

Center for Advanced Studies of Planetary Systems

1 Introduction

Over the last 10 years the field of exoplanet¹ research made a sharp transition from an "obscure hunt for ETs" to a precise scientific subject. This transition coincided with the discovery of the first exoplanet around a solar-type star, 51 Peg, but it was the logical result of long and coherent efforts to perfect the required observational techniques. The avalanche of exoplanet discoveries that followed gave us a whole new perspective in modern astrophysics. We now know that planetary systems are relatively common among cooler stars in our Galaxy, but the Solar system may be unusual in several respects. The latest addition to the list of exoplanets – the Earth-size planets – significantly broadened the range of systems where we could possibly find signs of biological activity.

Today the field of exoplanets has become one of the most dynamic, competitive and prestigious fields in astrophysics. It also became clear that further progress is only possible through a multi-disciplinary approach which brings together advanced modelling on different scales and today's state-of-the-art or future observations.

Below we briefly list some of the most important outstanding problems in the physics of exoplanets and point out how they can be approached by combining astrophysical methods with methodologies, data and models from adjacent research areas like Space Physics, Material Sciences, Geosciences etc. Then we briefly present on-going research in the departments participating in this application. In the following section we formulate specific scientific topics for the proposed Center for Advanced Studies of Planetary Systems (CASPS) and discuss the project feasibility and our international competitiveness in these areas. Finally we describe our national and international collaborations, present the proposed structure of CASPS and explain the need for the requested resources for achieving our goals.

2 Physics of exoplanets

In the coming years major international efforts will be directed toward understanding the formation and evolution of planetary systems. The emerging picture must be consistent with accumulated observational data on solar and extrasolar planetary systems. The combined progress in observations and theory should, among other things, provide us with reliable characteristics of exoplanets including their internal structure, the presence and parameters of their atmospheres, etc. We will also attempt to answer the question of how common our Solar system is among other planetary systems.

A very schematic scenario of planet formation around late-type stars (solar-type or cooler) consists of the following steps: (A) self gravity causes a cold molecular cloud

¹Exoplanets or extrasolar planets are planets outside our Solar system

to collapse into a disk and form a young stellar object in the center, (B) the remaining material in the disk forms solid particles (dust) that grow hierarchically to form planetesimals, (C) large planetesimals accumulate enough mass to be able to attract gas and dust gravitationally (core collapse scenario) or the whole disk cools to the point when it becomes gravitationally unstable and fragments into locally bound blobs of material continuing to form planets (gravitational instability scenario), (D) young planets interact with the remains of the disk and migrate to different orbits contributing to the destruction of the disk. The type of a newly formed planet (rocky, gas giant or ice giant) is determined by the initial distance from the central star and the amount of water available in solid form (ice). Unfortunately this scenario is too schematic for explaining/predicting the variety of properties found in extrasolar planetary systems. In particular it does not explain the high number of so-called hot Jupiters (gas giants very close to the parent star) and planets on very elongated orbits often found in other planetary systems. The ultimate problem of habitability of specific planets is presently unanswered, but this question has shifted to a more practical plane: both NASA and ESA are developing space observatories capable of detecting and measuring chemical compositions of planetary atmospheres and a list of plausible targets is urgently needed.

The existing scenarios of planet formation lack predictive power and we believe that the main reason for this is the lack of understanding of physical mechanisms determining crucial aspects of planet formation and evolution such as energy balance, chemistry and formation of solids, interaction with the disk and central star, etc. The existing observational data by itself is insufficient for addressing these issues. The observations of protoplanetary disks do not have sufficient spatial resolution and, with a few exceptions, the properties of planets are derived from indirect measurements like stellar radial velocity variations. Only by developing or improving models of important physical processes we can properly interpret the new advanced observations of planet-forming environments and compare them with characteristics of detected planets. Here is a deeper look at some crucial areas.

2.1 Planet birth places: stars and circumstellar medium

Planets form at a late stage of star formation when the remains of the protostellar cloud concentrate in a rather thin disk. The shape of a disk is determined by the gravity of the central star, the centrifugal force and internal pressure which is described by the local equation of state. Two main transport mechanisms are acting in a disk: mass is carried inwards (and thus the angular momentum must be transported outwards) and energy is transported to the disk or carried away from the disk by radiation. The presence of those mechanisms is proven by the detection of accretion of disk material on the central star, and observations of winds and radiation in the infra-red where the disk outshines the central star. None of these transport mechanisms is sufficiently well understood. For example, we do not know the origin of the viscosity that allows material to slow down in transiting to a smaller orbit and we have very little insight into the opacity sources controlling radiative transport at the temperatures and densities encountered throughout the disk.

The two unanswered questions which hold the keys to the transport problems are: the chemistry (in particular reactions leading to formation of complex molecules and solids) and the physical conditions (temperature and density) in the disk. Both chemistry and physical conditions are functions of time and location and they are closely linked. In the outer layers physical conditions are primarily controlled by radiation coming from the central star and leaving the disk, resulting in heating and cooling, respectively. Radiative heating and cooling happen at very different wavelengths and the efficiency of those processes depends on the optical properties of chemical species and dust particles present. The inner parts of the disk may be totally or partially obscured from incoming radiation and thus have very different temperature and conductivity than the surface. For the same reason the inner regions may not be accessible for direct observations but these are the regions where planetesimals form because solids tend to sediment toward the midplane of the disk. Chemical reactions are, of course, very sensitive to local density and temperature but they are also affected by the amount of high-energy photons. In the low temperature (between tens and a few hundred Kelvins) and low density ($< 10^8$ particles per cm^3) environment, UV and X-ray radiation may dissociate or ionize molecules in the surface layers opening new reaction channels and allowing interaction with the stellar magnetic fields. The latter will create turbulent motions due to the so-called magneto-rotational instability (MRI) which tends to help planet formation (see below).

