TABLE OF CONTENTS

SCIENTIFIC/TECHNICAL/MANAGEMENT SECTION

1. BACKGROUND AND OBJECTIVES

Under current and prior funding, my research group has developed numerical hydrodynamics and radiative transport techniques to study gravitational instabilities (GIs) of protoplanetary gas disks in three dimensions. GIs are interesting because they can produce significant mass transport, dramatically alter disk structure, mix and shock-process gas and solids, and assist in the formation of planets. Our modeling has now become sophisticated enough for us to include realistic radiative transport effects, environmental influences, and the interaction of GIs with the growth and processing of solid materials. This successor proposal describes our plans to extend this ongoing research, with the ultimate goal of integrating GIs into a comprehensive theory of disk evolution and planet formation.

1.1 Relevance to NASA Objectives

The simulations in this proposal will shed light on the evolution of protoplanetary disks, including the growth and processing of solids leading to planet formation, with application to the origin of our own and of extrasolar planetary systems. This supports NASA Strategic Goal #3, specifically Sub-goals #3C and 3D and Research Objectives #3C.1 and 3D.3. A more detailed discussion of Relevance is given in Section 4.

1.2 Background and Motivation

Circumstellar disks of Solar System size or larger are common around young stars during the first few million years of their existence, and stars accrete matter from these disks at substantial rates (Hartmann 1998, Calvet et al. 2000, Reipurth et al. 2007). Estimates of disk masses for young low-mass stars remain uncertain but range up to and above 0.1 $M_\odot$ (e.g., Eisner & Carpenter 2006), with ongoing accretion rates $\dot{M}$ typically between about 10^{-9} and 10^{-7} $M_\odot$/yr. Relative disk masses and $\dot{M}$'s for embedded objects could be higher (e.g., Osorio et al. 2003), and, during FU Orionis outbursts (Hartmann & Kenyon 1996), $\dot{M}$ may approach 10^{-4} $M_\odot$/yr or more. Disk evolution depends on angular momentum transport, with concomitant energy release and mass redistribution (Papaloizou & Lin 1995, Gammie & Johnson 2005). Magnetorotational instability (MRI) (Balbus & Hawley 1998) will occur in disk regions with high enough ionization fraction and produce vigorous turbulence, with effective $\alpha \sim 0.01$ (Balbus 2003), compatible with α-disk models for T Tauri disks (Dullemond et al. 2007). However, the MRI is unable to operate in regions with low ionization. Such "dead zones" (Gammie 1996) may span much of the prime region for gas giant planet formation from a fraction of an AU out to 10 AU or more (e.g., Glassgold et al. 1997, Sano et al. 2000, Reyes-Ruiz 2001, Matsumura & Pudritz 2003, 2006). This proposal concerns gravitational instabilities (GIs), which have long been recognized as an alternative to MRI for producing transport in astrophysical disks (Pringle 1981). Eruptions of GIs in dead zones (e.g., Armitage et al. 2001) raise the possibility of a "unified theory" for a variety of astrophysical phenomena associated with young stars and planet formation, including chondrule production and annealing of solids in spiral shocks, radial and vertical mixing, FU Orionis outbursts, and gas giant planet formation (Boss & Durisen 2005a,b, Boley et al. 2005, 2006).

When the Toomre (1981) Q-parameter becomes less than about 1.5 to 1.7 anywhere in a circumstellar disk, small perturbations grow within a few rotation periods. Q is $c_s\kappa/\pi G\Sigma$, where c_s is the sound speed, κ is the epicyclic frequency ($\sim$ the rotation frequency Ω in a nearly Keplerian disk), and Σ is the disk surface mass density. The growing perturbations have a predominantly trailing spiral character and transport angular momentum outward by gravitational torques (Larson 1984, Boss 1984, Durisen et al. 1986, Papaloizou & Savonije 1991, Laughlin & Bodenheimer 1994). Once fully developed, GIs infect the disk with nonlinear spiral structure over a broad range of radii (Laughlin et al. 1998, Nelson et al. 1998, 2000; Pickett et al. 1998, 2000, 2003). GIs can produce mass redistribution with sustained effective α's up to several hundreths or more (Pringle 1981, Gammie 2001, Lodato & Rice 2004, Rice et al. 2005, Mejía et al. 2005, Michael et al. 2007) and with even larger values during the onset of GIs (Boley et al. 2006). Work by our group supports the idea that GI transport in real disks is an intrinsically global phenomenon in many important respects and cannot be properly treated by a local α-like prescription (Laughlin & Rozyczka 1996, Balbus & Papaloizou 1999, Lodato & Rice 2005, Mejía et al. 2005, Boley et al. 2006, Cai et al. 2007). GIs will occur wherever a disk becomes sufficiently cold (c_s small) and/or massive (Σ large). This almost certainly applies to the embedded phase of both high and low-mass stars when infall from the collapsing protostellar cloud feeds mass into the disk at a rapid rate (e.g., Yorke et al. 1993, Laughlin & Bodenhiemer 1994, Yorke & Bodenheimer 1999, Vorobyov & Basu 2005, 2006, Kratter & Matzner 2007), and disks observed in the embedded phase can be quite massive relative to their central stars (e.g., Osorio et al. 2003). GIs may also occur in the outer regions of older disks (e.g., D'Alessio et al. 1999).

GIs also present an alternative to the core accretion plus gas capture scenario for gas giant planet formation (Pollack et al. 1996, Hubickyj et al. 2005, Durisen et al. 2007a, Lissauer & Stevenson 2007). The so-called "disk instability" theory posits that GIs cause disks to fragment dynamically into dense bound gas giant protoplanets (Kuiper 1951, Cameron 1978, Boss 1997, 1998, 2001, 2002a,b, Mayer et al. 2002, 2004). A discussion of the full debate between core accretion and disk instability goes beyond the scope of this proposal. Here, we focus on GIs as a disk process. Even from this narrower perspective, there are some critical issues. Although there is currently general agreement about the conditions necessary for disk fragmentation (Gammie 2001, Rice et al. 2003, 2005, Johnson & Gammie 2003, Mayer et al. 2004, Mejía et al. 2005, Michael et al. 2007), namely, that disks must simultaneously be sufficient cold or massive ($Q <$ about 1.5) and also cool sufficiently fast (cooling time $t_{cool} \sim P_{rot}$ or less, where P_{rot} is the orbital period), there is strong *dis*agreement about whether fragmentation occurs in 3D disks with realistic radiative cooling and equations of state. Some simulations of this type show fragmentation (Boss 2001, 2002a,b, 2004a, 2005, Mayer et al. 2007), but analytic arguments (Matzner & Levin 2005, Rafikov 2005, 2006) and other similar simulations (Nelson et al. 2000, Cai et al. 2006, Boley et al. 2006, Stamatellos & Whitworth 2007) indicate no fragmentation. The issues of clump longevity and numerical fragmentation are also somewhat murky (e.g., Nelson 2006, Pickett & Durisen 2007).

