Project D1:

Transition disks and planetary systems

Authors:

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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 the 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 (Shu et al. 1993; Alexander et al. 2006), or by embedded massive planets that carve deep gaps into the disk (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) that 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 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 had been noticed that the gap created by a single embedded planet is way too narrow to be in agreement with the observations. Given the problems with a single planet and evaporation models it has been proposed that the main observational features can be created by the presence of a system (three to four) of 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 larger 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. 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 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.

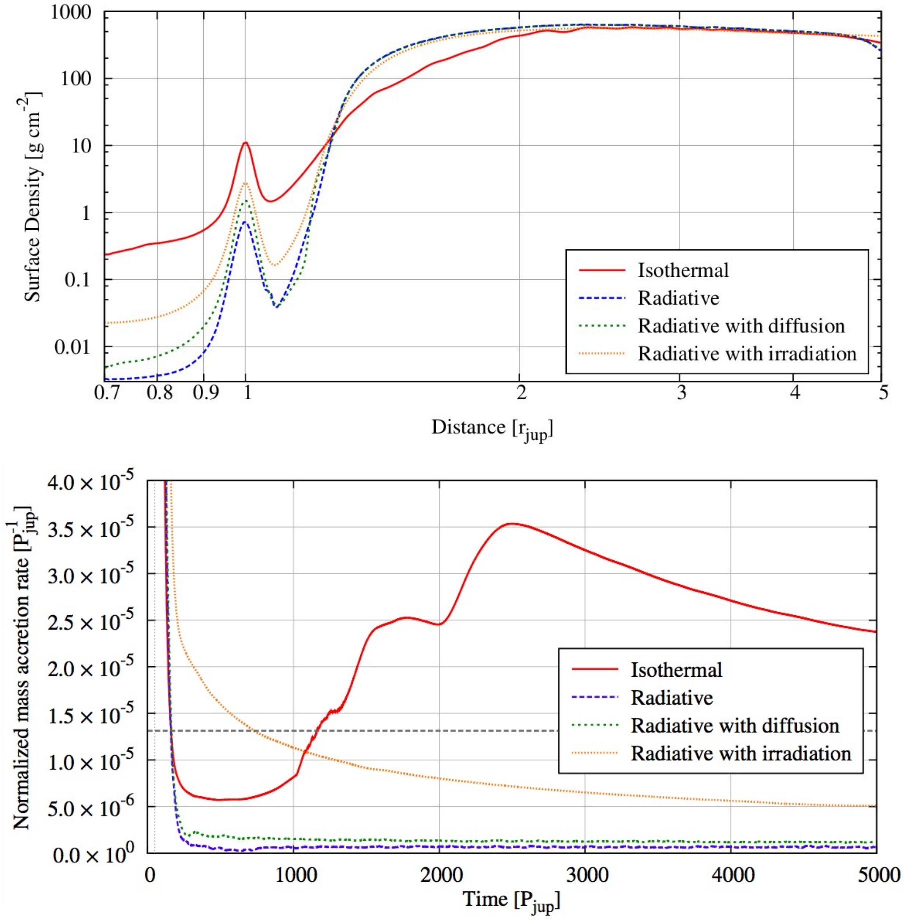

Figure 1: Radial density distribution (**top panel**) and time evolution of the mass accretion rate (**bottom panel**) into the inner hole of the disk for a $4M_{Jup}$ planet located at 5.2au in a transitional disk. Shown are curves for different thermodynamic treatments of the disk physics. Taken from: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

1.1.2 On the dust distribution in the disk around HL Tau

Upon publication of the spectacular image of the ring 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 decreasing

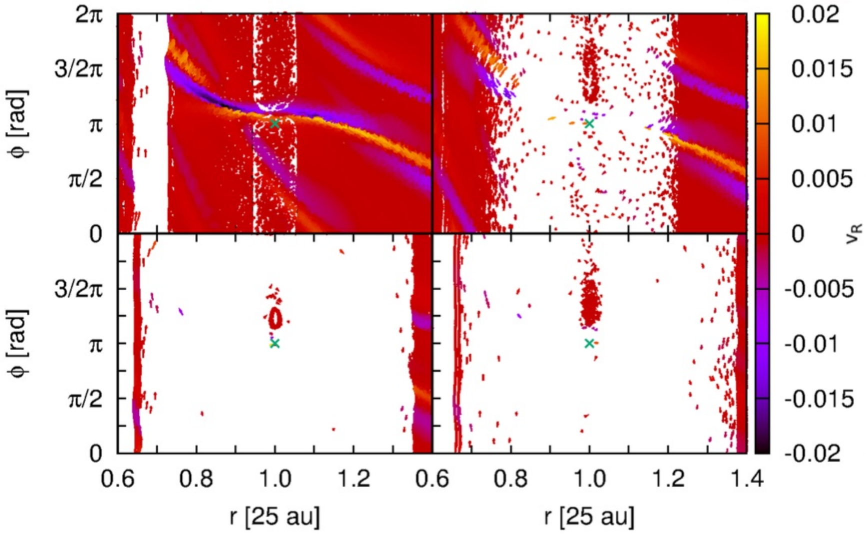

Figure 2: Particle distribution near the inner low mass planetary core location for mm- (**top left**), cm- (**top right**), dm- (**bottom left**), and m-sized (**bottom right**) particles at the end of the simulation. The velocity vectors of the particles with respect to the planet are shown and the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