Modern observational facilities like HST, Spitzer, VLT and VLTI provide some hints on disk dynamics and structure. Recent observations revealed the presence of warps and chemical stratification in some objects supporting theoretical model predictions, but the combination of available spectral and spatial resolutions is far from optimal and no firm manifestations of planet formation were found yet. In this respect the new sub-millimeter interferometer ALMA inspires some strong expectations. Relatively short wavelengths, large and adjustable baselines, huge photon collecting power and spectral resolution should be sufficient to detect and to follow disk structures throughout their orbital periods. Systematic studies of planet-forming regions with advanced facilities like ALMA combined with conventional detection techniques (e.g. radial velocity surveys) seems to be the direction of the future observational efforts in this area.

Studies of chemistry and energy transport at the conditions typical for a protoplanetary disk are theoretically and experimentally challenging but as long as those questions remain open any attempts to understand planet formation or to predict what kind of planetary systems will form from a given protoplanetary disk will be uncertain.

2.2 The planet formation process

The most plausible scenario of planet formation is a gradual growth of particles by chemical reactions and inelastic collisions (coagulation) followed by a gravitational accretion phase when particles reach sufficient mass. This process has to be quick as the destruction of the disk around a solar-type star takes only a few million years. Due to low temperatures and densities the first dust particles, once formed, become detached from the gas and may have different dynamics. In particular, they will tend

to sediment into the central plane of the disk creating chemical stratification. In order to keep on growing the newly formed "dust grains" have to gently collide with each other. Circumstances for such collisions can be provided by turbulence. Some of the mechanisms capable of creating turbulence (e.g. due to magneto-rotational instability) require partial ionization of matter and the presence of magnetic fields. Although some ionization can be created by the stellar UV and X-ray radiation in the surface layers, the exact level of turbulence or the disk magnetic fields is impossible to measure. In this context we primarily rely on MHD simulations. The first results (e.g. Johansen et al. 2007, *Nature* 448, 1022) seem to be promising in terms of facilitating further growth of solids trapped in turbulent vortices but much more sophisticated models must be developed to actually trace the evolution of the solids.

Another problem is the survival of solid particles in the size range between a few millimeters and a few centimeters. The gas component moves with sub-Keplerian velocities due to the presence of a radial pressure gradient. Solids have to go faster to stay on orbit and, therefore, they experience a constant headwind. Estimates show that breaking in this size range is so quick that any particle will plunge into the stellar surface within a few orbits. Another problem is the relative collisional velocities that tend to increase with size leading to fragmentation rather than to coagulation. The main unknown here is the actual atomic structure of the smallest particles limiting our ability to understand the chemical, mechanical and optical properties. The latter also compromises the interpretation of the observations: although we see signatures of dust in the spectra we cannot uniquely derive the mass distribution and structure of the grains.

The last stage of planet formation, gravitational accretion of gas, is critically important for the physical conditions on the future planet. This is the time when the chemical stratification occurs in the inner parts of a planet and, e.g., for an earth-like planet the dynamo starts operating in its core creating a planetary magnetic field. The inner structure also determines the efficiency of plate tectonics on these planets directly affecting the properties of their atmospheres.

Many of the properties mentioned above can be understood through ab initio calculations of dust grain formation and growth predicting mechanical, optical and magnetic properties of the solids. Additional experimental data comes from in situ studies of planets and small bodies in our Solar system.

2.3 Characterization of exoplanets

Characterization of an exoplanet includes determination of its orbit, mass, size, composition, properties of the parent star, etc. High-resolution spectroscopy has the potential to detect the atmosphere and study its chemical composition. In exceptional cases some of these data can be derived from indirect measurements (stellar radial velocity and transits, Knutson et al. 2007, *Nature* 447, 183). For objects on very short orbits that also show transits, extra information about the presence of some chemical elements in their (evaporating) atmospheres can be obtained already (Mandushev et al. 2007, *ApJ* 667, 195) but detecting "normal" atmospheres, measuring atmospheric composition

including possible indicators of biological activity requires reliable methods of registering and analyzing photons originating from or scattered by the planetary atmosphere. Such ambitious goals can only be achieved from space with projects like Darwin or TPF and Swedish universities and the Space Board are actively participating in the formulation and implementation of those projects as well as in the precursor missions like COROT and Gaia.

3 Center participants: current research relevant to the project

Below we give a short presentation of ongoing activities in the participating departments relevant to the outstanding problems outlined in the previous section.

3.1 UU: Astronomy and Space Physics

Planetary System group. In broad terms the goal of the research is to characterize the whole population of small bodies in the Solar System with respect to numbers, orbit and size distributions, dynamics, physical structure and chemical composition, and scenarios of formation and evolution. This population includes asteroids, comets, and the interplanetary and trans-Neptunian populations of the outer Solar System. Currently the main areas of research are as follows.

We model the outgassing of cometary nuclei – the process that gives rise to the observed gas and dust envelopes (coma) and tails (Davidsson & Skorov 2002, Icarus 159, 239; Davidsson & Skorov 2004, Icarus 168, 163). Outgassing is a main driver of cometary evolution and its accurate understanding provides a key to studying the pristine material of the nucleus preserved from the original protoplanetary disk. Therefore, detailed modelling of non-equilibrium processes associated with the outgassing is critical for the interpretation of data the Rosetta mission is expected to collect.