1.3 Objectives and Significance

In this proposal, we present accomplishments and ongoing efforts by our group toward clarifying our understanding of GIs as a transport and a planet formation mechanism in protoplanetary disks. Our most recent work on radiative transport in disks (see Sections 2.2 & 3.2) convinces us that rapid cooling due to convection (Boss 2004a, Mayer et al. 2007) does not occur (Rafikov 2006) and that fragmentation is generally unlikely in real disks. We therefore concentrate the proposed research on processes in non-fragmenting protoplanetary disks. Our 3D radiative hydrodynamics code with self-gravity is specifically designed for global simulations. We can simulate GI-active disks in 3D over significant time durations for a global range of radii, we can include radiative transport with realistic dust opacities and some forms of irradiation, we can employ a variety of equations of state, and we have many useful analysis tools. We propose to continue research in three general Project Areas – Environmental Effects, Gas-Solid Interactions, and the Unified Theory.

1.3.1 Project Area # 1: ENVIRONMENTAL EFFECTS

Research to date (Durisen et al. 2007a) indicates that GIs are sensitive to radiative and physical boundary conditions. The gas dynamics in the simulations proposed below will be done in 3D with our radiative hydrodynamics code.

Project 1a – Stellar Irradiation. As reviewed in Dullemond et al. (2007), at different stages of evolution, disks can be irradiated by starlight reprocessed by an infalling envelope (e.g., Chick & Cassen 1997), by light from its central star directly illuminating the topmost layers of the disk (e.g., Natta 1993, Chiang & Goldreich 1997, D'Alessio et al. 1998, 1999), and by UV from nearby hot stars (e.g., Johnstone et al. 1998). Often, the radiation we observe from disks around young stars is reprocessed starlight, and many of the interesting spectral features are formed in layers with complex thermal structure above the IR photosphere of the disk interior. These outermost layers are presently impractical to model in our 3D hydro calculations. Our simulations explicitly model the interiors of disks, usually optically thick, which contain most of the mass. We accommodate envelope irradiation in our code as an infrared flux shining down on the disk from above and find that its effects on GIs are complex and quite strong (see Section 3.2). As a first approximation suggested by new collaborator Hartmann, we can also treat stellar irradiation as a boundary IR flux from the upper layers (not modeled in the code) radiating down onto the lower layers of the disk. In this simple picture, the main difference from envelope irradiation would be the radial dependence of the irradiating flux. Cai and Co-I Steiman-Cameron already have some simulations of this type underway.

GIs produce strong spiral corrugation of the disk's IR photosphere. We do not yet know how far this extends into the upper hotter atmospheric layers exposed to starlight, because we have not yet been able to include these layers in our modeling. A changing strength of irradiation will feed back into the strength of GIs, their dominant modes, and the resultant mass transport (see Section 3.2). To get a handle on how surface distortions and shadowing might affect irradiation, we will perform 2D and 3D studies, with simplified physics, of the response of a hot upper layer to shock bores (Boley & Durisen 2006), the hydrodynamic structures in GI-active disks that distort the surface. We will then develop approximate ways to modulate IR irradiation in our full radiative 3D calculations due to surface distortions by GIs and study the resulting feedback. At the same time, we will attempt direct modeling of energy deposition by starlight in our 3D hydro calculations. A flawed preliminary effort by Mejía (2004) suggested that the effects on GIs could be severe. With our new-gained experience with ray methods (see Section 2.2), we will explore the possibility of including rays of illumination from the star hitting the disk upper layers, beginning with 2D equilibrium models similar to but simpler than those of D'Alessio et al. (1999). We will then adapt the scheme to 3D if possible or use the outcome of 2D models to heuristically impose realistic time variations in our IR illumination of the optically thick interior disks.

Project 1b – Infall. Another feedback mechanism for GIs is their interaction with infalling material. This can act directly as a mechanical boundary condition and source of mass accumulation leading to or sustaining unstable conditions, or it can act indirectly through irradiation by the accretion shock or by starlight reprocessed in the infalling envelope. Although we have already considered envelope irradiation, we have not applied ray methods to model the scattering and reprocessing of starlight by the envelope. This does not have to done in full time-dependent 3D, but could be treated in a 2D steady state to generate appropriate incoming IR boundary fluxes for IR irradiation simulations. We have so far included mechanical effects of infall and/or mass accumulation in only a few preliminary simulations. Simulations by Vorobyov & Basu (2005, 2006), with relatively crude modeling of the disk, suggest that, during the main infall phase, massive disks may undergo repeated bursts of GI activity which resemble FU Orionis outbursts. One way in which we plan to extend our current dead zone outburst models is to include disk-wide accumulation of mass though infall.

Project 1c – Binary Companions. By making a single star/disk system model using parameters deduced by Osorio et al. (2003), Cai et al. (2007) showed that the circumstellar disks in the L1551 IRS 5 binary system will be strongly GI active. The presence of a binary companion can have profound consequences for a disk (e.g., Lubow & Artymowicz 2000), but there have only been a few investigations of how interactions in binaries affect GIs in disks. Simulations by Nelson (2000) suggest that tidal stresses by companions tend to heat disks drastically and suppress GI instability and fragmentation, while those by Mayer et al. (2005) and Boss (2006) suggest that fragmentation can be enhanced under some conditions by binary perturbations. Collaborator Pickett plans to continue efforts already underway to include effects of binarity by centering our star/disk system in one lobe of a Roche potential and including the fictitious forces due to the accelerated frame in the hydro equations. We will later implement the gravitational back-reaction of the star/disk system on the companion star and irradiation of the outer disk edge by the companion star.

1.3.2 Project Area #2: INTERACTIONS OF GAS AND SOLIDS

As described in Section 2, we are currently coupling particle trajectory integration routines with our 3D radiative hydro code.

Project 2a – Planet Migration in a GI-Active Disk. Several effects are now known that can moderate the rate and even the direction of planet migration due to interactions with a disk (Papaloizou et al. 2007, Matsumura et al. 2007). By integrating the motion of a single massive particle, we will investigate how a planet migrates in a gravitoturbulent disk, i.e., one that is undergoing sustained GI activity, where heating by instability and radiative cooling achieve an overall balance (Gammie 2001, Lodato & Rice 2004, Mejía et al. 2005, Boley et al. 2006). Mayer et al. (2004) and Boss (2005) have examined migration in the context of fragmenting disks, a scenario we consider unlikely, and they report relatively modest migration. Our typical high-resolution 3D grids 512x512x64 in (r,ϕ,z) are comparable to those used successfully by Nelson & Papaloizou (2003, 2004) to study migration of planets with masses of 0.03 to 3 M_J (Jupiter masses) in global disks with MRI turbulence. Because our disks will be more massive, we may be restricted to treatment of the higher end of their mass range. The major differences between the MRI case and ours are that our disks are self-gravitating and that GI-induced turbulence is dominated by global modes.

