observations. **The B2 project aims at enabling the construction of a detailed chemical model of disk winds and atmospheres to directly compare with observations and provide a quantitative picture of the wind properties.**

As well as thermal winds driven by irradiation from the central star, the idea of magnetically driven winds has also been recently proposed. The classical magnetically supported/driven winds were developed to explain outflows from young stars, particularly in the class I phase. One set of these models were based on disk/magnetosphere interactions and mostly deal with the ideal MHD region of the disk (e.g. Shu et al. 2006, Ferreira et al. 2006). More recently, Bai et al. (2016), based on an extrapolation of the local calculations of Bai & Stone (2013) have suggested, however, that non-ideal MHD effects, may also cause a disk wind which may be launched from a much more extended region of the disk, overlapping/supporting/competing with photoevaporation to the dispersal of the disk. These authors suggest that these magnetically-launched disk winds may be so vigorous as to compete with photoevaporation for the dispersal of the disk. The mass loss rates from magnetic wind models are, however, highly uncertain as they are based on a number of assumptions that still need to be verified. In particular, the models require a minimum level of ionisation for the gas to be coupled to the magnetic field and assume that this may be delivered from far ultra-violet (FUV: 122-200nm) radiation ionising the atmosphere of a disk. The level of ionisation in the upper layer is currently estimated rather crudely as a fixed ionisation fraction of $f = 2 \times 10^{-5}$ in the form of carbon in the FUV layer, whose column density is chosen by default as $\Sigma_{FUV} = 0.03 g cm^{-2}$. This is based on results from Perez-Becker & Chiang (2011), who however only consider a simplified disk model. Crucially, these models do not include the contribution of the wind which itself may shield the disk atmosphere from the more energetic FUV photons, meaning that the currently used ionisation fractions may be overestimated. The models developed in this project will be able for the first time to provide a case-specific assessment of the level of coupling of the gas to the magnetic fields in the class II phase, taking into account the opacity provided by the wind itself. This is a fundamental ingredient to assess the possible role played by magnetic winds.

1.2 Chemical models of disks

Chemical models of gas in the protoplanetary and transition disks (TDs) are essential to pin down the initial conditions of the gas and dust from which planets form. Several sophisticated models have been and are continuously being developed to interpret the recent (e.g.) Herschel and ALMA observations of disks (e.g. Bruderer et al. 2015; Thi et al. 2013; Aresu et al. 2012; Meijerink et al. 2012; Woitke et al. 2010). These models however deal with with the dense parts of the disks, in rare cases extending to the bound disk atmospheres. Panoglou et al. (2012) have followed ionisation, chemical and thermal evolution within a steady state magneto-hydrodynamic disk wind solution and investigated various stages of young stellar objects (from Class 0 to Class II). No chemical model of a photoeveaporative TD wind as well as no time-dependent chemical model coupled with the dynamical evolution of a disk exist to date. This is a serious shortcoming for the identification of suitable wind tracers and more importantly wind diagnostics, to guide new observations and constrain disk dispersal models

The physical conditions valid for material in the bound disk itself are not appropriate for a disk wind. First of all winds are much less dense than the material in the bound disks. Even in the case of vigorous X-ray driven winds, the densities at the base of the wind are rarely above ten million hydrogen atoms per cubic centimetre, and they decrease roughly with the square of the distance (i.e. they behave roughly like Parker winds, see e.g. Owen et al. 2010; Font et al. 2004). The opacity in the wind is further reduced because they are depleted of dust, as only a fraction of the dust grains contained in the underlying disk are entrained in the wind (see Owen et al. 2011b, Hutschison et al. 2016ab and discussion in project C2). For these reasons molecules may have a much shorter lifetime and indeed parts of the gas in the wind will be completely photodissociated. For such physical conditions processes like surface chemistry, freeze-out etc. are not important, yielding a simpler problem, which bears less uncertainties compared with chemical models for colder and more opaque material in the bulk of the disk.

The chemical structure of the underlying bound disk is however still important, as it provides the initial conditions for the chemistry in the wind. Furthermore, the ionisation level in the upper layers as well as in the deep layers of the disk has recently been shown to be of outmost importance to the evolution and perhaps dispersal of disks, due to the role it plays in coupling the gas to magnetic fields. A minimum amount of coupling is indeed necessary for magnetic turbulence to take hold.

1.3 Disk Wind diagnostics

A number of disk wind tracers have been studied to date, both observationally and theoretically. To date however no diagnostic could be identified to directly measure the wind properties. Figure 1, taken from an upcoming review on transition disks by Ercolano & Pascucci (2017, to appear in Royal Society Open Science) shows an example of possible wind diagnostics, which are summarised in the caption.

We will divide our discussion on wind diagnostics into two parts, ionic and atomic species on the one hand and molecular species on the other.

Ionic and atomic species

The presence of disk winds has been confirmed via the observation of a few km/sec blue-shift in the line profiles of a number of tracers like [NeII] 12.8μm and [OI] 6300 (e.g. Pascucci et al 2007, Rigliaco et al. 2013) and a number of collisionally excited lines in the optical region (Natta et al. 2014).

We have demonstrated, however, that the [NeII] 12.8μm and the optical forbidden lines cannot be used to infer the underlying mass-loss-rates (e.g. Ercolano & Owen 2010, Ercolano & Owen 2016). For example, the intensity and the profile of the [NeII] 12.8μm line can be equally well fitted using an EUV (Alexander 2008) or an X-ray photoevaporation model (Ercolano & Owen 2010), as shown in Figure 2. The problem with the [NeII] line is that the Ne+ formation route can occur both via the removal of a valence electron in the fully-ionised winds driven by EUV radiation, but also by charge exchange of Ne++ with neutral H which is abundant in the quasi-neutral winds driven by X-ray. The problem with the [OI] 6300 line and all other optical collisionally excited lines considered to date is the strong temperature dependence imposed by the Boltzmann term in the emissivity. This means that these lines are mostly just tracing the hot layer of the wind heated by the EUV radiation and not actually tracing the bulk of the wind where it matters (Ercolano & Owen 2016), hence they cannot be used to infer mass-loss-rates or to constrain the wind driving mechanism.

This picture was further complicated by the recent high spectral resolution observations of Simon et al. (2016) who found that low velocity emission in [OI] forbidden lines, classically attributed to a slow-moving disk wind, is present in all T-Tauri stars with dust disks, even those classified as WTTs, but it is

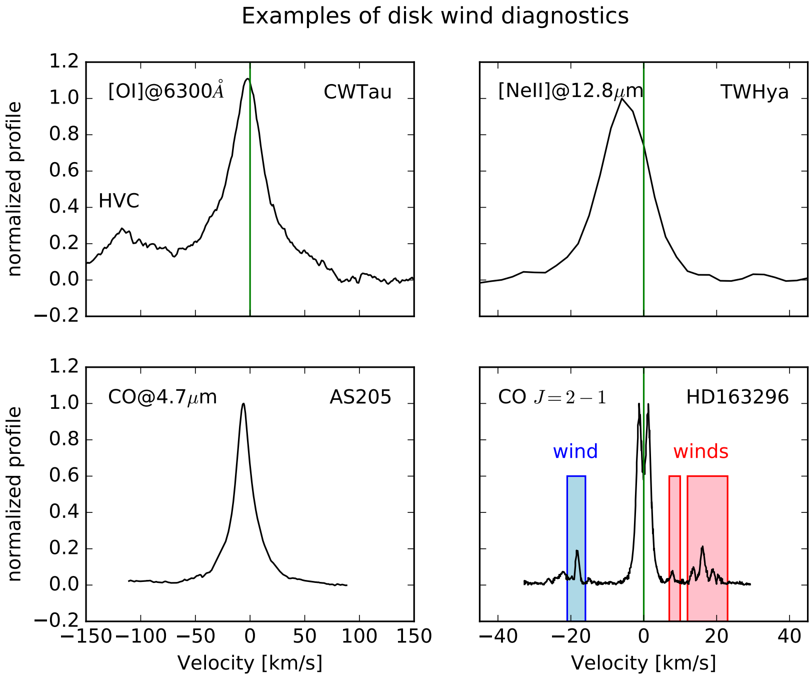

Figure 1: Examples of wind diagnostics. The [OI] 6300 Å profile of CW Tau is from Simon et al. (2016), note that the highvelocity component (HVC) is associated with fast jets. The [OI] 5577 Å transition is weaker than the 6300Å but shows a very similar low-velocity profile (Simon et al. 2016). The CO-M band profile of AS205 is from stacked CO rovibrational lines around 4.7μm (Banzatti & Pontopidan 2015). The [NeII] 12.8μm profile is the mean profile from Pascucci et al. (2011) and the CO J=2-1 profile of HD163296 is from Klaassen et al. (2013). All profiles, except that of AS205, are in the stellocentrc reference frame. Emission shifted in velocity with respect to the stellar velocity is indicative of unbound gas. This figure is taken from an upcoming review on transition disks by Ercolano & Pascucci (2017, to appear in Royal Society Open Science).

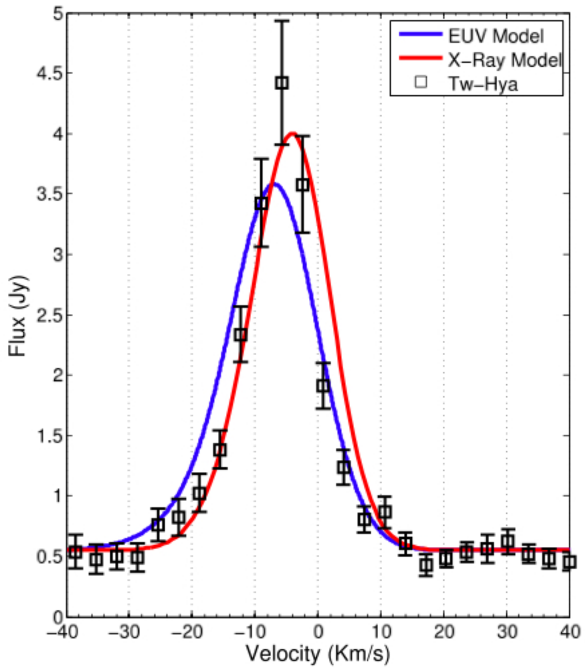

Figure 2: NeII 12.8μm line profile as predicted by the X-ray models of Ercolano & Owen (2010), red line, and by the EUV-only model of Alexander (2008), blue line, compared to the observation of TW-Hya by Pascucci et al. (2009), black line.

best fit by a superposition of a broad and a narrow component. Most of the broad component emission arises within 0.5AU and Simon et al. (2016) interpret it as being produced in a magnetically driven wind, given that the emitting region is well inside the gravitational potential well of the central star. The narrow component, which, unlike the broad component, is always present in also in transition disks, traces gas further away (0.5-5 AU) and is probably associated with photoevaporative winds.

The interpretation of the broad component as a tracer of a magnetic wind is however problematic for a number of reasons. The main problem is that one would need a very large scale height to overcome the fact that the emitting volume dominates as one goes to larger radius. Presumably a very large magnetic pressure would be needed to achieve this. Furthermore, if an hypothetical magnetic wind would have enough density to match the observed broad component, it may also absorb out all UV flux, which would then not be available to irradiate the wind at larger radii, hence being at odds with the observation of the narrow line component.

An alternative explanation could be that the broad component is not produced in the wind, but is emitted by bound material in the disk itself. The broad component, if coming from the inner disk, cannot have however a thermal origin. We have tested that with a new higher resolution set of hydrodynamical calculations, similar to those presented by Ercolano & Owen (2016), which extend further into the inner disk, to $r_{\rm in}$=0.04 AU. The line profiles for the high resolution hydrodynamical calculations are shown in Figure 3 for R=25000, which represent the resolution of the Rigliaco et al (2013) data, when the two component had not been resolved yet, and R=50000, which is more representative of the work of Simon et al. (2016). The R=50000 line profiles in our simulations do show broad wings at high disk inclinations. The wings are due to bound material in the inner disk. However the wings from our high resolution models are still much smaller (i.e. do not carry enough flux) than those detected by Simon et al. (2016). In fact in our calculations the line flux is completely dominated by the (unbound) emission at larger radii. This is easy to understand as the flux is proportional to density squared times the volume and the volume for an isothermal region in the disk scales like $R^{7/2}$

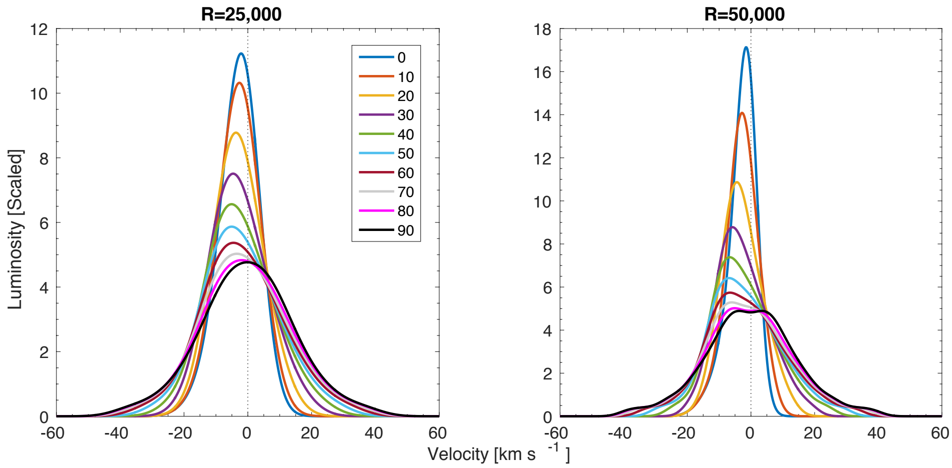

Figure 3: [OI] 6300 line profiles for the high resolution hydrodynamical calculations of Ercolano & Owen (2016) for R=25000 (**left panel**), which represent the resolution of the Rigliaco et al (2013) data, when the two component had not been resolved yet, and R=50000 (**right panel**, which is more representative of the work of Simon et al. (2016). In the left panel wings due to the bound material are clearly seen, but they are much smaller than those presented by Simon et al. (2016).

($R^2 \times H$). Given that the density does not fall off steeply enough in the heated region then the emission at larger radii dominates. For example a density profile set by the absorption of photons to a fixed column - indicative of our case - would fall of approximately as $n \propto 1/R$, provided the absorption is dominated at large radius.

Our calculations show nevertheless that bound material in the very inner disk can indeed produce broad wings. If the column of emitting bound material were larger then stronger wings would be produced. A non-thermal process acting at higher columns in the inner disk, as for example dissociation of the OH molecule, could indeed produce the missing flux in the wings. This could also be blue-shifted if the OH-layer extends to the base of the wind (see e.g. Gorti et al. 2011). As our codes currently lack chemistry we have been unable to test a non thermal origin of the broad component. This is however an important task, as if confirmed, there would be no need to invoke magnetic disk winds to explain the observations.

While a number of chemical models exist of the deeper, denser regions of disks, no model is currently available for the optically thinner disk winds. The work of Gorti, Dullemond & Hollenbach (2009), while carrying out detailed chemical calculations extending to the disk atmosphere, used a hydro*static* disk model which was analysed in a 1+1D fashion. Without hydro*dynamics* no predictions on line profiles can be made. Studying the kinematic of the emitting gas is the only way to constrain the origin and intensity of the disk wind and hence shed light on the driving mechanism behind the dispersal of disks and the formation of Type 1 transition disks.

Molecular species

Mid-infrared observations of molecular lines (e.g. CO) provide a new promising alternative to directly measure disk winds. Indeed recent observations suggest that these lines may be tracing a disk wind which is slow and partially molecular (e.g. Pontoppidan et al. 2011; Brown et al. 2013). The spectro-astrometric survey of molecular gas in the inner regions of protoplanetary disks using CRIRES, the high-resolution infrared imaging spectrometer on the Very Large Telescope (Pontoppidan et al. 2011), showed that for several sources the astrometric signatures are dominated by gas with strong non-Keplerian (radial) motions. These authors concluded that the non-Keplerian spectro-astrometric signatures are likely indicative of the presence of wide-angle disk winds. More observations of this type are planned after the update of the CRIRES instrument, which is expected to be completed by

2019. Observations with ALMA in molecular lines like e.g. CO J = 2-1 and J = 3-2 emission are also able to trace the presence of a wind (e.g.Klaassen et al. 2013, 2016). Molecular lines are sensitive to the mass loss rates since they sample a significant area of the wind launching regions. However the exploitation of molecular tracers is currently severely hampered by the lack of a suitable hydrodynamic wind model coupled to chemistry and to dust evolution models (which dominate the opacity in the wind) to interpret the observations.

Molecular tracers of outflow activity are common in the protostellar phase, they also probe a low velocity ($<$10 km/s) component whose intensity decreases while the opening angle increases going from the Class 0 through to the Class II phase (e.g. Frank et al. 2014 for a recent review). This slow wide-angle component, around a much faster jet, is naturally produced in MHD disk winds launched out to several AU (e.g. Pudritz et al. 2007, Panoglou et al. 2012). ALMA maps of outflow activity are corroborating this picture by providing the sensitivity to study in detail the faint Class II sources, see e.g. the CO disk wind surrounding the fast jet from the $\sim$4 Myr-old Herbig Ae star HD 163296 (Klaassen et al. 2013). Interestingly, the rough mass loss rate from the molecular wind is inferred to be similar to the mass accretion rate onto HD 163296 suggesting that winds contribute significantly to disk dispersal. Like optical forbidden lines, M-band CO ro-vibrational lines also show a broad and a narrow line emitting region (e.g. Banzatti et al. 2015) with FWHMs typically larger than the [OI] 6300 Å lines suggesting emitting gas closer to the central star (Simon et al. 2016). Blueshifts of $\sim$5 km/s are reported in 4 out of 7 single-peaked CO lines (Bast et al. 2011) while clear evidence of non-Keplerian motion is found in 2 out of the 16 sources observed with the spectro-astrometry technique (RU Lup and AS 205N, Pontoppidan et al. 2011). In the case of AS 205N, followup high-resolution ALMA observations also show deviations from Keplerian rotation in mm CO emission which could be due to a low velocity disk wind or tidal stripping by its companion AS 205S.

It is thus of outmost importance to understand how to distinguish the outflow signatures of a photoevaporating wind from those of a wide angle magnetically driven wind. Spectral line profiles are in this case helpful to determine the spatial location of the outflow, or of the region where the line originates. Comparison of profiles from transition disks and primordial disks are very helpful to shed light of the wind driving mechanism at different times. Indeed Ercolano & Owen (2010, 2016) and Simon et al. (2016) both discuss the expected and observed differences in the two cases. In general, a profile which shows a large component coming from unbound material at small disk radii ($<$ 0.5AU), for example is difficult to explain in terms of photoevaporation, where mass loss is only expected outside the so-called gravitational radius ($>$0.5AU), while, classically, magnetically driven wide angle winds are expected to come from the regions closer to the star.

1.4 Contributions of the team to the study of disk chemistry and ionisation

The study of chemistry in disk winds self-consistently with their atmospheres is pretty much uncharted territory, this also contributes to the fact that the determination of the ionisation level in disks is still based on simple models (e.g. Perez-Becker & Chiang, 2011). The team members have collectively large expertise in chemical and ionisation calculations of various environments including disks interiors as well as expertise in the development of photoevaporation models. This puts them in a prime position to be able to pioneer this work. The contributions of the PI Ercolano to the field of photoevaporatve winds can be appreciated from the work described in the previous section. In what follows, we briefly describe the state-of-the-art in the field of disk chemistry and ionisation, where the other team members of Project B2 have played an important role.

Chemical models of protoplanetary disks

Gas and solid chemistry play a key role in the evolution of planet-forming disks and in planet formation theories, and determine the original composition of (exo)-planets (Henning & Semenov 2013). Planets are formed in protoplanetary disks that evolve over typical lifetimes of a few millions years (Fedele et al. 2010) by viscous spreading (e.g., Hueso & Guillot 2005; Baillié & Charnoz 2014) combined with photoevaporation (Alexander et al. 2013). During that time, the dust grains coagulate to each other to reach the size of meter- then kilometre- sized bodies (Birnstiel et al. 2010, 2012). Those bodies can agglomerate into planets or participate to the late episodes of heavy bombardments, bringing material onto planetary atmospheres and surfaces. Detection of the main belt asteroids reinforces the idea that asteroids may have brought most of the water on Earth (Jewitt 2012). Another key role played by chemistry is to set the location of the disk region where water is frozen onto solids, the so-called ice zone. Beyond the water ice zone, giant gas planets like Jupiter can form after the rapid accumulation of solid cores of 10 Earth masses by the core-accretion model (Helled et al. 2014, Öberg et al. 2015a, Helling et al. 2014).

Contrary to their young counterpart 'hot-corinos' (Cazaux et al. 2003), a much limited amount of molecules have been detected in protoplanetary disks. The outer disk molecular inventory includes CO, CN, HCN, formaldehyde, C_2H, CS, CH_3CN, HCO^+ and after a lot of effort CH_3OH (e.g. Dutrey et al. 2014; Öberg et al. 2015b; Walsh et al. 2016). The low abundance of many of the molecules has been ascribed to a combination of photodissociation at the disk surfaces and freeze-out onto grain surfaces towards the disk mid-plane. Simple molecules such as H_2, HD, CO, CO_2, H_2O, C_2H_2, HCN, N_2H^+, and potentially CH_3OH, have been detected from the terrestrial planet-forming region of protoplanetary disks by high-resolution spectrometers from ground-telescopes and by the Spitzer Space Telescopes (Pontoppidan et al. 2014). The gas is sufficiently warm such that many molecules are formed by neutral-neutral reactions with activation barrier. The ro-vibrational transitions in the mid-infrared have the advantage that homonuclear species such as CO_2 or C_2H_2 can emit contrary to pure rotational transitions. In addition to those small species, Polycyclic Aromatic Hydrocarbons (PAHs) infrared emissions are prominently seen from disks around the UV-luminous Herbig Ae stars.

Carbonaceous compounds such as tholins may have been detected in an evolved disk (Debes et al. 2008, Köhler et al. 2008). The detected lines in both the inner and outer disk are emitted well above the mid-plane. Although the amount of detected species may be low, the chemical paths are not because of the large range of density, temperature, and UV field strength. Thermo-chemical disk models use a common unique network to model the entire disk. Many questions remain on the origin and survivability of complex organic molecules in protoplanetary disks in general and in the Solar Nebula in particular. We expect that grain surface thermal- and photoreactions (UV and X-ray) and high-energy particles play an important role in the formation of complex species in the disk regions where water can be frozen onto grains (Throop 2011, Ciesla & Sandford 2012, Walsh et al. 2014). The energetic radiation break molecular bonds producing reactive radicals and ions but stellar wind can inhibit the propagation of cosmic rays (Cleeves et al. 2013). Grain surfaces enhance considerably the probability for two species to meet and form other species. Throop (2011) and Ciesla & Sandford (2012) models do quantify neither the specific species that are synthesised nor their amount, but have demonstrated that complex organics can indeed form on the Solar Nebula grain surfaces. In addition Ciesla & Sandford (2012) results suggest that gas and dust transport in the Solar Nebula (and in disks) will interconnect disk regions with dissimilar physical and chemical environments.

Members of the PI group are active collaborators within the ProDiMo[2] consortium (see e.g. Thi et al. 2014; Woitke et al. 2016). ProDiMo is a software package to model static protoplanetary disks including gas phase, X-ray and UV-photo-chemistry, gas heating and cooling balance, disk structure and (dust & line) radiative transfer. Surface chemistry has been recently included (Thi et al., in preparation).

Ionisation in disks

An accurate calculation of ionisation-recombination balance in dense protoplanetary conditions is essential for understanding various fundamental problems, such as coupling of the gas with magnetic field (Li et al. 2014), accretion processes (Turner et al. 2014), chemistry (Semenov et al. 2004; Larsson et al. 2012) and dust evolution (Okuzumi et al. 2011b; Akimkin 2015). The charging of grains in such environments affects their interaction of surrounding ions and electrons (Okuzumi 2009;

[2] http://homepage.univie.ac.at/peter.woitke/ProDiMo.html

Weingartner & Draine 1999) and hence modifies the chemistry at the grain surface.

Both the ionisation and recombination processes can arise from several sources. Primary agents of ionisation in dense gas (at visual extinctions above $A_V \sim 10 - 30$ mag, where interstellar UV photons are absorbed) are X-rays, cosmic-rays (CRs), and the decay of radionuclides, leading to the ionisation fraction that decreases with density (Oppenheimer & Dalgarno 1974; Caselli et al. 2002; Maret et al. 2006). In disks around young, active stars the situation is complicated due to the presence of stellar X-rays (Glassgold et al. 1997) and the possible exclusion of low-energy CRs by protostellar winds (Cleeves et al. 2013b). Efficiency of stellar X-rays to ionize the circumstellar gas depends on the total fluxes and the hardness of the spectra (Igea & Glassgold 1999; Ercolano & Glassold 2013). Near the disk midplane, where X-rays and CRs are strongly attenuated, radioactive elements may substantially contribute to the electron fraction. In this case the ionisation rate is proportional to the abundance of the radioactive element and its decay rate (Umebayashi & Nakano 2009; Cleeves et al. 2013a): Short-lived radionuclides (SLR, mostly ^{26}Al with half-life 7.4×10^5 yr) contribute comparatively more than long-lived radionuclides (LLR, mostly ^{40}K with half-life 1.3×10^9 yr), but decay faster.

While the treatment of ionisation, despite the variety of ionisation sources, could be reduced to a single (total) ionisation rate, the description of recombination is less straightforward. At sufficiently high densities, where the dominant sink of free electrons and ions are dust grains, the recombination rate non-trivially depends on properties of the grains (Okuzumi et al. 2011a,b; Ivlev et al. 2016).

The grain charges are determined by different mechanisms operating in different regions of disks: In the disk atmosphere, the photoelectric emission from grains is a prominent charging mechanism, leading to positive charges (Weingartner & Draine 2001; Weingartner et al. 2006; Akimkin 2015). Not only stellar radiation, but also H_2 fluorescence induced by CRs can contribute to this (Ivlev et al. 2015). In the inner, midplane disk regions the photoemission becomes negligible, and the grain charges are determined by collection of electrons and ions from the surrounding weakly ionized gas, leading on average to negative grain charges.

Depletion of electrons in dense disk regions, caused by the presence of negatively charged grains, significantly reduces the degree of ionisation (Umebayashi 1983; Umebayashi & Nakano 1990; Nishi et al. 1991). As the ionisation controls the coupling of the gas to the magnetic field, and hence the development of the magnetorotational instability (MRI, e.g. Velikhov 1959, Balbus & Hawley 1991; Armitage 2015), dust is the essential ingredient for any MRI model. It has been shown that the grain size critically affects the size of a disk's "dead zone" (Sano et al. 2000; Salmeron & Wardle 2008; Bai 2011a,b; Dudorov & Khaibrakhmanov 2014).

Recently we have developed an exact analytical model which describes ionisation and dust charging in dense disk conditions, for arbitrary grain-size distribution (Ivlev et al. 2016). Unlike previously developed approaches (Ilgner & Nelson 2006; Okuzumi 2009; Fujii et al. 2011; Dzyurkevich et al. 2013; Mori & Okuzumi 2016), our model does not make assumptions on the form of the grain charge distribution, and enables convenient analysis of results in a general form, in terms of a few dimensionless numbers, which allows us to identify universality in the behavior of the charged species.

1.5 Project-related publications

Caselli P., Walmsley C.M., Terzieva R., Herbst E. *The ionization fraction in dense cloud cores*, 1998, ApJ, 499, 234. In this work we run chemical models and compared the results with observations to estimate the ionisation fraction and the cosmic ray ionisation rate for the first time in a statistically significant sample of dense cloud cores. These results have been used in recent theoretical work dealing with the propagation of cosmic rays in molecular clouds. The techniques developed in this papers will be useful to assess the ionisation structure of disks.

Caselli P., Walmsley C.M., Zucconi A., Tafalla M., Dore L., Myers P.C. *Molecular Ions in L1544. II. The Ionization Degree*, 2002, ApJ, 565, 344. We measure for the first time the ionisation fraction across a contracting low-mass dense cloud core with the help of a simple chemical network and comparison with observations of CO and protonated as well as deuteronated N2. Low ionisation fractions (1e-9) are predicted toward the core center, with a consequently short ambipolar diffusion time scale (comparable to the free-fall time scale). The techniques developed in this papers will be useful to assess the ionisation structure of disks and the relevance of non-ideal magnetohydrodynamics regimes.

Keto E., **Caselli P.**, Rawlings J. *The dynamics of collapsing cores and star formation*, 2015, MNRAS, 446, 3731. We construct a reduced chemical network for oxygen chemistry (including water and carbon monoxyde), include it into a hydrodynamical code of the evolution of Bonnor-Ebert (BE) spheres and compare the results with observations. For the first time, we demonstrate that dense cloud cores contract as unstable quasi-equilibrium BE spheres, while the singular isothermal sphere and Larson-Penston solutions for dense core contraction do not reproduce the observed line profiles. This was only computationally possible because the number of reactions was reduced to the core. A similar approach will be used in B1.

Ercolano, B. & Glassgold, A.E. *X-ray ionization rates in protoplanetary disks*, 2013, MNRAS, 436, 3446. In this paper we calculate the ionisation rate in protoplanetary disks using our MOCASSIN photoionisation and radiative transfer code and a realistic X-ray ionisation spectrum. The rates developed here are becoming the new standard for inclusion in chemical codes and for the calculation of dead-zones and magnetic coupling within protoplanetary disks. This paper represent the new state-of-the-art after the widely used Igea & Glassgold (1999) paper.

Ercolano, B., Drake, J.; Raymond, J., Clarke, C. *X-Ray-Irradiated Protoplanetary Disk Atmospheres. I. Predicted Emission-Line Spectrum and Photoevaporation*, 2008, ApJ 688, 398. In this paper we use the MOCASSIN code to present a first estimate of the magnitude of the X-ray photoevaporation process in protoplanetary disks. We obtain significant mass loss rates, showing the relevance of this process to the dispersal of disks. Before this work the importance of X-ray photoevaporation had not been recognised.

Ercolano, B., Clarke, C., Drake, J. *X-Ray Irradiated Protoplanetary Disk Atmospheres. II. Predictions from Models in Hydrostatic Equilibrium*, 2009, ApJ 699, 1639. We further develop our models to include the feedback of X-ray heating on the disk-structure in hydrostatic equilibrium, and obtain more accurate estimates of the photoevaporation rates, which confirm our previous conclusions that the X-ray photoevaporation process is a main player in the dispersal of disks. These calculations form the starting conditions for the full hydrodynamical investigations to Owen et al. (2010).

Ercolano B., Owen J. *Theoretical spectra of photoevaporating protoplanetary disks: an atlas of atomic and low-ionization emission lines*, 2010, MNRAS 406,1553. We postprocess the models of Owen et al. (2010) and obtain synthetic observations of atomic and low-ionisation emission lines to be compared with the observations. We show that our models compare favourably with the observations available at the time.

Ercolano B., Owen J. *Blueshifted [O I] lines from protoplanetary disks: the smoking gun of X-ray photoevaporation*, 2016, MNRAS 460. 3472 We produce new synthetic observations of a particularly promising diagnostic, and demonstrate that the observations available at the time (before Simon et al. 2016) are consistent with the photoevaporation model. We show however that this line cannot be used to measure mass-loss-rates and suggest that a thermochemical model of the wind launching region is necessary.

Ivlev, A. V., Padovani, M., Galli, D., **Caselli, P.** *Interstellar dust charging in dense molecular clouds: cosmic ray effects*, 2015, ApJ, 812,135. We calculate the dust charging in the atmosphere of protoplanetary disks and dense molecular clouds, showing that cosmic rays often provide a dominant contribution due to the locally generated UV field. This hitherto completely neglected charging mechanism is expected to critically affect the dust evolution in the disks.

Ivlev, A. V., Akimkin, V., **Caselli, P.** *Ionization and dust charging in protoplanetary disks*, 2016, to be published in ApJ. We develop an analytical model of ionization in protoplanetary disks. For a broad range of parameters and arbitrary grain size distributions, this enables self-consistent calculation of densities of the charged species and of the dust charges. The model can be easily included in available numerical codes following the dust evolution.

2. Objectives and work programme

2.1 Anticipated total duration of the project

36 months

2.2 Objectives

The overarching aim of this project is together with projects B1 and C2 to quantitatively characterise the dispersal mechanism of protoplanetary disks, leading to the formation of Type 1 Transition Disks. This will constrain the physical and chemical properties in the disk at the time of planet formation and provide case-specific limits to the timescales of formation and migration of gas giants, which must occur in a gaseous disks.

The intermediate goals that will lead to the achievement of the project main aim are:

1. Devise a chemical model appropriate for photoevaporative wind conditions which takes into account of the varying dust properties in the wind.
2. Directly measure the wind mass-loss-rates and profiles by comparing synthetic line profiles from the models to existing and upcoming observations.
3. Devise a chemical/ionisation model appropriate for protoplanetary disk atmospheres that self-consistently accounts for the shielding of stellar radiation from the wind. This will allow to assess the role of magnetic fields for launching a wind.