We study the dynamical transfer mechanisms that supply new comets from distant reservoirs into observable orbits, which – among other things – may help to clarify the origin of the Rosetta target comet, and to put measured chemical and isotopic compositions in perspective (Fouchard & Rickman et al. 2006, *Cel. Mech. Dyn. Astron.* 95, 299). We have also discovered that the trans-Neptunian population of the young Solar System was sensitive to stellar passages, which must have been important for the early supply of ice-rich bodies into the regions of the terrestrial planets, where they could have collided with planets providing material for oceans or atmospheres. Finally, we try to establish the observed cometary populations as well as possible in order to place further constraints on the source regions.

Observational and modelling studies of atmosphereless regolith-covered objects like Mercury, the Moon and asteroids are performed in order to interpret their surface composition, light scattering properties and microphysical characteristics (Warell & Blewett 2004, Icarus 168, 257; Warell et al. 2005, Icarus 180, 281). From this information studies of possible evolutionary paths that have brought the surfaces to their

present state may be carried out. One of the major drivers is to provide boundary constraints to deduce the formation model of Mercury, which has to explain, e.g., the origin of its large and massive core, iron-diluted upper mantle and crust and the presence of a magnetic field. The work carried out within the European Space Agency's GAIA mission involves classification and astrophysical parametrization of reflectance spectra of 300 000 minor bodies, to be used for improving our understanding the origin, dynamic and compositional evolution and interrelations between these types of objects (Warell & Lagerkvist 2007, A&A 467, 749).

These projects build the necessary background for understanding important processes in the formation and the evolution of planetary atmospheres and oceans due to impacts with smaller bodies.

Stellar Physics group There are very few places in the world with as many individuals actively engaged in research on stellar atmospheres and related astrophysics as in Uppsala. Expertise includes observation and modelling of surface inhomogeneities (star spots) often resulting from magnetic fields, as in the Sun; detailed studies of the composition of stellar atmospheres using models and observed spectra; the study of dynamical processes in stellar atmospheres including shocks and winds; chemistry in stellar winds including the dynamical effects of radiation acting on molecules and dust; and the study of inhomogeneities associated with subsurface convection as well as shocks and other nonlinear phenomena.

The basis of our research are the high-precision spectroscopic observations at different wavelengths. We have an extensive experience in carrying out complex observing programs and carefully analyzing the data. This experience is based on in-depth knowledge of the instruments we are using, as members of the group have been involved in development and commissioning of several ESO instruments like the UVES and the CRIRES on the VLT. Our data reduction package for echelle spectroscopy is used world-wide. Radial velocity follow-up observations of transiting exoplanet candidate systems detected in the HST SWEEPS survey (Sahu et al., 2007, Nature 443, 534) is a good illustration of our competence. All targets were much fainter than 18th magnitude. In Figure ?? we show examples of the HST photometry and UVES/FLAMES spectroscopy, the latter with signal-to-noise ratio of 4! Still we managed to detect radial velocity variations in binary systems and confirm systems with exoplanets.

We have pioneered the study of surface inhomogeneities on chemically peculiar (CP) stars and active solar-type stars by developing and applying the so-called Doppler Imaging (DI) technique, which allows re-construction of maps of inhomogeneous stellar surfaces from time series of high-resolution spectra. Today, this technique is actively used for studying chemical element distributions in A-type stars, magnetic activity in single and binary late-type stars, interaction in contact binaries, etc. Recently, we extended this technique to magnetic CP stars and demonstrated that we can reconstruct the surface distribution of magnetic vectors directly from observations without prior assumptions about field geometry (Piskunov & Kochukhov 2002, A&A 381, 736). The application of this technique to the observations of magnetic CP star 53 Cam immediately showed complex structures of the field (Kochukhov et al. 2004, A&A 414, 613).