Project 2b – Effects of Settling & Grain Growth on GIs through Radiative Physics. Dust opacity controls GIs through the cooling time scale $t_{cool} = \epsilon/\nabla \cdot F$, where ϵ is the internal energy density and $\nabla \cdot F$ is the divergence of the radiative flux. Our simulations to date use D'Alessio opacities (D'Alessio et al. 1998) which assume a distribution $\sim a^{-q}$ of particle radius a, with q usually 3.5, a minimum $a_{min} = 0.005$ μm, and an adjustable maximum a_{max}. Collaborator Calvet has the D'Alessio opacity routines and will provide tables with varied q, a_{min}, and a_{max} as needed. As in all GI simulations with radiative transport, our monochromatic treatment uses Rosseland and Planck mean opacities (see Boley et al. 2006, 2007b). As a_{max} is changed, the T-dependence of the mean opacities varies in a complex way that has considerable impact on GI strength (Cai et al. 2006). For instance, outer disks ($T < 100$ K) become more optically thick and inner disks more optically thin in the Rosseland mean as a_{max} is increased from 1 μm to 1 mm (see Figure 16 of Boley et al. 2006). Growth and settling of dust seems to occur at all observable phases of gas disk evolution (e.g., D'Alessio et al. 2001, 2006, Furlan et al. 2006, Hernandez et al. 2007, Dullemond et al. 2007). The theoretical connection between GI amplitudes and t_{cool} is also well established (e.g., Gammie 2001, Mejía et al. 2005, Durisen et al. 2007a).

Growth and settling of grains will have a profound influence on the occurrence and behavior of gas-phase GIs through the changing opacity. In an initial effort, we will decrease the dust opacity by a depletion factor $f(r,t)$ in accordance with growth and settling models of other researchers (e.g., Weidenschilling 1997, Dullemond & Dominik 2004, Johansen et al. 2006) to account for loss of grains due to growth and settling of centimeter and larger-sized particles. A next level of sophistication would be, as in D'Alessio et al. (2006), to introduce two vertical opacity regimes, one of "large" dust grains ($a_{max} \sim 1$ mm) confined within a fraction of a vertical scale height from the midplane and the other of "small" particles ($a_{max} \sim 1\mu$m) distributed throughout the gas. The fraction of solids in the two layers and the height of the large-grain layer could also be varied with time. In this case, the mass in both grain layers could be depleted to mimic the production of large particles (> centimeters) that no longer contribute significantly to the opacity. The large dust grains then represent an opacity-affecting population that is currently settling or is produced by collisions and commutation of the larger (> centimeters) settled particles. Once we have some experience from Project 2c below on how the large particles couple to GIs in our simulations, we could include feedback between the onset and strength of gas-phase GIs and the height, content, and r,ϕ-distribution of the large-grain opacity zone.

Project 2c – Stirring, Settling, & Particle Concentration. By integrating particles simultaneously with their SPH hydrodynamics, Rice et al. (2004, 2006) have already demonstrated that particles with meter size will be swept rapidly into GI structure by drifts due to gas drag and possibly lead to an accelerated rate of planetesimal formation. In some respects, this is similar to the idea that growth and settling lead to instability of a particle subdisk (e.g., Youdin & Goodman 2005, Johansen et al. 2006, Fromang & Papaloizou 2006). Unlike Rice et al., we plan to study a larger portion of parameter space and will have a proper treatment of radiative transport in our hydrodynamics. Initially, we will examine the gravitational buffetting of large particles that are not subject to gas drag (> 100's m) by the gravitoturbulence of a GI-active disk. We will determine how rapidly particles diffuse vertically and radially. Preliminary calculations suggest significant changes in orbit parameters within just five to ten orbits due to the global nature of GI turbulence. After exploring this regime, we will implement gas drag terms (Weidenschilling 1977, Haghighipour & Boss 2003) in the particle equations of motion and model particles ($\sim$ meter) that drift in response to gas drag. We then plan to include the back-reaction drag terms in the hydrodynamics and particle self-gravity. Methodologies for including particles are discussed in Section 2.3 and are already partially developed. All these particle-plus-hydro simulations will be 3D and global, because, as we have shown (Mejía et al. 2005, Boley et al. 2006, Cai et al. 2007), gravitoturbulence is dominated by low-order global modes and the vertical structure can be significantly disturbed (Boley & Durisen 2006).

1.3.3 Project Area #3: THE UNIFIED THEORY

Project 3a. – Bursting Dead Zones. As part of his dissertation, IU graduate student Boley is computing ultra-high-resolution, i.e, 512x1024x128 in (r,ϕ,z), 3D radiative hydro simulations of dead zones that have accumulated enough mass to undergo an outburst of GI activity. When GIs initiate from quiescent conditions, they often "burst" in just one (or several) low-order (few-armed) global modes (Mejía et al. 2005, Boley et al. 2006). These modes become extremely strong, driving the strongest shocks and hydraulic jumps that we typically see in GI simulations. This is of particular interest for chondrule production, annealing of solids, and mixing (see also Boss 2004b on mixing). Boley's current disk models for this problem are fairly massive ($\sim 0.15\ M_{\odot}$ from 1.5 to 10 AU) with an enhanced ring around 5 AU about 6 AU wide. This is not intended to be realistic, but to prejudice the outcome toward shock-processing of solids, as a test of concept. Fluid element trajectories will be analyzed to determine the shock conditions experienced by entrained dust (e.g., Desch & Connolly 2002) in collaboration with S. Desch (ASU). Boley already finds that it is difficult to achieve strong enough shocks because the cooling times in the opaque inner disk are long, and he is running companion cases where the dust opacity is artificially reduced, presumably by growth and settling (as in Hubickyj et al. 2005). With shorter t_{cool}, the shocks are stronger, but there is no indication of disk fragmentation. Mass inflow rates into the innermost disk are at FU Orionis levels.

Boley will complete this initial study under current funding. With the advice and consultation of new collaborator Hartmann, we will modify our bursting dead zone models in directions that seem the most promising for further study. For instance, if some settling of solids is necessary to lower t_{cool} in order for a bursting dead zone to process chondrules, this suggests a scenario where a quiescent dead zone grows in mass and cools as solids settle. The strong GI outburst that ensues may then simultaneously shock-process solids, drive a high mass inflow rate into the inner disk to trigger a visible FU Orionis outburst by thermal instability (Bell & Lin 1994, Hartmann et al. 2007), stir up the settled layer, accelerate planetesmal formation (Boley et al. 2005, Rice et al. 2006), heat and drain the dead zone back to stability, and allow the process to repeat again on a settling time scale. Obviously, this is very speculative, but we plan to use our growing collection of simulation tools to pursue these and other ideas.