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**. The CPU time used by this new code is shown in Fig. 3 for a standard test-problem. As can be inferred

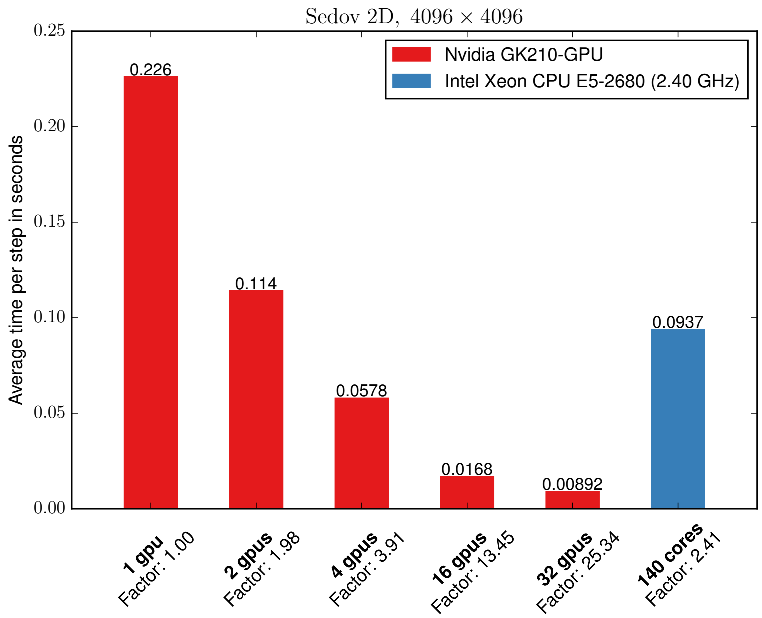

Figure 3: Computational time used for simulations using our new GPU-PLUTO code on the 2D Sedov test-problem using 4096 × 4096 gridcells. In red the values for the GPU-runs are displayed where multiple GPUs are connected via MPI. Each node of the system has 4 GPUs, so the results for 16 and 32 GPUs includes 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

Kees to Willy: Please add some text in each of the 10 publications below to argue what their relevance is to this project.

Kley, W. & Crida, A. (2008) *Migration of protoplanets in radiative disks*, Astronomy & Astrophysics, 487, 9.

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.

Kley, W., Bitsch, B. & Klahr, H. (2009) *Planet migration in three-dimensional radiative discs*, Astronomy & Astrophysics, 506, 971.

Müller, T. W. A. & **Kley**, W. (2013) *Modelling accretion in transitional disks* Astronomy & Astrophysics, 572, A61.

Ataiee, S., Pinilla, P., Zsom, A., **Dullemond**, C.P., Dominik, C. & Ghanbari, J. (2013) *Asymmetric transition disks: Vorticity or eccentricity?*, Astronomy & Astrophysics, 553, L3.

Picogna, G. & **Kley**, W. (2015) *How do giant planetary cores shape the dust disk?. HL Tauri system*, Astronomy & Astrophysics, 584, A110.

Kley, W. & Haghighipour, N. (2014) *Modeling circumbinary planets: The case of Kepler-38*, Astronomy & Astrophysics, 564, 72.

Stoll, M.H.R. & **Kley**, W. (2016) *Particle dynamics in discs with turbulence generated by the vertical shear instability*, Astronomy & Astrophysics, 594, A57.

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 are the birthplaces of planets: 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 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.

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 & 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 which we will expand our 2D density distribution by a vertical structure in hydrostatic equilibrium.

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.

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

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.

	Year 1	Year 2	Year 3	Sum
Conferences Postdoc	1500	1500	1500	4500
Conferences PIs	2000	2000	2000	6000
Working visits Heidelberg/TübingenMünchen	3000	3000	3000	9000
	6500	6500	6500	**19500**

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

4.1.2.5 Project-related publication expenses

We will publish in the **free European Journals** Astronomy & Astrophysics and Monthly Notices of the Royal Ast. Society.

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.

Kees to Willy: We might want to include a strong link to the project C1 (by Til) too, because we do dust stuff here, and C1 can provide recipes for the size distribution etc.

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 project is envisioned for the same reason. The postdoc of B2 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.

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)*

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. 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. As these simulations will require intensive computational effort and efficient codes, we plan to collaborate closely with Andrea Mignone (Torino, I) who is the developer of the PLUTO code. We will also strengthen ties to Dr. Pablo Benítez-Llambay (currently at Copenhagen, DK) who is the lead author of the FARGO-3D public code. 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[1] 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

[1] see http://www.bwhpc-c5.de/wiki/index.php/Category:BwForCluster_BinAC for a detailed description of the hardware.

will apply for additional computer time at the high performance computing center HLRS, located in Stuttgart, and at other centers in Germany.