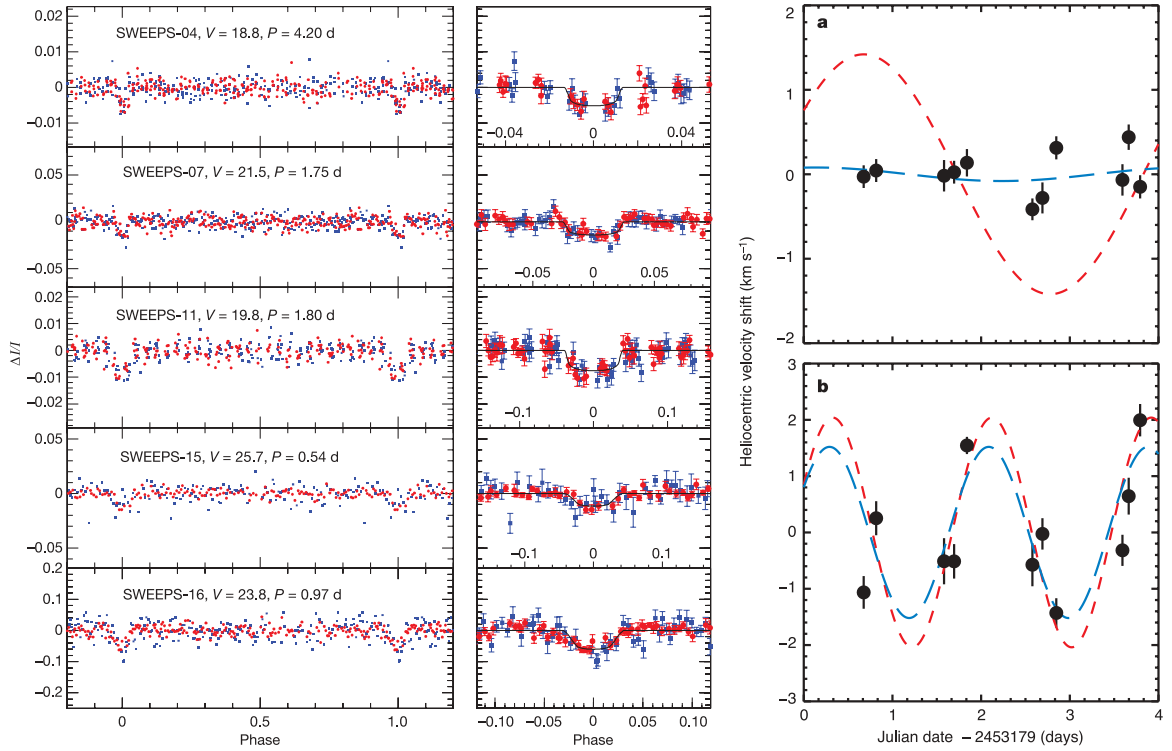


Figure 1: The left panel shows light curves of systems, candidates for hosting transiting planets. The middle panel is the zoom-in on the transits. The right panel shows radial velocity measurements for two systems: the top one with an exoplanet and the bottom one with a very small stellar companion (no planet).

The excellent quality of the data obtained for this project also allowed us to reconstruct the full 3D structure of the distribution of the chemical elements from the observations (Ryabchikova et al. 2002, A&A 384, 545). The derived depth dependence was successfully confirmed by the radial-velocity measurements of pulsations using spectral lines of different elements. We are working on applying similar techniques to study magnetic fields and thermal structure (footprints of the accretion flows) on the young stellar objects.

Long-term monitoring of chemical structures on the surface of α Andromeda revealed for the first time a "weather"-like evolution of Mercury clouds changing shape and location on a time scale of years (Kochukhov et al. 2007, Nature Physics, 3, 526). Such phenomena will have consequences on irradiation of protoplanetary disks and planets.

Magnetic fields play a major role in all stages of stellar evolution. The origin of the fields is a highly debated topic because observationally it is hard to distinguish between different possible dynamo mechanisms. In the special case of a close-binary system ER Vul with solar-type components, we were able to identify the relation between the tidal effects and the field generation mechanism leading to non-axisymmetric dynamo (Sokoloff & Piskunov 2002, MNRAS 334, 925). Several Jupiter-mass planets on very

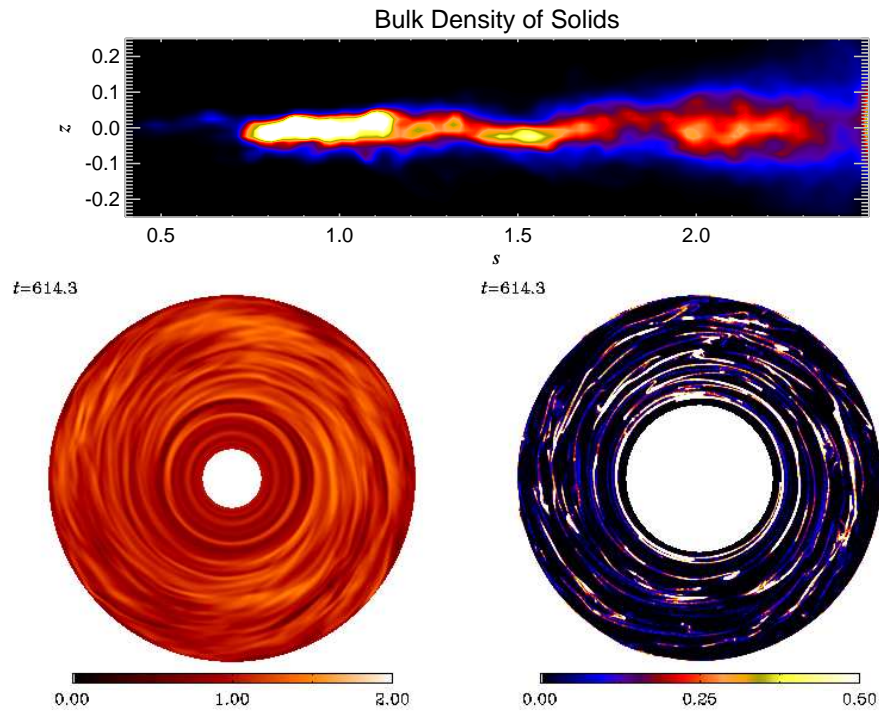


Figure 2: Magneto-hydrodynamical simulations of a turbulent protoplanetary disk computed by W. Lyra using the PENCIL code. The top panel shows the density of solids in a cut through the disk. Brighter colors show sedimentation of particles towards the middle plane. The bottom panels show the midplane density of the gas perturbed by the magnetic fields (left) and solids traced by a few million test particles (right). Concentrations of particles trapped by gas turbulence coincide with high-pressure regions in the gas (anticyclones). The bright areas indicate places where the density of solids reaches as high as 85 times the average density, increasing chances of coagulation. See also <http://www.astro.uu.se/~wlyra/planet.html>.

short orbits may create similar resonances and thus stimulate stellar activity.

Our studies of young stars (the so-called classical T Tauri stars) included high-resolution time series of spectroscopic data from the VLT and the theoretical modelling of the dynamo action and mass transport in inner part of the accretion disk. Observations help establishing the properties and geometry of the accretion flows and the winds (Stempels & Piskunov 2002, A&A 391, 595; 2003, A&A 408, 693) which were used to tune the parameters of the 3D MDH model (von Rekowski et al. 2003, A&A 398, 825; von Rekowski and Piskunov, 2006, AN 327, 340).