Project 3b. – Planet Formation. There are hybrid theories of gas giant planet formation that invoke hydrodynamic processes to accelerate core accretion (see, e.g., Klahr & Henning 1997, Klahr & Bodenheimer 2006). In particular, structures created by GIs in disks can be places where solids are concentrated and can grow quickly (Haghighipour & Boss 2003, Pickett & Lim 2004, Rice et al. 2004, 2006, Durisen et al. 2005). As all our proposed projects move forward, we will be attentive to applying our particle-plus-hydro techniques to conditions which seem favorable for accelerated core formation. It is difficult to be specific at this time, but we already know that GIs produce radial concentrations of mass and possibly even long-lived ring-like structures (Pickett et al. 2003, Mejía et al. 2005, Boley et al. 2006, Cai et al. 2007). We will be especially interested in looking at what happens to particles during a dead zone burst.

1.3.4 Limitations.

All these projects involve 3D hydrodynamics simulations using explicit time integration. For disk modeling, even with central holes, the Courant time-step-limitation of explicit hydrodynamics means that we typically only follow disk evolution over several to tens of outer disk rotations. Others who simulate dynamic instabilites in full 3D experience similar constraints. Using 20 outer rotations as a norm, simulations of disks for solar mass systems typically span about $2\text{x}10^4$ $(R_d/100\text{ AU})^{3/2}$ years, where R_d is the outer disk radius. For large R_d, we must sacrifice treatment of the inner disk by using a several AU central hole. Clearly we cannot yet follow the entire dynamic evolution of a protoplanetary disk nor model all the radiative and particle processes of interest at once in full 3D. With judicious experimentation, however, we can elucidate how these processes will interact with and affect GIs in disks. By following GI simulations to their asymptotic states, when these exist, we can extraploate the consequences over much longer times (e.g., Boley et al 2006).

2. TECHNICAL APPROACH AND METHODOLOGY

2.1 General

Nonlinear evolutions of disks undergoing GIs, even local thin-disk treatments (e.g., Johnson & Gammie 2003), are sufficiently complex that they must be done numerically. With the growing realization that GIs are intrinsically global 3D phenomena (Boley & Durisen 2006, Boley et al. 2006), that they are sensitive to the treatment of radiative transport (Durisen et al. 2007a), that real disks are affected by a variety of radiative environmental influences (Dullemond et al. 2007), and that gas-solid interactions may play a role on short time scales (Rice et al. 2004, 2006), useful contributions now require sophisticated approaches.

2.2 2D Star/Disk Equilibrium Models

We create starting models with a modified Hachisu-style (1986) self-consistent-field (SCF) code (Pickett et al. 2003, Mejía et al. 2005). We can produce axisymmetric (2D) star/disk equilibrium models with power-law surface density distributions $\Sigma(r) \sim r^{-p}$ for the disks and with a wide range of ratios of disk to stellar radius R_d/R_s of disk to stellar mass M_d/M_s. The SCF method requires that the pressure P is a function of density ρ only, so we use a polytropic relation, $P = K\rho^{\gamma}$ where K and γ are constant. By putting these models into a 2D version of our hydro code, we can adjust the temperature structure of the disk and carve out the central star. Cai recently developed the capability of reproducing Boss's (2002a,b) approximate analytic disks, while Boley is now able to accumulate disks slowly by accretion as in Mayer et al. (2004).

2.2 Radiative Hydrodynamics

Hydrodynamics. Our primary computational tool is a heavily modified version of the Pickett (1995) code, which solves the hydrodynamics equations to second-order accuracy in space and time on an (r,ϕ,z) cylindrical grid assuming reflection symmetry through the equatorial plane. It has an energy equation and includes a vonNeumann-Richtmeyer artificial viscosity to mediate shocks. Poisson's equation is solved on the grid by first Fourier transforming the density. The resulting 2D Poisson-like equations in r,z for each Fourier component of the potential is solved directly. This solver requires a boundary potential which is determined on the outer grid boundary by using a multipole expansion up to $m = l = 10$. Performance is comparable to that of other second-order schemes for 3D hydrodynamics (Bowers & Wilson 1991, Stone & Norman 1992, Boss & Myhill 1992, Smith *et al.* 1994). The code runs in parallel on shared memory machines in OpenMP and is now being parallelized in MPI to run on massively parallel machines with distributed memory. The excellent computational facilities available to our group are described in the *Budget Narrative* of this proposal. Up to now, we have kept the star fixed at the center of the grid coordinates. Michael, working with Pickett, is implementing routines which free the star and include its gravitational interaction with the disk. Pickett now is adding the capability of placing the star/disk system in the Roche lobe of a binary system. In recognition of the uncertainties introduced by the techniques embodied in any one code, we have code comparisons underway with other researchers (see Section 3.2).

Radiative Energy Transport: the Cai/Mejía Schemes. Mejía (2004) implemented 3D flux-limited radiative energy diffusion (Bodenheimer at al. 1990) with D'Alessio opacities in the optically thick part of our simulations. A boundary condition for the diffusion problem is provided by measuring the Rosseland mean optical depth τ vertically downward. The photosphere at $\tau = 2/3$ divides the disk into the optically thick interior and an optically thin atmosphere. The atmosphere is modeled explicitly for several reasons: Optically thin regions occupy a nonnegligible fraction of the disk volume (Cai et al. 2006), shock bores produced by GIs disproportionately heat the upper layers of stratified disks (Pickett et al. 2000, Boley & Durisen 2006), most forms of external irradiation are absorbed high in the disk atmosphere (Dullemond et al. 2007), and GIs are sensitive to vertical boundary conditions and irradiation (Cai et al. 2007). The Mejía scheme includes optically thin radiative cooling for $\tau < 2/3$, tallies radiation emitted upward and downward, and includes heating by upward moving photospheric photons. The radiant flux shining down on the photosphere is used to fit an Eddington atmosphere across the thin/thick boundary cell. The atmosphere is thus radiatively coupled to the optically thick region, and the Eddington fit sets the boundary condition for the flux-limited diffusion solver. Cai made several improvements and allowed for external downward IR irradiation at the top of the grid. Thin/thick radiative coupling is only incompletely captured by the Cai/Mejía schemes, as shown in Figure 1 by comparison with an analytic solution (based on Hubeny 1990). They both produce an overcool atmosphere with a sharp temperature drop near the photosphere. Nevertheless, the Eddington fit guarantees the correct boundary flux to within a few percent, i.e., the correct amount of heat is removed from the optically thick interior.