2.3 Work programme including proposed research methods

As will be detailed in what follows, a number of steps are required to further develop our methods to be able to deal with the problem at hand. Nevertheless as an example we have applied our chemical

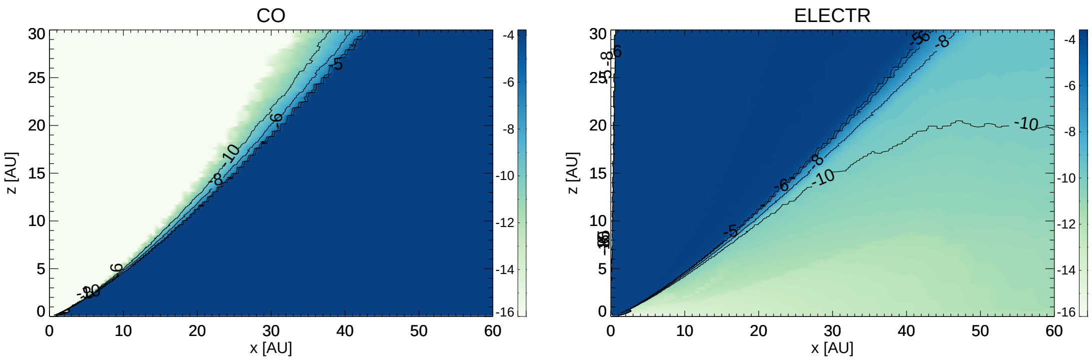

Figure 4: CO (left) and e^- maps from our toy chemical model applied to the Owen et al. (2010) wind solutions. See text for details

model to the standard wind solution from Owen et al. (2010). Figure 4 shows maps of the CO and of the electrons resulting from our toy model.

Some interesting features are already visible from this toy calculation, most notably that CO survives in the atmosphere of the disk and at the base of the wind, where it can be launched.

We use now the simple calculation above to describe the limitations of the current methods, which we aim to lift in this project.

1. The model makes simple assumptions for the irradiating spectrum of the central star (we assume here a radius and effective temperature of 2.076 R_s and 3862 K for the central star, which are appropriate for a $0.7 M_\odot$ star at 1 Myr age, Baraffe et al. 1997, 2002).
2. Only thermal effects of X-rays on the gas temperature are taken into account (i.e. the X-ray ionisation rate to 0) and the current chemical network does not include specific X-ray chemistry.
3. A standard dust opacity model was used to attenuate the FUV (Ossenkopf & Henning, 1994). As the models depend strongly on this a tailored dust model is necessary.
4. The H_2 and CO self-shielding calculation assumed constant 0.5 and 1e-4 abundances. This overestimates the true shielding, so a more realistic model would need to iterate the chemical model with updated shielding coefficient from the previous iteration.
5. The chemical model is the KIDA 2015 release, which is a gas-phase chemical network, but it takes the formation of H_2 on grain surface and charge exchange with grains into account. The network however does not include double or higher ionisation states, which would be produced by X-rays. Freeze-out of gas phase species are also not considered, while this is not a problem in the warm atmosphere and wind of the disk, it produces unrealistically high CO abundance in the mid-plane.
6. The chemical network is solved time-dependently, and evolved to 1 Myr, which is longer than most of the chemical timescales at typical disk densities (although this is not always true in the atmosphere). The abundances shown are then roughly equilibrium abundances (especially since no grains surface chemistry is considered). Time-dependence is likely to play a role in the modeling of the tenuous disk atmospheres and winds.

2.3.1 Research tools and inputs

The KIDA (http://kida.obs.u-bordeaux1.fr) code will be used as a starting point, as this is continuously updated, based on new experimental and theoretical work on rate coefficients. From this, we will extract a reduced network (as recently done in Kong, Caselli et al. 2015 for the particular case of massive star forming regions), where the chemistry of simple and abundant species such as CO, OH, O, C, C+, ... is followed with the same accuracy as with the more comprehensive network. We will then add important disk wind tracers such as Ne, Ar and their ionised forms, as well as X-ray chemistry based on work already described in the literature (e.g. Glassgold et al. 2007; Meijerink et al. 2012; Akimkin et al. 2013).

This chemical network will be inlcuded into the MOCASSIN+KROME, to solve the geometry independent radiative transfer through gas and dust, including photoionisation and chemical calculation including X-rays. PI Ercolano has been working on coupling her 3D Monte Carlo photoionisation and dust radiative transfer code MOCASSIN (Ercolano et al. 2003, 2005, 2008b) to the KROME package (Grassi et al. 2014), to perform arbitrary chemical calculations (Ercolano & Grassi, 2017, in preparation). Simple photoionisation benchmarks from the set of Pequignot et al. (2001) have already been successfully performed with the new coupled version, and a toy network has also been introduced, which is however inadequate for any realistic modelling of disk chemistry. The development of an appropriate chemical network to be included into MOCASSIN+KROME is indeed one of the first tasks of the work program described below.

The advantage of using this new code compared to existing chemical codes for disks, is that it allows a fully self-consistent treatment of the radiative transfer and hence radiation field attenuation through dust and gas. The code is fully 3D (but can work in 2D) and it can handle complex, multi-component and space-varying dust grain models.

MOCASSIN (without KROME) has already been used to post-process hydrodynamical calculations of photoevaporating disks (e.g. Ercolano & Owen 2010, 2016) to produce synthetic spectral line profiles of atomic and ionised species in the wind and atmosphere.

The abundances calculated with MOCASSIN+KROME will then be further post-processed using the popular RADMC-3D code, developed and mantained by Prof. Dullemond (PI of project D2) or the MOLLIE (Keto et al. 2004) or the LIME (Brinch & Hogerheijde 2010) codes, which have also already been used by members of our B2 team for other projects.

2.3.2 Work Program

The project will develop along a path of growing complexity. It is possible that some of the tasks in the last stage (time-dependance) may be carried over to the next funding period. While this complex project will be led by the postdoc, the PIs and collaborators will also take an active part in the work. One of the PIs of this project has extensive experience in devising efficient and reliable reduced networks (see e.g. Keto & Caselli 2008, 2010; Keto, Rawlings & Caselli 2014), while one of the collaborators and the other PI are leading effort in the ionisation structure and radiative transfer of disks (e.g. Ivlev et al. 2016, Glassgold & Ercolano 2013, Ercolano et al. 2008,2009).

2.3.2.1 Months 1-12

The reduced network. A first task for this project is to simplify the gas-grain chemistry by reducing the chemical network to the minimum number of reactions needed to properly follow the formation/destruction of important species (in particular Hydrogen, Carbon, Oxygen as well as simple C-, O-bearing molecules) and the electron abundance or ionisation fraction. The reduced chemical network will be benchmarked against comprehensive chemical networks to make sure that the abundances of important (diagnostic) species such as C^+, C, O, CO are well reproduced in the range of conditions appropriate for evolved and transitions disks. This will imply running the comprehensive and reduced networks in a grid of physical conditions by varying temperature, density, and UV/X-ray fluxes. As lines of Ne ([NeII], [NeIII]) and Ar ([ArII]) are good tracers of disk winds (e.g. Pascucci 2007, Szulágyi et al. 2012), Ne and Ar will be included in the chemical code.

Particular attention will be dedicated to the inclusion of X-rays and the identification of the regions within the disk where X-rays, FUV photons and cosmic-rays (CRs) dominate the chemical and thermal properties. Typical assumption is that the X-ray spectrum is given by the bremsstrahlung spectrum ($I_\nu \simeq 1/E \times exp(-E/kT)$ on the 0.1 - 10 keV energy range (e.g. Glassgold et al. 2007, Aresu et al. 2011, Meijerink et al. 2012). The observed luminosity ranges are $L_X = 10^{29} - 10^{31}$ erg/s (based on the Taurus survey, Güdel et al. 2007). The X-rays heat up the gas with 10-40% efficiency (UV heating has only a few per cent efficiency).

Impinging X-rays may ionise the disk or wind material via primary or secondary ionisation. Primary ionisation may produce a single or multiple electrons due to the Auger effect. Their energy range depends on the shell from which the Auger electron originates. The rate coefficient is given by the integral of the product of the X-ray energy spectrum and the ionisation cross section of the element (see e.g. Meijerink 2012, equation A.13). Secondary electrons might have keV energies, capable of $\sim$20-30 hydrogen ionisation. In fact the secondary electron ionisation rate per H nucleus is higher than the primary by an order of a magnitude, thus often only the secondary ionisations are considered in chemical models (e.g. Ádámkovics et al. 2011, Bruderer 2012). The exact expressions and the peak electronic ionisation cross sections are given in Ádámkovics et al. (2011).

Chemical models in the literature deal differently with X-ray reactions. The Semenov et al. (2010) and associated papers (Akimkin et al. 2013) model these reactions as an additional contribution to cosmic ray ionisation reactions (i.e. the rate is given by $R = \alpha \times (\zeta_{CR} + \zeta_X)$). Bruderer et al. (2012) accounts for only the secondary ionisation. Finally, Meijerink et al. (2012) take both the primary and secondary ionisation into account, as described above (see also Table 3 in Henning & Semenov 2013).

X-rays affect the chemistry in various ways: (i) X-rays might directly ionise H (while FUV radiation does not), initiating H_2 formation via the H-path. In high temperature regions, where the grain surface H_2 formation is less efficient, this reaction might contribute significantly to the total H_2 formation rate. (ii) Secondary electrons interacting with H_2 produce H_2^+ that quickly reacts with a further H_2 to form H_3^+ or reforms H_2 via charge transfer with neutral H. This can lead to H_3^+ abundances as high as 10^{-8}. This then initiates efficient ion-neutral reactions which e.g. result in efficient H_2O production (see e.g. Meijerink et al. 2012). Furthermore, the heating effect might also increase the rate of neutral-neutral reactions with reaction barriers. (iii) H_3^+ initiates ion-molecular reactions which keep molecular abundances high even at high temperatures (if X-rays are present, compares to only FUV). (iv) Ne, Ne+, Ar and Ar+ have ionisation potentials 21.56, 40.96, 15.76 and 27.63 eV respectively. They are only ionised due to X-rays or X-ray induced fast electrons. Therefore, their ionisation is an indicator for X-rays and, as already mentioned, these species will be included in our chemical models. (v) Enhanced CO destruction through reaction with He^+, which has an ionisation energy of 24.6 eV (CRs can also ionize it). (vi) Other observational tracers (suggested by Meijerink 2012) are: H_2O, Ne^+, C/C^+ ratio,O^+.

Finally, while X-rays are unlikely to interact at the low column densities of the wind they are crucial for the chemistry in the underlying disk material, which feeds the wind.

2.3.2.2 Months 13-18

Line diagnostics from chemical models. Once the reduced network is benchmarked and tested, it will be included in the MOCASSIN-KROME code by the co-PI Ercolano. The MOCASSIN-KROME code will be used to obtain the chemical abundances, while, radiative transfer codes available at the PI Institute (RADMC-3D[3] and LIME[4]) will be used to obtain fluxes in dust continuum and lines to then perform simulated observations and compare with available data and/or make predictions for future observations. We note that at this stage the chemical models will still use an unrealisticly simple dust model. However this step is important to guide us towards interesting diagnostics and to help us refine our chemical model. This step to obtain synthetic observations will be repeated every time a

[3] http://www.ita.uni-heidelberg.de/ dullemond/software/radmc-3d/

[4] http://www.nbi.dk/ brinch/index.php?page=lime

significant update is performed on the model.

At this point we will already be able to further investigate the nature of the broad-component of the neutral hydrogen emission, for which we have suggested a non-thermal origin coming from OH dissociation in the bound inner disk regions. Even if our models our not final, they can already be used to assess the plausibility of our proposed scenario.

In this second part of the project, we will also explore the effect of varying initial conditions, taking into account effects of accretion, vertical mixing and magnetic disk wind on chemistry following prescriptions by Heinzeller et al. (2011). Often low metal elemental abundances are assumed (H_2 molecular, C^+ ionised) or the chemical network is initially evolved to simulate the conditions of the parent cloud. Depending on what kind of disk wind model is considered, the wind starts to dominate the mass loss rate at different times. For example, EUV winds tend to be efficient at late times, thus the initial chemical composition might not matter, while the X-ray winds might dominate the mass loss over accretion in early times, and thus the initial chemical abundances might matter (see review of Alexander et al. 2014, page 483 end of section 2.3). Furthermore, several papers shows that the radial movement of material and the vertical mixing affect the chemistry in disks, i.e. by lowering concentration gradients and enhancing abundances of NH_3, CH_3OH, C_2H_2 and sulphur-containing species (e.g. Ilger et al. 2004, Semenov et al. 2010, Heinzeller et al. 2011). If the chemical timescales are long compared to the disk wind dynamic time, then the disk composition will affect the wind as well. Thus, we will model the effects of the radial accretion flow and vertical mixing (although the later is more important, see Semenov 2010) on the disk chemistry (even if these motions are not included in the original simulation). As the MOCASSIN simulations start from an alpha-disk model, we will take this disk structure to model the vertical mixing and accretion similarly as was done by Heinzeller et al. (2011).

2.3.2.3 Months 19-24

Dust evolution. The chemical model assumes initially that dust grains can be approximated by one-size particles of 0.1μm in diameter and that the dust-to-gas mass ratio is fixed. However, this assumption is completely inappropriate for disk winds. Indeed as explained in detail in project C2 of this proposal, the maximum grain size that can be entrained in the wind at a given radial distance from the star results from the local force balance between the drag force, gravity and the centrifugal force. A further complication is that the underlying distribution of grains is also not constant and varies as a function of disk radius and vertical distance from the mid-plane, due to the effects of grain growth, fragmentation, settling and drift. A detailed model of the spatially and time-varying grain abundances and size distributions in the wind is however essential for the chemical model, since grains provide the bulk of the opacity in the FUV. The third task of the Postdoc employed for this project will be to include spatially-varying grain abundances and size distributions provided by project C2 into the chemical code, at different evolutionary times, to properly account for dust opacities in the wind. Also the effects of different dust grain properties on the chemical composition will be explored at this point. At MPE, we are already studying the effect of varying grain-size distribution on the ionisation structure of disks (Ivlev et al. 2016).

This step will be further decomposed into levels of increasing complexity. We will begin with decoupling the time and space evolution of the grains. We will then compare the timescales involved and asses whether the time-evolution of the dust must be treated self-consistently or if we can work with snapshots.

An important **milestone** at the end of this step will be a case specific assessment of the ionisation level in the atmospheres of disks. The irradiating spectra used for the models will be obtained in co-operation with the team of project A2. We will make our results immediately available to the international community as this is a crucial ingredient for the development of MHD calculations. This will also help us assess under what conditions, if any, one can expect that a significant component of observed outflow emission may be indeed magnetically driven.

2.3.2.4 Months 25-36

Time-dependent chemistry. It is unclear at this stage if equilibrium chemistry is an appropriate approximation for disk winds. The material flows at a few km/sec and as it moves along the wind streamlines it is subject to changes in density and radiation field. It is possible that time dependent calculations will be necessary for this problem, where the dust properties in the chemical code will be provided by the time-dependent calculation of the dust evolution described in C1. This will be the final task of the Postdoc employed for this project, who will first study the time scales of the various physical/chemical processes (e.g. photochemistry, accretion, mixing, wind) and quantify the validity of equilibrium chemistry.

After this, the whole team will work together with the B1 and the C2 teams to couple time-dependent gas-grain chemistry and dust evolution. Depending on the level of complexity required, part of this final step may be carried out in the second funding period.

Once the machinery to efficiently calculate chemical models of disks and their atmospheres/winds is in place, it will also be useful to explore possible observational signatures of the theoretical models developed in projects C1, D1 and D2. Depending on the exact timeline we expect to do this either at the end of the first funding period or at the start of the second.

2.3.2.5 Summary of the Work Program

The Gannt chart below summarises the approximate time-line of the B2 project:

Year 1: (i) focus on the chemical network update, to make sure that all the most recent reaction rates will be included. This will be done by comparing our code with KIDA[5], the kinematic database for astrochemistry, as well as with comprehensive literature research. (ii) Include detailed ionisation processes, taking into account the effects of ionisation-recombination from FUV and CRs. (iii) Include X-ray chemistry based on the extensive literature work available as well work done within the ProDiMo code. (iv) Finalise the reduced chemical network, including Ne and Ar, and test/benchmark it.

Year 2: (i) inclusion of reduced chemical network in MOCASSIN-KROME. (ii) Calculation of the chemical-physical model, which will then be used as input in radiative transfer code to produce dust continuum emission and line fluxes. (iii) Comparison with observations and further update of chemical code based on observational constraints. (iv) Study of the effect of changing the grain size from mono-disperse (0.1 μm) to MRN grain-size distribution (Mathis et al. 1977) or evolved-MRN distributions (e.g. Zhao et al. 2016; Ivlev et al. 2016). (v) ionisation level calculations. (vi) Calculation of an updated chemical-physical model, which will then be used as input in radiative transfer code to produce dust continuum emission and line fluxes. Comparison with observations.

Year 3: (i) study of time scales of various processes in chemical and dynamical model. (ii) Benchmark of time-dependent reduced chemical code. (iii) Inclusion of time-dependent chemistry in dynamical model. (iv) Calculation of an updated chemical-physical model, which will then be used as input in radiative transfer code to produce dust continuum emission and line fluxes. Comparison with observations.

Continuous Assessment of New Diagnostics Jointly with the B1, C2 and A1 team members as well as with our external collaborators Prof. Henning and Prof. van Dishoeck, we will regularly compare our models to the observations via the production of synthetic spectra. This will allow us to promptly identify and characterise new wind diagnostics and allow us to use the observations to measure the crucial wind properties of mass loss rate and wind profile, which have a large impact on the formation and evolution of planetary systems.

[5] http://kida.obs.u-bordeaux1.fr

TASK NAME	Year 1	Year 2	Year 3
The reduced network	- update chemical model - include detailed ionisation processes - insert X-ray chemistry - finalise reduced network		
Line diagnostics from chemical models		- inclusion of chemical code in MOCASSIN by B1 - radiative transfer - comparison with observations	
Dust evolution		- from mono-disperse to grain-size distribution - grain-size from C2 - radiative transfer - comparison with observations	
Disc ionisation		- case-specific ionisation rate	
Time-Dependent chemistry			- study of time scales of various processes - benchmark of time-dependent chemical code - inclusion of time-dependent chemistry in dynamical model - radiative transfer - comparison with observations

Figure 5: Gannt chart for B2. More details have been outlined in the previous section.

2.4 Data handling

We will make the sets of line profiles for the different wind and disk characteristics publicly available in electronic format on the public partition of the Research Unit server. The reduced and full networks will also be made available at the end of the first funding period, when they will have reach their final form.

2.5 Other information

Not Applicable

2.6 Information on scientific and financial involvement of international cooperation partners

Not applicable

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4. Requested modules/funds

4.1 Basic Module

4.1.1 Funding for Staff

We require funding for one Postdoc to work jointly at the MPE with Prof. Caselli and at the LMU in the group of Prof. Ercolano. A Postdoc with at least some experience of astrochemistry would be certainly desirable to work on this complex project. The Postdoc will receive scientific support form the PIs, but also from experienced astrochemists and plasma physicists (e.g. Dr. Ivlev, Dr. Thi) at the Centre for Astrochemical Studies led by Prof. Caselli at the MPE.

In case of an award Dr. Szücs, currently working at the MPE in the group of PI Caselli, has expressed interest in taking on the position. His expertise in this field would be very beneficial to the achievement of the aims of this project.

4.1.2 Direct Project Costs

4.1.2.1 Equipment up to EUR 10,000, Software and Consumables

Theoretical numerical research can only be done when sufficient and appropriate computational facilities are available. While production runs will be done on supercomputer facilities, a substantial part of the work in this project is code development. Testing these codes on realistic problems requires a workstation for the postdoc students – which is beyond the standard base equipment (Grundausstattung). We therefore request a workstation-grade desktop computer for the PhD position for 3 000 €.

4.1.2.2 Travel Expenses

Travel within the Research Unit is handled in project Z. In addition we request funding for conference travel for the personnel and one Applicant. This includes one national (1.000 €) and one international (1.500 €) conference trip per year, totalling 2.500 € per person per year.

For this project this totals 5.000 € per year for the postdoc and one Applicant, which is in total 15.000 €.

4.1.2.3 Visiting Researchers (excluding Mercator Fellows)

During the course of the project 2 one week long visits to our main international collaborator, Dr. T. Grassi (Copenhagen). This includes airfare and 6 overnight stay 1200 € (2.400 € for 2 visits)

4.1.2.4 Project-related publication expenses

We request 750 €/year (total 2250 €) for publication expenses.

5. Project requirements

5.1 Employment status information

Paola Caselli, Director at the Max Planck Institute for Extraterrestrial Physics (MPE) – permanent
Barbara Ercolano, Professor at the Ludwig-Maximilians-Universität München – permanent

5.2 Composition of the project group

Alexei Ivlev, Dr, permanent scientist at the MPE Wing Fai, Thi, Dr, postdoctoral assistant at the MPE

5.3 Cooperation with other researchers

5.3.1 Planned cooperation on this project

5.3.1.1 Collaborating researchers for this project within the Research Unit

This project is intimately linked to project B1 (PI Ercolano) and to project C2 (PI Ercolano). It requires the input from the radiation-hydrodynamic models from B1 as well as the MOCASSIN-KROME code which is developed by the PI Ercolano for B1 and B2 (with different immediate objectives). It also requires input from project C2 (PI Ercolano) and will work closely with T. Birnstiel (C1, C2) for help in the implementation of the dust models. The irradiating spectra used for the models will be obtained in co-operation with the team of project A2. The synthetic spectra will be compared with observations with the help of the A1 team (PI Testi) and our external collaborators Prof. Henning and Prof. van Dishoeck.

This can also provide the final machinery to projects D1 and D2 to calculate the chemical abundance of molecules. These can then be used for line transfer calculations, which are essential to probe the gas and the kinematics of Type 2 TDs.

5.3.1.2 Collaborating researchers for this project outside of the Research Unit

Dr. Grassi, the author of the KROME package has already helped Prof. Ercolano with the implementation of KROME into MOCASSIN and is expected to help further in implementing the new networks and optimising the chemistry routine (inclusion, for example, of a better equilibrium chemistry option. It is envisioned that Dr. Grassi will play regular visits to our group.

5.3.2 Researchers with whom you have collaborated scientifically within the past three years

Maite Bertran (INAF-Osservatorio Astrofisico di Arcetri), Aaron Boley (University of British Columbia), Sandra Brünken (University of Cologne), Stephanie Cazaux (University of Groningen), Cecilia Ceccarelli (Univ. Grenoble Alpes), Francesco Fontani (INAF-Osservatorio Astrofisico di Arcetri), Thomas

Hartquist (University of Leeds), Izaskun Jimenez-Serra (Queen Mary University London), Eric Keto (Harvard-Smithsonian Center for Astrophysics), Marco Spaans (University of Groningen), Jonathan Tan (University of Florida), Stephan Schlemmer (University of Cologne), Charlotte Vastel (Université de Tulouse), Malcolm Walmsley (INAF-Osservatorio Astrofisico di Arcetri) Niederhofer (STSci, USA); M. Hilker (ESO, Garching); N. Bastian (U. Liverpool, UK); M. Guarcello (U. Palermo, Italy); M. Tazzari (U. Cambridge, UK); A. Natta (Florence, Italy); R. Alexander (U. Leicester); D. Hubber (LMU); J. Dale (U. Hertfordshire, UK); C. Koepferl (LMU); I. Bonnell (U. St. Andrews, UK); A. McLeod (ESO, Garching); D. Boneberg (U. Cambridge, UK); R. Parker (U. Liverpool, UK); R. Wesson (UCL, London, UK); M. Barlow (UCL, London, UK); A. Glassgold (u. Berkeley, USA); C. Manara (ESA, Noordwjik, Netherlands); A. Danekhar (CfA, Harward, USA); Q. Parker (Sidney, Australia); S. Casassus (U. de Chile, Santiago, Chile); I. Pascucci (U. Arizona, USA); A. Bevan (UCL, London, UK).

5.4 Scientific equipment

The CAS centre led by Prof. Caselli has available computer facilities for visiting scientists and students. CAS has its own cluster: an HPC cluster comprising of 25 nodes with 20 cores and 128 GB memory each; 4 nodes with 20 cores and 256 GB memory each (Infiniband, 50 TB storage, Login-Node, Batch-System; 2 Compute nodes, i.e. 2 nodes with 20 cores and 512 GB (10 TB storage).

The group of Prof. Ercolano has two own computer clusters comprising

- 2 CPU Intel Xeon X5650 (Westmere, beginning 2010, 2.66 GHz) 6 cores each 12 cores total (24 virtual) 74 GB ram.
- 4 CPU Intel Xeon E7-4850 (Ivy Bridge, beginning 2014, 2.30 GHz) 12 cores each 48 cores total (96 virtual) 660 GB ram.

Further computational power is provided through the C2PAP facility of the Excellence Cluster to which the group has guaranteed time. This comprises 126 nodes, each node with 2 CPU Intel Xeon E5-2680 (Sandy Bridge, beginning 2012, 2.7 GHz) 8 cores each 16 cores total (32 virtual) 64 GB ram. Note that while the future of the Excellence Cluster Universe is uncertain, the C2PAP facilities will be in any case supported by the LMU.

The facilities at the Leibniz Rechenzentrum (LRZ) , with the iDataPlex HPC System HYDRA with Intel Ivy Bridge processors (3500 nodes with 20 cores at 2.8 GHz each are also available to us.

Project C1:

Trapping the dust: planet formation ‘hotspots’ in Transition Disks

Authors:
Applicants: T. Birnstiel (LMU)
C.P. Dullemond (ZAH Heidelberg)
Co-Applicants: W. Kley (U. Tübingen), L. Testi (ESO), E. van Dishoeck (MPE/Leiden), Th. Henning (MPIA)

Requested positions: 1 PhD student

Abstract:
In the core accretion scenario of planet formation dust grains must grow many orders of magnitude in size from micron sizes to thousands of kilometres. However, based on our current understanding of the physics of planet formation, several processes seemingly prevent or stall the growth towards larger bodies: (1) collisional growth is inefficient above $\sim$meter-sizes, (2) fast radial migration removes solid particles on very short time scales, (3) large particles need to locally accumulate above the canonical dust-to-gas ratio in order to trigger gravoturbulent formation of planetesimals, and (4) radial migration of pebble-sized particles renders the accretional growth of planetesimals inefficient. Observations of transition disks suggest that they provide the environments, where all of these issues can be solved: trapping and growth of solid particles in the pressure bumps in the gas distribution of transition disks can provide the large enough particles at high enough densities to trigger gravoturbulent planetesimal formation. Additionally, the trapped particles are not drifting away, meaning they can be efficiently accreted onto the growing planetesimals. It is the goal of this proposal to investigate the trapping, planetesimal formation, and planetesimal growth processes in these apparent ‘planet formation hotspots’ in transition disks with numerical simulations.

1. State of the art and preliminary work

State of the art: Transition Disks and Planet Formation

With over to 3000 detected planets, it is striking that we still do not understand how planets form. Their building blocks, the *planetesimals* form in gas disks around young stars, where colliding dust grains form ever-larger aggregates. But this growth is not without limits: larger particles quickly drift towards the star and collide at speeds that shatter them to pieces, long before gravity can bind them together. The mechanisms involved in the assembly and transport of these building blocks remain some of the biggest mysteries of planet formation.

Over the last couple of decades, observations of protoplanetary disks have revolutionized the field of planet formation. This started with surveys of disks (see the review of Williams & Cieza 2011) and continued with ever better imaging campaigns (e.g., Andrews & Williams 2007; Brown et al. 2009, and many others). Early imaging results of Brown et al. (2008) and Brown et al. (2009) revealed for the first time depleted inner cavities in disks that were previously just suspected from the spectral energy distributions. These disks with holes were initially thought to be in the process of transitioning from a gas rich disk to a gas poor disk (e.g., Clarke et al. 2001) and thus termed *transition disks* (see Espaillat et al. 2014; Alexander et al. 2014, and references therein).

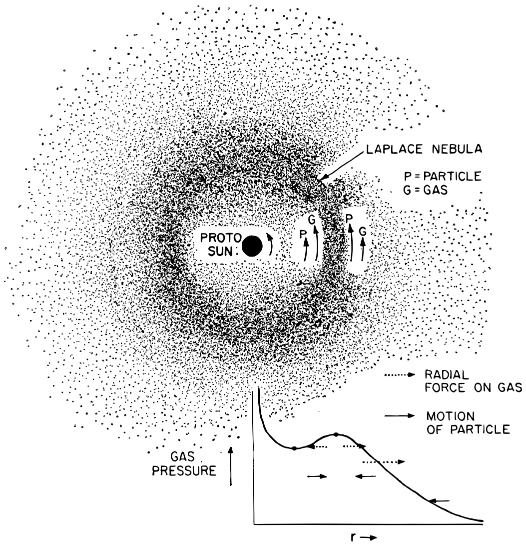

Figure 1: Accumulation of solid particles in pressure bumps. Taken from Whipple (1972).

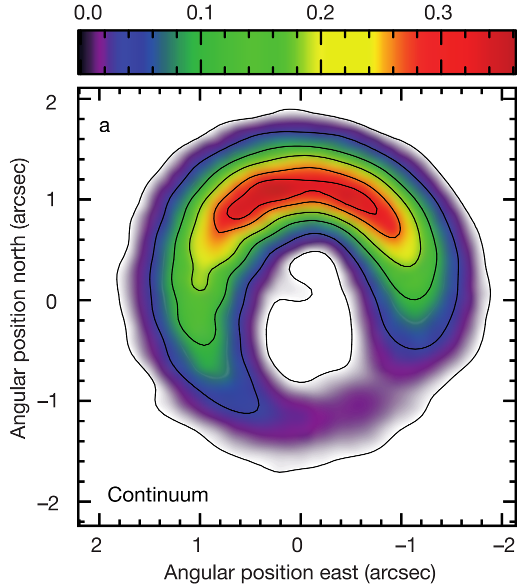

Figure 2: Continuum imaging of a ring-like accumulation of dust in the transition disk HD 142527. Taken from Casassus et al. (2013). Units are in Jy/beam.

As statistics and theoretical models improved, it became clear that this cannot be the full story: some of the inner holes were found to be clearly too large and the disk accreting too vigorously to be explainable by current models of photoevaporation (i.e. Type 2 TDs, Owen et al. 2010, 2011). Other explanations were discussed, such as particle growth (Dullemond & Dominik 2005; Tanaka et al. 2005; Birnstiel et al. 2012a) or gap opening by planets (Paardekooper & Mellema 2004, 2006; Rice et al. 2006; Pinilla et al. 2012a; Zhu et al. 2012). Most of these models have in common that some mechanism (e.g., photoevaporation, planet-disk-interaction, or others) produce a pressure maximum in the distribution of the gas. Solid particles that have collisionally grown to macroscopic sizes experience fast radial migration towards higher gas pressure (Whipple 1972; Weidenschilling 1977; Nakagawa et al. 1986). Already Whipple (1972) suggested that particles moving due to this effect can become *trapped* in a pressure maximum, as depicted in Figure 1 taken from his paper. A recent image of such a ring-like transition disk (in this case showing also azimuthal asymmetry), from Casassus et al. (2013) is shown in Figure 2.

Statistical analysis of the occurrence rates and properties of transition disks suggested that there are two families of transition disks: a family of small accretion rate / small hole sizes / small disk mass and another family of larger hole sizes accompanied by larger disk masses and higher accretion rates (Owen & Clarke 2012). In this proposal we refer to the former as Type 1 Transition Disks and the latter as Type 2. While the possibly diverse *origins* of transition disks are still obscure, the observations at face value already show us something even more interesting: large fractions of the solid contents of the disks can be contained near the inner edge of the outer disk. These cavity edges should therefore be prime regions for the formation of planetesimals or even planets. As such, transition disks are not only interesting probes of disk evolution or disk dispersal, but may allow us to study in detail what role pressure bumps are playing in the formation of planets.

In 2013, we proposed that the dust trapped in a slightly lopsided gas disk (i.e. an azimuthal pressure bump) can become extremely concentrated in that azimuthal over-density (see Birnstiel et al. 2013). In the same year, we were part of a team that published and analyzed ALMA observations of the disk Oph IRS 48 that showed such an extreme asymmetry, as predicted by the models (see van der Marel et al. 2013). It is widely accepted that the dust accumulations in pressure bumps (whatever their formation mechanism may be) are prime regions – *hot spots* – of planet formation: accumulation of particles in pressure bumps (e.g., Kretke & Lin 2007) prevents them from drifting away and shortens the growth time scales of dust particles allowing further growth (Brauer et al. 2008b). Accumulation of these particles can trigger the streaming instability which needs particle accumulations and particles of the right sizes to operate (Youdin & Goodman 2005; Johansen et al. 2007). Vortices further support the accumulation to critical densities (Barge & Sommeria 1995; Klahr & Henning 1997; Raettig et al. 2015) or even the direct formation of earth sized objects (Lyra et al. 2009).