Full 3D MHD simulations of protoplanetary disks around solar-type stars are carried out in collaboration with NORDITA. The first results show the effects of turbulence due to magneto-rotational instability on the dynamics of boulders embedded into the disk (de Val-Borro et al. 2006, MNRAS 370, 529; Lyra et al. 2007 A&A in press) as illustrated in Figure ???. We are also constructing local thermodynamic models of a disk based on detailed treatment of radiative transfer, chemistry and phase transitions

(Regandell et al. in preparation).

Stars are the source of most of the "heavy" elements necessary for life, from carbon to iron and beyond. Edvardsson, Gustafsson, Eriksson and collaborators have systematically used solar-type stars to explore the gradual build-up of chemical elements in the disk of the Galaxy. Although we expect the most reliable abundance determinations from these not so luminous stars, an extension to the sub-giants showed the abundances obtained to be as consistent and precise; this is significant because age determinations for subgiants are much more accurate than for solar-type stars. Abundances are determined also for other important groups of stars: Eriksson, Gustafsson & Wahlin have recently obtained data from the infrared spectrometers at the VLT and Gemini telescopes for carbon stars in different dwarf galaxies in the Local Group. A study of hydrogen-poor carbon stars in very late evolutionary stages (R CrB stars, Asplund et al. 2000, *A&A* 353, 287) has also been carried out. The oldest stars known, the metal-poor Halo stars, preserve dynamical and elemental-composition information about the conditions from the time when, or maybe even before, the Galaxy was formed. The high-resolution spectra are obtained as part of an international collaboration. One of the most remarkable results is the discovery of HE 0107-5240, by far the most metal-poor giant star known today with an overall metallicity of about 1/200 000 of the Sun (Christlieb et al. 2002, *Nature* 419, 904; 2004, *ApJ* 603, 708). An interesting, and unanswered question, is whether planets form around extremely metal-poor stars.

The late evolutionary stage when stars burn hydrogen and helium in concentric shells surrounding an inert core and appear as Asymptotic Giant Branch (AGB) stars, is of great importance for stellar evolution, nucleosynthesis and mass loss. AGB stars contribute significantly to the building material for new generations of planets. During the past few years Höfner and collaborators (2003, *A&A* 399, 589) have constructed an advanced radiation-hydrodynamics code, combining frequency-dependent radiative transfer with a detailed description of dust formation. The code allows consideration of effects of molecular line-blanketing, leading to a much more realistic representation of atmospheric structures and synthetic spectra. In addition, Freytag and Höfner (2007, *A&A* submitted) have recently developed the first prototypes of 3D radiation-hydrodynamical models of the full stellar mantle and atmosphere of AGB stars ("star-in-a-box") to study the influence of giant convection cells on atmospheric dust formation and wind acceleration. These models are an extension of the pioneering attempts to model red supergiant atmospheres (Freytag et al. 2002, *Astron. Nachr.* 323, 213). The description of physical and chemical processes and numerical methods involved in these calculations are now applied to detailed modelling of disks and planet formation (Regandell, 2007 in preparation).

Eriksson and Regandell search for circumstellar disks in young star-forming regions using the LABOCA bolometer camera on the APEX sub-millimeter telescope. The Atacama Pathfinder EXperiment is an ALMA prototype telescope situated close to the ALMA site in Chile at a height above 5,000 meter so that a large part of the far-IR spectrum is accessible. We successfully imaged parts a young star-forming region in Serpens at 870 μm during the first round of Swedish APEX-time after the commissioning of LABOCA. The observational data has recently arrived and are just being

analyzed. At these wavelengths one sees the emission from the cool dust in the disks. When these data are combined with maps at near- and mid-IR wavelengths as well as with the X-ray data for the central stars (XMM observations in collaboration Alex Brown from Boulder Colorado) one can derive several characteristics of the disks. Another even younger star forming region will be imaged in the 2nd round of LABOCA observations. The detected targets will be studied in detail when ALMA telescope becomes operational.

The vast majority of the detected planetary host stars are of intermediate, solar-type temperature (F, G or K type). For these systems one has established a correlation between the amount of heavy elements in stellar atmosphere and the presence of gas giant planets (e.g. Heiter & Luck 2003, *AJ*, 126, 2015; Fischer & Valenti 2005, *ApJ*, 622, 1102). However, most stars in our Galaxy (about 75%) are cool and faint “red dwarfs” (M dwarfs). Several such stars have recently been found to host planetary systems (e.g. Bonfils et al. 2007, *A&A* 474, 293). We are developing advanced models for M dwarf stars including an improved description of the molecular transitions. The models will be verified by comparison to high resolution observations. A further application of these improved models will be the interpretation of direct observations of planets, allowing us to study their chemical compositions. Planets around M dwarfs are the best candidates for such observations, because the contrast between light coming directly from the central star and reflected by the planet is smallest. A good understanding of the stellar spectrum is crucial for interpreting the planetary spectra. The lowest-mass planets, i.e. with masses most similar to the Earth, have been detected orbiting M dwarfs (e.g. Udry et al. 2007, *A&A* 469, 43). Such planets will likely be the targets for the search for signatures of biological activity in their spectra (see e.g. Segura et al. 2005, *Astrobiology* 5, 706) and the correct interpretation of the planetary spectra will only be possible if we have good knowledge of the parent star.