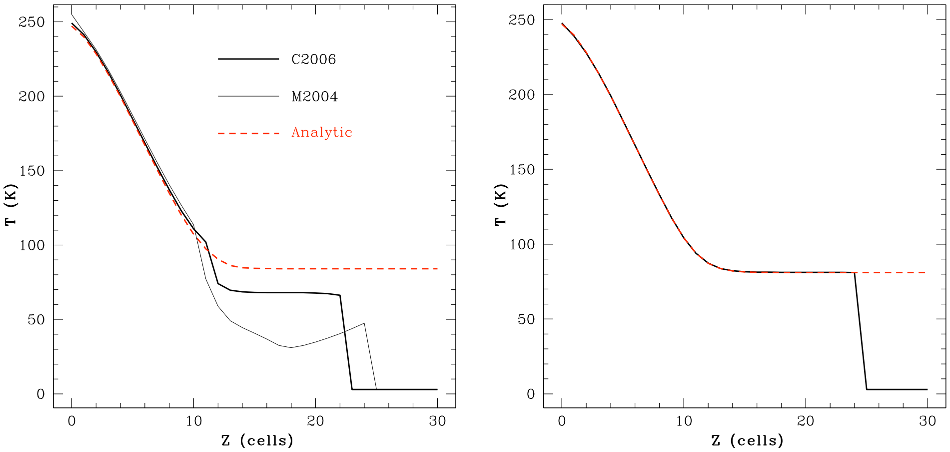

Figure 1. (Left Panel) Comparison of the temperature distributions given by the Mejía (2004) (light grey) and Cai (2006) (solid black) radiative cooling algorithms with an analytic steady-state solution for a slab (red dashed). (Right Panel) The same for the new BDNL scheme (Boley et al. 2007b). The discontinuities at vertical cell 12 are the photosphere; the ones near vertical cell 25 are the boundary above which no radiative physics is done.

Radiative Energy Transport: the BDNL Scheme. During current funding, a major advance in our techniques has been the development and testing of a new radiative scheme. Inspired by a yet unsuccessful effort to implement the Heineman et al. (2006) multi-ray radiative transfer scheme in cylindrical coordinates, Boley produced the hybrid BDNL scheme (Boley et al. 2007b). The vertical direction is solved by a one-ray discrete ordinate method over the whole thin/thick regime. For cooling in the energy equation, the ray solution is used to compute the z-contribution to the flux divergence for all τ. Flux-limited diffusion is still used to transport energy and compute flux divergence in the r and ϕ directions for the optically thick regions. As shown in Figure 1, the BDNL scheme reproduces the analytic temperature distribution to high accuracy. Results are similarly good for the vertical radiative flux. We also demonstrate as part of our tests that our routines model convection when convection should occur and that convection does not lead to substantially reduced cooling times.

Equation of State. Using local thin-disk shearing box simulations, Gammie (2001) showed that disks of ideal gas with a ratio of specific heats $\gamma = 5/3$ will fragment into dense bound clumps when $t_{cool}\Omega < 3$ or so. This criterion has been confirmed by 3D simulations (Rice et al. 2003, Mejía et al. 2005). Rice et al. (2005) found that, if γ is reduced to

7/5, the fragmentation occurs more easily, namely, for $t_{cool}\Omega < 12$ or so. Yet-unpublished simulations by Michael with our own code confirm this. It thus becomes important to include a proper gas equation of state (EOS), if we wish to determine whether a disk will fragment. Over temperatures of interest, we expect the H_2 EOS to make a transition from 5/3 to 7/5 behavior. Current collaborator Hartquist (U. Leeds) worked with us (Boley et al. 2007a) to compute correct H_2 EOSs for various assumptions about the ortho/para hydrogen ratio. As shown in Figure 2, the dynamic response of a GI unstable disk, as measured by the adiabatic index Γ_1, can be severely affected by H_2. Piecewise approximations (dashed curve in Figure 2) may produce a reasonable $e(T)$ but result in sharp features in Γ_1 that might make a disk artificially susceptible to fragmentation. We have implemented the new H_2 EOSs into our code, together with helium, heavy elements, and dust.

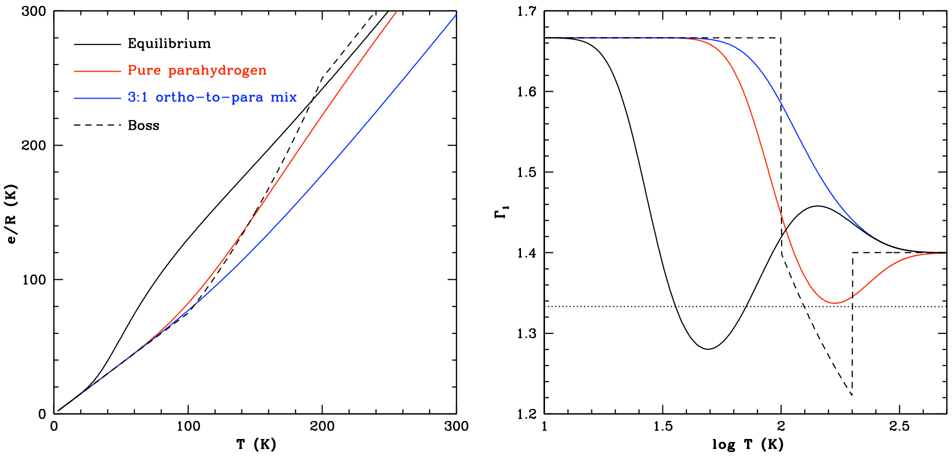

Figure 2. The equation of state for molecular hydrogen. (Left Panel) The correct internal energy for various assumptions about ortho-to-para hydrogen, plus the interpolation used by Boss (2007a). (Right Panel) The adiabatic Γ_1 for these internal energies.

2.3 Other Computational Tools

Analysis of Modes, Torques, & Stresses. In the asymptotic state of GI-active disks, where heating and cooling are balanced, strongly nonlinear turbulence infects the whole disk (Pickett et al. 2003, Mejía et al. 2005, Boley et al. 2006). Fourier decomposition of the density allows us to determine amplitudes and pattern periods for dominant modes even when they are difficult to discern by visual inspection. Important evidence that GI mass transport is dominated by low-order global modes, as reported in Section 3.2 below, was obtained in this way. For Boley et al. (2006. 2007b), we developed new analysis tools which allow us to measure the gravitational and, to a lesser degree, hydrodynamics stresses from stored simulation data, as done in 2D by Gammie (2001) and in SPH simulations by Lodato & Rice (2004, 2005). This has permitted accurate computation of effective α's due to gravity for comparison with analytic predictions (Pringle 1981, Gammie 2001).

Fluid Element Tracing & Shock Detection. Our hydro code is Eulerian and grid-based. For studies of chondrule formation by GI-induced shocks (Boley et al. 2005), we need to know the thermodynamic history of Lagrangian fluid elements. Boley now uses the velocity field calculated by the hydro code in real time to integrate trajectories of select fluid elements during a computation. The kinematic problem is not difficult in itself, but post-analysis of the thermal histories to determine whether entrained dust will be processed in shocks is rather tricky. Boley has made considerable progress. We plan to use these data, under current funding, to look at shock-processing of dust and time-dependent gas-phase chemistry with our current collaborators Hartquist and Desch, respectively.