Another revolution in the field of planet formation came not from the observational, but from the theoretical side. It was shown that small particles can very effectively be accreted onto planetesimals under the right conditions when gas drag effects increase the effective cross section of the accreting body (Ormel & Klahr 2010; Lambrechts & Johansen 2012). It has turned out that this process – termed *pebble accretion* – can be dominant over the late-stage oligarchic growth and giant impact growth if the flow of pebbles can be controlled (Levison et al. 2015), although the exact ratio of mass that is accreted via planetesimals and via smaller particles is still under investigation, as is the efficiency of the process (see Guillot et al. 2014; Visser & Ormel 2016; Owen & Kollmeier 2016). But there is a problem with this and that is the fact that planetesimals seem to be formed big (Morbidelli et al. 2009, Klahr et al., submitted to Nature) with sizes around 100 km. This happens to be the size at which pebble accretion onto the planetesimals is particularly inefficient (Visser & Ormel 2016). If the pebbles do not drift away from the accreting planetesimal and even accumulate near them, this problem could be overcome.

In other words: planetesimals likely form 100-km-sized bodies, but only if over-densities of pebble sized objects are present. Further growth of planetesimals of this size is inefficient unless there is a large reservoir of particles of the right sizes available to be accreted. Pressure bumps, such as the ones observed in transition disks provide the right conditions to solve all of these problems.

Several authors have already investigated the dynamics of particles in and around planetary gaps in disks. Some of the recent work includes Paardekooper & Mellema (2004, 2006), Rice et al. (2006), Lyra et al. (2009), Zhu et al. (2012), Gonzalez et al. (2012), Ataiee et al. (2013), or Picogna & Kley (2015), to name just a few. Most of these works have in common, that they follow only small particles that are not growing in size and they do not follow planetesimals or their growth at the same time. These works are mainly aimed at explaining the observed properties of transition disks, but surprisingly little work has been done to understand how transition disks – or pressure bumps in general – regulate the formation of planets or planetesimals. Some authors (e.g., Chatterjee & Tan 2014, and following papers in that series) have pointed out how pressure bumps and planet formation can trigger each other, leading to a inside-out planet formation scenario. This is a promising scenario to explain for example the systems with tightly packed inner planets discovered with the Kepler Mission (Fang & Margot 2012). However the details of what happens to the dust and larger bodies in the pressure bump has not been subject of a dedicated study yet.

With this proposal, we want to build on our expertise on dust evolution and particle trapping in protoplanetary disks to study the formation of planetesimals in pressure bumps, their further evolution due to dynamics, interaction with the gas disk, interaction with other planetesimals, and growth due to accretion of pebbles.

The goal of this proposal is to understand how planetesimal and planet formation proceeds in pressure bumps and to find out if transition disks are indeed the hot-spots of planet formation that we think they are.

Preliminary Work

Both Applicants have extensive experience in the physics of particle growth and dynamics of dust particles (e..g Dullemond & Dominik 2005; Brauer et al. 2008a; Zsom & Dullemond 2008; Birnstiel et al. 2010, 2012b; Drążkowska & Dullemond 2014, see Birnstiel et al. 2016 for a recent review) as well as in disk structure and evolution (e.g., Dullemond et al. 2001, 2002; Dullemond & Dominik 2004; Dullemond & Monnier 2010; Birnstiel et al. 2015, and many others). Furthermore, C.P. Dullemond has been supervising or contributing to several works on planet-disk-interaction, vortex-formation, and planet-vortex-interaction (Regály et al. 2012; Ataiee et al. 2013, 2014).

More recently, a collaboration between the Applicants of this proposal and the group of Dr. Hui Li at Los Alamos National Labs (LANL), USA has been established. Dr. Hui Li has been pioneering the field of vortex formation in the context of protoplanetary disks (Li et al. 2001, 2000). Furthermore, the LANL group has extensive experience in hydrodynamical modeling and more recently in modeling dust dynamics via tracer fluids (e.g., Fu et al. 2014; Jin et al. 2016).

Dr. T. Birnstiel has worked on two-dimensional models of dust evolution, treating particle growth, fragmentation, turbulent mixing and vertical settling. Preliminary results of this are shown in Figure 3 in the left column. Similar work on this, but in the radial/azimuthal dimensions is ongoing as part of the collaboration with the LANL group. The right hand side panels in Figure 3 show a proof of concept simulation where gas dynamics as well as dust dynamics of around 100 different particle sizes are taken into account. Subroutines for simulating particle growth and fragmentation have been developed and are currently being tested.

To continue this work on particle growth in two dimensions as well as work on other related topics, Dr. T. Birnstiel has recently been awarded an *ERC Starting Grant* which will start in March 2017 at the LMU Munich. By becoming part of this Research Unit, Dr. Birnstiel will share the progress and the resulting data with the research group wherever other projects of the Research Unit profit from it. This includes, but is not limited to, the dust density distribution $\rho_{\mathrm{dust}}(r, z, a)$ as function of distance to the star r, height above the mid-plane z, and particle size a and similar results from the radial/azimuthal models.

1.1 Project-related publications

Birnstiel, T., **Dullemond, C.P.**; Brauer, F.: *Gas and dust evolution in protoplanetary disks*, 2010, A&A 513, 79. In this paper we present the basic code for the evolution of the disk and the dust. The latter follows the dust coagulation, fragmentation, settling and radial drift of the dust.

Sándor, Z.; Lyra, W.; **Dullemond, C.P.**, *Formation of PlanetaryCores at Type I Migration Traps*, 2011, ApJ, 728, L9. Here we performed detailed N-body calculations of multi-planet systems with migration torques. This experience helps us with determining the dynamics of pebbles as they approach the planet. The migration torque is then replaced by gas friction.

Birnstiel, T.; Klahr, H.; Ercolano, B.: *A simple model for the evolution of the dust population in protoplanetary disks*, 2012, A&A 539, 148. In this model the flow of pebbles from the outer disk regions into the inner planet forming disk regions is studied, and an easy to use model derived.

Birnstiel, T.; Andrews S.M.; Ercolano B.: *Can grain growth explain transition disks?*, 2012, A&A, 544, A79. We showed that particle coagulation in itself can successfully create observed transition disk signatures at infrared wavelengths, but fails to produce the central cavities at (sub-)millimeter wavelengths.

Pinilla P.; Benisty M.; **Birnstiel, T.**: *Ring shaped dust accumulation in transition disks*, 2012, A&A, 545, A81. We presented the first model that explained transition disks trough a combination of particle growth and transport processes and the pressure trap created by a giant planet.

Ataiee, S.; Pinilla, P.; Zsom, A.; **Dullemond, C. P.**; Dominik, C.; Ghanbari, J.: *Asymmetric transition disks: Vorticity or eccentricity?*, 2013, A&A, 553, L3. We demonstrated how asymmetries in dust disks can be produced by vortices or by disk eccentricity and how these methods cause very different dust density contrasts.

van der Marel N.; van Dishoeck E.F.; Bruderer S.; **Birnstiel, T.**; Pinilla P.; **Dullemond, C.P.**, et al.: *A Major Asymmetric Dust Trap in a Transition Disk* 2013, Science, 340(6), 1199. First observation of an extremely lopsided dust disk that was interpreted as trapping of solids in a vortex-like structure.

Ataiee, S.; **Dullemond, C. P.**; Kley, W.; Regály, Zs.; Meheut, H.: *Planet-vortex interaction: How a vortex can shepherd a planetary embryo*, 2014, A&A, 572, A61. We studied how a vortex interacts gravitationally with a migrating planet or with a planet that is created inside the vortex.

van der Marel, N.; Pinilla, P.; Tobin, J.; Van Kempen, T.; Andrews, S.; Ricci, L.; **Birnstiel, T**: *A Concentration of Centimeter-sized Grains in the Ophiuchus IRS 48 Dust Trap*, 2015, ApJL, 810, L7. A follow-up of previous IRS 48 observations at longer wavelength, confirming that the larger particles are even more strongly concentrated in the trap as smaller particles.

Pinilla, P.; Klarmann, L.; **Birnstiel, T.**; Benisty, M.; Dominik, C.; **Dullemond, C.P.**: *A tunnel and a traffic jam: How transition disks maintain a detectable warm dust component despite the presence of a large planet-carved gap*, 2016, A&A 585, A35. Here the dust coagulation and trapping model is extended to explain the shape of pre-transitional disks via incomplete trapping, coagulation and fragmentation near the water ice line.

2. Objectives and work programme

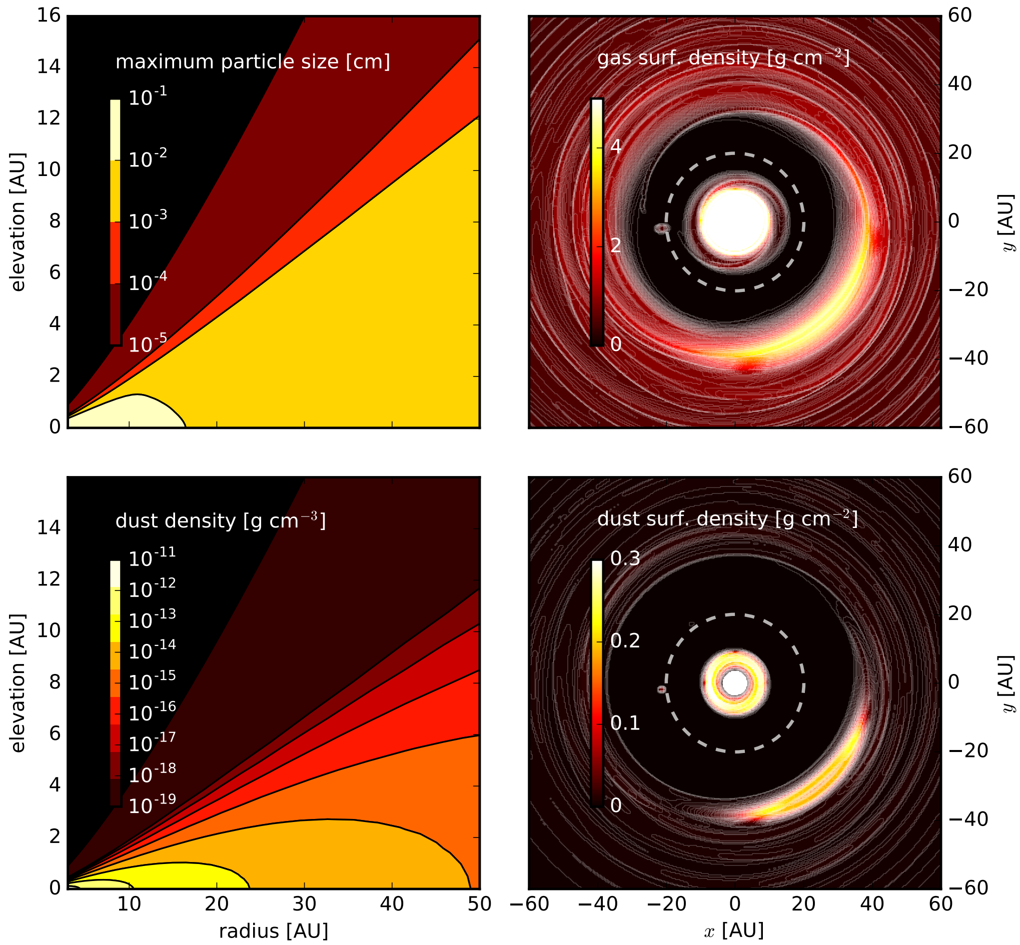

Figure 3: Proof-of-concept models for 2D dust evolution simulations. The panels to the **left** show the radial/vertical distribution of solids (**bottom**) and maximum particle sizes (**top**) where both coagulation and vertical transport processes are treated at each point of a 2D grid. The panels on the **right** show radial/azimuthal results of the LA-COMPASS code (in normalized code units, resolution of 1024$\times$1536) that is now able to treat 100s of particle sizes and their size evolution. The **top** panel shows the distribution of gas surface density where a planet, orbiting on the dashed line, carves a gap and forms a pressure bump outside of its orbit. The pressure bump becomes Rossby unstable and the resulting vortex efficiently traps larger particles. The distribution of 0.09 mm sized particles is shown in the **lower right**.

2.1 Anticipated total duration of the project

36 Months

2.2 Objectives

The goal of this project is to investigate the growth and dynamics of planetesimals and of forming planets in pressure bumps of transition disks. The scientific questions we want to answer are:

- How effectively can planetesimals be formed in pressure bumps?
- What properties of the pressure bumps are compatible with observational properties of protoplanetary disks? How effective can planet(esimal) formation be in transition disks? At what efficiency will it start violating observational properties of observed disks?
- Is growth via mutual collisions or accretion of pebble sized dust the dominant mode of planetesimal growth in transition disks?
- What role does the dynamical evolution play – how large can planetesimals grow before their dynamics either leads to destruction or causes them to leave their birth places? Related: how will a newly formed planet in the bump move around the remaining pebbles? Will there be observational signals of such a planet in the shape of the dust concentration and its polarized signature (such as the offset between the sub-mm continuum and polarized intensity, see Kataoka et al. 2016)?
- How does the origin of the pressure bump (e.g. viscosity bump, photoevaporation, or planet) affect these scenarios?
- How does the situation change with various parameters such as the extent of the pressure bump, the turbulence strengths or in particular with vortices in case the pressure bump becomes Rossby wave unstable?

2.3 Work programme including proposed research methods

2.3.1 Research Methodology

In this project, we will couple the evolution of small solid particles via recipes of gravoturbulent planetesimal formation to the growth and dynamical evolution of planetesimals. To do this, we will will employ two different methodologies: first, we will use simplified gas disk structure models (i.e. hydrostatic disks). Therefore, we will be able to concentrate on the dust processes and the planetesimal formation and dynamical evolution processes in more detail. This methodology will encompass phase I and II (cf. Section 2.3.3.1 and Section 2.3.3.2). The second approach in phase III (cf. Section 2.3.3.3) will include detailed hydrodynamical processes but therefore necessarily simplifying other aspects such as the dust evolution. This simplification, however, will be based on the results of phase I and II (and the ERC project of Dr. Birnstiel) and will thus *not* be based on ad-hoc assumptions.

2.3.2 Research Tools and Inputs

For this project, we will be using the following tools:

- A dust evolution code, either the open-source code `twopoppy` (Birnstiel et al. 2012b), described below, or if needed, the gas+dust disk evolution code of Birnstiel et al. (2010).

- A N-body integrator. For this we will use the open-source code `REBOUND` (Rein & Liu 2012), which offers a wide variety of integration schemes and flexible options to include additional forces or add/remove particles.
- A disk hydrodynamical code with Lagrangian particles. The foundation of this will be the custom version of the `PLUTO` code from (Picogna & Kley 2015). We will use this code or future versions of it in phase III (Section 2.3.3.3) and implement the growth processes developed in phase I and phase II.
- For comparison with dust continuum observations, we will employ the 3D monte carlo radiative transfer code `RADMC-3D` that was developed by the Applicant Prof. Dullemond. Scripts to directly run the `RADMC-3D` dust radiative transfer calculation with the input from the dust evolution code of Applicant Dr. Birnstiel are available. These include opacity calculations as well as hydrostatic equilibrium iteration with dust-settling-mixing solutions for each particle size.

2.3.3 Research Plan

2.3.3.1 Phase I: Planetesimal formation and simple gas structures

The student will begin by getting acquainted with the astrophysics of disks and planet formation on the one side and and with the numerical methods on the other side. The initial setup will be an axisymmetric pressure bump profile. For this, we will start with a parametrized, stationary pressure bump in our one dimensional dust/gas code `twopoppy`[1] (Birnstiel et al. 2012b). Further gradual improvements will include an α-disk evolution (already implemented in the code) where the pressure bump forms due to parametrized variations in the α-viscosity (Kretke & Lin 2007). This will allow us to look at time-dependent trapping processes, e.g. for pressure bumps with a finite life time. If necessary, the viscous radial evolution of the gas density could also be treated using 1D hydrodynamics to account for deviations in the rotation profile near the bump.

The student will then implement a subroutine that converts small dust particles to planetesimals whenever the right conditions are fulfilled. Similar methods have already been used by the Applicants (Drążkowska & Dullemond 2014, and Klahr, Birnstiel, Lenz, in prep.). We will employ Eq. 12 of Drążkowska & Dullemond (2014), which is a fit to detailed numerical results of Bai & Stone (2010) consistent with other works on planetesimal formation in the context of the streaming instability (e.g., Johansen et al. 2009b). Based on the local metallicity and the resulting planetesimal formation efficiency, dust mass will be removed via a sink term and the resulting mass in planetesimals will be tracked (without further evolution of the planetesimals at this point). The particle size distribution can be reconstructed using the methods published in Birnstiel et al. (2015). Should we find that the accuracy of this method is not sufficient (i.e. if the results are very sensitive to one of the approximations done here), then we could switch to an implementation of the code presented in Birnstiel et al. (2010). This will be more accurate and more detailed, but also significantly slower but not prohibitively slow as the N-body dynamics of the later stages of the project will be more limiting. The calculations outlined above will lay the foundation of the next parts of the proposed research plan:

- They provide the accretion rate of dust particles into the pressure bump.
- They provide the size distribution of the particles entering the pressure bump.
- The subroutine will calculate how much of the available dust is transformed into planetesimals.

Using the code at this stage, we will already be able to publish a first paper describing the methods and our results on planetesimal formation rates comparing to previous works in this direction (e.g., Drążkowska & Dullemond 2014; Krijt et al. 2016). Some mechanisms creating pressure bumps have

[1] `http://birnstiel.github.io/two-pop-py/`

a finite life time, such as zonal flows, or pressure bumps at the edges of dead zones. Using bumps of finite life time will allow us to investigate the efficiency of particle trapping in time-dependent pressure maxima and their possible relation to Type I transition disks, which is a significant improvement over previous works such as Pinilla et al. (2012b) and Pinilla et al. (2013). By linking this to existing millimeter wave radio-surveys (e.g., Pascucci et al. 2016 and references therein as well as previous surveys such as Ricci et al. 2010) in collaboration with project A1 we will be able to test which bump amplitudes, bump sizes, and life times are producing results consistent with (1) dust continuum observations and (2) dust disk life times[2]. This way, we will be able to exclude or constrain some of the theoretically proposed mechanisms, such as zonal flows (e.g., Johansen et al. 2009a; Dittrich et al. 2013; Bai & Stone 2014) based on their life times or amplitudes.

At this point, we can connect to project C2: the results of this project C1 provide the evolution of the dust-to-gas ratio and the particle sizes in the pressure bump. In the case of a pressure bump created via photoevaporation, these two quantities define how much dust and of what particle sizes will reach the base of the evaporative flow and can hence be entrained in the wind. At the same time, the models of photoevaporative mass loss rates resulting from project C2 can be used in this project: the gas flowing off the disk surface will have a substantially lower dust content due to vertical settling of the dust particles. By removing mostly gas, the photoevaporation process increases the dust-to-gas ratio in the pressure bump, hence possibly triggering the planetesimal formation process. As part of this project, we will test to what extend photoevaporation can modify the planetesimal formation rates during the late stages of disk evolution.

2.3.3.2 Phase II: N-Body dynamics and planetesimal evolution

In Phase I, planetesimals are formed at a given rate based on calculations of the dust evolution code, however the forming planetesimals are just kept on record and are not evolving further. Phase II of this proposal aims at improving upon this. At the beginning of the project, we will use the modular, and easy to use N-body integrator `REBOUND`[3] (Rein & Liu 2012). The fact that both `twopoppy` and `REBOUND` have python interfaces simplifies linking them: based on the planetesimal formation rates and the gas and dust surface densities from `twopoppy`, particles (planetesimals) can be created in `REBOUND`. Initially, planetesimals might be tracked individually, but as their number increases, we will likely need to switch to a super-particle approach, where one individual particle in the code represents a larger number of physical planetesimals.

The gas and dust density distribution is still assumed to be axisymmetric at this point, but an analytical vertical distribution of the density will be assumed to create a 3D density distribution: the gas will be assumed to be in hydrostatic equilibrium, while the dust will be in a mixing-settling equilibrium (Fromang & Nelson 2009).

At this point of the proposal, there are two parallel directions in which the simulation tools will be improved, linking to two different scientific directions: one focuses on more detailed gas dynamics that has links to project C2 and will be discussed below in Section 2.3.3.3. In this phase II of the research plan we will focus on the N-body treatment of the planetesimals and related science questions (to clarify: pebbles are treated as a fluid).

Based on the dust particle sizes and the 3D distribution of dust and gas developed above, we can calculate the accretion rate of pebbles onto the planetesimals. This will use the prescriptions of Ormel & Klahr (2010), Visser & Ormel (2016) and related works. Based on these rates, calculated/updated at appropriate time intervals, the mass of the N-body particles (in the `REBOUND` code) will be increased and the total mass of accreted dust particles will be removed as sink terms in the `twopoppy` code. This way the evolution of planetesimals and of the dust distribution affect each other:

Planetesimals (1) form based on the local metallicity and (2) grow via pebble accretion of dust particles of the right sizes. Dust, on the other hand, is removed by both of these effects, but possibly and to

[2] The text highlighted in green refers to the connection of this project to other projects of this Research Unit.
[3] `http://github.com/hannorein/rebound`

a smaller extend replenished by fragments. If these dust removal processes are efficient no further planetesimals will be formed since the metallicity in the bump will be kept below critical values. As another consequence, the reduction in dust mass might also reduce the particle sizes which further minimizes the amount of particles contributing to planetesimal formation. This latter effect will, however also decrease the efficiency at which the dust is accreted onto the planetesimal. Based on this, various outcomes of the early stages of planet formation could be imagined:

- Planetesimals form but then prevent further planetesimal formation, instead efficiently growing via pebble accretion (and possibly oligarchic growth at the same time).
- Planetesimal formation may be too efficient: many planetesimals form leaving little amounts of dust to be accreted onto the planetesimals. At this point dynamical and collisional evolution of planetesimals may become the dominant driving force.

As this shows, it will be extremely interesting to see how the formation of larger bodies proceeds in the hot-spots of planet formation in transition disks. This project so far already incorporates aspects of gas dynamics, collisional evolution and dynamics of small dust particles and N-body dynamics, a seemingly challenging combination. However, we would like to point out that the methods and codes we use for this are well established: the `REBOUND` code for example allows scientifically relevant calculation with only a few lines of code. It offers a wide variety of well tested and well documented integrators and a simple object-oriented approach to handle additional forces or close encounters. The `twopoppy` code as well can be run with only a hand full of lines of code and well reproduces the results of complicated coagulation codes. Combining these codes offers a student interesting quick successes but still the opportunity to gradually learn the numerical methods and also the physical processes used and assumed "under the hood" of these codes.

At the end of this phase II of the project, we anticipate at least one more publication that describes the numerical setup and explains the findings of a parameter study. With this study, we will be able to calculate planetesimal formation rates under various trapping conditions and study how the general outcome but also the detailed size distribution of planetesimals varies with disk parameters. We will also test under which conditions an analytical treatment of the involved effects, based on rate equations, can be found. Follow up studies can include improved collision models, effects of turbulence on the planetesimal distribution and many other effects. At the same time, we can use the existing links to the radiative transfer code `RADMC-3D` to investigate the observability of the simulated pressure bumps, for example to see if the presence or absence of planetesimal formation causes observationally distinct signatures and compare against current or upcoming observations in collaborations with project A1.

2.3.3.3 Phase III: Breaking the Symmetry

So far the distribution of both dust and gas has been assumed to be symmetric. As observations show us, this is indeed the case in many transition disks, as well as in disks with small scale axisymmetric structure, such as HL Tau (ALMA Partnership et al. 2015; Carrasco-González et al. 2016), TW Hydrae (Andrews et al. 2016; Tsukagoshi et al. 2016), or HD 97048 (van der Plas et al. 2016). These observations prove that the approach of the phases I and II of this project is extremely relevant. However, other observations spectacularly show strong asymmetries in the dust continuum emission (e.g., Casassus et al. 2013; van der Marel et al. 2013) or even offset asymmetries when comparing sub-mm continuum to polarized intensity (see Kataoka et al. 2016). It is suspected that these asymmetries arise from a strong pressure bumps which can become unstable to the Rossby instability (e.g., Li et al. 2001; Lyra et al. 2009). The resulting vortex then represents an azimuthal pressure maximum and is therefore able to azimuthally trap particles, further concentrating them (e.g., Barge & Sommeria 1995; Klahr & Henning 1997; Lyra et al. 2009; Birnstiel et al. 2013; Lyra & Lin 2013). In this phase III of the project, we therefore want to study the formation of planetesimals and their growth towards larger bodies in non-axisymmetric disks. This opens the possibilities to study a wide range of interesting scenarios:

First of all, it allows to study how the formation of a vortex in a pressure bump changes the outcome from phase II: is planetesimal formation more efficient inside a vortex? If so, are planetesimals growing by pebble accretion less efficient compared to a symmetric pressure bump? How does the ratio between planetesimal formation rate and planetesimal growth rate change if a vortex is formed? How are the planetesimal dynamics changing from the gravitational interaction with the vortex?

Secondly, the (at least) three possible origins of the pressure bump can make a difference:

1. How does a viscosity transition (via turbulence) affect the formation and growth rates as well as the dynamical / collisional evolution?
2. How does the gravitational forcing of a giant planet influence the dynamics of either the dust or the planetesimals?
3. Is a pressure bump caused by photoevaporation more closely resembling item 1 or 2 or entirely different? The hydrodynamical models developed in project B1 (PI Ercolano) will be used to tackle this question.

Can we find structural differences that allow us to observationally distinguish between the possible causes of a pressure bump?

The main addition in this phase III of the project is the hydrodynamical aspect where we switch from a quasi-stationary disk structure to actual hydrodynamics. While this opens an enormous range of interesting topics to investigate, it comes at significant numerical changes and challenges that make this the most risky part of the project. However, we would like to stress, that the thesis of the PhD student is not decisively dependent on this part of the project. Even if this phase III turns out to be numerically too challenging or cannot be finished within the duration of the PhD program, phase I and II offer plenty of applications and publications for a PhD thesis. Some of the aims of phase III may be then carried over to the second funding period of the Research Unit.

The addition of hydrodynamics cannot be easily added on top of the python code that employs `REBOUND` and `twopoppy`. Furthermore, long integration times of 2D hydrodynamical simulations are computationally very expensive, in particular if the dust phase and N-body particles are to be evolved at the same time. Therefore, complexity needs to be reduced in other aspects of the model. We will therefore simplify the treatment of dust coagulation: we will reduce the dust to a single fluid with either a fixed particle size that is representative of the particle sizes trapped in a pressure bump in phase I and II of this project. The best way in which this can be mimicked (for example using a radially varying particle size for the dust fluid) will be tested as part of the ERC project and are difficult to envision at this point.

To treat the new aspects (2D hydrodynamics, 2D dust dynamics) we will switch to the `PLUTO` code[4]. Our collaborator, Prof. Kley and his former postdoc Dr. Picogna (now in the group of Prof. Ercolano) have developed a particle integrator for the `PLUTO` code (see Picogna & Kley 2015). Furthermore, the treatment of dust as a tracer is already implemented in `PLUTO` (although not yet officially supported, some testing will be needed). This part of the proposal will therefore be done in close collaboration with the Tübingen group and with members of the ERC group at Munich. It is anticipated that the three setups will (due to their increasing complexity) be done in the order as itemized above. The setups and results produced in projects C2 (PI Ercolano), D1 (PI Kley) and D2 (PI Dullemond) by that point will guide this work. Project C2 deals with dust entrainment in a photoeavporative wind, while projects D1 and D2 focus respectively on planet-disk interactions and non-axysymmentric features in transition disks.

It is envisioned that this phase of the project (and to some extend also phase II) will lay the foundation for future studies in this Research Unit as it gives rise to several follow-up studies where several

[4] `http://plutocode.ph.unito.it`

aspects can be improved upon beyond this ground-laying work: this includes improvements of the collisional evolution of small dust grains in the bump, the treatment of pebbles in a particle-based approach, or by using hydrodynamical setups that are more advanced in their treatment of thermodynamics or radiation-hydrodynamics, to name just a few.

2.4 Data handling

The model results of this project as well as the relevant results of the ERC group will be shared with other members of the Research Unit using the Research Units dedicated server.

Furthermore, we will publish all data, scripts, and where possible the simulation codes necessary to reproduce the results presented in the publications of this project. To this end we will either use available options of the publishers and/or use Zenodo[5] to ensure reproducibility, long-time availability, and the possibility to reference the data.

2.5 Other information

None

2.6 Information on scientific and financial involvement of international cooperation partners

None

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[5]Zenodo is a free open science repository funded and supported by the European Commission and managed by the CERN data center. See `https://zenodo.org`.

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4. Requested modules/funds

4.1 Basic Module

4.1.1 Funding for Staff

We request funding for 1 PhD position (75% E13) to be stationed at the LMU Munich and be supervised by Dr. Birnstiel and co-supervised by Prof. Dullemond.

4.1.2 Direct Project Costs

4.1.2.1 Equipment up to EUR 10,000, Software and Consumables

Theoretical numerical research can only be done when sufficient and appropriate computational facilities are available. While production runs will be done on supercomputer facilities, a substantial part of the work in this project is code development. Testing these codes on realistic problems requires a workstation for the two PhD student – which is beyond the standard base equipment (Grundausstattung). We therefore request a workstation-grade desktop computer for the PhD position for 3 000 €.

4.1.2.2 Travel Expenses

Travel within the Research Unit is handled in project Z. In addition we request funding for conference travel for the personnel and one Applicant. This includes one national (1.000 €) and one international (1.500 €) conference trip per year, totalling 2.500 € per person per year.

For this project this totals 5.000 € per year for the PhD student and one Applicant, which is in total 15.000 €.

4.1.2.3 Project-related publication expenses

We request 750 € per year (a total of 2 250 €) for publication expenses, mainly to support open access options or whenever necessary, publication in non-free journals.

5. Project requirements

5.1 Employment status information

Dr. Birnstiel, Tilman, ERC Starting Grant holder (starting: March 2017) at the Ludwig-Maximilians-Universität Munich. Hiring process for tenure-track W2 professorship at LMU Munich ongoing, anticipated starting date: February-March 2017
Prof. Dr. Dullemond, Cornelis Petrus. W3 Professor (permanent) at Heidelberg University.

5.2 First-time proposal data

N/A

5.3 Composition of the project group

Munich: Only the Applicant TB will work directly on the project; group members of the ERC Starting Grant group led by the Applicant TB will share results where needed.
Heidelberg: Only the Applicant CPD.

5.4 Cooperation with other researchers

5.4.1 Planned cooperation on this project

5.4.1.1 Collaborating researchers for this project within the Research Unit

The student of this project, stationed in Munich, will greatly benefit from the numerical expertise within the Research Unit, in particular the hydrodynamical and N-body expertise in Tübingen and in Heidelberg. The simulation results and setups will also be exchanged with project C2 (PI Ercolano) and the implications of the results, in particular, the radiative transfer model output, will be compared against available and upcoming observational campaigns of project A1 (PI Testi) and our external collaborators Prof. van Dishoeck and Prof. Henning. This will encompass modelled emission of both (sub-)mm continuum and scattered light. This project will also benefit from frequent exchange with projects D1 (PI Kley) and D2 (PI Dullemond) particularly the planet-disk interaction models and the Lagrangian particle modules for the `PLUTO` code. Vice-versa, D1 in particular will benefit from the dust and collision models created in this project. Project B1 will provide us with the hydrodynamical models for photoevaporating disks, to allow us to investigate dust growth in pressure bumps formed at the inner edge of the outer disk.

5.4.1.2 Collaborating researchers for this project outside of the Research Unit

We will collaborate with the ERC-funded group of the Applicant Dr. Birnstiel, which will run parallel to the Research Unit.