3.2 Institute of Space Physics (IRF² Uppsala)

The space plasma physics group at the Swedish Institute of Space Physics in Uppsala explores the plasma universe reachable by in situ observations. The overall scientific goal is to identify, model and understand the main processes in ionized gas in the Solar System. The major hardware experience at the IRFU includes instruments for investigation of DC and wave electric fields, and plasma density and temperature. The current major satellite missions with IRFU involvement include Cluster (four ESA satellites investigating the terrestrial magnetosphere, science phase started early 2001, The Cluster and PHOENIX missions, Dordrecht: Kluwer 1997.), Cassini (NASA, arrived to Saturn and Titan in 2004) and Rosetta (ESA, successfully launched March 2004, cometary science phase 2014-2015). Previously we have supplied instruments for the Swedish Viking, Freja and Astrid-2 spacecraft. All these satellites have a full complement of instrumentation for detailed in situ plasma observations in different regions

²IRF is a national research facility which is not part of any university but its Uppsala division is located in Ångström Lab and has close ties with the University through education and research

of the planetary systems. Together with international partners we have considerable experience in observing and modelling complex plasma systems.

Previous studies of interest to this application include our investigations of terrestrial ionospheric outflow. Observations by Viking and Freja have shown how ions of ionospheric origin can be energized to energies well above escape velocity. Statistical studies of observations, together with theoretical work and Monte Carlo simulations, have also shown which electromagnetic wave characteristics in a collisionless plasma are important for the energy transfer causing this energization. This is a typical study for our team in the sense that the investigation includes comparison between in situ observations, and theory combined with simulations. The first plasma and density observations in the ionosphere of Titan, made by our team with our Cassini instrument, show a similar outflow from this body, although caused by other mechanisms (Wahlund et al., *Science*, vol 308, 986, 2005).

The Cluster project is a unique four-satellite ESA cornerstone mission. This mission gives the first chance ever to truly separate spatial and temporal effects in the collisionless terrestrial magnetospheric plasma. Using Cluster we are now investigating boundaries in space plasmas (the bow shock and the magnetopause), subsequent energy transport to lower altitudes, and the concentration of this energy to cause, for example, auroras. Of particular interest are studies of energy conversion and transport associated with magnetic reconnection, and the structures and dynamics associated with turbulence. For example, we have for the first time in any turbulent plasma observed Alfvén vortices (Sundkvist et al., *Nature*, vol 436, 825, 2005) and again for the first time in any turbulent plasma observed magnetic reconnection (Retin et al., *Nature Physics*, Vol 3, 235, 2007).

Using space as a laboratory without walls, the Physics in Space group at the Swedish Institute of Space Physics performs model experiments that test fundamental laws of nature in ways not possible in ground-based laboratories. Specific focus is placed on non-linear interactions, turbulence, dynamical processes and self-structuring of space matter and radiation, for better understanding and prediction of planet Earth's interaction with its space environment, the physics in turbulent layers in space and the upper atmosphere, and identification of possible anthropogenic turbulence in the ionosphere due to electromagnetic radiation from man-made sources. Using innovative radio methods based on concepts developed in modern radio astronomy and quantum optics, systematic studies of electromagnetic radiation from space are performed in order to explore the physical mechanisms behind the collective, non-thermal electromagnetic radiation that is generated in the Earth's magnetosphere, the Solar corona, and other space plasma in our planetary system.

Study of a very low-density plasma requires a special mathematical treatment. With the help of in-house developed computer code for solving the full multidimensional Boltzmann-Vlasov-Maxwell equations, turbulent interactions in magnetized space plasma are modelled and compared with experiments. In this work, extensive use is made of the UPPMAX and SweGrid high-performance computer clusters and visualisation engines.

3.3 UU: Condensed matter theory

In fields such as materials science, electronics, mechanical engineering and bioscience, not to mention physics and chemistry, the keywords "first principles" and "ab initio" are constantly encountered. The principal idea of these keywords is to regard a many-atom system as a many-body system composed of electrons and nuclei, and to treat everything on the basis of first principles of quantum mechanics, without introducing any empirical parameters. Hence the theory can be predictive and does not rely on experimental input.

The activities of the Condensed Matter Theory Group (CMT) involve theoretical modeling of materials in general, including metals, magnetic materials, surfaces, catalytic properties, superconductors, and semiconductors. The models used are based on density functional theory, total energy calculations, electronic structure, optical and phonon spectra, molecular dynamics simulations, Monte Carlo simulations and analytical work with model Hamiltonians. Methods used for the electronic structure/optical or phonon spectra and total energy studies are: linear muffin-tin orbital methods (atomic spheres approximation, full charge density and full potential), linear and non-linear augmented plane wave methods (including non-collinear theory), alloy theory using the coherent potential approximation, plane wave pseudopotentials codes like VASP (Vienna ab-initio Simulation Package) and gaussian basis functions based computer code like TURBOMOLE. Issues that are addressed are connected to hardness and elasticity of materials, structural phase transitions, optical properties, magnetic phase transitions, alloy formation, catalysis, interlayer exchange interactions, surface and interface magnetism. Some of recent work done at CMT group include discovery of a "post-stishovite" α - PbO_2 -like phase of SiO_2 (Nature 388, 362, 1997), predictions of two superhard titania phases (Nature, 410, 653, 2001; Phys. Rev. Lett. 87, 275501, 2001), and theoretical study of the stability of the *bcc* phase of iron at conditions of Earth's core (Phys. Rev. Lett. 84, 3638, 2000; Nature 424, 1032, 2003), discovery of new materials for spintronics i.e dilute magnetic semiconductor (Nature-Materials 2, 673 (2003)). Our spintronics paper has been listed on the top 3 cited-papers-list in the all fields of material science for last two years and it is No.1 cited paper in Nature Materials to-date (No. of citations 330 as of October 2007).