Particle Integration Routines. Large particles, like planetesimals and planets, are unaffected by gas drag but will respond to the fluctuating gravitational field of the GI turbulence. For Projects 2c and 3b, we will use a fifth-order Runge-Kutta, with an embedded fourth-order scheme for error estimation, to integrate the trajectories of between 10^5 to 10^6 particles or more in conjunction with computation of the hydrodynamics. The hardest part of the integration is interpolating the gravitational force due to the gas to the current positions of the particles, while only knowing the potential at the cylindrical grid points. By using a modified Shepard's method (Renka 1988), Michael can now interpolate all force components to within parts in 10^4. This is over an order of magnitude better than with conventional interpolation schemes. We are now testing particle stirring by the fluctuating gravitational field of a GI-active disk. For the planet migration Project 2a, we will add the potential from the planet to the hydrodynamic calculation, with smoothing of the planet's potential around the planet on a scale of several grid cells. For Projects 2c and 3b, we will examine particles (centimeters to meters sizes) that experience significant gas drag and drift. This requires the addition of gas drag forces to the particle integration (Haghighipour & Boss 2003). To account for particle self-gravity and the back-reaction on the hydrodynamics of the drag on the particles, we will envision the integrated particles as a sample of a much larger population and use a kernel estimation method (Monaghan 1992), similar to that implemented by Youdin & Johansen (2007), to calculate back-reaction forces and particle densities at hydrocode grid cells. The densities will be added to the gas density when computing potentials for the particle and gas integrations.

3. PERCEIVED IMPACT AND PRIOR ACCOMPLISHMENTS

3.1 Perceived Impact

Gas-phase GIs are one of the major processes that can occur in protoplanetary disks. Even if they do not produce planets directly, they are likely to play an important role in disk evolution and the planet formation process (Boss & Durisen 2005a,b, Durisen et al. 2007a). Simulations by our group have been instrumental (e.g., Pickett et al. 1998, 2000) in demonstrating the critical importance of thermal physics for controlling the amplitude and outcome of GIs, as originally suggested in Goldreich & Lynden-Bell (1965) (see also Tomley et al. 1992, 1994). Much of the research under current funding has been devoted to understanding whether direct planet formation by GIs (Boss 1997, 2001, 2002a,b, Mayer et al. 2004, 2007) is possible for disks undergoing realistic radiative cooling (Cai et al. 2006, Boley et al. 2006, Boley et al. 2007b). Because GIs are sensitive to cooling, they are sensitive to the boundary conditions for energy transport. 3D radiative hydrodynamics is difficult, and we have tried to lead the way by painstaking work on treatment of optically thick and thin boundaries in our simulations. We are convinced that, for the conditions in current simulations of realistic radiative cooling, direct disk fragmentation into planets should not occur. Instead, we suspect that planet formation is assisted by the interaction of gas-phase GIs with embedded solids (Haghighipour 2005, Durisen et al. 2005, Rice et al. 2004, 2006). Understanding of planet formation and other phenomena which may be distantly or directly related to planet formation, like chondrule production, annealing of solids, and FU Orionis outbursts, requires study of how GIs interact with solids and how the radiation environment and opacity changes due to settling affect and modulate GIs. This proposal addresses all these areas. In addition, we will examine planet migration in the background of a GI-active disk and explore how GIs are affected by a binary companion. For all these problems, we will be performing global 3D simulations using our latest, well-tested radiative routines.

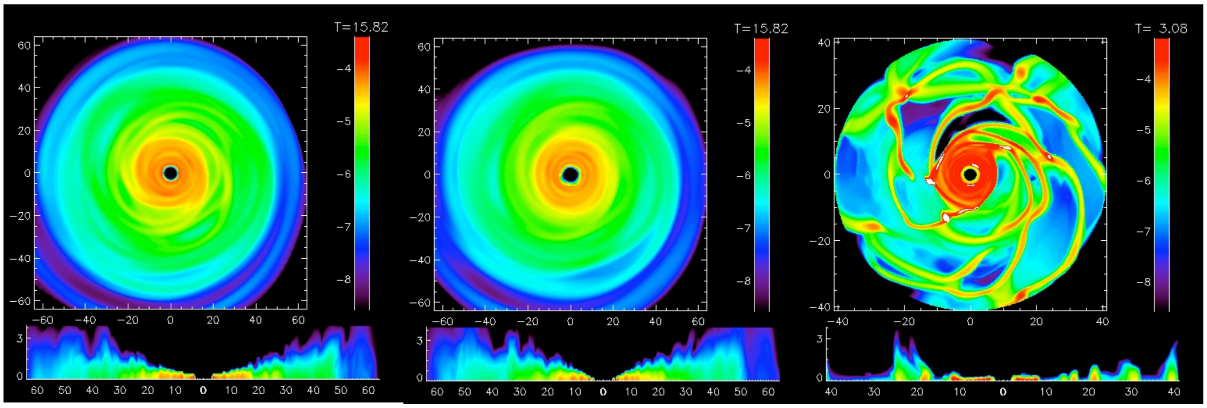

Figure 3. Logarithmic color-scale of the midplane density and meridional cross-sections for three simulations. Length units are in AU. The starting model for all three cases is a 0.07 $M_\odot$ disk of $\gamma = 5/3$ ideal gas with an initial radius of 40 AU orbiting a 0.5 $M_\odot$ star. For the left two images (130 AU on a side), the initial surface density is $\Sigma \sim r^{-1/2}$. (Left Panel) The disk at time $t = 15.8$ orp $\approx$ 4,000 yr evolved with the Mejía (2004) scheme (Boley et al. 2006). (Middle Panel) The same disk at the same time evolved with the BDNL radiative scheme (Boley et al. 2007b). (Right Panel) A $\Sigma \sim r^{-1}$ disk at $t = 3.1$ orp evolved with idealized $t_{cool} = 0.6$ orp cooling (MIchael et al. 2007). The box in this panel is 80 AU on a side.

3.2 Accomplishments under Current Funding.

Publications, Presentations, & Student Participation. Since the start of current funding on June 30, 2005, our group has published two review articles (Boss & Durisen 2005b, Durisen et al. 2007a), five referred journal articles (Cai et al. 2006, Boley & Durisen 2006, Boley et al. 2006, Pickett & Durisen 2007, Boley et al. 2007a), one popular science article, and one refereed paper in a conference proceedings (Boley et al. 2005). Another invited review is in press (Durisen 2007), another journal article has been accepted (Boley et al. 2007b), one is under review (Durisen et al. 2007b), and ten contributed posters or talks have been given at meetings. The PI gave five invited talks on "Disk Hydrodynamics" at a workshop on disks in Vidago, Portugal that will become a chapter in a book. The PI is also scheduled to give a review talk and co-author a review paper for the meeting on *Structure Formation in the Universe* in Chamonix, France in May 2007. The PI repeated the Vidago lectures at Indiana University and will repeat them again at MPI-Astronomy in Heidelberg, Germany in June 2007. Additional journal articles are in an advanced stage of preparation (Cai et al. 2007, Michael et al. 2007). Since June 2005, one Ph.D. dissertation (Cai 2006) has been completed, and two others are in progress (Boley and Michael). Boley is supported by a NASA GRSP Fellowship. Undergraduate J.W. Lord participated in our research during Summer 2006 as part of IU Astronomy's NSF-funded REU program.