5.4.2 Researchers with whom you have collaborated scientifically within the past three years

We list only true collaborations, not all co-authors on publications from large consortia.
S. Andrews (CfA, Harvard), S. Ataiee (Uni Bern), X.-N. Bai (CfA, Harvard), A. Banzatti (STScI, Baltimore), M. Benisty (IPAG, Grenoble), C. Brinch (University of Copenhagen), J. Carpenter (Caltech), C. Carrasco-González (UNAM, México), C. J. Chandler (NRAO, USA), E. Chapillon (Univ. Bordeaux), F. Ciesla (The University of Chicago), L. I. Cleeves (University of Michigan), E. Di Folco (Univ. Bordeaux), C. Dominik (University of Amsterdam), J. Drazkowska (Zürich University), A. Dutrey (Univ. Bordeaux), B. Ercolano (LMU München), M. Fang (Purple Mountain Observatory, China), M. Flock (JPL, Caltech), J. H. Girard (ESO, Chile), U. Gorti (SETI Institute), N. Grosso (Université de Strasbourg), G. Guidi (INAF Arcetri, Italy), S. Guilloteau (Univ. Bordeaux), Th. Henning (MPIA, Heidelberg), G. Herczeg (Kavli Institute Beijing), M. Hogerheijde (Leiden University), D. Hollenbach (SETI Institute), N. Huelamo (Centro de Astrobiología, Spain), A. Isella (Rice University), A. Johansen (Lund Observatory), A. Juhász (Institute of Astronomy, Cambridge), M. Kama (Leiden Observatory), A. Kataoka (Heidelberg University), H. Klahr (MPIA Heidelberg), L. Klarmann (University of Amsterdam), W. Kley (Universität Tübingen), R. Kuiper (Uni Tübingen), H. Linz (MPIA Heidelberg), H. Meheut (CEA, France), M. Min (University of Amsterdam), P. Mollière (MPIA Heidelberg), M. Momose (Ibaraki University), C. Mordasini (Universität Bern), R. Murray-Clay (UCSB), T. Muto (Kogakuin University), A. Natta (Dublin Institute for Advanced Studies),

K. Öberg (CfA, Harvard), S.-J. Paardekooper (Queen Mary University of London), P. Pinilla (Leiden Observatory), A.-M. Piso (CfA, Harvard), V. Piétu (IRAM, France), A. Pohl (MPIA Heidelberg), K. M. Pontoppidan (STScI, Baltimore), L. Pérez (MPIfR Bonn), J. P. Ramsey (Copenhagen), Zs. Regály (Konkoly Observatory, Hungary), L. Ricci (CfA, Harvard), V. Roccatagliata (LMU, Munich), D. Semenov (MPIA Heidelberg), A. Sicilia-Aguilar (University of St Andrews), S. Stammler (Heidelberg University), M. Tazzari (ESO), R. Teague (MPIA Heidelberg), L. Testi (ESO), C. Thalmann (ETH Zurich), J. Tobin (Leiden Observatory), N. Turner (JPL, Pasadena), T. Tsukagoshi (Ibaraki University), N. Turner (JPL, Pasadena), A. Uribe (Coll. Charlston), C. Walsh (Leiden Observatory), D. Wilner (CfA, Harvard), Z. Zhu (Princeton University), J. de Boer (Leiden Observatory), M. de Juan Ovelar (Liverpool John Moores University), R. van Boekel (MPIA Heidelberg), E. F. van Dishoeck (Leiden Observatory), T. van Kempen (Leiden Observatory), N. van der Marel (Leiden Observatory)

5.5 Scientific equipment

At ZAH we have access to the bwFor cluster at Tübingen. All members stationed at LMU will have access to high performance computing clusters at the Leibnitz Rechenzentrum (`lrz.de`).

5.6 Project-relevant interests in commercial enterprises

None

5.7 Additional information

None

Project C2:

Gone with the wind: dust entrainment in photoevaporative winds

Authors:
Applicant: B. Ercolano (LMU)
Co-Applicants: T. Birnstiel (LMU), C. Dullemond (ZAH, Heidelberg), T. Henning (MPIA)
Cooperation Partners: J. Owen (Princeton, USA)

Requested positions: 1PhD student

Abstract:
The search for the smoking gun of disk dispersal via photoevaporative winds, leading to the formation of Type 1 TDs, has until now failed to identify suitable diagnostics. Quantitative spectroscopy of YSOs to search for blue-shifted emission lines produced in the wind relies on an accurate characterisation of the thermochemical properties of the winds. A central ingredients for the chemical calculations is the dust content of the wind as micron sized grains provide the dominant opacity channel in the far-ultraviolet. Furthermore small particles are important players in the temperature balance of the gas via the photoelectric process.

We will use realistic radiation-hydrodynamic models of photoevaporative winds coupled to dust evolution models for the underlying grain distribution in the disk, to calculate the dust entrainment in winds to feed to chemical models. The observability of the emission and scattering due to the dust grains in winds from edge-on disks, a potential new diagnostic, will be estimated for current and upcoming facilities (e.g. SPHERE, JWST) both for Herbig Ae stars and for their fainter T-Tauri counterparts.

1. State of the art and preliminary work

The dispersal of protoplanetary disks plays a crucial role in the planet formation process, and leads to the formation of Type 1 TDs. While photoevaporation from the central star has been proposed as the dominant disk-dispersal mechanism around low-mass stars (e.g., Clarke et al. 2001), to date the only direct evidence of a wind is the detection of blue-shifted line emission from some of the sources. The lines include [NeII] 12.8μm, [OI] 6300 and a number of other optical forbidden lines, which can be matched with more or less success by photoevaporation models (e.g., Hartigan et al. 1995; Alexander 2008; Rigliaco et al. 2013; Natta et al. 2014; Pascucci & Sterzik 2009; Schisano et al. 2010; Ercolano & Owen 2010, 2016; Simon et al. 2016). These lines however can only probe the wind on very local scales and they cannot be inverted to obtain mass loss rates, which are crucial to pin down the dominating mechanism driving the disk photoevaporative wind (i.e. EUV, FUV or X-ray - or a combination). Different driving mechanism induce more or less vigorous mass loss at different disk radii, which can have dramatic effect on planet formation, both at the times of planetesimal assembly and for the later dynamical evolution of planet(esimal)s (e.g., Alexander & Pascucci 2012; Ercolano & Rosotti 2015, or the discussion in projects B1 and B2). Projects B1 & B2 aim at identifying and using new spectroscopic diagnostics to quantitatively measure the mass loss rate and profile in disk winds. In order to achieve these aims a chemical model of the wind will be constructed in B2 using the wind structures from radiation-hydrodynamic calculations performed in B1 and the dust model developed in this project (C2)[1].

Chemistry is sensitively affected by the dust distribution in the wind and in the underlying disk atmosphere, but to date only rough estimates exist (e.g., Owen et al. 2011; Hutchison et al. 2016a,b). While the results of these works are not yet to the stage that they can be used in the chemical models, they demonstrate that a non-negligible population of small grains, which dominate the opacity in the FUV, are expected to be entrained in the winds.

Owen et al. (2011) demonstrated that in the case of Herbig Ae/Be stars with an EUV-driven wind, the wind selectively entrains grains of different sizes at different radii, resulting in a dust population that varies spatially and increases with height above the disk at radii larger than about 10 AU. This is a result of the streamlines topology, which extend roughly radially out. At near infrared wavelengths this variable grain population produces a 'wingnut' morphology which may have already been observed in the case of PDS 144N (Perrin et al. 2006). The work of Owen et al. (2011) could not however reproduce the colour gradient of the observations, which show redder emission at larger heights above the disk. Owen et al. (2011) suggested that the inconsistence may be due to the fact that the synthetic images are dominated by emission from the smallest grains entrained in the flow. Grain growth in the underlying disk, neglected in the Owen et al. (2011) calculations, would reduce the population of small grains there and may provide a solution to the colour problem. The grain size evolution in the underlying disk needs to be taken into account in future simulations.

While it is currently not clear if the PDS 144N observations can be explained by dust entrainment in a photoevaporative wind, the work of Owen et al. (2011) has clearly demonstrated that a significant amount of small grains (which dominate the opacity in the FUV) do populate disk winds, hence playing an important part in the chemistry there and at the base of the flow.

More recently Hutchison et al. (2016a,b) investigated the question of dust entrainment in protoplanetary disks using smoothed particle hydrodynamics (SPH). While their models are very idealised (non-rotating, plane-parallel disks), their simulations seem to support most of the conclusions reported in the semi-analytical work of Owen et al. (2011). The Hutschison et al. models also only consider an a EUV-driven wind, in order to simplify the calculations.

1.1 Dust-entrainment in winds: two modelling strategies

In this section the two approaches to model dust-entrainment in winds mentioned above are described in more detail. The limitations of both approaches are also discussed, thus highlighting the knowledge gap that our project is aiming to fill.

1.1.1 Analytical approach

Owen et al. (2011) post-processed radiation-hydrodynamical simulations of photoevaporating disk winds around Herbig Ae/Be stars in order to study the distribution and observational appearance of dust grains entrained in the wind. Their approach involved three steps: (i) (radiation)-hydrodynamical calculations of the photoevaporative wind; (ii) calculation of the dust profile distribution in the wind; (iii) radiative transfer calculation of the dust distribution to infer the observational appearance.

As the work of Owen et al. (2011) was motivated by the observations of several edge-on disks around Herbig stars, which showed extended emission above and below their midplane at NIR wavelengths (e.g., Padgett et al. 1999; Perrin et al. 2006), these authors focussed in step (i) on EUV-driven winds (e.g. Hollenbach et al. 1994; Font et al. 2004; Alexander et al. 2006a,b). Indeed Herbig stars have generally a much lower X-ray luminosity relative to their bolometric luminosity, compared to T-Tauri stars, raising questions on what the driving radiation may be for these intermediate mass stars. For that reason Owen et al. (2011) chose to adopt the hydrodynamic EUV wind solution of Font et al.

[1] The text highlighted in green refers to the connection of this project to other projects of this Research Unit.

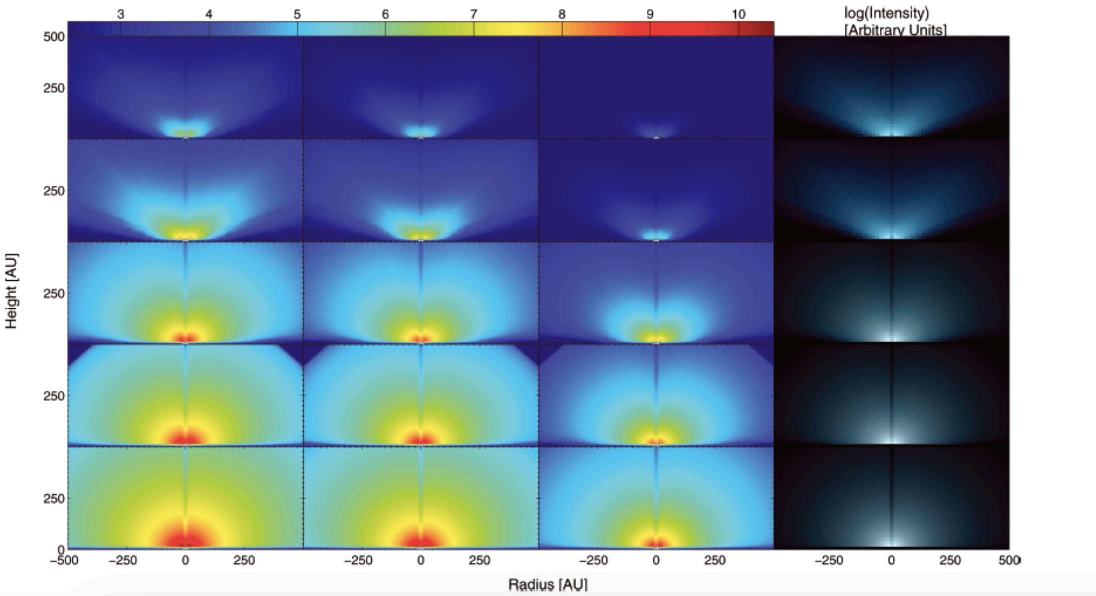

Figure 1: Image from Owen et al. (2011): Synthetic images for disk models with irradiating fluxes ϕ = $1e41....1e45 phot/sec$, the **first column** shows the image in the H band, the **second column** displays the K band and the **third column** displays the L band. The **fourth column** displays a red green blue composite image (L,K and H bands, respectively). The images are individually scaled so that there is a 5 dex spread between the brightest pixel and the darkest. All images assume that the disk is edge-on, therefore the stellar emission is blocked out by the presence of the optically thick disk.

(2004), which is simple and scalable, hence allowing them to investigate a wider range of parameter space. As we will see in Section 2, this option is not suitable for T-Tauri stars we wish to model here, where the X-ray photoevaporation model needs to be considered. X-ray driven photoevaporative winds, are shown to be two orders of magnitude stronger than EUV-winds around T-Tauri stars.

In step (ii) Owen et al. (2011) calculated streamlines from the base of the flow to the edge of their grid from the solutions obtained in step (i). Along each of the streamlines the balance between the drag force, gravity and the centrifugal force was then calculated for a given grain size: a positive net force was interpreted as grains of that size being entrained in the flow from that location.

The density distribution of dust grains in the wind was then calculated and post-processed by means of radiative transfer in step (iii) . Figure 1 shows the synthetic images obtained from the models of Owen et al. (2011) in L,K & H band and composite, which were then compared with the observations of Perrin et al. (2006).

While the calculations of Owen, Ercolano & Clarke show that indeed a significant amount of small grains can be expected in photoevaporative winds, they present however some serious limitations that make them unsuitable for application to our Research Unit tasks. First of all, these calculations are limited to the EUV-case only. The X-ray photoevaporation case, which is likely dominant amongst T-Tauri stars, is completely different and significantly more complex than the EUV case.

Another important shortcoming of Owen et al. (2011) is that they do not account for dust evolution in the underlying disk. An MRN (Mathis et al. 1977) size distribution with standard gas-to-dust ratio of 100 is assumed everywhere in the disk. The resulting dust density and size distribution in the wind is thus necessarily incorrect. Given the central role played by dust grains for the chemistry (see project B2), our project will couple dust evolution in the underlying disk to the wind entrainment problem for the X-ray driven winds around T-Tauri stars.

1.1.2 Numerical approaches

The dynamics of dust grains in protoplanetary disks can be studied either by directly integrating the orbits of a large number of dust 'super-particles' (that sample the local properties of the dust population) or by solving the collisionless Boltzmann equation for the particle distribution function. For a population of very small (tightly coupled with the gas) dust particles, the Boltzmann equation can be reduced to the zero pressure fluid equation (Cuzzi et al. 1993; Garaud et al. 2004). This 'two-fluid' approach has been used to study planet-disk interactions (e.g., Paardekooper & Mellema 2004, 2006; Zhu et al. 2012). This is however limited to a single population of small particles, it cannot account for the full velocity distribution of the grains at a single location, and it is not able to capture strong density gradients. The particle approach has the great advantage to follow the evolution of solid particles with different physical properties, perfectly recovering the dust dynamics in the limit where the grains are decoupled from the gas (Youdin & Johansen 2007; Miniati 2010; Bai & Stone 2010). This method has also been applied successfully to the study of planet disk interaction adopting both SPH and grid-based codes (Fouchet et al. 2007, 2010; Ayliffe et al. 2012; Lyra et al. 2009; Zhu & Stone 2014). Grid codes are generally preferred because they do not introduce a large artificial viscosity that can affect the evolution of low-mass planets. Moreover, the accuracy needed to properly model the evolution of the gas and dust component in a protoplanetary disks is strongly dependent on the choice of the grid geometry (Lyra et al. 2009; de Val-Borro et al. 2006), requiring more computational effort in a cartesian grid than in a cylindrical or spherical one.

Dr. Picogna, who is currently employed as a postdoc in the group of PI Ercolano, has implemented a population of dust particles in the modern grid-based code PLUTO (Mignone et al. 2012) that can evolve both in a cylindrical and spherical coordinate system (Picogna, Stoll & Kley, in prep.). This approach is thus ideal to study the evolution of different dust particle populations in protoplanetary disks. As detailed in the next section, this method, coupled with the photoevaporation model implemented in PLUTO, will be adopted to self-consistently model dust particles entrained into the wind from the disk atmosphere for a number of selected cases.

In their recent work of Hutchison et al. (2016a,b) used a new algorithm to treat a wind in an SPH code. The wind is treated using unequal-mass, one-fluid SPH. Using new techniques developed by the authors, they are able to simulate two-fluid dynamics in highly stratified atmospheres. The work currently represents only a proof of concept, suggesting, however, that these novel techniques may in the future be applied to study interesting aspects of gas and dust dynamics in the wind. At present, however, the models are very idealised, approximating disks and winds by a thin, non-rotating, plane-parallel atmosphere. This technique is thus not yet mature to be used for the purposes of our project.

1.2 Project-related publications

Birnstiel, T.; Dullemond, C.P. & Brauer, F.: *Gas and dust evolution in protoplanetary disks*, 2010, A&A 513, 79. In this paper we present the basic code for the evolution of the disk and the dust. The latter follows the dust coagulation, fragmentation, settling and radial drift of the dust.

Birnstiel, T.; Klahr, H. & **Ercolano, B.**: *A simple model for the evolution of the dust population in protoplanetary disks*, 2012, A&A 539, 148. In this model the flow of pebbles from the outer disk regions into the inner planet forming disk regions is studied, and an easy to use model derived.

Birnstiel, T.; Andrews, S.; Pinilla, P. & Kama, M.: *Dust Evolution Can Produce Scattered Light Gaps in Protoplanetary Disks*, 2015, ApJL 813, L14. Here we applied the vertical steady state settling mixing distribution to calculate the observational appearance of simulated disks.

Ercolano, B.; Drake, J.; Raymond, J. C.; Clarke, C. C.: *X-Ray-Irradiated Protoplanetary Disk Atmospheres. I. Predicted Emission-Line Spectrum and Photoevaporation*, 2008, ApJ 688, 398. We present mocassin two-dimensional photoionization and dust radiative transfer models of a prototypical T Tauri disk irradiated by X-rays from the young pre-main-sequence star. In this work a first estimate of X-ray photoevaporation rates is given, hinting at the relevance of this process for disk dispersal

Ercolano, B.; Clarke, C. C.: Drake, J.; *X-Ray Irradiated Protoplanetary Disk Atmospheres. II. Predictions from Models in Hydrostatic Equilibrium*, 2009, ApJ 699, 1639. In this follow-up paper we take into account the response of the disk structure to the X-ray heating and demonstrate that even in this case the X-ray photoevaporation rates remain substantial. A hydrostatic solution is reached iteratively with the full photoionisation problem.

Owen, J. E.; **Ercolano, B.**; Clarke, C. J.; Alexander, R. D. *Radiation-hydrodynamic models of X-ray and EUV photoevaporating protoplanetary disks*, 2010, MNRAS, 401, 1415. Starting from the hydrostatic solutions of Ercolano et al. (2009), we perform the first radiation-hydrodynamic solution of an X-ray irradiated disk. Robust mass-loss-rates and profiles are calculated for this model, suggesting that X-ray drive the dispersal of disks.

Owen J., **Ercolano B.**, Clarke C. *Protoplanetary disk evolution and dispersal: the implications of X-ray photoevaporation*, 2011a, MNRAS, 412, 13. We explore the role of X-ray photoevaporation in the evolution and dispersal of viscously evolving T Tauri disks. Our models confirm that X-rays play a dominant role in the evolution and dispersal of protoplanetary disks giving rise to the observed diverse population of transition disks, including some of those with massive outer disks, some of those with gas in their inner holes and some of those with detectable accretion signatures.

Owen J., **Ercolano B.**, Clarke C. *The imprint of photoevaporation on edge-on disks*, 2011b, MNRAS, 411, 4103. We perform hydrodynamic and radiative transfer calculations of a photoevaporating disk around a Herbig Ae/Be star to determine the evolution and observational impact of dust entrained in the wind. We find that the wind selectively entrains grains of different sizes at different radii resulting in a dust population that varies spatially and increases with height above the midplane.

Owen J., Clarke & **Ercolano B.** *On the theory of disk photoevaporation* 2012, MNRAS, 422, 1880. We derive analytical scaling relations and derive estimates for the total mass-loss rates, as well as discussing the existence of similarity solutions for flows from primordial and transition disks. In this paper we catch a first glimpse at a new process for the clearing of the very last stages, which we name "thermal sweeping".

Ercolano B., Owen J. *Blueshifted [O I] lines from protoplanetary disks: the smoking gun of X-ray photoevaporation*, 2016, MNRAS 460. 3472 We produce new synthetic observations of a particularly promising diagnostic, and demonstrate that the observations available at the time (before Simon et al. 2016) are consistent with the photoevaporation model. We show however that this line cannot be used to measure mass-loss-rates.

2. Objectives and work programme

2.1 Anticipated total duration of the project

36 months

2.2 Objectives

In this project we aim to determine the dust content and size distribution of photoevaporative winds for a range of stellar, disk and wind parameters, using realistic descriptions for grain evolution in the underlying disk.

This will allow us to :

1. Build a dust model for photoevaporative winds to be used in astrochemistry and radiative transfer calculations (see B2).
2. Estimate the observability and observation characteristics of the dust phase in photoevaporative winds.

2.3 Work programme including proposed research methods

In this project we will first use the semi-analytical approach described in Section 1.1.1 coupled to models for the evolution of dust grains in the disk in order to efficiently produce dust entrainment models for the complete set of X-ray photoevaporation wind solutions calculated in project B1. The dust models will then be passed on to project B2 (chemical models), incrementally as they are calculated.

There are several reasons for choosing the semi-analytical approach over fully numerical approaches (SPH or grid-based). First of all, semi-analytical approaches are much more efficient for our aims. We will make use snapshots from the hydrodynamical calculations, since, to first order, the grain entrainment problem can be decoupled from the photoevaporation problem. Indeed dust grains entrained in the wind do now provide tangible extinction at X-ray frequencies, hence the wind structures and rates are not sensitive to the dust distribution in the wind. The dust entrainment calculation can thus be performed by post-processing snapshots of the radiation-hydrodynamic calculations, allowing us to use the same wind solution and changing (e.g.) the underlying dust distribution in the disk, according to different models and prescriptions.

It is perhaps worth mentioning that the dust evolution in the underlying disk is however strongly coupled to the evolution of the gas in the disk. A full radiation-hydrodynamic simulation of the gas and dust which also simultaneously solves the dust coagulation and drift is however beyond what is currently feasible. It is however possible to perform a gas radiation hydrodynamics calculation which includes dust particles, not accounting for coagulation (e.g. Picogna, Stoll & Kley, in prep.). If time allows, we will perform a number of such (expensive) calculations to compare with the semi-analytical ones. This is particularly important for transition disk models, where the dust may be pushed back away from the inner edge of the disk due to the pressure gradients in the gas, thus resulting in a lower dust content in TD winds, compared to full disks. These models are also relevant to the study of dust trapping in pressure bumps, performed in project C1. In any case, a more comprehensive set of these simulations will be performed during the second funding period of the Research Unit.

2.3.1 Grain sizes and abundances at the base of the wind

One key element of this project is to investigate the impact of the underlying grain population on the population of grains entrained in photoevaporative winds. To this end we will use the state of the art coagulation code from Birnstiel et al. (2010) which solves for the evolution of the particle distribution due to coagulation, fragmentation, and erosion, as well as radial transport by drift, mixing, and gas advection. The resulting particle size distribution $\Sigma_d(t, r, a)$ is then a function of distance to the star r, particle size a, and time t. Treating the growth in a vertically averaged way (i.e. using surface densities instead of volume densities) is generally a good approximation since vertical settling and mixing time scales are short for growing particles. However, for this project, the vertical distribution of particle sizes is important as it determines the sizes and abundances of particles at the base of the photoevaporative flow.

At the beginning of the project, we will use vertical distributions of particles that are in a steady state between mixing and settling, such as derived by Fromang & Nelson (2009). These are simple analytical equations, which need to be numerically integrated for each particle size. This technique is already available and has been used for calculating the observational appearance of simulated disks e.g. in Birnstiel et al. (2015) and many other works. This should give a good first representation of the particles that are present at the base of the flow.

At a later point, these prescriptions can be updated with a more sophisticated treatment of coagulation and transport processes: at high dust-to-gas ratios small grains can be “trapped” closer to the mid-plane due to frequent collisions with other particles (Krijt & Ciesla 2016). When photoevaporation has preferentially depleted the gas, thus raising the dust-to-gas ratio in the disk, this effect could potentially affect the amount of small dust grains that are mixed up to the base of the photoevaporative flow. The results of Krijt & Ciesla (2016) can be used to estimate this effect. Some time during the second year of this project, we expect the ERC group of T. Birnstiel to have a working 2D dust coagulation and transport model which will allow us to check for differences between the earlier approaches (steady state distributions) and models that take the time evolution and collisional processes into account.

2.3.2 Research Tools and Inputs

For this project we will need the following tools:

1. Photoevaporative wind solutions for EUV-driven models for T-Tauri and Herbig stars. These are easily computable using the models that are described in the literature (e.g., Font et al. 2004).
2. Photoevaporative wind solutions for X-ray photoevaporated models. These will be provided from project B1.
3. One-dimensional dust growth models. These codes are published and available within the group: simulation code of Birnstiel et al. (2010) and the parameterized model of Birnstiel et al. (2012). The one dimensional results will be coupled to prescriptions of vertical mixing (e.g., Fromang & Nelson 2009)
4. Two-dimensional dust evolution results/parameterisation from the ERC-funded projects of Dr. Birnstiel.

5. A 3D radiative transfer code to post-postprocess the wind models with the calculated grain populations. For this we can use the streamlined version of the MOCASSIN code developed by the PI (see description below) and/or use of the RADMC-3D code developed and maintained by Prof. Dullemond.

2.3.3 Research Plan

The work proposed here will be carried out by a PhD student supervised by Prof. Ercolano (LMU) with the help of Dr. Birnstiel (LMU), who will advice, respectively, on the dust entrainment calculations and the coupling with the dust evolution models for the underlying disk.

The project will proceed in stages of increasing complexity. We will start by setting up a framework that can be benchmarked against available calculations and progressively add new elements, as they become available from other projects. The plan has been designed to fit a PhD student, who will have the opportunity to develop a new theoretical model as well as acquainting her/himself with standard numerical techniques (e.g. radiation-hydrodynamics, dust evolution models, radiative transfer).

The most important science product from this project is the set of grain models developed for the X-ray driven wind. These are needed by project B2 for the chemical calculations, as the dust grains dominating the opacities in the FUV are not equally distributed in the wind (see e.g., Owen et al. 2011; Hutchison et al. 2016a,b) and they thus affect the chemistry in the wind differently in different parts.

2.3.3.1 Preparatory Work

The methodology described in Owen et al. (2011), has been used in the group of the PI Ercolano to develop a suit of codes which take the gas density and velocity of the EUV-only wind and the stellar irradiation spectrum as an input and calculate the dust density and size distribution in the wind.

The resulting codes are the product of first a bachelor and then a master student project in the group of PI Ercolano. The aim of the bachelor project performed by George Dadunashvilli in 2013 and of the master project performed by Denis Mehmedov in 2014, was to asses the role played by dust growth in the underlying disk on the appearance of the wind in the case of the EUV-only driven wind from the Herbig star studied by Owen et al. (2011). The projects were motivated by the failure of the Owen et al. (2011) models in reproducing the colour gradient in the observations of PDS 144N (e.g., Perrin et al. 2006), which show redder emission at larger heights above the disk.

The main results of the two projects can be briefly summarised as follows.

In the case of an EUV-only wind, the removal of small grains from the disk atmosphere due to grain growth produces an overall reduction in the total dust density in the wind. This can be seen in Figure 2, where the dust density distribution in the wind is compared for the case of an underlying disk grain size distribution following a standard MRN (Mathis et al. 1977) and for a truncated MRN. The colours of the wind are also affected by the removal of small grains in the disk, but not enough to reproduce the observations. A comparison of different calculations for different grain size cut-offs are shown in Figure 3.

There are a number of problems with these preliminary results however. First of all a full exploration of the parameter space, even if only for the EUV-only case is beyond the scope of bachelor or even master projects. This is one of the reason why these results have yet to be published. Furthermore an unrealistically simplified approach to including the effects of grain growth was used. Simply a cut-off was applied to the minimum grain size in the MRN distribution of the underlying disk. This led to the fact that we have been limited to a maximum cut-off of 0.73mum. A cut-off at larger sizes would have led to a virtually dust-free wind. This is unrealistic since the growth of grains in a more realistic coagulation model leads to a larger population (by number) of a few micron-size grains compared to a standard MRN which is truncated at say 1mu.

Nevertheless, the legacy of these projects is a suite of codes, which were benchmarked in detail, and

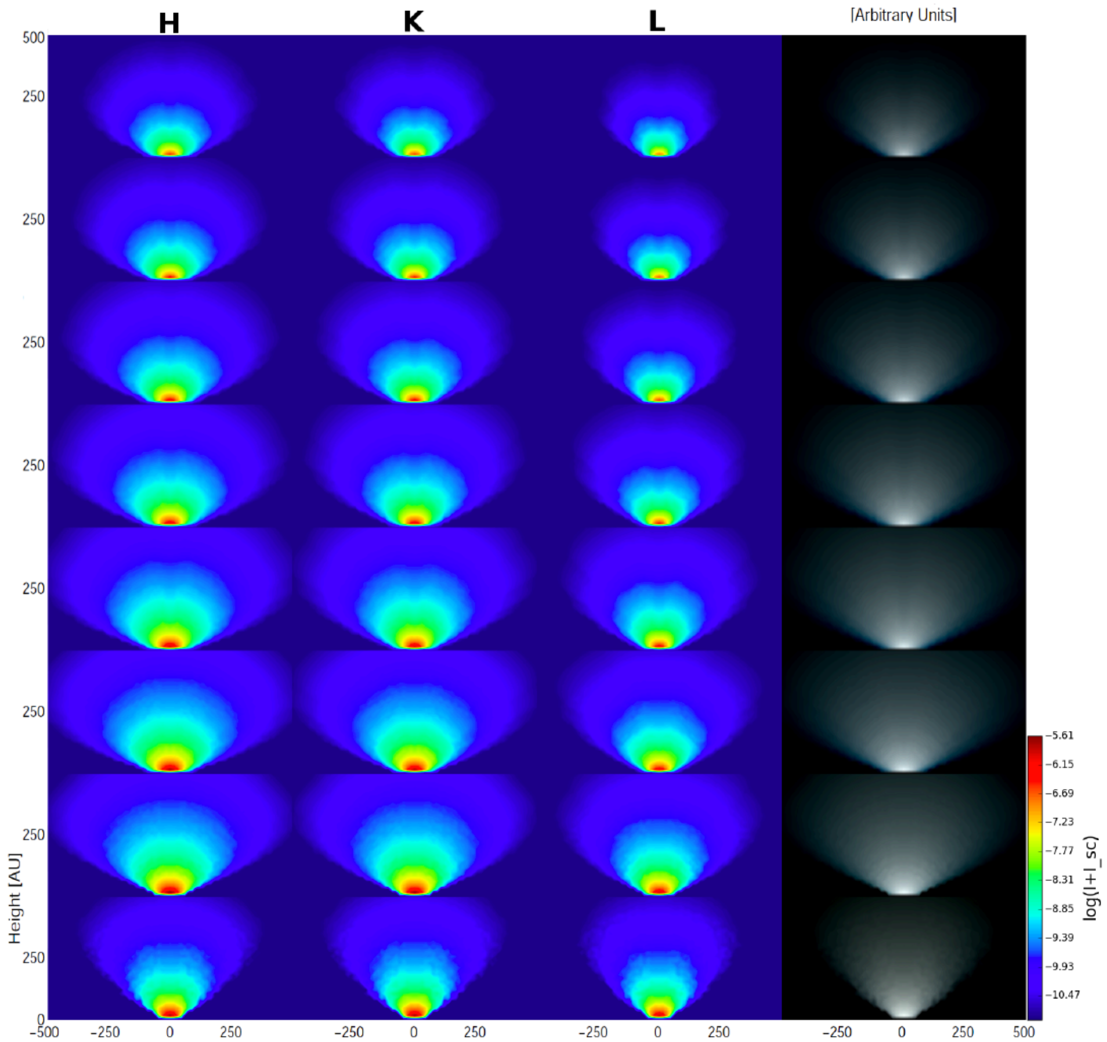

Figure 2: Effect of sequential truncation of MRN on the image. **Columns, from left to right respectivley:** H: (1.5 - 1.8)μm, K: (2 - 2.4)μm, L: (3 - 4)μm. Rows from top to bottom correspond to MRN in the disk with respectively: a_{min} = 5, 10, 20, 42.4, 86, 170, 360, 730 nm and a_{max} = 1mm. **First three columns of all rows** are normalized such that there are 5 dex between the brightest value in the L band of all images, representing the white pixel and the black pixel. Figure taken from the LMU Master Thesis of Denis Mehmedov, 2015.

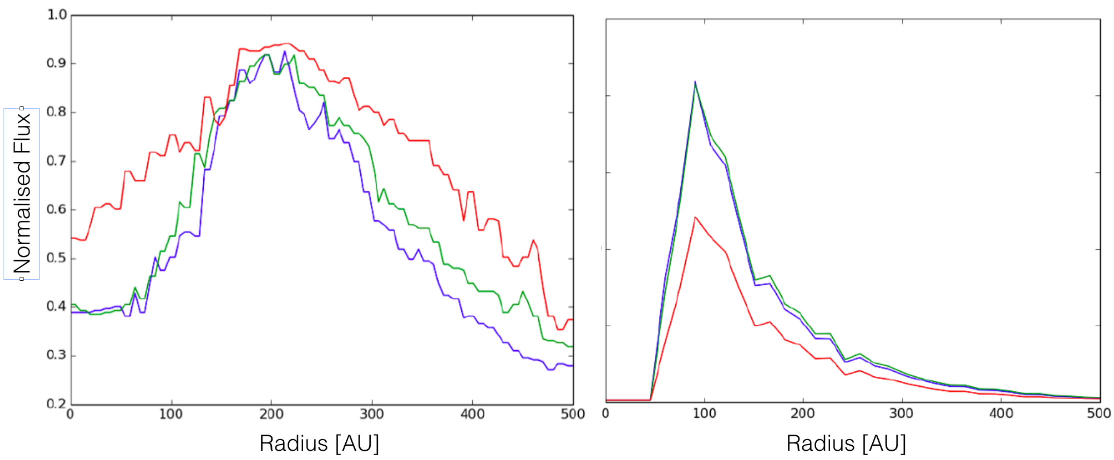

Figure 3: **Left Panel:** Color plot of the slice at 100AU in the observational images extracted from Perrin and Graham (2006). **Right Panel:** The same for out simulation with the maximum truncation of the MRN (a_{min}=730nm). Figure taken from the LMU Master Thesis of Denis Mehmedov, 2015.

result now much improved compared to the Owen et al. (2011) tools. These can be used as a starting point and upgraded by the PhD student employed for the project.