One of the main current activities at the CMT group is high pressure research. A vast number of extremely interesting and fundamental physical and chemical changes in solids have been reported in high pressure experiments. Theory was for a long time far behind the experimental development. However, today we are witnessing a very strong improvement in theoretical work in predicting certain properties of solids even before they are observed in experiments. As an example, we are looking at important issues of structural and magnetic properties of Fe bearing MgSiO_3 and MgO system under very high pressure using ab initio quantum mechanical calculations. The structural properties of pure MgO and MgSiO_3 are now well understood but the effect of impurities such as Fe is not very well known and also there exist some contradictions in the results obtained by the recent experiments. Fe is one of the abundant metals in the Earth's core and exists as impurities in mantle silicate minerals and oxides. Thus, the

magnetic properties of iron impurities in silicate minerals and oxides play a crucial role in determining the properties of the Earth's mantle mineral such as rheology, electrical and thermal properties etc. For this reason, ab initio calculations can provide a very good estimates of parameters which are fundamental to understanding the physics and chemistry of the Earth's mantle.

Another interesting ongoing project is to look at the optical properties of solids and clusters. Depending on the iron content the small silicate grains in circumstellar environment could be a dominant source of opacity thus having a decisive influence on radiative energy transport and mass transport in these regions. Here, we are using an ab initio optical code which is developed in our group. One of the materials which we have already studied is carbon/graphite and it is one of the important elements in stellar dust. Graphite can be regarded as an archetype of layered crystals. Intraplanar sp^2 bonding leaves a singly occupied orbital at each C atomic site, and intraplanar π orbitals are formed from these p states, causing the semi-metallic character of the solid. Hexagonal graphite has an abnormally large c/a ratio ($c/a = 2.7259$). This gives rise to a large anisotropy in the structural and electronic properties. The carbon atoms in the basal plane are bound together by strong covalent bonds (σ), whereas the binding between the adjacent planes is weak and caused by van der Waals bonds. As a result, the interlayer nearest neighbour distance between the atoms (3.35 \AA) is much larger than the in-plane nearest neighbour distance (1.42 \AA). This rather unique formation of π and σ orbitals in graphite also strongly influences the optical properties. The typical anisotropy of the dielectric function obtained in calculations is due to the difference in the optical matrix elements for the two different polarizations, which is a result of the anisotropic crystallographic and electronic properties of graphite.

We have also looked the optical properties of a more complex material based on carbon, C_{60} . The imaginary part of computed dielectric function also compares very well with the experiment. These calculations gives us confidence that we can go one step forward and look the optical properties of small carbon clusters and we have found a significant change in optical properties depending on the size of cluster. Now in future we are planning to do size dependent electronic, structural and optical properties of crystalline and cluster structures. We are going to focus on materials which are related to present proposal. These systems include $Mg_{2x}Fe_{2(1-x)}SiO_4$, $Mg_xFe_{(1-x)}SiO_3$, Ti_xO_y , SiO_2 , Al_xO_y , C and SiC.

3.4 Geosciences

Many of the basic problems in understanding early formation of metallic cores in terrestrial planets remain unresolved. For example, while the chemical composition of the Earth's outer core and its liquid character is assigned to the presence of light elements, there is no answer to how these were actually introduced in the core. In the homogeneous accretion model, the process of core formation is described as the melting of iron in a silicate crystalline mantle and its sinking into the core. Unfortunately the proposed models of this process raise more questions than they give answers reflecting the lack of accurate information on mineral physics and chemistry of iron and iron alloys involved

in the process of core formation, particularly in their early stages. Within the project "Physics and Chemistry of Iron in the Earth's Core" we focus on structural, magnetic and transport properties of iron and iron alloys at high pressures and temperatures. We have developed a new synchrotron radiation-based technique for studying partial melting at very high pressures (Andraut et al. 2006, High Pressure Research 26, 267) and applied it to the Fe-S binary system. Currently we are investigating the thermal conductivity of hot and compressed iron in a diamond anvil cell using laser heating at conditions similar to those in the cores of young terrestrial planets.

4 Specific scientific goals

Research carried out at the Uppsala Astronomy Department is presently quite diverse and we see CASPS as an opportunity to focus on the fields which are mutually beneficial and where we have extensive expertise. These areas of expertise include spectroscopic and polarimetric observations, 1D and 3D static and hydrodynamic modelling, semi-empirical modelling (inverse problems), radiative transfer in multi-dimensions, atomic, molecular and dust opacities, quantum-mechanical descriptions of line formation, physics and history of small bodies in the solar system. In addition we identified the leading groups at other departments or neighboring institutes that fit the goals of the proposed center. Among these the Institute of Space Physics carries out in situ studies of planets, rings and atmospheres (e.g. Titan) in the solar system, the Condensed Matter Theory group runs ab initio calculations of the structural, mechanical, chemical and optical properties of the smallest dust particles consisting of up to few hundred atoms and the Geosciences perform experimental and theoretical characterization of material in planetary cores. Such restructuring of scientific priorities coincides with a generation shift at the Department with 7 leading scientists retiring within the next 7-9 years, but it will not happen overnight. In this respect, external resources will give us possibilities for scientific renewal with an opportunity for the future scientific leaders to establish themselves internationally while completing important on-going projects. This will also give Sweden a leading institution working in the field of planetary research. This strategy was presented in the recent international evaluation of research at Uppsala University (KOF) and it received strong support in the final report of the panel.