Realistic Radiative Cooling. The development of the new and better BDNL radiative cooling algorithm and rigorous testing of our new and old routines against anayltic solutions (Section 2) are highlights of work under current funding. Boley et al. (2007b) reran the post-burst phase of the Boley et al. (2006) simulation to demonstrate, as shown in Figure 3, that the new routines give essentially the same answer as the old routines. Our now well-tested algorithms, both old and new, are consistent with the analytic arguments of Rafikov (2005, 2006) that the planet forming regions of disks with realistic dust opacities do not cool fast enough to fragment. Our code is capable of detecting and modeling convection, and convection does not lead to rapid cooling. We challenge all researchers in this field to demonstrate that their radiative codes can pass our tests. Another important result from our work on radiatively cooled simulations is confirmation (Boley et al. 2006) that transport by GIs in non-fragmenting disks is dominated by low-order global spiral modes (see also Balbus & Papaloizou 1999, Mejía et al. 2005).

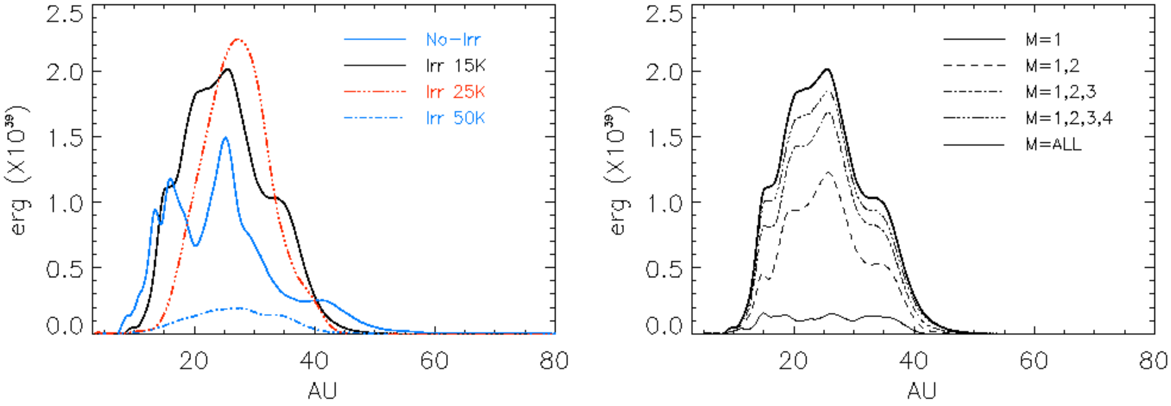

Figure 4. Gravitational torques at late times in simulations of the same disk as in the left two panels of Figure 3 with radiative cooling and envelope irradiation (Cai et al. 2007). (Left Panel) A comparison of the torques for different values of the irradiation temperature T_{irr}. (Right Panel) A decomposition of the torque into contributions by spirals with different numbers of arms for $T_{irr} = 15$ K. Global two-armed modes contribute half the torque and produce the dominant features in the torque profile.

Envelope Irradiation, Metallicity, & Grain Size. Cai (2006) completed his dissertation on the effects of irradiation from a surrounding envelope, as represented by a uniform σT_{irr}^4 IR flux shining vertically downward. Cai used the 0.07 $M_\odot$ Mejía (2004) disk with an $r^{-1/2}$ surface density distribution orbiting a 0.50 $M_\odot$ star and our standard D'Alessio opacities with $a_{max} = 1\mu$m. As reported by Cai et al. (2007), in disks evolved over 15 outer rotation periods (about 3,800 years) with $T_{irr} = 15$ and 25 K, the amplitude and effective α's of the GIs decrease as T_{irr} increases, and the disks are farther from fragmentation than the non-irradiated case. This is not surprising, because at $T_{irr} = 25$ K, ten times more energy is irradiated into the disk than is released by GI-activity. On the other hand, as shown in the left panel of Figure 4, the torques (and mass inflow rates) are *larger* for $T_{irr} = 15$ and 25 K than for $T_{irr} = 0$ K. We find that this occurs because irradiation selectively suppresses higher-order multi-armed spiral modes, while leaving the dominant two-armed modes unaffected. This is further evidence that it is the global low-order modes that are most effective at producing mass and angular momentum transport. The right hand side of Figure 4 illustrates the point quantitatively by decomposing the torques by azimuthal mode number. When T_{irr} is increased to 50 K late in the 25 K run, all the GIs damp on a cooling time. These results are motivation for Project 1a. GI transport is strongly affected by irradiation and will respond on the time scale t_{cool} to spatiotemporal variations in T_{irr} due to shadowing effects in stellar irradiation. Substantial modulation of the mass transport is possible.

When Cai et al. (2006) recomputed the $T_{irr} = 15$ K case with metallicity Z ranging from 1/4 to 2 solar for the same a_{max}, he found that, as Z increases, t_{cool} increases and GI amplitudes decrease. No fragmentation was seen in any simulation. This is very different from Boss (2002a) who found fragmentation for Z ranging from 0.1 to 10. Increasing a_{max} to 1mm weakens GIs and increases t_{cool}. Cai et al. (2007) also studied the evolution of a disk with parameters chosen to match the α-disk model for one of the circumstellar disks in the L1551 IRS 5 system as determined by Osorio et al. (2003). Despite intense irradiation

(120 K), this disk is violently unstable in a global low-order mode. This result is part of the motivation for Project 1c.

Shock Bores. Boley et al. (2005) and Boley & Durisen (2006) have shown that the strong corrugation of the disk surface due to GIs noticed in our earlier work (Pickett et al. 2000, 2003) is due to spiral "shock bores", with the combined characteristics of both shocks and hydraulic jumps (Martos & Cox 1998). Large-scale transient breaking waves occur with vertical "jumps" of a scale height or more, and strong mixing on orbit period time scales occurs over even greater radial distances (see also Boss 2004b). As described in Boss & Durisen (2005a,b), as well as in the Boley papers, eruptions of GIs associated with gas giant formation may have produced the spiral shocks responsible for chondrule melting in the Solar Nebula.

Initial Conditions & Equation of State Comparisons. Michael is completing a large suite of simulations using an artificial volumetric cooling rate $\Lambda = \epsilon/t_{cool}$, with constant t_{cool}, as in Mejía et al. (2005). He has varied $t_{cool}\Omega$, the initial power-law surface density, the assumed value of the adiabatic γ, and the nature of the initial perturbation (Michael et al. 2007). We agree with the Gammie (2001) fragmentation criterion of $t_{cool}\Omega <$ about 3 for $\gamma = 5/3$ (right panel of Figure 3) and with an increase of this limit to about 10 to 12 for $\gamma = 7/5$ (Rice et al. 2005). This is direct evidence that, contrary to a recent criticism by Boss (2007b), our code does detect fragmentation when it really should occur. As a subproject, Michael is simulating the inner disk region at much higher resolution to test whether ring formation in the inner disk (Mejía et al. 2005, Durisen et al. 2005, Boley et al. 2006) is real or a numerical artifact.