2.3.3.2 Months 1-12

The student will start by producing wind solution for the EUV case from the work of Font et al. (2004), which may be applicable to Herbig stars. For that she/he will use the standard version of the PLUTO code (Mignone et al. 2007, 2012) in two-dimensional mode. Note that no additional column density/Stroemgren radius calculations need to be used in order to implement the Font et al. (2004) solutions for EUV winds. This solution simply treats the wind as an isothermal gas with sound speed, $c_s = 10\,\mathrm{km\,s^{-1}}$. The number density at the base of the wind is also fixed and is a simple function of radius, mass of the central star, gas sound speed and ionising stellar flux (Hollenbach et al. 1994; Font et al. 2004; Alexander & Armitage 2009). We will be able to validate our solutions with those in the literature, which is an important step, particularly in a project led by a PhD student.

The student will then proceed to calculate the dust distribution in the wind, under simplifying assumptions for the underlying dust distribution in the disk as in Owen et al. (2011). In brief, streamlines from the base of the flow to the edge of the grid will be computed and along each of them, the force balance between the drag force, gravity and the centrifugal force will be calculated. A positive net force on a grain along the streamline will indicate that the grain is entrained.

Once dust abundance and size distributions have been obtained for the wind, radiative transfer calculations will be performed to produce synthetic continuum observations at several disk inclinations. These first models will be benchmarked against the solutions of Owen et al. (2011). Note that we have developed a streamlined version of our MOCASSIN code which was used to produce the images in Owen et al. (2011), as well as in the subsequent bachelor and master thesis projects. However the RADMC-3D code developed by Prof. Dullemond (co-speaker to the Research Unit) is also available to us for comparison.

After the benchmarking tests, we will be sure that we have developed a solid framework which can now be applied, for the first time, to the calculation of the dust component entrained in an X-ray driven photoevaporative wind. The wind solutions of Owen et al. (2010, 2011, 2012) and Ercolano & Owen (2016) are readily available and they could provide a starting point, until new wind solutions become available form project B1. This may however not be necessary as the new wind models for the X-ray case are already being calculated by Dr. Picogna, who is employed to do the preparatory work for project B1. It is therefore likely that an initial set of high resolutions new X-ray wind solution may already be available to the student right from the start of project C2.

As the first dust models for the X-ray driven wind become available they will be immediately passed on to project B2 (Astrochemistry), for inclusion in the chemical models to be then updated when the new models including dust evolution in the disk become available (see next section).

We will perform new radiative transfer calculations of the dusty X-ray driven wind to produce synthetic continuum observations and provide a first estimate of the observability of such winds with current/future instrumentations. Our results may motivate observational campaigns led by collaborators (e.g. the group of Prof. Henning), the outcome of which, however does not influence the success of the research aims of our projects.

2.3.3.3 Months 13-24

At this point we will be in a position to significantly improve on this work by considering more realistic grain abundances and size distributions for the underlying disk.

We will first couple the grain entrainment calculations to simple prescriptions of dust evolution (e.g., Birnstiel et al. 2012) obtained from the one-dimensional models of Birnstiel et al. (2010). The one dimensional models describe the evolution of dust that is mostly in the mid-plane, i.e. well below the base of the wind, where the grains may be entrained from. The Birstiel, Klahr & Ercolano (2012) prescriptions will then need to be coupled to vertical mixing prescriptions (Fromang & Nelson 2009) in order to estimate the grain distributions at the wind-launching location, obtained from the hydro simulations. While this is not optimal, it is the standard approach used in this field as a two-dimensional model of dust evolution is still lacking. As an example the observational appearance of simulated disks is generally calculated in this way (e.g., Birnstiel et al. 2015).

Complementary to this project the ERC-funded team led by Dr. Birnstiel aims to develop new two-dimensional (both radius-height and radius-azimuth) dust evolution models. When these new models become available, the student will work closely with Dr. Birnstiel to include elements of these new results in our calculations.

As the first new models which account for grain evolution in the underlying disk become available for a few selected cases, they will be implemented in the astrochemistry models of project B2. In collaboration with the postdoc employed for project B2, we will then compare the resulting chemical models with those obtained in the previous year, which assumed a standard MRN distribution for the underlying disk. This will allow us to estimate the effects due to the coupling of grain evolution and grain entrainment in the wind on the chemical abundance in the wind and disk atmosphere. This step is important to establish to what degree of complexity this coupling should be performed in further calculations in order to ensure accurate results.

2.3.3.4 Months 25-36

In this last year of the first funding period the whole machinery will be in place. We will now be able to apply it to a wide parameter space of disk winds, producing sets of dust models to be passed on to project B2 for the optimised chemical calculations.

At this stage we will also connect with project C1, where models of disks with dust traps are to be developed. The question to be asked is “What is the effect of dust traps in the underlying disk on the grain entrainment? Can one expect signatures of this process to be observed either in the continuum emission in the wind or in the molecular lines observations?”. The reverse question is also interesting:”What is the effect of photoevaporation on the evolution of the underlying dust grains?”. If the wind removes the gas, but the dust has grown to large enough sizes that they are not dragged along (because they have settled below the base of the wind) then the dust-to-gas ratio in the disk will be increased, possibly triggering the streaming instability, and thus possible planet formation, albeit in a somewhat later stage of disk evolution (Throop & Bally 2005, e.g.).

We will perform comprehensive dust radiative transfer calculations of the obtained structures (with and without dust traps) to compare with available observations or to make more detailed observability predictions, which may further guide future observing proposals. We will join forces with expert collaborators on scattered light observations (e.g. Prof. Henning, Prof. Dullemond) to plan new proposals, however we stress that failure to obtain new observations as well as eventual non-detections do not preclude the main aim of this project to be achieved, i.e. the development of dust models and dust distributions in photoevaporative winds.

Furthermore, as detailed in a previous section, we plan to compare and contrast the efficiency of dust entrainment for disks at different evolutionary stages. In order to do that we will use grids of TD disks from model B1 with cavities of various sizes, where the streamline topologies are different from those of full disks.

If time allows, the student will collaborate with the postdoc employed for project B1 to produce full hydrodynamical simulations of disk winds, where the dust component in the disk and wind is treated as particles (e.g. Picogna & Kley 2016). As we discussed in the previous sections of this proposal, these calculations are computationally expensive and therefore we will only be able to perform a limited number of them. Nevertheless they may be useful as a piecewise comparison to the simpler methods previously developed by the student in the project.

A more comprehensive set of simulations, performed via the semi-analytical and (for a smaller sample) the numerical method, will be performed in the second funding period. These will also include photo-evaporating disks with gaps opened by giant planets (e.g., Rosotti et al. 2013, 2015) and other types of asymmetries, for which the models developed in projects D1 (PI Kley) and D2 (PI Dullemond) will provide the starting conditions.

2.4 Data handling

The model data-grids will be made available on the Research Unit dedicated server for use within the team. Furthermore we will provide a set of diagnostic models to guide observers in the wider community, which will be placed on the public partition of the server. This public data will include sets containing the full size distribution at every 2D point, as well as sets of the mean/minimum/maximum grain sizes (the mean averaged in different ways), as well as synthesised images in different bands which can be directly compared to observations.

2.5 Other information

Not Relevant

2.6 Information on scientific and financial involvement of international cooperation partners

Not Relevant

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4. Requested modules/funds

4.1 Basic Module

4.1.1 Funding for Staff

We require funding for one PhD (75% E13) student for three years to be supervised at the LMU by Prof. Ercolano.

4.1.2 Direct Project Costs

4.1.2.1 Equipment up to EUR 10,000, Software and Consumables

Theoretical numerical research can only be done when sufficient and appropriate computational facilities are available. While production runs will be done on supercomputer facilities, a substantial part of the work in this project is code development. Testing these codes on realistic problems requires a workstation for the PhD student – which is beyond the standard base equipment (Grundausstattung). We therefore request a workstation-grade desktop computer for the PhD position for 3 000 €.

4.1.2.2 Travel Expenses

Travel within the Research Unit is handled in project Z. In addition we request funding for conference travel for the personnel and one Applicant. This includes one national (1.000 €) and one international (1.500 €) conference trip per year, totalling 2.500 € per person per year.

For this project this totals 5.000 € per year for the PhD student and one Applicant, which is in total 15.000 €.

4.1.2.3 Visiting Researchers (excluding Mercator Fellows)

During the course of the project a one week long visits to our main international collaborator, Dr J. Owen (currently at Princeton University, will move to Imperial College London in 2017). This includes airfare and 6 overnight stay 1200 €

4.1.2.4 Other Costs

None

4.1.2.5 Project-related publication expenses

We request 750 €/year (total 2250 €) for publication expenses.

4.1.3 Instrumentation

None

4.1.3.1 Equipment exceeding EUR 10,000

None

4.1.3.2 Major Instrumentation exceeding EUR 100,000

None

5. Project requirements

5.1 Employment status information

Barbara Ercolano, Professor at the Ludwig-Maximilians-Universität München (permanent)

5.2 First-time proposal data

Not Relevant

5.3 Composition of the project group

5.4 Cooperation with other researchers

5.4.1 Planned cooperation on this project

5.4.1.1 Collaborating researchers for this project within the Research Unit

The project will use the wind models calculated in project B1 (PI Ercolano) and then feed back the results to project B2 (PI Caselli, Ercolano), where a chemical model of the wind and atmosphere will be developed. Dr. Birnstiel will provide guidance on the implementation of existing and new dust evolution models and, in the one-dimensional case, also helping us to link them to vertical mixing prescriptions. Models for two-dimensional dust evolution of the underlying disk will be provided by the ERC-funded group of Dr Birnstiel. In the third year of the Research Unit we will connect with project C1 (PI Birnstiel & Dullemond) to use the dust distributions in the underlying disks. The project will also feed back to C2 providing the grain entrainment to establish the effects on dust evolution in the disk (e.g. streaming instability). Stellar properties to guide the models will be obtained with the help of the team from project A2 (PI Preibisch). Observational constraints will be obtained in collaboration with experts working on project A1 (PI Testi) and our external collaborators Prof. Henning and Prof. van Dishoeck. At the end of the first funding period, if time allows, or in the second funding period, we plan to investigate the effects of non-axisymmetric underlying disks, for which the models developed in projects D1 (PI Kley) and D2 (PI Dullemond) will provide the initial conditions.

5.4.1.2 Collaborating researchers for this project outside of the Research Unit

Dr. James Owen, currently at Princeton University, from 2017 at Imperial College London, has performed the original semi-analytical calculations of dust-entrainment in the wind together with the PI of this project (Owen et al. 2011). He is also an expert in radiation-hydrodynamics models of photoevaporating winds (e.g., Owen et al. 2010, 2011, 2012) and is expected to pay frequent visit to Munich to actively participate in our project.

We also plan to use the 2D dust evolution models which will be constructed within the ERC- funded group of Dr. Birnstiel, which will run parallel to the Research Unit.

5.4.2 Researchers with whom you have collaborated scientifically within the past three years

R. Alexander (U. Leicester), S. Andrews (Harvard, USA), X. Bai (Harvard, USA), A. Banzatti (STScI Baltimore, USA), M. Barlow (UCL, London, UK), N. Bastian (U. Liverpool, UK), M. Benisty (IPAG Grenoble, FRA), A. Bevan (UCL, London, UK).D. Boneberg (U. Cambridge, UK), I. Bonnell (U. St. Andrews, UK), J. Carpenter (California Institute of Technology), C. Carrasco-González (UNAM, MEX), S. Casassus (U. de Chile, Santiago, Chile), P. Cazzoletti (MPE, DEU), J. Dale (U. Hertfordshire, UK),

A. Danekhar (CfA, Harward, USA), C. Dominik (Univ. Amsterdam, NLD), C. Dullemond (Univ. Heidelberg, DEU), A. Dutrey (Univ. Bordeaux, FRA), M. Fang (Purple Mountain Obs., CHN), M. Flock (JPL, USA), A. Glassgold (U. Berkeley, USA), U. Gorti (SETI Institute, USA), M. Guarcello (U. Palermo, Italy), S. Guilloteau (Univ. Bordeaux, FRA), T. Henning (MPIA, DEU), M. Hilker (ESO, Garching), M. Hogerheijde (Leiden Observatory, NLD), D. Hubber (LMU), A. Isella (Rice Univ., USA), A. Johansen (Lund Univ., SWE), M. Kama (Leiden Observatory, NLD), A. Kataoka (Univ. Heidelberg, DEU), H. Klahr (MPIA, DEU), C. Koepferl (LMU), H. Linz (MPIA, DEU), C. Manara (ESA, Noordwjik, Netherlands), A. McLeod (ESO, Garching), R. Murray-Clay (UCSB, USA), A. Natta (DIAS, IRL), F. Niederhofer (STSci, USA), R. Parker (U. Liverpool, UK), Q. Parker (Sidney, Australia), I. Pascucci (U. Arizona, USA), P. Pinilla (Leiden Observatory, NLD), A. Piso (Harvard, USA), A. Pohl (MPIA, DEU), L. Pérez (MPIfR, DEU), L. Ricci (Harvard, USA), V. Roccatagliata (LMU, DEU), K. Rosenfeld (Harvard, USA), D. Semenov (MPIA, DEU), M. Tazzari (U. Cambridge, UK), R. Teague (MPIA, DEU), L. Testi (ESO), C. Walsh (Leiden Observatory, NLD), R. Wesson (UCL, London, UK), D. Wilner (Harvard, USA), Z. Zhu (Princeton U., USA), M. de Juan Ovelar (Liverpool Univ., GBR), R. van Boekel (MPIA, DEU), E. van Dishoeck (Leiden Observatory, NLD), N. van der Marel (Leiden Observatory, NLD), K. Öberg (Harvard, USA),

5.5 Scientific equipment

The group of Prof. Ercolano has two own computer clusters comprising

- 2 CPU Intel Xeon X5650 (Westmere, beginning 2010, 2.66 GHz) 6 cores each 12 cores total (24 virtual) 74 GB ram.
- 4 CPU Intel Xeon E7-4850 (Ivy Bridge, beginning 2014, 2.30 GHz) 12 cores each 48 cores total (96 virtual) 660 GB ram.

Further computational power is provided through the C2PAP facility of the Excellence Cluster to which the group has guaranteed time. This comprises 126 nodes, each node with 2 CPU Intel Xeon E5-2680 (Sandy Bridge, beginning 2012, 2.7 GHz) 8 cores each 16 cores total (32 virtual) 64 GB ram. Note that while the future of the Excellence Cluster Universe is uncertain, the C2PAP facilities will be in any case supported by the LMU.

The Leibniz Rechnung Zentrum (LRZ) is also available to us, where still larger facilities are available with somewhat more constrained and longer queues.

Project D1:
Transition disks and planetary systems

Authors:
Applicants: W. Kley (U. Tübingen), C.P. Dullemond (ZAH, Heidelberg)
Co-Applicants: L. Testi (ESO), E. van Dishoeck (MPE/Leiden), T. Henning (MPIA)

Requested positions: 1 Postdoc

Abstract:
Transitional disks (TDs) presumably occur in the later phases of the evolution of protostellar disks around young stars and show a depletion of flux from the inner, central parts of the disk. One variety of such disks display a lack of radiation in the mid-infrared wavelength regime which is interpreted as large inner holes in their dust distribution. Nevertheless they show significant gas accretion signatures coming from the central inner region. It has been suggested that for these type of TDs this inner cavity might be created by the presence of one or more planets that cleared out the inner disk region. In this project we shall follow this line of thought and will perform multi-dimensional hydrodynamic studies to clarify the dynamical impact of planets on TDs in order to prove (or disprove) the existence of planets in such disks. The studies will include gas dynamics, dust particles, embedded planets, radiation transport and irradiation from the central star.

1. State of the art and preliminary work

Observationally, transition disks are characterized by a lack of flux in the few μ-meter (near/mid IR) range as seen in the spectral energy distributions (SEDs) of young stars. This flux deficit is typically associated with 'missing' dust having temperatures of 200-1000 K (Calvet et al. 2002; D'Alessio et al. 2005) corresponding to the inner regions of accretion disks. Despite this lack of dust, there are nevertheless still signatures of gas accretion in several systems with large inner (dust) holes that are a few tens of AU wide.

The observational properties of transitional disks and the modeling attempts up to date have been reviewed recently by Owen (2016) and we mention here only the main aspects relevant to this project. As described in the general introduction to this collaborative research proposal, the origin of the inner disk clearing has been basically attributed to two different processes: either photoevaporation from inside out through high energy radiation from the central young protostar (e.g. Shu et al. 1993; Alexander et al. 2006), or by embedded massive planets that carve deep gaps into the disk (e.g., Varnière et al. 2006). Now, as outlined in the introduction, TDs appear to come in two flavors, mm-faint disks with low mm-fluxes, small inner holes ($\lesssim$ 10au), and low accretion rates onto the stars ($\approx 10^{-10} - 10^{-9}$ $M_\odot$/yr) and mm-bright-disks with large mm-fluxes, large holes ($\gtrsim$ 20au), and high accretion rates $\approx 10^{-8}$ $M_\odot$/yr (Owen & Clarke 2012) to which we refer here as Type I and Type II disks, respectively.

While photoevaporation is certainly at work in some systems (Type I TDs) it is believed that it can only operate for systems with a sufficiently low mass accretion rate below $10^{-8} M_\odot/yr$ and is otherwise quenched by the accretion flow (Owen & Clarke 2012). At the same time the persistence of gas accretion within the inner (dust) holes is taken as an additional indication that other mechanisms should operate that create these gaps (Manara et al. 2014). The very likely mechanism for this second class of TDs is related to the growth of planets in the disks, because young planets embedded in their nascent disks will not only open a gap in the gas disk but they will create an even stronger depletion of the dust near the planetary orbit (Paardekooper & Mellema 2004).

Consequently, it has been suggested early on that the presence of a massive (Jupiter-sized) planet might be responsible for the gap creation (Varnière et al. 2006; Rice et al. 2006), but at the same time it has been noticed that the gap created by a single embedded planet is significantly narrower than observations of transition disks suggest. Given the problems with a single planet and the photoevaporation models, it has been proposed that the main observational features can be created by the presence of a system of (three to four) massive planets. Following this line of thought, Zhu et al. (2011) and Dodson-Robinson & Salyk (2011) performed numerical simulations and argue that transitional disks are in fact *Signposts of young multi-planet systems*. In this scenario the embedded planets act as a 'barrier' for the gas flow through the disk allowing some gas to enter the inner region, causing the observed accretional features near the star, while the dust is filtered out at the pressure maximum just beyond the outer edge of the gap and cannot enter the inner disk regions. Following this line of thought theoretical models with embedded planets and dust in disks have been constructed to match the observed spectral energy distributions in the sub-millimeter (de Juan Ovelar et al. 2013; Pinilla et al. 2015). However, even though the disk is modeled via two-dimensional (2D) hydrodynamical simulations in this case the dust motion is not self-consistent and based on the azimuthally averaged disk models using a 1D dust evolution model of Birnstiel et al. (2010).

New ALMA observations in special wavelength bands focusing on CO-vibrational lines have allowed to determine the gas content in the inner disk region in more detail. These results show that the inner disk gas depleted by factors of about 10^2 (van der Marel et al. 2015) or even to a factor of 10^4 with gas holes about a factor 2-3 smaller than the dust gaps (van der Marel et al. 2016) which is taken as another example of massive planets in disks (Ho 2016). The conclusion that all or the majority of Type II TDs are shaped by massive planets has been questioned recently by Dong & Dawson (2016) who argue that there may not be enough giant planets to explain all observed Type 2 TDs, see also Cumming et al. (2008) for the occurrence rate of massive planets at larger separations. The solution to this problem is either that current numerical models of planet-disk interactions are too inefficient at gap opening compared to Nature, or that Type II TDs are intrinsically rare objects, rather than common and sort-lived objects, as is probably the case for their Type I counterparts. Considering that the arguments of Dong & Dawson (2016) are based on analytical approximations on gap widths and sizes that are based on isothermal models and do not consider any dust motion it may well be that the theoretical models have not reached the degree of sophistication necessary to produce reliable results.

As pointed out above, despite this strong belief that planets play an important role in shaping transition disks, there is still a lack of theoretical modeling to be able to make detailed comparison with observations. The most advanced simulations are those of Zhu et al. (2011) who model a system of up to 4 massive planets embedded in a 2D flat disk. Their studies suggest that only the presence of several planets will result in a strong depletion of the gas in the inner disk. However, there are several short-comings. The simulations treat the disk in the isothermal approximation, they are only 2D and neglect the vertical structure, and no accretion luminosity of the planets was considered. Despite these limitations the most important constraints may be the omission of dust particles in the simulations, which is important as it is the dust emission that is actually observed in many cases.

In any event, as mentioned in the recent review by (Owen 2016): *if we understand the specific planet-disk signature, then we may be able to use the observations of transition disks to observationally probe planet formation*. In this project we aim exactly at this twofold goal: We will construct new self-consistent models for Type II TDs that contain a system of embedded planets that will allow us to determine the role that planets play in shaping TDs in general, and obtain at the same time a deeper understanding of the planet formation process. Given that many of the above issues, as well as our modeling techniques, may also apply to the newly emerging class of “Multi-Ringed Disks” (such as HL Tau, TW Hydra, HD 163296, BP Piscium, etc., see Introduction text of this Research Unit), we will also include these objects in our scope.

To this purpose we will perform a series of time-dependent, multidimensional hydrodynamical simulations to study in detail the impact of a planetary system on the ambient disk. In these new studies we will go beyond the isothermal approach used by most of the studies and will add radiative transport, including irradiation from the central star. Secondly, the motion of embedded dust particles will be followed simultaneously with the gas which allows to study in detail the gas motion and dust filtration process at the gap's outer edge as a function of particle size. Thirdly, we will perform simulations in full 3D that allows us to study the gas overflow across the planets in detail and makes the stellar irradiation more realistic. The results of the simulations will be used to calculate emission properties to be compared to the observations.

1.1 Preliminary work

The PI of this project has ample experience in modeling accretion disks with embedded planets, starting from single embedded planets to a system of planets evolving into a resonant configuration. Initially two-dimensional (2D) studies in the isothermal approximation were performed and later full 3D studies including full radiative transfer. A summary of the topic of planet-disk interaction with references to several works of the PI is given in a review article in Annual Rev. of Astronomy & Astrophysics by Kley & Nelson (2012). The evolution of two massive planets embedded in a disk has been studied in Kley et al. (2004) where we were interested in the resonant capture process. In Kley & Dirksen (2006) we studied the impact of circular embedded planets on an outer disk, and in Kley et al. (2009) we studied the planet-disk interaction in full 3D radiative disks. In the past years a study on the physics of transitional disk with one embedded massive planet has been conducted Müller & Kley (2013), and recently hydrodynamical simulations with embedded dust particles have been performed Picogna & Kley (2015); Stoll & Kley (2016). Here, we list some of our recent work relevant to this project.

1.1.1 On the accretion flow in Transitional Disks

In Müller & Kley (2013) two-dimensional hydrodynamical simulations using the grid-based code FARGO for disks with a single embedded planet were performed. In addition to the standard isothermal models we constructed models that include viscous heating, radiative cooling from the disk surfaces, radiative diffusion in the disk midplane and stellar irradiation in the energy equation in order to have more realistic models and estimate the importance of the disks thermodynamics on the flow. The mass flow rate into the gap region depends, for given disk thermodynamics, non-monotonically on the mass of the planet. Generally, more massive planets open wider and deeper gaps which would tend to reduce the mass accretion into the inner cavity. However, for larger mass planets the outer disk becomes eccentric (Kley & Dirksen 2006) and the mass flow rate is enhanced over the low mass cases. As a result, for the isothermal disks the mass flow into the inner gap is always comparable to the expected mass flow of unperturbed disks $\dot{M}_{\rm d}$, while for radiative disks the mass flow is very small for low mass planets ($\leq 4\,M_{\rm jup}$) and about 50 % of $\dot{M}_{\rm d}$ for larger planet masses. The radial surface density distribution and the mass accretion rate into the inner disk cavity is shown in Fig. 1 for the $4\,M_{\rm jup}$ planet located at 5.2au for different treatments of the disk thermodynamics. As shown in the upper panel, the isothermal model shows by far the highest gas density in the inner disk region, while the radiative models fall well below it. Including stellar irradiation brings the models somewhat in between the purely isothermal and radiative case. This gas density distribution is reflected in the mass accretion rate onto the star displayed in the bottom panel of Fig. 1. In addition, for the radiative disks the critical planet mass for the disk to become eccentric is much larger than in the purely isothermal case. In Müller & Kley (2013) we simulated only single embedded planets on fixed circular orbits but we could show that massive embedded planets can reduce the mass flow across the gap considerably, and that the disk thermodynamics plays indeed a decisive role in determining the gas fraction entering the inner hole.

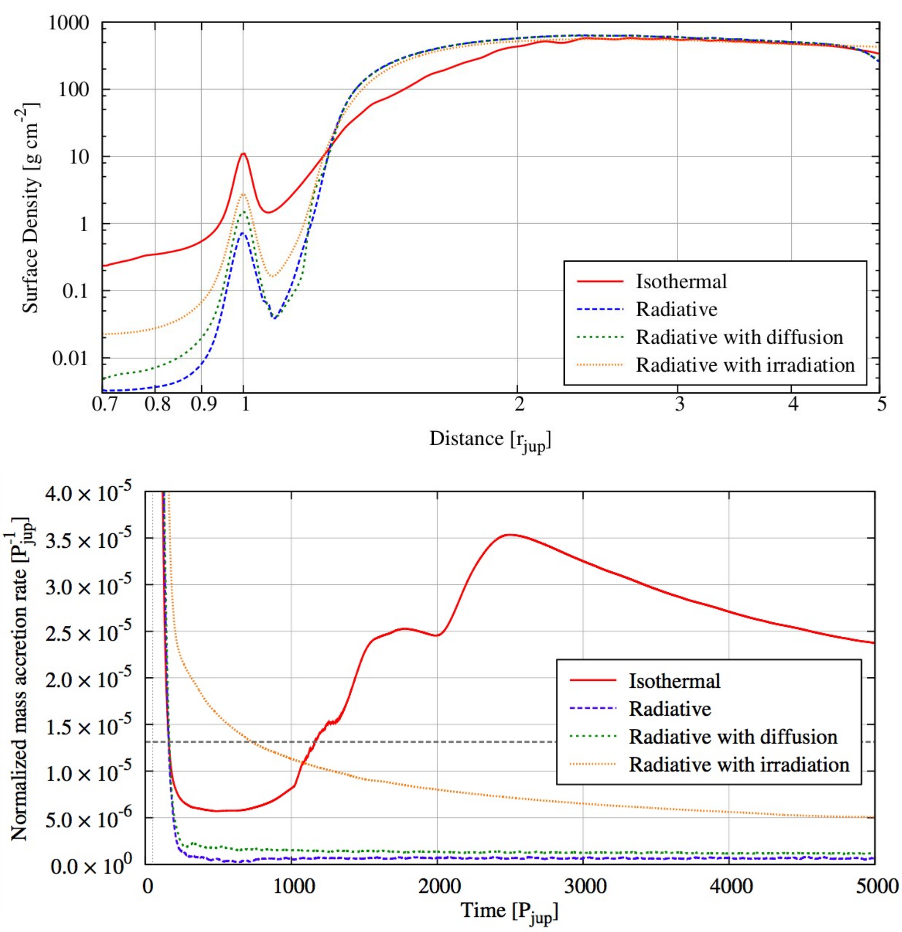

Figure 1: Radial density distribution (**top panel**) and time evolution of the mass accretion rate (**bottom panel**) into the inner hole of the disk for a $4M_{Jup}$ planet located at 5.2au in a transitional disk. Shown are curves for different thermodynamic treatments of the disk physics. Taken from: Müller & Kley (2013)

1.1.2 On the dust distribution in the disk around HL Tau

Upon publication of the spectacular image of the "Multi-Ringed Disk" system in the HL Tau disk by the ALMA Partnership (ALMA Partnership et al. 2015), we performed hydrodynamical simulations of the disk around HL Tau with embedded planets and dust particles (Picogna & Kley 2015). There, we followed the evolution of a population of dust particles treated as Lagrangian particles simultaneously with the hydrodynamics, in two-dimensional locally isothermal disks where two equal-mass planets are present. The planets were kept in fixed orbits and they did not accrete mass. We found that the outer planet plays a major role in removing the dust particles in the co-orbital region of the inner planet and in forming a particle ring which has a steeper density gradient close to the gap edge with respect to the single-planet scenario, which promotes the development of vortices. The ring and gap width depend strongly on the planetary mass and particle stopping times of the particles, i.e. how well they couple to the gas motion. For the more massive cores the ring clumps into few points that are able to collect a high mass fraction. In summary we found that the features observed in the HL Tau system can be explained through the presence of two massive cores that shape the dust disk where the inner planet has a mass of the order of $0.07M_{Jup}$ and the outer one of the order of $0.35M_{Jup}$. These values can be significantly lower if the disk mass turns out to be less than previously estimated. By

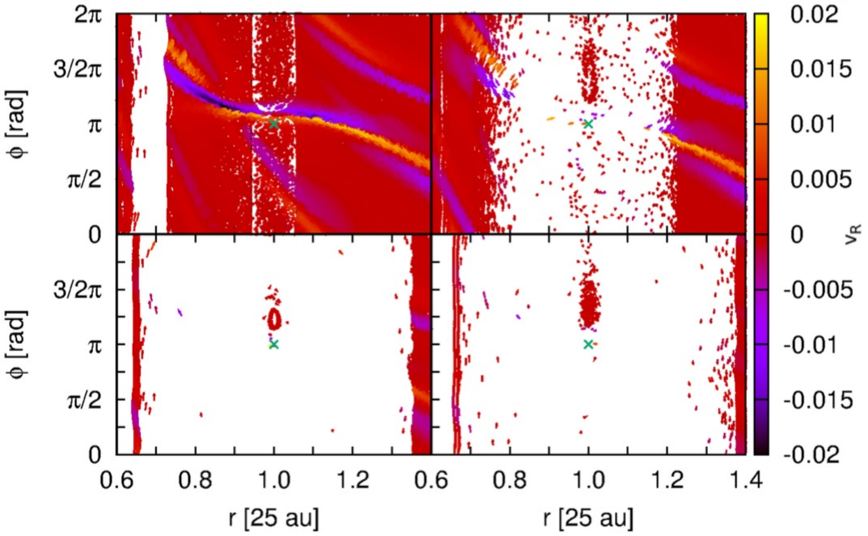

Figure 2: Particle distribution near the inner low mass planetary core location for mm- (**top left**), cm- (**top right**), dm- (**bottom left**), and m-sized (**bottom right**) particles at the end of the simulation. The velocity vectors of the particles with respect to the planet are shown and the colour scale shows the relative radial velocity. Taken from: Picogna & Kley (2015)

decreasing the disk mass by a factor of 10, we obtain similar gap widths for planets with a mass of $10M_{Earth}$ and $20M_{Earth}$ for the inner and outer planets, respectively. Although the particle gaps are prominent, the expected gaseous gaps are barely visible. The final distribution of dust particles of different sizes is shown in Fig. 2, clearly the gap width depends on the size or better the dimensionless stopping time of the embedded particles, see eq. (4) below. For very small particles that couple well to the gas (top left panel) there is no strong gap visible while for larger, not so well coupled particles a strong gap will be opened in the dust distribution. Obviously this filtering effect will play a major role in determining the dust distribution in transitional disks as well.

1.1.3 Circumbinary disks and GPU-computing

In a closely related project we studied the evolution of disks around a central binary star (circumbinary disks, CBs) and followed the migration process of embedded planets (Kley & Haghighipour 2014, 2015). This work is conceptually similar to the transitional disk case in that multiple objects (here two stars - in the TD case a few planets) are surrounded by an outer disk which which is truncated due to the torques acting by the embedded bodies. In both cases there is nevertheless a transfer of mass into the inner central region. The CB-disk simulations were performed for 2D flat-disk configurations using the binary parameter of the Kepler-38 and Kepler-34 system. In addition to locally isothermal runs we included in some models viscous heating, and radiative cooling (Kley & Crida 2008).

To run such CB-disk and TD models as mentioned above (Müller & Kley 2013) takes typically several 1000 dynamical timescales (e.g. orbit of the binary/planets) to bring the system into quasi-equilibrium. For standard codes, even using the FARGO-algorithm, this requires considerable computer time, see also the comments in Zhu et al. (2011). Hence, within the framework of a Diploma/PhD-Thesis, we have recently developed a completely new implementation of the PLUTO-code to run on Graphics Processor Units (GPUs). Presently, full 3D viscous hydrodynamics is included and for 2D disks we have implemented radiative effects as well. In a first application we studied the dynamical friction process (Thun et al. 2016) and will submit a new paper on the dynamics of circumbinary disks shortly. The CPU time used by this new code is shown in Fig. 3 for a standard test-problem. As can be inferred

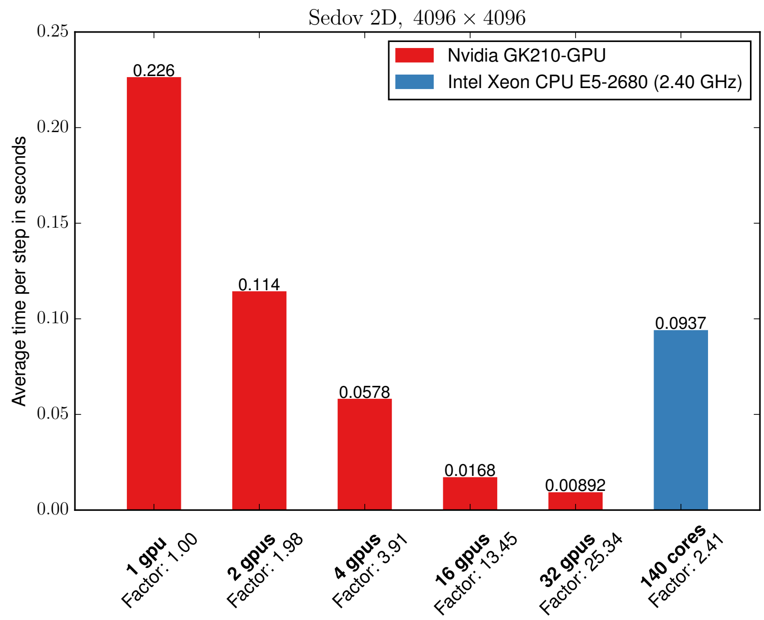

Figure 3: Computational time used for simulations using our new GPU-PLUTO code on the 2D Sedov test-problem using 4096×4096 gridcells. In red the values for the GPU-runs are displayed where multiple GPUs are connected via MPI. Each node of the system has 4 GPUs, so the results for 16 and 32 GPUs includes MPI communication between different nodes. The blue column refers to an MPI simulation on 5 nodes with 28 cores each.

from the plot, the new GPU-code runs on one GPU card in our new cluster (see Sect. 5.5) as fast as the pure MPI-version on about 60 cores. In this project we plan to use this code in addition to the publicly available versions of the FARGO and PLUTO code.

1.2 Project-related publications

Kley, W., & Dirksen, G., *Disk eccentricity and embedded planets*, 2006, A&A, 447, 369. In this paper we demonstrate how a massive planetary companion can make an outer disk eccentric. The applied methods and results are relevant at least for Task 1 of the project.

Kley, W. & Crida, A. (2008) *Migration of protoplanets in radiative disks*, Astronomy & Astrophysics, 487, 9. In this paper we present a detailed study of the importance of an improved thermodynamical treatment on the migration problem. The presented methods are directly relevant to the first Task of the project that deals with 2D disks including radiative transport and cooling.

Gorti, U., **Dullemond**, C. P. & Hollenbach, D. (2009) *Time Evolution of Viscous Circumstellar Disks due to Photoevaporation by Far-Ultraviolet, Extreme-Ultraviolet, and X-ray Radiation from the Central Star*, Astrophysical Journal, 705, 1237. In this paper we describe a method on how to evolve viscous disks with photoevaporation due to high energy radiation. This porcess is important to clear out in inner regions particularly for type I TDs but may play a role for type II disks as well.

Kley, W., Bitsch, B. & Klahr, H. (2009) *Planet migration in three-dimensional radiative disks*, Astronomy & Astrophysics, 506, 971. In this paper we study the interaction of an embedded planet with the disk in full 3D including radiative transport. This paper is relevant as demonstrate the importance of radiative transport on planet disk interaction and we introduce here the treatment of radiative transport and the Fargo-algorithm in 3D hydrodynamics.

Kolb, S. M.; Stute, M.; **Kley**, W. & Mignone, A., *Radiation hydrodynamics integrated in the PLUTO code*, Astronomy & Astrophysics, 559, A80. In this paper we describe the implementation of a new full 3D radiation module to the PLUTO-code using flux-limited diffusion including irradiation from the central star via ray-tracing. The new modules have been made available via webserver to the computational astrophysics community and are relevant for this project in particular Task 3.

Müller, T. W. A. & **Kley**, W. (2013) *Modelling accretion in transitional disks* Astronomy & Astrophysics, 572, A61. This paper shows our experience with modeling the dynamics of transition disks. In this paper the gas flow through the planet-induced gap is studied using various treatments of the disks thermodynamics. This is very relevant for the type 2 TDs which usually still have substantial accretion onto the star and have inner disks.

Ataiee, S., Pinilla, P., Zsom, A., **Dullemond**, C.P., Dominik, C. & Ghanbari, J. (2013) *Asymmetric transition disks: Vorticity or eccentricity?*, Astronomy & Astrophysics, 553, L3. This paper shows our work on how a massive planet can make the disk asymmetric (lopsided) in two independent ways: by making the disk eccentric or by creating a vortex. We show how to distinguish observationally between these two scenarios. It is relevant with respect to the consideration of dust and hydrodynamics and is an example of how we make a link between modeling and observations.

Picogna, G. & **Kley**, W. (2015) *How do giant planetary cores shape the dust disk?. HL Tauri system*, Astronomy & Astrophysics, 584, A110. In this paper we present 2D disk simulations that simultanously evolve the disk, embedded planets and dust particles. It shows very clearly the different behaviour of gas and dust and the importance of incorporating both at the same time.

Kley, W. & Haghighipour, N. (2014) *Modeling circumbinary planets: The case of Kepler-38*, Astronomy & Astrophysics, 564, 72. The dynamical evolution of circumbinary disks with embedded planets is calculated. We show that a migrating planet can naturally be stopped at the inner disk gap close to the observed position. The paper is relevant as the overall dynamics of the system (i.e. several bodies interacting with a disk) is similar to the problems to be treated here.

Stoll, M.H.R. & **Kley**, W. (2016) *Particle dynamics in discs with turbulence generated by the vertical shear instability*, Astronomy & Astrophysics, 594, A57. In this paper we describe the evolution of dust and gas for 3D accretion disks. The methodology applied here is important for the Task 3 of this project.

2. Objectives and work programme

2.1 Anticipated total duration of the project

3 years.

2.2 Objectives

The ultimate goal of this project is to investigate whether Type 2 TDs and/or Multi-Ringed Disks are signposts of (multiple) planet formation: i.e. can the observed features of these disks be explained by an ensemble of embedded planets and what can we learn in this case about the nature of the planets? Earlier models have tried to explain TD holes with multi-planet systems, but their conclusions are inconclusive due to missing essential physics, such as dust dynamics, radiative cooling and full 3D flow. In this project we plan to bring the modeling of Type II TDs and Multi-Ringed Disks that contain a system of embedded planets to a new level of realism that allows robust predictions. To this purpose we will perform a series of time-dependent, multidimensional hydrodynamical simulations to study in detail the impact of a planetary system on the ambient disk. The new studies will first include realistic thermodynamics of the gas by adding radiative transport and including irradiation from the central star. Secondly, the motion of embedded dust particles will be followed which allows to study the gas dynamics and dust filtration process at the gap's outer edge. Thirdly, we will perform simulations in full 3D that allows us to study the gas overflow across the planets in detail and makes the stellar irradiation more realistic. The results of the simulations will be used to calculate emission properties to be compared to the observations in collaboration with the A1 (PI Testi) team. A selection of the developed models will also be used by subprojects B1 (photoevaporation PI Ercolano), B2 (chemistry PI Caselli & Ercolano), C1 (PI Birnstiel & Dullemond) and C2 (PI Ercolano).The models will be used to investigate the effects of planet-gaps in the disk on photoevaporation (B1), search for chemical signature of planet-induced gaps (B2), explore the effects of these gaps on dust traps (C1) and on the final dust entrainment in the wind (C2)[1].

2.3 Work programme including proposed research methods

The hydrodynamical simulations will make use of the FARGO- and PLUTO-codes. Using the spatial distribution of the dust and gas we will use the radiative transport code RADMC-3D for making observational predictions from our models. The project will contain the following steps:

1) *2D hydrodynamical simulations of protoplanetary disks with multiple embedded planets*
To connect to existing multi-planet simulations of Zhu et al. (2011) and our own (Müller & Kley 2013) the first hydrodynamical models will be performed for flat 2D locally isothermal disks that contain several planets. In a parameter study the planetary masses will be varied systematically, and the resulting equilibrium density configurations will be analysed. The 2D isothermal models will be extended by including viscous heating, radiative cooling and transport based on Kley &

[1] The text highlighted in green refers to the connection of this project to other projects of this Research Unit.

Crida (2008) and Müller & Kley (2012). For these models first emission maps will be calculated using the RADMC-3D code (Dullemond 2012).

2) *Dust evolution in 2D dimensional disk simulations with embedded protoplanets*
Dust particles will then be added to these models whose motion is determined by the frictional forces between gas and particles, that depends on the particle size and the gas density of the disk. In parameter studies the disk mass, the planet mass and the particle radii will be varied in order to determine the dust depletion factor within the central cavity relative to the gas accretion rate as a function of particle size and planet masses. Additionally we will determine the accumulation point of the dust in the outer remaining disk and check for possible asymmetries. For this work we shall extend the methods developed in Picogna & Kley (2015).

3) *Full three dimensional disk simulations with embedded protoplanets*
From the 2D-runs the most promising parameter sets will be selected to perform full 3D time dependent hydrodynamical simulations using the PLUTO-code. These simulations will yield new results of the mass overflow across the planetary obits and allow for small inclinations of the planets. Using the resulting gas and dust spatial density distribution the RADMC-3D code will be applied for making observational predictions from our models. This can be used for both, continuum and line emission.

2.3.1 Tools for the proposed project

As the projects includes complex numerical hydrodynamical simulations we plan to perform simulations with different numerical tools (codes) in order to crosscheck our results. Experience has shown that the usage of different codes on the same physical problem in parallel allows the elimination of numerical issues and improves the reliability of the results considerably. Specifically we plan to use the FARGO and PLUTO codes that are publicly available and have already been used and updated in our research groups.

FARGO-code For the 2D simulations we plan to use the ADSG version of FARGO (Masset 2000; Baruteau & Masset 2008) updated by Müller & Kley (2012). This code uses a staggered mesh finite difference method to solve the hydrodynamic equations. The velocities are updated with the source terms using a first-order integrator with operator splitting, while the advective terms are treated by a second-order upwind algorithm (van Leer 1977). A special treatment of the angular velocity advection allows for much larger time-steps to be used (Masset 2000). In this version of FARGO we have implemented radiative cooling and stellar irradiation (Müller & Kley 2012). The position of embedded objects is calculated by a fifth-order Runge-Kutta algorithm. For the 3D simulations we plans to utilize the new GPU-version FARGO3D (Benítez-Llambay & Masset 2016) that is based on similar numerical algorithms as the standard 2D version extended to 3D. Both codes are publicly available.

PLUTO-code For the 2D and 3D simulations we plan to use the PLUTO-code (Mignone et al. 2007). Pluto solves the hydrodynamic equations using the finite-volume method which evolves volume averages in time. To evolve the solution by one time step three substeps are required. First the cell averages are interpolated to the cell interfaces, where then in a second step a Riemann problem is solved. In a last step the averages are evolved in time using the interface fluxes. Different reconstructions and limiters can be used. Recently, we have extended the most recent version 4.2 of PLUTO to run on GPUs using the CUDA-language. In this new GPU-PLUTO version the prime integrators of the standard PLUTO-code are included. Presently, the new GPU-code has implemented full 3D hydrodynamics including viscosity in different coordinate systems (cartesian, cylindrical, and spherical). Extensive test-runs show identical results to the standard MPI-version of PLUTO on various test-problems, with much increased overall performance (see Fig. 3). This new code can ideally be used on the new GPU-cluster available within the bwHPC initiative of the state of Baden-Württemberg, see Sect. 5.5.

2.3.2 Work plan

The work plan consists of several sub-projects that follow the general outline of the overall project goals. It consists of multi-dimensional hydrodynamical simulations with increasing complexity. It is conveniently divided into the following three Tasks:

Task 1 *2D hydrodynamical simulations of protoplanetary disks with multiple embedded planets*
In this first part of the project we plan to perform 2D simulations of flat accretion disks with multiple embedded planets. To become familiarized with the topic and connect to the existing simulations by Zhu et al. (2011) in the first stage the simulations will be in the locally isothermal approximation. These simulations will be performed simultaneousy with the FARGO-code and with our new GPU-PLUTO code for selected parameter sets similar to those chosen in Zhu et al. (2011). For comparison to our own work (Müller & Kley 2013) we will run a few single planet calculations for planets of varying mass in the isothermal case. Having verified the accuracy of our treatment, in particular ensure agreement between the two codes used, we shall extend the simulations directly with important physics. One strong handicap of many existing single-multi-planet simulations is the assumption of an isothermal gas. However, near the inner edge of the disk the gas flows into the inner cavity on more radial orbits and has to expand and real gases tend to cool upon this expansion, additionally the gas can cool more efficiently near the disk's inner edge because it becomes optically thin. Due to the inability to cool when being transferred into the inner hole of the disk the gas flow will typically be overestimated significantly as shown in our direct comparison simulations (Müller & Kley 2013) and displayed in Fig. 1. We will add internal and external heating processes by including viscous effects and irradiation by the central star as introduced in our previous works (Kley & Crida 2008; Müller & Kley 2012, 2013). Cooling from the disk surfaces will be calculated via suitable averaging of the opacity from the midplane temperature (energy) of the disk which is the quantity that is evolved in 2d disk simulations.

Some of the required physics is presently been introduced into the GPU-version of the PLUTO code but will need further testing and development. For the initial density distribution we plan to use exponential power-laws that follow from viscous disk evolution

$$\Sigma(r) = \Sigma_c \left(\frac{r}{r_c}\right)^{-\gamma} \exp\left[-\left(\frac{r}{r_c}\right)^{2-\gamma}\right] \tag{1}$$

that is frequently used by interpreting observational data on protoplanetary disks (Williams & Cieza 2011) and TDs (see e.g. van der Marel et al. 2015). In eq. (1) r_c is the critical radius where the surface density equals Σ_c and γ is the power-law slope. For these fully radiative simulations the planet masses will be varied and they will be able to accrete material from the disk environment. Initially the planets are held fixed on their orbits but will then be allowed to move according to the forces acting on them by the star, the other planets and the disk material. The disk self-gravity will most likely not be important but its influence on the planetary dynamics will be checked.

For the obtained density structures we will calculate synthetic images and spectra using our RADMC-3D code. For this we will expand our 2D density distribution by a vertical structure in hydrostatic equilibrium. The resulting observables (images, position-velocity maps and spectra) will be compared with VLT-SPHERE and ALMA data of real Type II TDs and Multi-Ringed Disks through collaboration with project A1. This comparison will also include new ALMA data from the ALMA Large Programme on Multi-Ringed Disks (Andrews, Perez, Dullemond & Isella, ALMA proposal ID 2016.1.00484.L), which was ranked A, and for which we expect a large flood of data starting around the summer of 2017.

In this task we expect a strong collaboration with project D2 that also contains a part where simulations of single embedded objects in 2D disks will be studied. The focus in D2 will be on

Brown Dwarf or M star companions, possibly on strongly eccentric orbits. However, technically there are several similarities, making a strong collaboration beneficial for both projects.

Task 2 *Dust evolution in 2D dimensional disk simulations with embedded protoplanets*

As outlined in the preliminary work, the motion of dust particles in disks is strongly influenced by the presence of embedded planets in the disk. A planet creates a gap in the disk where the density and hence pressure is lowered with respect to the ambient disk. At the gap edges there are maxima in the pressure distribution of the disk created. The altered radial pressure gradient has an impact on the motion of the dust particles in the disk as they feel the changing pressure gradient. At the outer gap edge the pressure gradient is positive which leads to an super-Keplerian azimuthal flow velocity while beyond the pressure maximum the gradient is negative again. On the other hand unperturbed dust particles do not feel the pressure gradient but move with speeds equal to the Keplerian orbital angular velocity. This difference in velocities of the gas and the dust particles leads to drag forces between them and to a collection of dust particles near the outer edge (pressure maximum) of the gap. This effect is illustrated for two embedded planets in Fig. 2 for the disk around HL Tau. The inner edge of a transition disk is in structure very similar to the outer edge of a planetary gap in fact identical if the gap is created by a few planets. Hence, dust particles will be filtered there according to their sizes (see Fig. 2).

In this second task of the project the motion of embedded dust particles will be followed simultaneously with the hydrodynamical evolution of the disk. This has not been done yet in the context of transitional disks. A postprocessing version of this was done by Ataiee et al. (2013) in their analyses of dust in vortices, but that was for a single dust grain size only and not done simultaneously with the hydrodynamics. Also, it did not study particles small enough to be dragged inward through the gap. Individual Langragian particles of different size will be added to the hydrodynamics of the disk, and they will move under the influence of the gravitating objects (star and planets) and experience the gas drag. The equations of motion for a dust particle due to these forces are then given by

$$\frac{d\vec{x}_p}{dt} = \vec{u}_p \qquad \text{and} \qquad \frac{d\vec{u}_p}{dt} = \vec{f} - \frac{\vec{u} - \vec{u}_p}{t_s}\,, \tag{2}$$

where $\vec{f}$ contains the external forces acting on the particle (gravitational attraction due to the star and the planets), $\vec{u}$ denotes the velocity of the gas and $\vec{u}_p$ of a dust particle, and t_s is the so called stopping time. Our focus will be on particles in the Epstein-regime for which the mean free path of the gas molecules is typically greater than the particle cross section and t_s is given by (Epstein 1924)

$$t_s = \frac{1}{\sqrt{8/\pi}}\,\frac{r_p \rho_p}{\rho_g c_s}\,. \tag{3}$$

Here, r_p is particle radius, ρ_p the particle bulk density, ρ_g the gas density, and c_s is the sound speed. In case other drag forces (Stokes-regime) become necessary it is relatively straight forward to implement those, for example using the methods suggested in Haghighipour & Boss (2003). As expected, the drag force depends on the particle and gas properties and to estimate its importance it is convenient to define the dimensionless stopping time by

$$\tau_s = t_s \Omega_K \tag{4}$$

where Ω_K is the Keplerian angular frequency. From eq. (2) it is clear that particles with small dimensionless stopping times will be well coupled to the gas such that $\vec{u}_p \approx \vec{u}$. On the other hand, for very large τ_s (for example bigger particles with larger r_p) they will be decoupled and do not feel the gas. Hence, the most important parameters are those for which $\tau_s \approx 1$. We have implemented the time integration of eqs. (2) into the 2D FARGO-code (Picogna & Kley 2015) and into the 3D-PLUTO code (Stoll & Kley 2016) using the semi-implicit method of Bai & Stone (2010) with eq. (2) written in cylindrical coordinates. We plan to implement the particle solver also into our GPU-PLUTO code. After having performed the necessary test calculations to verify the accuracy of the integrator detailed parameter studies will be performed in order to calculate the efficiency of dust filtering at the inner edge of the disk. This will allow us to determine the dust depletion factor in the inner hole as a function of the planet masses, dust and disk properties. In the first stage of the project we will assume that the local (surface) density of the dust is still much lower than the gas density and neglect the dynamical back-reaction of the dust onto the gas. In case the dust becomes highly concentrated this assumption will break down and we then plan to include the back-reaction of the dust onto the gas.

In this part of project we aim at following the dust kinetics and dust trapping in TDs. For sufficiently low viscosity disks we expect that non-axisymmetric features (vortices) may form within the disk such that dust may accumulate there (Ataiee et al. 2013). This fits well into the topic of non-axisymmetric TDs to be studied in project D2, as some of them display lopsided dust emission believed to be due to a huge dust-trapping vortex. Hence, the study of non-axisymmetric features in disks will be studied in close collaboration between the postdocs of project D2 and D1.

Task 3 *Full three dimensional disk simulations with embedded protoplanets*
In this part of the project we will extend the previous 2D simulations to full 3D. From our own first experience in performing simulations for transitional disks (Müller & Kley 2013) in only 2D we know that many dynamical timescales of the disk will have to be calculated. Hence, we expect full 3D simulation to extremely costly concerning CPU-resources. Hence, we plan to use new, recently developed codes that run very efficiently on GPU-processors. In particular, for these type of simulations we plan to utilize our newly developed 3D GPU-PLUTO code (Thun et al. 2016) to speed up the simulations. Of course, comparison test simulation using the standard MPI-version of PLUTO or the new FARGO3D code for GPUs, as described in Benítez-Llambay & Masset (2016) will be performed. For more details on such codes see Sect. 2.3.1.

Despite the possible improvements in computational speed full 3D simulations will be very demanding in computational resources. To alleviate this problem at least partly we plan to run dedicated models for selected parameter sets that we expect from the 2D simulations of the previous tasks to be the most promising. In a first step we plan to compare a few selected examples for isothermal setups and calculate the differences between 2D and 3D results. From recent studies of a pair of giant embedded planets that capture each other in mean motion resonance there should not be such a large difference between isothermal 2D and 3D results (André & Papaloizou 2016) if both planets are located in the midplane of the disk. We will check this for a few selected cases using the coplanar setup. Then we plan to extend this study to non-coplanar planetary orbits and and investigate the influence of small inclinations between the planets and the disk. For this part of the project we again plan intensive collaboration with project D2, because there 3D simulations with high inclinations will be studied.

After successful isothermal simulations we will include radiative transfer and viscous heating in full 3D. Here, we plan rely initially on our implementation of radiative transfer and stellar irradiation for the PLUTO code (Kolb et al. 2013). Here, the radiative transport is using the flux-limited diffusion approximation while stellar irradiation is modeled directly using a ray-tracing method. As indicated already in Müller & Kley (2013) we expect significant differences between the isothermal and fully radiative cases, as indicated in Fig. 1 for the 2D case and with single embedded planet.

Obviously in Tasks 2 and 3 we will also, like in Task 1, compare our results with observed objects – see Task 1 for the procedure.

2.3.3 Time frame

The project is devided into 3 Tasks with increasing complexity. To become familiar with the whole topis the first task starts initially with isothermal disks that are extended to the radiative case including irradiation. In this task the irradiation and radiative transfer within the disk need to be added to the GPU-PLUTO-code while simulations using the FARGO-code could be started basically from the beginning. In the second Task dust particles will need to be added to the GPU-PLUTO-code, while our availlable FARGO has particle motion already implemted its performance and accuracy need to be checked. The third Task is the most advanced as the radiative transport would have to be included into our GPU-PLUTO code but simulations with FARGO-3D can be started more or less directly after the applicability of the implemented radiation module for our purposed has been thoroughly tested.

Knowing about the difficulties that may occur with multidimensional hydrodynamical simulations we estimate for each Task a minimum of one year. Hence, the proposed work will definitely fill the 3 year funding period and part of the work, particularly from Task 3 might even have to be taken over into the next funding period.

2.4 Data handling

The model data we produce will be made immediately available online, once the corresponding paper is accepted.

2.5 Other information

Not relevant.

2.6 Information on scientific and financial involvement of international cooperation partners

Not relevant.

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4. Requested modules/funds

4.1 Basic Module

4.1.1 Funding for Staff

Given by the complexity of the project we request 1 Postdoc E13 position for three years, to be based at the Institute of Astronomy and Astrophysics at the University of Tübingen.

4.1.2 Direct Project Costs

4.1.2.1 Equipment up to EUR 10,000, Software and Consumables

Theoretical numerical research on multi-dimensional hydrodynamics can only be done when sufficient and appropriate computational facilities are available. While production runs will be done on supercomputer facilities, a substantial part of the work in this project requires testing and code-development. Testing performance and accuracy of these codes on realistic problems requires a high end workstation including a high end graphics card suitable for GPU computing. Here we apply for a NVIDIA TESLA K40 card together with the workstation. This is beyond the standard base equipment (*Grundausstattung*). We therefore request one workstation-GPU desktop computer for 6000 Euro.

4.1.2.2 Travel Expenses

Participation at at least one conference per year, or similar is anticipated for the postdoc. In addition to travel funds for conferences for the PIs, regular mutual working visits at Heidelberg/Tübingen/München are planned.

Travel within the Research Unit is handled in project Z. In addition we request funding for conference travel for the personnel and one Applicant. This includes one national (1.000 €) and one international (1.500 €) conference trip per year, totalling 2.500 € per person per year.

For this project this totals 5.000 € per year for the Postdoc and one Applicant, which is in total 15.000 €.

4.1.2.3 Visiting Researchers (excluding Mercator Fellows)

	Visit 1	Visit 2	Sum
Dr. Zsolt Regaly (Konkoly Observatory, Hungary)	1000	1000	2000
Prof. Andrea Mignone (University Torino, Italy)	1000	1000	2000
	2000	2000	**4000**

4.1.2.4 Other Costs

Not applicable.

4.1.2.5 Project-related publication expenses

We request 750 €/year (total 2250 €) for publication expenses.

5. Project requirements

5.1 Employment status information

Kley, Wilhelm: Prof. Dr., full Professor with tenure at the University of Tübingen, Institute for Astronomy & Astrophysics

Dullemond, Cornelis P.: Prof. Dr., full Professor with tenure at the University of Heidelberg, Institute for Theoretical Astrophysics

5.2 First-time proposal data

5.3 Composition of the project group

The project is a joint activity of the Computational Astrophysics group (CPT) at the Institute of Astronomy and Astrophysics of the University of Tübingen (IAAT), and the Institute for Theoretical Astrophysics (ITA) which is part of the Zentrum für Astronomie (ZAH) at the University of Heidelberg. The PIs Kley and Dullemond were both members of the past DFG research group *The Formation of Planets: The Critical First Growth Phase* (FOR 759) and plan to join their expertise and collaborate within this project. Within their groups at the IAAT and ITA the following scientists work presently in a research field related to this project:

- Kley, Wilhelm, Prof. Dr. — *Professor, IAAT (CPT)*
- Dullemond, Cornelis P., Prof. Dr. — *Professor, ITA (ZAH)*
- Kuiper, Rolf, Dr. — *Emmy Noether Group Leader, IAAT (CPT, DFG)*
- Schäfer, Christoph, Dr. — *Research Assistant, IAAT (CPT)*
- Thun, Daniel, Dipl.Phys. — *PhD student, IAAT (CPT, DFG)*

Emmy Noether Group Leader Rolf Kuiper has recently extended his activities into the field of planet formation and is an an expert in computational astrophysics. Research assistant Christoph Schäfer has ample experience in the field of planet formation and with GPU-computing. They both can give helpful advice to the Postdoc. The PhD student Daniel Thun has developed the GPU version of the *PLUTO*-code and can give helpful advice on related questions.

5.4 Cooperation with other researchers

5.4.1 Planned cooperation on this project

5.4.1.1 Collaborating researchers for this project within the Research Unit

A strong collaboration within this Forschergruppe will be carried out with the postdoc of project D2. Projects D1 and D2 have several methods in common, in particular both employing 2-D and 3-D (radiation-)hydrodynamics of protoplanetary disks. On the technical side both postdocs are envisioned to collaborate closely. The first two sub-projects of D2 are also topically somewhat overlapping with project D1: focusing on planet-disk interaction as an explanation for Type 2 TDs. The differences are: in D2 we focus on single massive companions, presumably low mass stars rather than planets, while project D1 focuses more on multiple planet-mass companions. Secondly, D2 focuses on finding the origin of strong deviations from circular symmetry, in part by making the companion's orbit strongly eccentric. Finally, D2 aims at explaining the extremely tilted inner disks of several Type 2 TDs, which is not a goal of D1.

A strong collaboration with project C1 (PI Birnstiel & Dullemond) is planned on two levels: first of all recipes for dust distributions may be obtained from C1 which may be included in our models. Secondly the models developed here will provide inputs for C1, aiming to explore pressure bumps of diverse nature

For comparison to observations, we will collaborate strongly with the groups of Th. Henning (MPIA), E. van Dishoeck (MPE/Leiden), who have expertise and data of/from SPHERE and ALMA. Also collaboration with the A1 (PI Testi) project is envisioned for the same reason. The postdoc of B2 (PI Caselli & Ercolano) will be working a lot with 3-D diagnostic radiative transfer modeling, so a collaboration on the technical side can be helpful here as well.

Finally, some of the models developed here will be used by project B1 (PI Ercolano) to investigate the effects of planet-induced gaps on the disk dispersal model, and by project C2 (PI Ercolano) to test wether the dust entrainment in the wind of photoevaporating disks with planets is also affected.

5.4.1.2 Collaborating researchers for this project outside of the Research Unit

The following external researchers will be involved to some degree in the work on this project:

- Benítez-Llambay, Pablo — *Niels Bohr Institute Copenhagen (DK)*
- Bitsch, Bertram — *Lund University (S)*
- Mignone, Andrea — *Torino University (I)*
- Regaly, Zsolt — *Konkoly Observatory, Budapest (HU)*

Pablo Benítez-Llambay (currently at Copenhagen, DK) is the co-developer of the FARGO-3D code and we plan to collaborate with him on numerical and physical aspects using this code. Former PhD student Bertram Bitsch is now a postdoctoral researcher in Lund (Sweden). His expertise in planet-disk simulations and torque-formulae for migration will be helpful for the project. We have already collaborated with Andrea Mignone when adding a new radiation module to the PLUTO-code. Andrea Mignone (Torino, I) is the developer of the PLUTO code. His expertise will be useful in further extending our 3D GPU-PLUTO code. With Zsolt Regaly from Budapest both PIs have long standing successful collaborations in the proposed research field in all relevant aspects: planet formation, celestial mechanics and computational astrophysics. We plan to continue the collaboration with them in this project. In addition collaboration with the groups of M. Benisty (Grenoble/Santiago) and C. Dominik (Amsterdam) is envisioned for the comparison to observational data with ALMA and SPHERE.

5.4.2 Researchers with whom you have collaborated scientifically within the past three years

The PIs have worked with the following scientists in research fields related to planet formation. Only more senior scientist and postdocs are listed, no PhD students.

Baruteau, C. (University of Toulouse, F); Bitsch, Bertram (Lund Observatory, S); Blum, Jürgen; Schräpler, Rainer (both Universität Braunschweig); Dullemond, Cornelis, P. (Universität Heidelberg); Haghighipour, Nader (Institute for Astronomy, University of Hawaii, USA); Masset, Frederic (University of Mexico); Meru, Farzana; Papaloizou, J.C.P. (both University of Cambridge, GB); Mignone, Andrea (University of Torino, I); Nelson, Richard and Paardekooper, S.J. (University of London, Queen Mary, GB); Regaly, Zsolt (University of Budapest, H); Rein, Hanno (University of Toronto, Canada); Vorobyov, Eduard (University of Vienna, A);

S. Andrews (CfA, Harvard), E. van Dishoeck (MPE Garching, Uni Leiden), C. Dominik (UvA, Amsterdam), A. Natta (DIAS, Dublin), L. Testi (ESO, Garching), J. Carpenter (Caltech, Pasadena), C. Chandler (NRAO, Socorro), A. Isella (Rice Uni, Houston), L. Ricci (Caltech, Pasadena), N. Calvet (Uni Michigan), S. Corder (ALMA), J. Greaves (Uni St. Andrews), N. Turner (JPL, Pasadena), A. Uribe (Coll. Charlston), Z. Regaly (Konkoly Obs, Budapest), A. Juhasz (Cambridge), R. Klessen (Uni-Heidelberg), R. Kuiper (Uni Tübingen), C. Brinch (University of Copenhagen), M. Benisty (Uni Grenoble), P. Pinilla (Tucson), C. Mordasini (Uni Bern), G. Guidi (ESO), M. Tazzari (ESO), L. Perez (MPIfR, Bonn), H. Linz (MPIA), A. Sargent (Caltech, Pasadena), L. Mundy (University of Maryland), S. Storm (University of Maryland), J. Lazio (JPL, Caltech), W. Kwon(Korea Astronomy and Space Science Institute), T. Muto (Kogakuin University), M. Momose(Ibaraki University), T. Tsukagoshi (Ibaraki University), L. Klarmann (Uni Amsterdam), H. Klahr (MPIA, Heidelberg), S. Ataiee (Uni Bern), M. Fukagawa (NAOJ Japan), H. Shibai (Osaka University), T. Hanawa (Chiba University), K. Murakawa (Osaka Sangyo University), J. Ramsey (Uni Kopenhagen), J. Drazkowska (Uni Zürich)

5.5 Scientific equipment

The project requires, at least for the full hydrodynamical simulations, a considerable amount of CPU-time. For this we rely on own as well as outside resources. For testing purpose computing time will be available on local PC clusters (institute and university clusters). Here we have dedicated GPU-systems available as well as smaller clusters.