Unified Theory for Chondrules, FU Orionis Outbursts, & Planet Formation. During current funding, Boley determined that the Mach number distribution of shocks encountered by fluid elements in fully developed gravitoturbulence roughly follows a Boltzmann law. This does not produce enough chondrule forming events. So, if chondrules form through GI-induced shocks, it must happen in a burst. Boley has been devoting most of his recent efforts to producing ultra-high resolution simulations of a bursting dead zone (see Sections 1.3.3 and 2.3).

Numerical Issues & Code Comparisons. Two code comparisons are underway that we plan to complete by the end of current funding. In collaboration with Boss and Pickett, Cai has reproduced the Boss (2002a,b) initial disk and perturbation conditions and then integrated this disk with our Cai/Mejía routines. The initial perturbation damps substantially after a few rotations. When we try to run the simulations with an approximation to Boss's own radiative boundary conditions, the simulation produces clumps. However, there are some strange numerical behaviors in the latter run that must be understood before we can draw any conclusions. Through Mejía and now Boley, we are also participating in the Wengen Tests led by L. Mayer (U. Zurich), where the same highly unstable disk is being evolved isothermally by many different codes. This comparison verifies that, contrary to comments in Boss (2007b), our code reliably detects fragments in simulations where fragmentation should occur (see also Mejía et al. 2005, Pickett & Durisen 2007). Boley has recently tested higher-order boundary potential routines in our code and reaches the same conclusion.

4. RELEVANCE

The proposed research involves 3D radiative hydrodynamics simulations of GIs in protoplanetary disks with the goal of understanding how these disks evolve and how GIs influence the process of planet formation. We will continue ongoing studies of how the physical and radiation environment affects GIs and how GIs influence the processing, mixing, and growth of solids leading to extrasolar planet formation. These simulations will also be directly relevant to the early evolution of our own Solar Nebula and the conditions under which the planetesimals and planets of our own Solar System formed. The origin of planets and planetary systems is a specific focus of the Origins Program. Our work directly supports NASA Strategic Goal #3, specifically Sub-goals #3C and 3D by advancing or knowledge and understanding of the origins of our own and of extrasolar planetary systems, as detailed in NASA Research Objectives #3C.1 and 3D.3, respectively. The proposed research will also be relevant to future developments in ground-based and space-based observational capabilities for resolving disk structure in nearby star forming regions.

5. RESEARCH PLAN AND MANAGEMENT STRUCTURE

5.1 Plan of Research Work

YEAR ZERO (Current Funding): *July 1, 2007 to June 30, 2008.*

Some efforts under current funding substantially overlap initial phases of the proposed research. Only the overlap areas are mentioned here.

PROJECT AREA #1: **1a.** Stellar Irradiation. Complete simulations with an r-dependent T_{irr} to mimic stellar irradiation and shadowing effects. **1b.** Infall. No planned activity. **1c.** Binary Companions. Complete implementation of centering the star/disk in a Roche potential and perform some production runs.

PROJECT AREA #2: **2a.** Planet Migration. Begin studying planet migration in a GI-active (gravitoturbulent) disk. **2b.** Feedback of Settling on Radiative Cooling. Begin simplest treatments of how settling affects GIs. **2c.** Stirring, Settling, & Concentrating. Use the combined particle-plus-hydro code to study gravitational buffetting and stirring of moderate-sized planetesimals by a gravitoturbulent disk without particle gravity or gas drag.

PROJECT AREA #3: **3a.** Bursting Dead Zones. Complete current runs and their analysis. **3b.** Planet Formation. Complete simulations testing the reality of the "rings" reported in Durisen et al. (2005).

YEAR ONE: *July 1, 2008 to June 30, 2009.*

PROJECT AREA #1: **1a.** Complete work on $T_{irr}(r)$. Begin to study how shock bores affect the upper disk atmosphere and begin efforts to develop a ray method for treating stellar irradiation. **1b.** Compute simulations with ongoing infall. **1c.** Continue Roche lobe simulations.

PROJECT AREA #2: **2a.** Complete the planet migration study. **2b.** Begin implementing heuristic treatments of settling. **2c.** Implement gas drag into the particle integration.

PROJECT AREA #3: **3a.** Simulate bursting dead zones with infall and/or settling. **3b.** Introduce particles into dead zone simulations.

YEARS TWO & THREE: *July 1, 2009 to June 30, 2011.*

Because the anniversary date of this successor proposal is so far in the future, we have combined the last two years.

PROJECT AREA #1: **1a.** Do simulations that modulate irradiation in response to GI vertical structure and also implement a ray approach to stellar irradiation. **1b.** Continue infall modelling. **1c.** Implement gravitational and radiative coupling of star/disk systems with the binary companion.

PROJECT AREA #2: **2a.** No activity. **2b.** Continue and complete studies of heuristic settling models. **2c.** Implement gas drag back-reaction and particle gravity.

PROJECT AREA #3: **3a, 3b.** Continue as seems appropriate.

5.2 Management Structure and Personnel

Principal Investigator R.H. Durisen. The PI assumes overall management and coordination for all the proposed research throughout the funding period. In Years Zero to Two, the PI will provide day-to-day direction of both the Co-Investigator and the Research Assistant. When he retires in Year Three, he will transfer most day-to-day activity to the Co-I. The PI will maintain contact throughout with his former doctoral students insofar as they remain active in work on related problems.

Co-Investigator T.Y. Steiman-Cameron. The Co-I is a Senior Scientist at IU and a former doctoral student of the PI who has extensive research experience with gas and particle disk dynamics. He will have primary responsibility for the irradiation, infall, and dead zone projects (Projects 1a, 1b, and 3a). After RA Michael completes his dissertation, the Co-I will share with the PI responsibility for continuation at IU of Projects 2b, 2c, and 3b. To that end, he will co-direct with the PI the research for the student who replaces Michael as RA. Starting in Year Three, the Co-I will take over routine supervision of the RA.

Graduate Research Assistant S. Michael. Michael's dissertation concerns Projects 2a, 2b, 2c, and 3b, and he will have primary responsibility for this research under the direction of the PI. After he finishes, continuation of Projects 2b, 2c, and 3b at IU will divide among the Co-I, the PI, and a graduate RA to be determined. Michael will complete Project 2a.

Collaborator M.K. Pickett. Pickett is an Associate Professor of Physics at Lawrence University and former doctoral student of the PI. She has been and continues to be an external member of the Research Committee for all of the PI's recent doctoral students. She will have primary responsibility for Project 1c but will consult with us on aspects of all projects as needed.

Collaborator L. Hartmann. Hartmann is a Professor of Astronomy at the University of Michigan. He will provide consultation and advice on all aspects of this research, but especially on Projects 1a and 3a.

Collaborator N. Calvet. Calvet is a Professor of Astronomy at the University of Michigan. She will provide consultation and advice on the treatment of radiative physics in Project 1a and 2b. Specifically, she will provide us with dust opacities as needed.

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The literature on the various subtopics in this proposal has become enormously large. The PI has only cited classic, recent, and/or representative papers and review articles. He apologizes to the reviewer if some of his or her favorite works are omitted.

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