We have special access to computing resources supplied within the State of Baden-Württemberg (Baden-Württemberg High Performance Computing - Coordinated Compute Cluster Competence

Centers: bwHPC-c5). A part of this initiative is the new BinAC-system[2] that has just gone online at the University of Tübingen and is dedicated to Astrophysics and Computer Science only. BinAC offers over 236 CPU nodes with dual Intel Xeon E5-2630v4 each. Moreover (and especially suited for our GPU-*PLUTO*-code) the cluster also offers 60 GPU nodes with dual Nvidia Tesla K80 (with two GK210 GPU chips each). Additional resources are available with bwHPC-c5 at the ForHLR-cluster at the Steinbuch Centre for Computing (SCC) in Karlsruhe. If further resources will be required we will apply for additional computer time at the high performance computing center HLRS, located in Stuttgart, and at other centers in Germany.

[2]see `http://www.bwhpc-c5.de/wiki/index.php/Category:BwForCluster_BinAC` for a detailed description of the hardware.

Project D2:

Origin of complex non-axisymmetric structures in Type 2 Transition Disks

Authors:

Applicants:	C.P. Dullemond (ZAH, Heidelberg), W. Kley (U. Tübingen)
Co-Applicants:	E. van Dishoeck (MPE), T. Henning (MPIA), L. Testi (ESO)
Cooperation Partners:	R. Klessen (ZAH), M. Fukagawa (NAOJ), M. Benisty (Grenoble)

Requested positions: 1 Postdoc

Abstract:
Transition disks have recently been shown to display spectacular structures such as large scale spirals, blobs, tilts etc. These features indicate that highly dynamic processes are going on in these disks, allowing us to test our understanding of the physics of protoplanetary disks. This project aims to understand these structures in terms of dynamic models of disks.

1. State of the art and preliminary work

With the spectacular new capabilities of observatories in the millimeter wavelength range (ALMA) and at optical wavelengths (Subaru and VLT coronographic imagers, most recently: VLT-SPHERE), protoplanetary disks are found to be much more complex than previously thought. Until only a few years ago observations of protoplanetary disks were consistent with the idea of them being mostly axi-symmetric rotating structures around young stars.

Recent observations have now shown this picture to be false, in particular for transition disks. Many such disks, while remarkable in their own right due to their large inner holes (see project **D1**), are even more remarkable due to their often-present strong deviations from axisymmetry. At millimeter wavelengths, spatially resolved with ALMA, all transition disks show a strong dust emission ring just beyond the inner hole. Several of them, in particular the sources HD 142527 and Oph IRS 48, show this ring to be strongly lopsided: one side being clearly much brighter than the other side (Casassus et al. 2013; van der Marel et al. 2013). These appear to be vortices created by the Rossby wave instability (Regály et al. 2012). This raises the exciting possibility that these are *dust-trapping vortices*, predicted to play an important role in planet formation (Barge & Sommeria 1995; Klahr & Henning 1997).

At optical and near infrared wavelengths many of these sources show another remarkable and unexpected feature: grand design spiral waves (e.g. the sources HD 135344b, MWC 758, HD 100453). While $m = 1$ spiral waves were expected as a result of newborn planets embedded in these disks, the spirals observed in many Type 2 transition disks are symmetric $m = 2$ modes, making them look like the galaxy M51. The origin of these spirals is still hotly debated and planetary/stellar companions (Dong et al. 2016) and gravitational instabilities (Tomida et al. 2016) are often suggested to be at their origin, as is residual infall into the disk (Lesur et al. 2015). Recently an even more unorthodox and intriguing scenario was proposed: The bright ring of scattered light (the illuminated inner rim of the outer disk as seen with the Subaru and VLT telescopes) of HD 142527 has two conspicuous dark spots on almost opposite sides. Marino et al. (2015) were able to show with 3-D radiative transfer modeling that these dark spots are most likely the shadows cast by an inclined small inner disk. If this scenario is confirmed, HD 142527 (and possibly HD 100453 and other transition disks) is an "inclined disk inside a disk" (a warped disk). According to Montesinos et al. (2016) these two shadows on opposite sides of the bright rim may even be the origin of the $m = 2$ spiral waves, caused by the brief loss of pressure in these shadows. This is an intriguing possibility, as it would indicate that Type 2 transition disks may be related to warped disks, and perhaps be the origin of the misalignment effects seen in many exoplanetary systems with the Rossiter-Mclaughlin effect.

But how can the inner disk have a different rotation axis as the outer one? Is this a result of an inclined planet or brown dwarf orbiting inside the gap? For HD142527 a companion star is known to exist, but it is at the current epoch still rather close to the main star compared to the size of the cavity, so it is not directly clear that this companion is responsible for the large cavity. Or is this due to late accretion of different angular momentum molecular cloud material? Thies et al. (2011) suggest this scenario to explain misaligned exoplanetary systems. It might also explain misaligned outer disks. Or could the Kozai-mechanism caused by a companion at large radii cause this?

These enigmatic non-axisymmetries in Type 2 TDs offer a unique opportunity to test our understanding of the physical processes occurring in these disks. The features appear to be highly organized, not random. This suggests that a strong and well-defined physical mechanism is at work. If we identify this mechanism (or these mechanisms), we do not only solve the mystery of these non-axisymmetric features, but also get a better understanding of the dominant physical processes at work in these disks. It is hoped that this may allow us to get a better understanding of the process of planet formation. For instance, several attempts have been made to explain the spiral structures by embedded planets (Muto et al. 2012; Benisty et al. 2015; Pohl et al. 2015), though it turns out that planetary spiral features are usually single-armed ($m = 1$) instead of the double-armed ($m = 2$) spirals often seen. Also the giant central cavity of Type 2 TDs were investigated in the context of gap-opening planets, though it turns out that this is not easy and requires at least multiple planets to work (Zhu et al. 2011). The bright dust rings with often lopsided geometry seen in Type 2 TDs strongly suggest dust trapping at work. These rings are consistent with the radial dust trapping suggested by Whipple (1972), and the lopsidedness appears to be a result of dust trapping in a huge vortex (Barge & Sommeria 1995; Klahr & Henning 1997; Birnstiel et al. 2013; Ataiee et al. 2013; Zhu & Stone 2014; Baruteau & Zhu 2016). What is the origin of these dust traps remains unsolved. Regály et al. (2012) suggest that this is a result of a change in viscosity in the disk at the outer edge of the “dead zone”. They find not only a strong ring-shaped pressure bump forming (which can trap dust), but they see this ring also periodically becoming lopsided by forming a giant anti-cyclonic vortex. The formation of such vortices was first reported by Lovelace et al. (1999), and it seems that with Type 2 TDs we now see evidence for their existence. Given that dust tends to get trapped in these vortices, an exciting question is whether these vortices are the birthplaces of new planets.

The goal of this proposal is to understand the origin of the non-axisymmetric features in Type 2 TDs from the perspective of gas dynamics. Particular emphasis will be put on “non-standard” dynamics such as out-of-plane companions and secondary infall. Ultimately we wish to find out if Type 2 TDs are rare outliers or not, and if they teach us something about the formation of planets or are too exotic to do so.

1.1 Preliminary work

As a preparation for this project we have conducted several small preliminary investigations in the context of Bachelor projects. We are also involved in several collaborations involving VLT-SPHERE scattered light images of Type 2 TDs as well as ALMA observations.

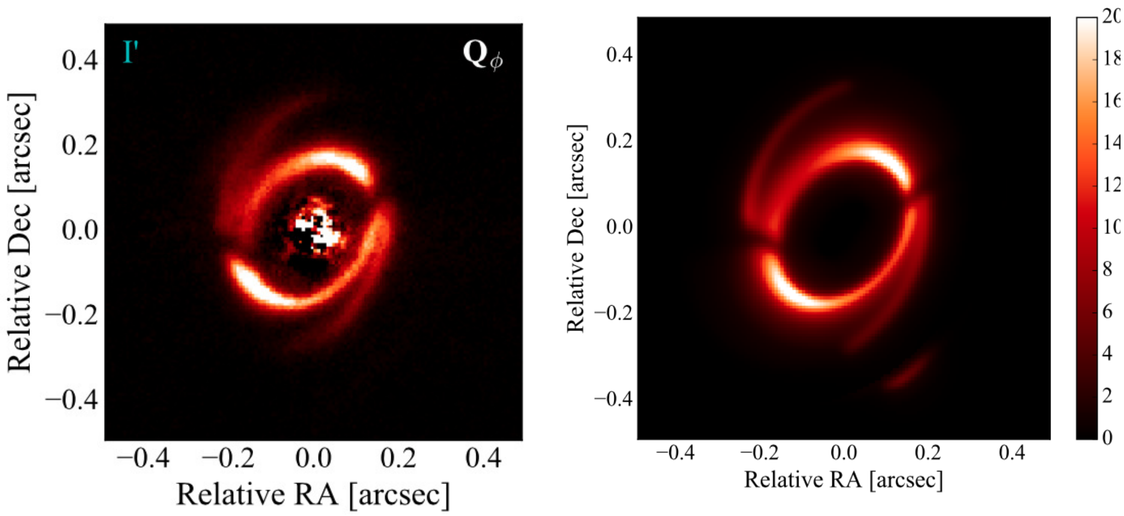

Figure 1: Polarized scattered light observations of the Type 2 TD HD100453. **Left:** Actual observations with VLT-SPHERE in the I' band. **Right:** Synthetic model image made with the MCMax Monte Carlo code. From: Benisty et al. (2016).

1.1.1 VLT-SPHERE observations of Type 2 TDs

Th. Henning, one of the collaborators on this project, is involved in VLT-SPHERE scattered light image observations of Type 2 TDs. A particularly spectacular example, where the PI was also involved in, is the very recent image of the Type 2 TD HD 100453 (Benisty et al. 2016). This is a Transition Disk with an inner disk spanning out to 1 AU, and an outer disk spanning between 20 AU and 45 AU. It features a prominent $m = 2$ spiral pattern originating from a bright ring that features two bright arcs (presumably due to the scattering phase function) and two dark spots (presumably due to the shadowing caused by an inclined inner disk, as in HD 142527 (Marino et al. 2015)). The observed polarized intensity and the synthetic model image are shown in Fig. 1. The synthetic image was made with the MCMax radiative transfer code, and the setup involved in tilted inner disk that produced the shadow features on the ring, and parameterized spiral features.

1.1.2 ALMA observations of Type 2 TDs

Dr. Akimasa Kataoka has been a postdoc at the ITA since April 2015 on his own JSPS-Fellowship grant. During this period he successfully applied for substantial ALMA time to observe the Type 2 TD source HD 142527 using the newly available polarization mode. The observations we obtained have turned out to be quite spectacular (Fig. 2). The strongly lopsided arc-shaped dust emission was already well known since (Casassus et al. 2013). But the shape of the polarized light image contains a huge amount of additional information. Please note that it is not the purpose of this project to investigate how to use this new technique of polarized thermal emission at millimeter wavelengths. This is the topic of another – completely separate – DFG proposal that was submitted in the summer of 2016 (DFG DU 414/17-1). Here we merely show the kind of objects we study and the type of observations we are involved in, which will (in addition to published data from other groups) serve as observational evidence for the complex disk geometries seen in Type 2 TDs.

The PI has also been involved in an ALMA observational study of the source IRS 48 from the team of Ewine van Dishoeck, where an even stronger lopsided dust emission was found (van der Marel et al. 2013).

The PI and collaborators on this project are continuing involvement (and leading) of such observa-

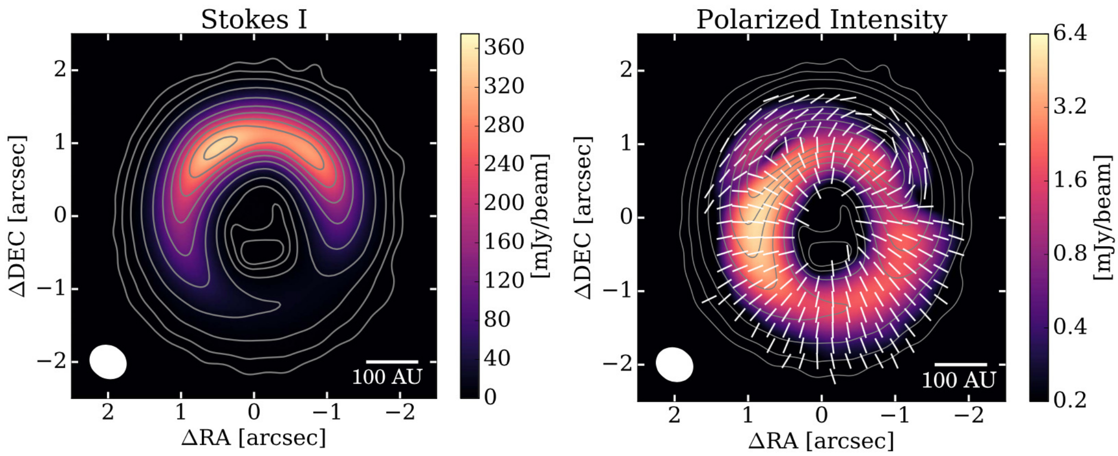

Figure 2: ALMA Observations of the Type 2 TD HD 142527. **Left:** The continuum (Stokes I component) at 850 μm showing the well known arc-shaped structure believed to be dust trapped in a Rossby-vortex. **Right:** The polarized intensity with the polarized direction overlayed. From: Kataoka et al. (2016).

tional campaigns.

1.1.3 Preliminary models of out-of-plane companion-disk interaction

Out-of-plane planet disk interaction models have been made by Bitsch & Kley (2011) and Bitsch et al. (2013) using a fully 3-D radiation hydrodynamics grid-based code. The focus here was on intermediate mass planets inducing moderate disk warps, and the aim was to understand inclination damping and migration. Other work include Xiang-Gruess & Papaloizou (2013) who employ a Smooth Particle Hydrodynamics code to study the effect of such an inclined companion on the disk structure, and back on the planet. Also here the planet mass was intermediate and the induced warps were moderate.

For the present purpose we need to go to more extreme cases: higher inclinations, higher planet masses, and focusing on the change of the appearance of the disk shape to be able to compare this with observed Type 2 TDs.

As a preliminary test case for such modelling, we performed a set of simple models using the Smooth Particle Hydrodynamics code Gadget-2. We set up an initially smooth planar disk, but add a low mass companion on an inclined circular orbit. The orbit crosses the disk twice each orbital period. The results of one such model is shown in Fig. 3. As time passes by, this process opens up a strong gap in the disk. The gravitational torque of the planet on the inner and outer disk, however, cause both to precess. The inner disk precesses faster than the outer disk. As a result, the inner and outer disks become tilted with respect to each other (they are no longer co-planar). The "warp" can be seen in all three panels of Fig. 3, but the tilt between inner and outer disk is only seen in the middle panel, which is a snapshot at 50000 years. This model was initially set up by Dr. Daniel Harsono and further developed and applied by Matthew Herbst during his Bachelor thesis project. These results show that for a brief period the inclined companion can lead to tilted inner/outer disks, but eventually the outer disk aligns with the plane of the planetary orbit, and the inner disk disappears by viscous accretion. This viscous accretion appears to be strongly boosted by excessive numerical viscosity due to too few SPH particles. This excessive viscous accretion also appears to be the cause of the very bright outer disk ring. This is presumably not realistic, so this simulation can merely serve as a proof-of-concept. Much higher resolution models have to be made, with more careful testing of the viscosity of the model.

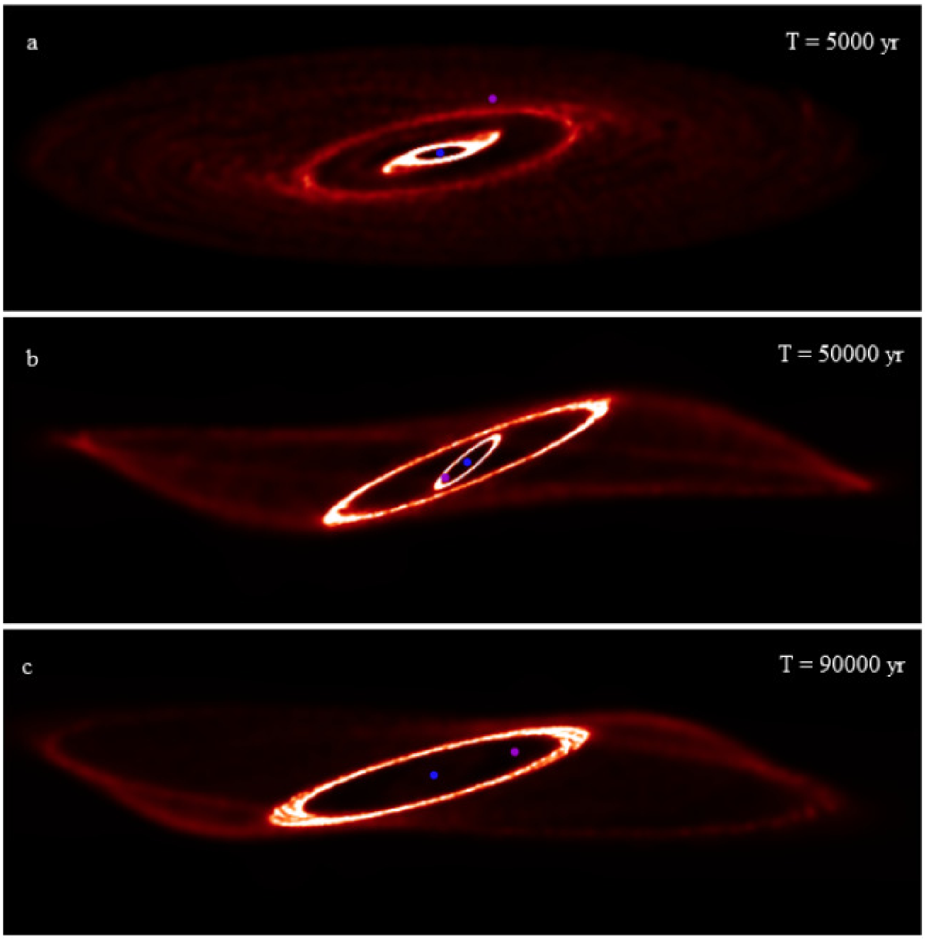

Figure 3: Time snapshots of the shape of a circumstellar disk disrupted by an inclined planetary companion passing through the disk twice each orbit. The star is blue, the planet is purple. The gas SPH particles are shown in shades of red (low column density) and yellow (high column density). The star has a solar mass. The planet orbital inclination is 33 degrees, the semi-major axis 40 AU, the mass 0.01 $M_{\odot}$. The disk is initially 200 AU in radius and has a mass of 0.01 $M_{\odot}$. The surface density is shown as a projection with respect to a camera. The angle of the camera is not the same in each snapshot, but chosen such that the warp in the disk is better seen. From: Bachelor Thesis by Matthew Herbst, Heidelberg University, 2016.

1.1.4 Preliminary models of secondary disk formation

As a proof of concept for the secondary accretion of material from a low mass molecular cloudlet we performed a simple set of grid-based numerical hydrodynamic models. The model setup is a rectangular grid of $256 \times 256 \times 64$ cells covering $10 \times 10 \times 2.5$ kAU (one kAU = 1000 AU). The initial cloud setup is a simple Gaussian shaped spherical cloud:

$$\rho(\mathbf{r}) = \rho_0 + (\rho_1 - \rho_0)\exp\left(-\frac{|\mathbf{r}-\mathbf{r}_{\rm cl}|^2}{2D_{\rm cl}^2}\right) \tag{1}$$

where ρ_0 is the background density, ρ_1 is the initial peak density at the cloud center, $\mathbf{r}_{\rm cl}$ is the initial location of the cloud and $D_{\rm cl}$ is the cloud initial size. The temperature is kept constant at all times and locations, such that the sound speed is 1 km/s. The gas velocity at all locations in the grid is initially the same everywhere, but will of course change due to the gravitational pull of the star and the hydrodynamics of the gas. The star is kept at a fixed location $\mathbf{r}_*$ at the center of the box, and the cloud motion has a non-zero impact parameter b with respect to the star. The gravitational potential of that star was smoothed, but only very mildly so:

$$\Phi(\mathbf{r}) = -\frac{GM_*}{(|\mathbf{r}-\mathbf{r}_*|^8 + r_{\rm smooth}^8)^{1/8}} \tag{2}$$

The 8th power was chosen to minimize the effect of smoothing on the solution, essentially limiting the smoothing only to the few cells around the star. We used a 3-D Riemann-solver hydrodynamics code (developed by the PI many years ago for the purpose of a lecture on numerical hydrodynamics, but not public). The main parameters of the model are the size of the cloud $D_{\rm cl}$, the initial position of the cloud $\mathbf{r}_{\rm cl}$, the Mach number of the velocity $\mathcal{M}$ and the impact parameter b. Using this setup and code, a series of models were made in the context of the Bachelor thesis of Manuel Kramer during the summer of 2016. One such model is shown in Fig. 4. This result shows that such a secondary cloud accretion tends to produce disks with strong one-armed spiral structure at large scales. Which shape is seen depends not only on the parameters, but also on the timing of the snapshot. The geometries can vary a lot. The ones seen in Fig. 4 are reminiscent of some geometries seen at large scales around several Type 2 TDs. We also made synthetic scattered light images that can be directly compared to data. An example is shown in Fig. 5. This image bears resemblance to the arc-shaped envelope around the disk of the Transition Disk star AB Aurigae as imaged by Grady et al. (1999).

1.2 Project-related publications

Birnstiel, T., **Dullemond, C.P.** & Brauer, F., *Gas and dust evolution in protoplanetary disks*, 2010, A&A 513, 79. In this paper we present the basic code for the evolution of the disk and the dust. The disk evolution is followed using the time-dependent viscous disk equations, the dust part follows the dust coagulation, fragmentation, settling and radial drift of the dust.

Ataiee, S., **Dullemond, C.P.**, **Kley, W.**, Regaly, Z., & Meheut, H. *Planet-vortex interaction: How a vortex can shepherd a planetary embryo*, 2014, A&A, 572, A61. This paper is an example of our work on how a planet is interacting with a non-axisymmetric transition disk featuring a huge vortex.

Ataiee, S., Pinilla, P., Zsom, A., **Dullemond, C.P.**, Dominik, C., & Ghanbari, J., *Asymmetric transition disks: Vorticity or eccentricity?*, 2013, A&A, 553, L3. This paper shows our work on how a massive planet can make the disk asymmetric (lopsided) in two independent ways: by making the disk eccentric or by creating a vortex. We show how to distinguish observationally between these two scenarios. It is an example of how we make a link between modeling and observations.

Müller, T.W.A., & **Kley, W.**, *Modelling accretion in transitional disks*, 2013, A&A, 560, 40. This paper shows our experience with modeling the dynamics of transition disks. In this paper the gas flow through the planet-induced gap is studied, which is very relevant for the type 2 TDs which usually still have substantial accretion onto the star and have inner disks.

D. Thun, R. Kuiper, F. Schmidt, **W. Kley**, *Dynamical friction for supersonic motion in a homogeneous gaseous medium*, 2016, A&A, 589, A10. Since we will be dealing with extremely inclined companions interacting with the disk in part of this project, the experience gained in this paper will be used.

Bitsch, B., & **Kley, W.**, *Evolution of inclined planets in three-dimensional radiative discs*, 2011, A&A, 530, 41. This paper shows our experience with modeling out-of-plane 3-D planet-disk interaction. This paper focused mostly on how the disk damps the inclination of the planet, and focused on small inclinations and masses lower than about half a Jupiter mass. In this proposal we will shift our attention to more extreme cases, as suggested by the large observed disk tilts of up to 70 degrees, and focus on how the disk shape is changed as a result.

Kley, W., & Dirksen, G., *Disk eccentricity and embedded planets*, 2006, A&A, 447, 369. This was the original paper demonstrating how a massive planetary companion can make a disk eccentric.

N. van der Marel, E.F. van Dishoeck, S. Bruderer, T. Birnstiel, P. Pinilla, **C.P. Dullemond**, T.A. van Kempen, M. Schmalzl, J.M. Brown,

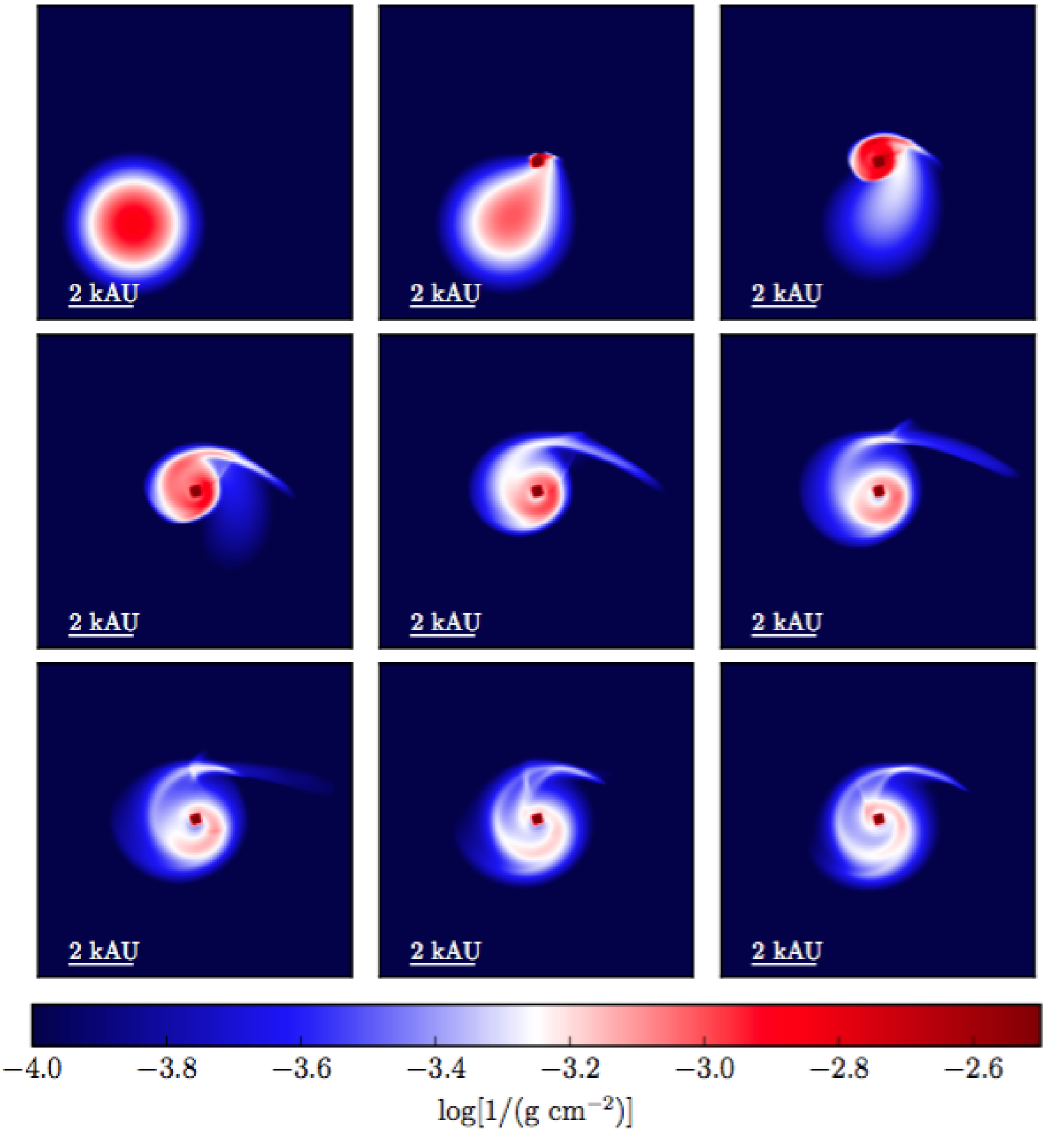

Figure 4: Time sequence of off-center accretion of a small low-mass spherical Gaussian molecular cloud by a star. The star is at the center, the cloud moves initially from left to right. The star is kept fixed, i.e. the cloud mass is small compared to the star mass. Time snapshots (**from left to right, top to bottom**) are with 4.8×10^3 years intervals. The color bar is surface density in $\mathrm{g\,cm^{-2}}$. The star mass is 1.4 $M_\odot$, the Mach number of the cloud velocity with respect to the star. From: Bachelor Thesis by Manuel Kramer, Heidelberg University, 2016.

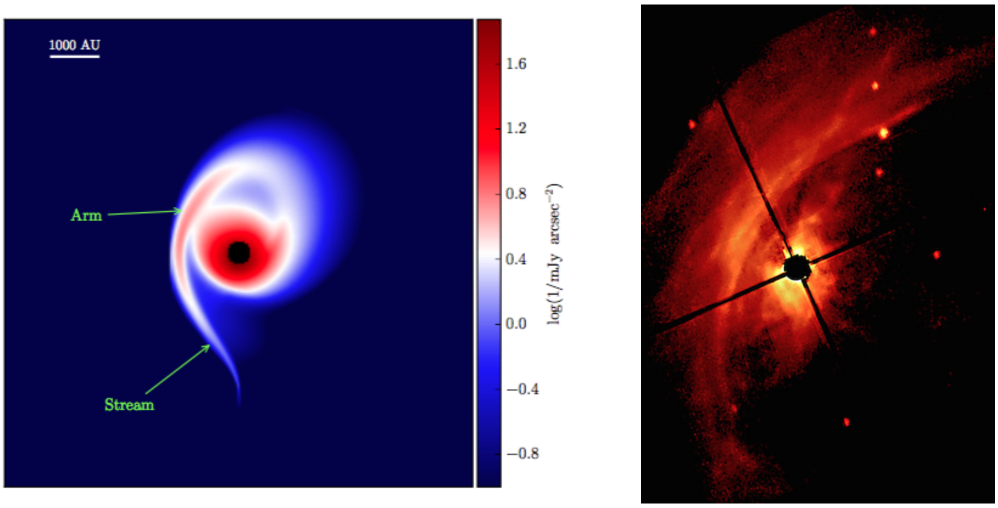

Figure 5: **Left:** Scattered light synthetic image computed for a snapshot of the simulations of an off-center accretion of a small low-mass spherical Gaussian molecular cloud by a star. The color bas unit is mJy/arcsec^2. From: Bachelor Thesis by Manuel Kramer, Heidelberg University, 2016. **Right:** Observed scattered light image of the arc-shaped envelope around the Type 2 TD star AB Aurigae by P. Kalas (Grady et al. 1999).

G.J. Herczeg, G.S. Mathews, V. Geers, *A Major Asymmetric Dust Trap in a Transition Disk*, 2013, Science, 340, 1199. This was the first discovery paper of a dust trapping vortex, and still is the best example of such an object so far. The role of the PI was the interpretation of the discovered lopsided dust clump as evidence for a dust-trapping vortex.

M. Benisty, T. Stolker, A. Pohl, J. de Boer, G. Lesur, C. Dominik, **C.P. Dullemond**, M. Langlois, M. Min, K. Wagner, T. Henning, A. Juhász, P. Pinilla, S. Facchini, D. Apai, R. van Boekel, A. Garufi, C. Ginski, F. Ménard, C. Pinte, S.P. Quanz, A. Zurlo, A. Boccaletti, M. Bonnefoy, J-L. Beuzit, G. Chauvin, M. Cudel, S. Desidera, M. Feldt, C. Fontanive, R. Gratton, M. Kasper, A.M. Lagrange, H. LeCoroller, D. Mouillet, D. Mesa, E. Sissa, A. Vigan, J. Antichi, T. Buey, T. Fusco, D. Gisler, M. Llored, Y. Magnard, O. Moeller-Nilsson, J. Pragt, R. Roelfsema, J-F. Sauvage, F. Wildi, *Shadows and spirals in the protoplanetary disk HD 100453*, 2016, A&A in press. This is the paper presenting the spectacular scattered light image of HD 100453 with the ring, the two shadows and the two perfect spirals (the SPHERE image shown in Fig. 1). The PI is closely associated with several members of the SPHERE consortium who made this observation, and is co-author of this paper having contributed theoretical interpretations.

A. Kataoka, T. Tsukagoshi, M. Momose, H. Nagai, T. Muto, **C.P. Dullemond**, A. Pohl, M. Fukagawa, H. Shibai, T. Hanawa, K. Murakawa, *Submillimeter Polarization Observation of the Protoplanetary Disk around HD 142527*, 2016, ApJ, 831, L12. This paper shows the power of ALMA observations of lopsided disks.

2. Objectives and work programme

2.1 Anticipated total duration of the project

3 years.

2.2 Objectives

This project aims to study the *dynamics* of non-axisymmetric Type 2 TDs, with the goal of trying to learn from these spectacular "disk dynamics laboratories" of Nature. The origin of these strange structures, including single- and double-armed spirals, heavy gas+dust rings with lopsided asymmetry, inclined/warped inner/outer disk geometry, is not yet understood. We plan to carry out numerical hydrodynamic simulations to test a variety of possible explanations for these non-axisymmetric features.

Concretely, we intend to study:

1) The effect of one or more planetary and/or brown dwarf companions on the disk, in particular focussing on the effect of their eccentric and/or out-of-plane orbits on the disk. Could this open

up a large gap as observed? Could the out-of-plane orbit lead to precession of the inner disk with respect to the outer disk, and thus explain the inclined inner disk with respect to the outer disk?

2) Are the arc-shaped features in Type 2 TDs really a proof of there being an anticyclonic, dust-trapping vortex, or can disk eccentricity induced by a massive enough companion cause equally strong density contrast along the ring (see e.g. Kley & Dirksen 2006)? We have investigated this question in the past (Ataiee et al. 2013) and came to the conclusion that the contrasts along the ring were not strong enough to match the strong asymmetry seen in HD142527 and IRS 48 (at that time the only two ALMA-confirmed lopsided disks). However, Ragusa et al. (2017) calls this conclusion in question, at least for HD 142527. By assuming a particularly massive companion (i.e. a stellar companion) they appear to be able to create rather strongly lopsided rings with contrasts along the ring of up to a factor of 10, even without dust trapping. With the exception of IRS 48 they conclude that all other famous lopsided TDs (HD 142527, HD 135344b, SR 21, DorAr 44 and LkHα 330) can be explained by just disk eccentricity, without a dust-trapping vortex. A reinvestigation from our side is necessary to find out who is right, where we would use a grid-based method, as opposed to Ragusa et al. (2017), who use an SPH method.
3) What is the effect of photoevaporation on a tilted inner/outer disk configuration? The irradiation of the inner edge of the outer disk can take place without extinction by the inner disk, and so it would be expected to be extremely effective. How long would it take to destroy the outer disk by photoevaporation?
4) Is Rossby-wave instability really the main reason for the lopsided heavy rings seen in Type 2 TDs? If so, why are some sources *much* more lopsided than others? Could this be a time-sequence effect (the vortex becoming stronger and weaker periodically as seen in the simulations by Regály et al. (2012)), or must it be an intrintic effect?
5) Can the outer disks have originated from late-time infall of gas+dust from a passing low-mass molecular cloud filament? Could this explain the tilted/warped inner/outer disk geometry seen in several Type 2 TDs? What would the remnants of this cloud look like at large scales? Could this explain the arc-shaped large scale features seen arouns several Type 2 TDs? Can this secondary infall explain the spiral waves seen in many Type 2 TDs, and how would the tilted angular momentum vector affect this compared to Lesur et al. (2015)?

2.3 Work programme including proposed research methods

2.3.1 Tools for the proposed project

For this project we will require the following main tools:

1) **A 3-D hydrodynamics modeling code.** Depending on which of the above subquestions we wish to address, the requirements for the hydrodynamics code will be different.
   - For the study of the effects of a massive companion on the disk we will resort to the FARGO-3D code by Pablo Benítez-Llambay and Frederic Masset[1]. This code is very flexible, has parallellization and GPU acceleration implemented, and is well documented.
   - For models of how a severely out-of-plane companion affects the dynamics of the disk, the classical grid-based codes may not be suitable. Fixed-grid codes, when applied to disks that are not aligned with the grid, tend to cause numerical precession and artificial alignment. These effects can easily dominate over the real precession and alignment effects, making the results very unreliable. Even if these numerical effects are kept small by using a large numerical resolution, due to the large number of orbits that have to be modeled, they can still become problematic. Lagrangian hydrodynamics codes would be more suitable for this problem, in particular because this problem is dominated by orbital dynamics and gravitational torques. The simplest of this class of methods is the Smooth Particle Hydrodynamics (SPH) method. The Gadget-2 SPH code (Springel 2005) would be a suitable option. Perhaps even

[1] `http://fargo.in2p3.fr`

better would be the Arepo code (Springel 2010), since it has the orbital dynamics of an SPH code, but the hydrodynamics of a grid-based Riemann solver: it uses dynamic Voronoi cells comoving with the fluid to solve the finite volume problem. SPH codes are, however, a bit easier to handle, so we will start with that type of code, and switch to Arepo if the advantage to effort ratio turns out to be large enough.

- For the problem of external capture of a low-mass molecular cloud fragment, an SPH code will not really be suitable, because to reproduce the large scale geometry of the remnant of that cloud, a too large number of SPH "particles" is required (because even very low density remnants would scatter light and remain visible). An SPH code does not have the required dynamic range in density. For this we therefore resort to a Riemann Solver. We could use again Arepo, but since we wish to post-process the results with a scattered-light radiative transfer code, better and smoother images can be produced with a fixed grid. Which code we use will depend on the candidate for the position. But two popular publicly available Riemann codes that could be suitable are RAMSES (Teyssier 2002) and PLUTO (Mignone et al. 2007). The RAMSES code has a working moment-based radiative transfer module included for radiation-hydrodynamic modeling.

In Heidelberg and Tübingen there is ample experience with all five codes mentioned here.

2) **A 3-D diagnostic radiative transfer code.** The radiative transfer modeles used in the hydrodynamics codes for radiation hydrodynamics are generally not suited for diagnostic radiative transfer: i.e. the computation of synthetic images and spectra. It is necessary to apply a separate 3-D radiative transfer code to post-process snapshots of the model. We have in-house software for this: the popular publicly available RADMC-3D code package (Dullemond 2012). This software allows us to compute scattered-light images based on Monte-Carlo simulations using the full Müller matrix phase function for randomly oriented dust particles. The code also self-consistently computes the dust temperatures in the disk, using the Bjorkman & Wood (2001) Monte-Carlo algorithm, and thus allows for self-consistent spectral energy distribution calculations. Finally, the code also allows for the computation of molecular line maps from the hydrodynamics model. The observations of molecular line maps are a way to infer the dynamics of these disks.

2.3.2 Work plan

The work plan consists of several sub-projects that aim to explain the non-axisymmetric features mentioned above. In each of these sub-projects we will not only do the (radiation-)hydrodynamic modeling, but also compare their predicted appearances (using RADMC-3D) with the copious VLT/SPHERE and ALMA observations of these objects. With ALMA, in addition to continuum data, we will use line data to constrain the dynamics. Access to these data will be in part through public data, and in part through collaboration with observational teams. The PI is member of several ALMA consortia, as well as external member of the SPHERE disk consortium.

1. **Companion inside the disk: The in-plane 2-D case**
The first project will be a "simple" start up project. We will use the FARGO-3D code to model the effect of a single, massive companion, either on a circular or eccentric, but always in-plane, orbit on the circumstellar disk. At first we will do just 2-D (r, ϕ) models and revisit and reproduce older models that we have already done in the past (Kley & Dirksen 2006; Ataiee et al. 2013). We will then employ larger companion masses and see if we can reproduce the lopsidedness of a factor of 10 found by Ragusa et al. (2017). They use an SPH code. Such codes are known to be more numerically viscous than grid-based codes. It is known that a strong viscosity in the disk tends to drive eccentricity, so perhaps viscosity is also responsible for the formation of the strong arc-shaped overdensities. A verification with a grid-based code is therefore important to be able to make strong conclusions. A next application of these in-plane companion-disk interaction models will be to test if these models can explain the huge radial range of the gap. Many Type 2 TDs have inner disks of only about 1 AU radius and outer disks starting beyond

many tens of AU (in the extreme case of HD 142527 the inner disk is about 10 AU in radius while the outer disk starts beyond 120 AU). Can a single companion cause this? And will there still be gas flowing through the gap? What is the effect of a possible orbital eccentricity of the companion on the disk? What kind of gap *shape* does the companion produce? In scattered light observations of the star HD 142527 (Rodigas et al. 2014) it is clearly seen that the outer edge of the gap is eccentric with respect to the position of the star (though that does not exclude the possibility of its arc-shaped ALMA continuum peak being due to dust trapping in a vortex), with the star being to the north of the center of the disk. Also this outer edge appears to be a bit ragged (also seen in an earlier image by Rameau et al. 2012). Can this eccentricity and these irregularities (deviations from a perfect keplerian ellipse) be understood in the context of a companion-disk interaction model? This sub-project will be done in close collaboration with the postdoc of project D1, as that project is specialized on planets in disks. Project D1 focuses on multi-planet systems being responsible for the cavity in Type 2 TDs because single planets have not been proven to be able to explain TDs. Here we focus on Brown Dwarf or M star companions, possibly on strongly eccentric orbits. Yet, technically there are several similarities, making a strong collaboration beneficial[2]. To make the connection to the observations, in particular the scattered-light images of Type 2 TDs, we will make use of our RADMC-3D code. We will have to turn the 2-D models into 3-D using a gaussian vertical structure model as in Juhász et al. (2015). It will be critical to treat the thermodynamics, in particular near the shocks of the spiral waves caused by the companion, as the sudden heating by a shock will puff up the disk and thus increase the intercepted stellar light (see Dong et al. 2015). We will employ a simple recipe for the heating/cooling in our 2-D hydrodynamics models following Müller & Kley (2013) and Pohl et al. (2015). Near the shock the assumption of vertical hydrostatic equilibrium may not be warranted, but the differences may not be too large (see discussion for the case of planetary companions by Dong et al. 2015). Once these predicted scattered light images are made, their comparison to actual observed images will be done through our collaboration with project A1, as well as with the MPIA (through Prof. Henning). At this point the comparison with ALMA observations would focus mostly on the observed gas inside of the dust hole (such as e.g., van der Marel et al. 2016), again in collaboration with project A1 as well as with Prof. van Dishoeck, but detailed comparisons will not be done as these would require us to delve into the CO chemistry which we wish to avoid, to save time for the following sub-projects.

2. **Companion inside the disk: The in-plane 3-D case**
   One of our prime interests is to study the strongly warped disks (or more precisely: the strongly inclined inner disks) that appear to be responsible for the strange shadows in some Type 2 TDs. This will be the task of the next sub-project. But as a warm-up, the postdoc will gain some experience with 3-D disk modelling in a slightly less challenging setting. So in this sub-project we will redo some of the models of the previous sub-project in full 3-D. For the heating/cooling we will attempt to convert the simple recipe to a form that can be used in these 3-D settings as well. With these 3-D models will then be able to see if the hydrolic shock-bore effect of (Boley & Durisen 2006) (and discussed in the context of observability of spiral waves in Dong et al. 2015) significantly affects the predicted observed scattered light images from the first sub-project. This might well be the case, since in this project we will study massive companions that are expected to create strong perturbations in the disk. We will, also here, collaborate strongly with project D1. While D1 will concentrate more on improving the realism and accuracy of the 3-D simulations, our project here will focus on extending them to more extreme cases (strong eccentricities of a massive companion).

3. **Companion inside the disk: The out-of-plane case**
   Since we know by now that many TDs are warped, it is entirely natural to investigate what happens to the disk if the star has a companion (planetary or stellar) that has orbital elements

[2] The text highlighted in green refers to the connection of this project to other projects of this Research Unit.

carrying it out of the plane of the disk. Could such a configuration cause the inner/outer disk to precess and explain the weird warped/tilted disk systems such as HD 142527 and HD 100453? To model this problem we will resort to another kind of hydrodynamics code. We will start with the SPH code Gadget-2, set up the problem starting from the simulations we did previously (see preliminary work) and improve those calculations in various ways. First, we will use many more particles, and compute our models on a computer cluster. We will carefully investigate the viscosity effects and how they scale (reduce) with increasing number of SPH particles. We will then move to the Arepo code, which uses the same underlying data infrastructure as Gadget-2, so that the switch to Arepo should be reasonably doable. We will investigate if this code has, for the same number of sampling points ("particles") a lower (and therefore more realistic) numerical viscosity. The first investigation of the results can be done by computing quantities such as tilt angle, disk eccentricity etc, which can be directly compared to the equivalent observed quantities. A more detailed comparison to the observations will again require radiative transfer. In principle we are then again faced with the problem of radiation hydrodynamics (see above). For this kind of highly complex geometries it might be not yet feasible to do this. In Gadget-2 this kind of radiative transfer (Flux-limited diffusion) is not yet built in. In Arepo such a method is implemented (Petkova & Springel 2011), but testing its feasibility for the kind of models discussed here might be too time-consuming. We might try, but we might also use a simple power law as a function of distance. However, for the scattered-light observations we again use RADMC-3D. The Arepo grid is, however, a Voronoi grid. This is not yet built in into RADMC-3D. We will therefore instead regrid a snapshot from Arepo on an oct-tree cartesian adaptive mesh before inserting this into RADMC-3D. Alternatively we might use the recently Voronoi-enabled MOCASSIN code of Prof. Ercolano. In Project D1 mild inclinations of planetary mass companions are modelled, while here we focus on extreme inclinations of stellar mass companions. In the latter case the star, being too massive, is unlikely to be forced back into the plane of the disk; instead the disk is likely to be torqued by the companion. Like in the previous sub-projects, we will collaborate with project A1 when comparing our simulations with observed Type 2 TDs.

4. **Tilted disks: The effect of Photoevaporation**
   The UV and X-ray photons from the star may photoevaporate the disk (see projects B1 and B2). It is known from model calculations that, once the stellar radiation can impinge directly onto the inner edge of the disk, the photoevaporative destruction can accelerate dramatically (coined "thermal sweeping" by Owen et al. 2012). In normal disks without warping this requires the entire inner disk to vanish. Once it is vanished, the sweeping begins and the outer disk quickly vanishes too. With the tilted Type 2 TDs, however, we have an interesting new situation: due to the tilt of the inner disk, the stellar photons can reach the inner edge of the outer disk unobstructed (barring two small shadows where the two disk planes intersect). The question is therefore: should we expect these outer disks to be subject to thermal sweeping, and if so, how rapidly would this destroy the outer disk? And is this time scale consistent with the statistics of known tilted TDs? We will take the tilted disk models of the previous subproject and pick a time snapshot. We will then subject this to a radiative transfer calculation of UV and X-ray photons. We will collaborate with Prof. Barbara Ercolano, and use her MOCASSIN code for this (Ercolano et al. 2003, 2005, 2008b). This will then give an estimate of the typical volume of heated gas in this outer disk edge, and with this we will *estimate* what the evaporation rate will be, using the same approach as in Ercolano et al. (2008a, 2009). We will not model this evaporation directly, because the geometry is full 3-D and this is presumably too numerically expensive. However, we might, in addition, make a 2-D (r, z) axisymmetric model of the outer disk without inner disk (i.e. ignoring the two shadow spots by the inner disk) and do a run similar to the 2-D models of Owen et al. (2012) to see what the time scale will be. This sub-project will benefit strongly from a collaboration with the postdoc of project B1, since he/she will work with hydrodynamic models of photoevaporative winds. In particular the 2-D axisymmetric approximation model can presumably be set up quite easily by the postdoc of project B1.

5. **Secondary infall of a low-mass molecular cloudlet**
   Next we will explore the idea that the tilted disk geometry seen in HD 142527 and HD 100453 could be as a result of late infall of fresh envelope material with a different angular momentum axis than the earlier primordial collapsing cloud from which the star has formed (the scenario by Thies et al. 2011, but now applied to disks). We will employ the PLUTO or RAMSES code in cartesian coordinates and set up a model of the kind we already started in the preliminary work (see above). We will improve on these models in several ways. First we will perform models with much higher resolution. Second we will start the cloud much farther from the star. This all requires modeling on a substantial computer cluster. In our initial models we will ignore the inner disk and focus only on the formation of the outer disk from the capture of the cloudlet. To test whether the geometries we find are not too strongly affected by the gridding, we will repeat some models with the same setup, but randomly rotated with respect to the grid. The resulting outcome should ideally become the same (apart from being rotated). We will compute the scattered light images using RADMC-3D and compare these images with observed images of these disks in the optical and near-infrared, particularly focusing on the large scale structure, what people tend to call the "envelope". We may also compute images at other wavelengths, as well as molecular line maps, and compare with what is present in the literature. For instance, for AB Aurigae the envelope structure (see Fig. 5) has been studied in quite some detail at many wavelengths, including molecular lines (Semenov et al. 2005). Likewise for HD 100546, which also shows an arc-shaped envelope (Ardila et al. 2007).

6. **Secondary infall: interaction with pre-existing disk**
   As a follow-up of sub-project 5 we consider the case that the secondary infall may not just simply *create* a new "outer disk", but collide onto a *previously existing* outer disk (of better: a full disk including inner and outer part in the same plane) with a completely different angular momentum direction. This would lead to violent hydrodynamic effects, and might torque the rotation axis of the pre-existing disk initially to a third direction (neither parallel to the initial disk, nor to the angular momentum axis of the infalling material). A calculation of this process is challenging, and grid codes such as RAMSES and PLUTO may not be the most suitable. SPH codes or Arepo might be better suited. We will presumably first try this kind of modeling with the SPH code Gadget-2. The problem with the dynamic range in density described in subproject 5 is not an issue here, because we will not focus on the large scale low-density regions ($\gtrsim$ 1000 AU), but on the intermediate scales ($\simeq$ 100 AU) where the collision between the infalling material and the pre-existing disk occurs. SPH modelling, with all its caveats, does give a quick-look result relatively easily, even for complex geometries. And since the problem of torques induced onto the outer disk is mainly a matter of angular momentum exchange between gas parcels, and less a matter of the detailed hydrodynamic phenomena such as shocks, this quick-look approach with SPH will be a good starting point. We will compare our results with what modelers from the star-formation community tend to find in their much larger scale simulations. An in-house collaboration with the group of Prof. Ralf Klessen at the ITA will be helpful here. If we will find the time, and if we find it necessary, we may switch at some point to the Arepo code. The Arepo code shares the same Input/Output formats with the Gadget-2 code, so the switch, while undoubtedly challenging, will not be as difficult as switching to an entirely independent code. We will be able to use the same setup scripts and post-processing tools.

7. **Revisit the Rossby-wave instability**
   Finally, if we still have time, we will (in strong collaboration with D1) revisit the the Rossby-wave instability origin of the observed vortices, comparing the different scenarios of inner hole formation against each other (planets, massive companion, inclined companion, photoevaporation): do they all predict these vortices? And are vortices and spirals predicted simultaneously or mutually exclusively? The relation to dust-trapping makes a connection to project **C1** natural. Project D1 aims, among other things, to follow the dust kinetics and dust trapping in TDs. This fits well into the topic of non-axisymmetric TDs, as some of them display lopsided dust emission

believed to be due to a huge dust-trapping vortex. This sub-project will thus be either lead by the postdoc of D1 or by the postdoc of this project.

2.3.3 Time plan

We are aware that this is an ambitious set of projects. It is likely that some of these projects will have to be carried over to the second funding period of the Research Unit. Some subprojects may also become obsolete, given that this is a very fast evolving and somewhat unpredictable field, with new data appearing regularly. A slight overbooking of sub-projects is therefore part of the plan. Nevertheless, a rough time plan would look as follows:

- **Year 1:**
  Sub-project 1 and 2 will both be based on relatively state of the art techniques and methods, and with close collaboration with project D1 we estimate that both together will take about 1 year.
- **Year 2:**
  Sub-project 3 will be challenging, especially if a new code (Arepo) has to be learned and applied to a problem that has not yet been modeled with Arepo before. We can expect the unexpected. It could take the whole year. If, however, time permits, then we will attempt to also start with sub-project 4. This project, being at a slightly less high priority, will be done as a side project, and may spill into phase 2 of the Research Unit.
- **Year 3:**
  By this time the data from observations will probably be so much advanced that we may already be able to estimate which of the sub-projects 5, 6 and 7 should gain priority at this point. We may then either focus entirely on that single sub-project during this last year, or we pick 2 of them and work on them half a year each. The remaining sub-project(s) will then, if still current, spill over into phase 2 of the Research Unit.

2.4 Data handling

The model data we produce will be made immediately available online, once the corresponding paper is accepted.

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4. Requested modules/funds

4.1 Basic Module

4.1.1 Funding for Staff

We request 1 Postdoc E13 position for three years, to be based in Heidelberg.

4.1.2 Direct Project Costs

4.1.2.1 Equipment up to EUR 10,000, Software and Consumables

Theoretical numerical research can only be done when sufficient and appropriate computational facilities are available. While production runs will be done on supercomputer facilities, a substantial part of the work in this project is code development. Testing these codes on realistic problems requires a workstation – which is beyond the standard base equipment (*Grundausstattung*). We therefore request one workstation-grade desktop computer for 3000 Euro.

4.1.2.2 Travel Expenses

Travel within the Research Unit is handled in project Z. In addition we request funding for conference travel for the personnel and one Applicant. This includes one national (1.000 €) and one international (1.500 €) conference trip per year, totalling 2.500 € per person per year.

For this project this totals 5.000 € per year for the Postdoc and one Applicant, which is in total 15.000 €.

4.1.2.3 Visiting Researchers (excluding Mercator Fellows)

This project strongly ties to observations of Type 2 TDs in scattered light (with VLT-SPHERE), thermal millimeter dust emission (with ALMA) and gas lines (with ALMA). We collaborate internally with Prof. Ewine van Dishoeck (on the ALMA data) and Prof. Thomas Henning (on the scattered light data). Over the last few years we have also strongly collaborated (and published several common papers) with Dr. Myriam Benisty and Prof. Carsten Dominik, both strongly involved in the VLT-SPHERE project. Recently we have started also a collaboration with Prof. Misato Fukagawa, who is strongly involved in both ALMA observations and Subaru scattered light images of transition disks. Early access to new data from these projects is very advantageous for our project, since it would allow us to tune our models to data about a year before the data become public, giving us a head-start over competitors. We will also continue our strong collaboration with Dr. Akimasa Kataoka, who will be moving to Tokyo in April 2017. For travel to/form Dr. Kataoka we will not ask funding here, because that travel will be funded through the Humboldt Foundation.

We therefore ask for 2.000 € travel money for Prof. Misato Fukagawa (Japan), 1.000 € for Dr. Myriam Benisty (Grenoble) and 1.000 € for Prof. Carsten Dominik (Amsterdam), totalling 4.000 €.

4.1.2.4 Other Costs

4.1.2.5 Project-related publication expenses

We request 750 €/year (total 2250 €) for publication expenses.

5. Project requirements

5.1 Employment status information

Prof. Dr. Dullemond, Cornelis Petrus. W3 Professor (permanent) at Univertiät Heidelberg.
Prof. Dr. Kley, Wilhelm. W3 Professor (permanent) at Univertiät Tübingen.

5.2 First-time proposal data

5.3 Composition of the project group

The main work will be done by the requested postdoc, in close collaboration with the PI C. Dullemond and co-PI W. Kley. When it comes to comparison with observations, close collaboration with the teams of Th. Henning and E. van Dishoeck will occur. For the late stage infall modelling we will collaborate with the Star Formation group of R. Klessen at the same institute of the PI (ITA).

5.4 Cooperation with other researchers

5.4.1 Planned cooperation on this project

5.4.1.1 Collaborating researchers for this project within the Research Unit

A key to the success of this project will be the comparison of the models to observations of Type 2 TDs. Access to the latest VLT-SPHERE images in scattered light is guaranteed through collaboration with the group of Thomas Henning. Access to the latest ALMA data is guaranteed through the groups of Leonardo Testi (see also project A1) and Ewine van Dishoeck. Direct collaboration with the PhD students from project A1 (PI Testi) is forseen to help with the comparison of our models with these ALMA data. The postdoc of B2 (PI Caselli & Ercolano) will be working a lot with 3-D diagnostic radiative transfer modeling, so a collaboration on the technical side can be helpful here as well. This collaboration will also provide chemistry input for the abundances of molecules that can be traced with ALMA to determine the kinetics of the disks.

A strong collaboration within this Forschergruppe will be carried out with the postdoc of project D1. Projects D1 (PI Kley) and D2 have several methods in common, in particular both employing 2-D and 3-D (radiation-)hydrodynamics of protoplanetary disks. On the technical side both postdocs are envisioned to collaborate closely. The first two sub-projects of D2 are also topically somewhat overlapping with project D1: focussing on planet-disk interaction as an explanation for Type 2 TDs. The differences are: in D2 we focus on *single massive* companions, presumably low mass stars rather than planets, while project D1 focuses more on multiple planet-mass companions. Secondly, D2 focuses on finding the origin of strong deviations from circular symmetry, in part by making the companion's orbit strongly eccentric. Finally, D2 aims at explaining the extremely tilted inner disks of several Type 2 TDs, which is not a goal of D1.

A connection with project C1 (PI Birnstiel & Dullemond) is foreseen as the models developed here will provide inputs to explore pressure bumps of diverse nature.

A connection to project B1 (PI Ercolano) will be established when we intend to apply the photoevaporation models of B1 to the case of an outer disk photoionized/evaporated by the star, as a result of free irradiation due to the inclined inner disk.

5.4.1.2 Collaborating researchers for this project outside of the Research Unit

External collaboration with M. Benisty (Grenoble/Santiago) and C. Dominik (Amsterdam) is envisioned for the task of comparison to observational data with ALMA and SPHERE. In addition, collaboration with M. Fukagawa (Nagoya, Japan) and A. Kataoka (NAOJ, Japan) and other Japanese colleagues involved in studies of transition disks, is envisioned. The PI has established strong scientific links with these groups, in particular recently in the study of Type 2 TDs with ALMA, both from a modeling perspective and from ALMA observations.

We will also strengthen ties to Dr. Pablo Benítez-Llambay (currently at Copenhagen) who is the lead author of the FARGO-3D public code.

5.4.2 Researchers with whom you have collaborated scientifically within the past three years

Close collaboration is in boldface. The rest is due to large common consortia.
S. Andrews (CfA, Harvard), E. van Dishoeck (MPE Garching, Uni Leiden), C. Dominik (UvA, Amsterdam), A. Natta (DIAS, Dublin), L. Testi (ESO, Garching), J. Carpenter (Caltech, Pasadena), **C. Chandler (NRAO, Socorro),** A. Isella (Rice Uni, Houston), L. Ricci (Caltech, Pasadena), N. Calvet (Uni Michigan), S. Corder (ALMA), J. Greaves (Uni St. Andrews), **N. Turner (JPL, Pasadena),** A. Uribe (Coll. Charlston), **Z. Regaly (Konkoly Obs, Budapest), A. Juhasz (Cambridge), R. Klessen (Uni-Heidelberg), R. Kuiper (Uni Tübingen), C. Brinch (University of Copenhagen), M. Benisty (Uni Grenoble), P. Pinilla (Tucson), C. Mordasini (Uni Bern),** G. Guidi (ESO), **M. Tazzari (ESO), L. Perez (MPIfR, Bonn),** H. Linz (MPIA), A. Sargent (Caltech, Pasadena), L. Mundy (University of Maryland), S. Storm (University of Maryland), J. Lazio (JPL, Caltech), W. Kwon (Korea Astronomy and Space Science Institute), **B. Ercolano (Uni München), T. Muto (Kogakuin University),** M. Momose(Ibaraki University), **T. Tsukagoshi (Ibaraki University),** L. Klarmann (Uni Amsterdam), **H. Klahr (MPIA, Heidelberg), S. Ataiee (Uni Bern),** S. Paardekooper (Queen Mary University of London), M. Fukagawa (NAOJ Japan), H. Shibai (Osaka University), T. Hanawa (Chiba University), K. Murakawa (Osaka Sangyo University), **J. Ramsey (Uni Kopenhagen), J. Drazkowska (Uni Zürich)**

5.5 Scientific equipment

The project requires a considerable amount of CPU-time. For production runs we will rely on outside resources.

We have special access to computing resources supplied within the State of Baden-Württemberg (Baden-Württemberg High Performance Computing - Coordinated Compute Cluster Competence Centers: bwHPC-c5). A part of this initiative is the new BinAC-system[3] that has just gone online at the University of Tübingen and is dedicated to Astrophysics and Computer Science only, and is accessible for researchers from Heidelberg. BinAC offers over 236 CPU nodes with dual Intel Xeon E5-2630v4 each. Additional resources are available with bwHPC-c5 at the ForHLR-cluster at the Steinbuch Centre for Computing (SCC) in Karlsruhe. If further resources will be required we will apply for additional computer time at the high performance computing center HLRS, located in Stuttgart, and at other centers in Germany.

[3] see `http://www.bwhpc-c5.de/wiki/index.php/Category:BwForCluster_BinAC` for a detailed description of the hardware.

Project Z:
Coordination of the Research Unit

Coordinators:
Main Speaker: Prof. Dr. Barbara Ercolano (LMU)
Vice Speaker: Prof. Dr. Cornelis P. Dullemond (Uni Heidelberg)

Requested positions: 50% secretary position

1. General

As outlined in the main part of the proposal, in this Research Unit (RU) we plan several measures to strengthen collaboration and interaction between the different nodes. Among these are frequent visits between partner institutes and the participating nodes, regular Video-conferences, regular (twice a year) meetings of the members of the RU, and joint invitations of guests/visitors. Additionally, we plan to organize an international meeting and invite review speakers from outside, and we plan for a summerschool for students and interested young scientists within the first year of the RU funding period.

Travel *within* the Research Unit is organized here in Project Z, while project-specific travel and external guests are organized in each project separately.

2. Funding Request for Project Z

To estimate our requested funds as listed below we have assumed the following personnel involved in the RU: 5 PhD students, 4 Postdocs, 7 Principle investigators (PIs), 2 senior collaborators, in total 18 people.

2.1 Network management

- **Secretarial support:**
  The organization and (financial) management of all these activities requires a dedicated person dealing with these duties. This person can at the same time organize the official web-pages for the RU, as well as organize the meetings, school and conference. This position has the following requirements: Work relatively independently, English language skills and basic computer skills. We apply for a E8 position for 50% part-time.
  23.550 € × 3 70.650 €

- **Consumables:**
  For regular expenses of the management (printing costs, postal services, toner, copying materials, etc..) we request 1000 € per year.
  1000 € × 3 3.000 €

2.2 Travel and meetings within the Research Unit

In the individual project descriptions we have only included travel funds for direct collaboration between or within (if two nodes are involved in one project) the individual projects, referring primarily to longer term visits of approximately a week.

Additionally, we plan here for occasional short term visits (collaboration) between scientists, which we plan to organize through this central budget. Funds for regular meetings of the RU are also organized centrally.

For travel within Germany we assume on average 200 Euro per train return ticket per person and 100 Euro per day for lodging and food.

We estimate the following amounts (which are totals over 3 years):

- **Full network meetings.**
  We plan for two two-day meetings per year for the whole RU (in total 18 participants; 400 € per person and meeting). On average we plan to invite one international guest per meeting (800 € travel, 2×100 € lodging and food).
  (400 € × 18 + 1000 €) × 2 × 3 — 49.200 €

- **Tutorials and Lectures.**
  As an extension to the first two full network meetings during the first year, we intend to add two more days for tutorials and lectures. This means that the students and postdocs will stay for two more days, as well as two of the PIs (in addition to the local PI(s)) as lecturers.
  (200 € × 9 + 200 € × 2) × 2 — 4.400 €

- **Collaboration:** *Short term visits to other nodes within the RU.*
  We plan on average 2 visits for about 2 days per person and year (i.e. in total 400 EUR per person and visit).
  400 € × 2 × 18 × 3 — 43.200 €

- **Working visits:** *Working visits of RU-personnel within the RU.*
  We plan on average one working visit for about 2 weeks per person and year (i.e. in total 1400 EUR per person and visit). We have 9 RU-funded personnel.
  1400 € × 1 × 9 × 3 — 37.800 €

- **International school:** *An international summer / winter school on disk physics.*
  We intend to organize an international summer / winter school on disk physics during the second year, with an emphasis on, but not limited to, TDs. We will apply for the Bad Honnef programme, which would give funding. But to provide additional support for external international students with little means, we apply for 10,000 €.
  10.000 € × 1 — 10.000 €

- **International conference:** *An international conference on TDs.*
  We intend to wrap up the RU with an international small size conference on the topic (roughly 60 participants). We apply for 30,000 € for this.
  30.000 € × 1 — 30.000 €

- **Family support measures:**
  To support members who wish to travel with a caretaker for their small children to face-2-face meetings within the Research Unit, we request 1500 € per year.
  1500 € × 3 4.500 €

2.3 Central Computing Facility

We request a multicore machine to carry out part of the theoretical work. This is necessary for mid-size production runs of some of the bigger model calculations. This will give a unified computation environment for the entire Research Unit, making it easier to combine/connect models from different sub-projects. The machine will be accessible to all members of the Research Unit. The total cost of the machine (see attached quote) is 30.000 €, to be spent in the first year. The hosting and the maintenance will be provided by the University Observatory at the LMU.
30.000 € × 1 30.000 €

2.4 Summary of Project Z

The total funds requested for Project Z are summarized in the following table.

	Year 1	Year 2	Year 3	Total
Management	24.550	24.550	24.550	73.650
Travel and meetings	49.300	54.900	74.900	179.100
Computing Facility	30.000	0	0	30.000
Total: (EUR)	103.850	79.450	99.450	282.750

Grand Total for project Z: *282.750 €*