During the first three to four years of the CASPS activities we plan to concentrate our research on the following topics. They were identified during a series of presentations of the research carried out at the participating departments and through examination of the international research initiatives (for the history of selection visit also <http://www.astro.uu.se/~piskunov/Linne2007>). The selection criteria were: topics of high scientific importance with to-date relatively low competition and where we have international-level expertise.

- **Global models of protoplanetary disks.** We will produce multi-component 3D MHD models of circumstellar disks taking into account the energy transport by radiation. The components will include gas, dust and protoplanets.

Wavelength-dependent treatment of radiation will allow proper account of heating and cooling. These models will be used for studying the dynamics of the disk including mass transport, mutual effects of gas and solids, concentration of planetesimals, migration of planets, planet growth and gap opening in the disk. This work will be done by further developing and adopting the PENCIL code which we are using already now and by extensively using the national computing resources available via Swedish National Infrastructure for Computing (SNIC). A large grid of models will be needed to probe the parameter space covered by the observations of the planet-forming regions, in particular those that will become available with the next generation instruments for the VLTI (e.g. PRIMA) and ALMA. The model database will serve as a foundation to study and improve the numerical schemes and to generate synthetic observables to be compared with the observations. Such comparison will be used to improve the models to the level where they can be used for reliable interpretation of the observations and prediction of planet properties based on characteristics of the protoplanetary disk.

- **Magnetic fields and structure formation in protoplanetary disks.** Magnetic fields presumably affect the mass and angular momentum transport in a protoplanetary disk as a whole. They may also be responsible for generating turbulent motions facilitating local agglomeration of planetesimals. Close to the star, around the co-rotation radius, stellar fields control the accretion flows and winds leaving the disk. Thus, we plan to study stellar and disk field generation and interaction with matter on different scales. The goal will be to understand the role of magnetic fields in steering the motions of gas and solids and growth of dust particles and see if those effects can be observed. On the observational side we will continue perfecting instrumentation capable of detecting and measuring magnetic vectors (the so-called full Stokes polarimeters, including the one being developed for the ESO HARPS instrument). We will also continue carrying out observations of stellar magnetic fields for stars of different temperatures and ages in order to understand the dependence of the field origin on the stellar parameters and possible effects of planets on stellar magnetic activity. Attempts will be made to detect fields inside the disks.

On the theoretical side we will focus on the role of magnetic fields in structure formation in the disks. This can be done with a "local box" setup of the MHD simulations where we follow material in a co-rotating coordinate system. Due to the higher resolution compared to global simulations we will take into account such processes as variable resistivity caused by partial ionization of gas and dust particles by high-energy radiation and cosmic rays. Such simulations have also application to the analysis of in situ measurements of magnetic and electric fields in the rings of Saturn by the Cassini mission.

- **Local physical conditions and dynamics in the planet forming regions.** In order to confront our models with the observations we must generate synthetic observables (e.g. spectral energy distribution, high-resolution spectra, spectropo-

larimetry). This requires the solution of the radiative transfer problem through dynamic media in 3D. The necessary techniques to solve such problems have been developed in Uppsala but the realistic computation of opacities will require a massive effort. On one side we need to derive accurate temperature and density profiles across the disk with resolution much better than we can afford during global calculations. Global models will serve as the initial guess while the refinement will be done in 1- or 2-dimensions but with a much more realistic equation of state, improved opacities and a larger number of frequencies. In order to extend the applicability of our equation of state to very low temperatures we need to compute the partition functions for several hundred species that are present in significant amounts. For the solids the formation cannot be treated in equilibrium and will require a separate effort. We rely on the expertise of the CMT group to investigate the following properties of solids: (i) how the optical properties depend on the cluster sizes; (ii) at which cluster size the systems reach their bulk properties; (iii) the sticking probabilities; (iv) the diffusion of pure Fe in $\text{Mg}_{2x}\text{Fe}_{2(1-x)}\text{SiO}_4$ and $\text{Mg}_x\text{Fe}_{(1-x)}\text{SiO}_3$ in order to understand whether or not these systems can become iron rich; (v) the formation of Ti_xO_y and Al_xO_y clusters. The results are crucial for computing realistic opacities and particle growth in our MDH models.

- **Planet formation: evolution of planetary cores and atmospheres.** Once the mass and size of a proto-planet have reached the ratio that allows it to withstand the tidal forces it starts actively accreting surrounding material quickly increasing the density of its core. Regarding the initial evolution of the core, studies of the changes of its chemical, structural and magnetic properties will be one of the goals of our efforts. We will carry out combined experimental and theoretical studies aiming at the quantitative description of differentiating processes, and at the determination of properties of iron and its alloys at pressure-temperature conditions corresponding to those during formations of cores of terrestrial planets. Diverse high-pressure experimental techniques will be complemented and guided by the first-principle molecular dynamics simulations and density functional theory. Experiments will utilize high-pressure technology of diamond anvil cell combined with laser heating. Scientific goal is to study processes of partial melting and chemical differentiation in iron-rich systems in the presence of volatile species in order to determine freezing-point depression relative to pure iron, siderophile-element partitioning etc. Structural and electronic/magnetic properties of various crystalline iron-rich phases at high pressures and temperatures will be studied to understand the formation and evolution of planetary magnetic fields. Characterization of processes and materials at extreme conditions requires advanced micro-analytical techniques applied in-situ. We will utilize state-of-the-art synchrotron radiation based techniques - x-ray diffraction, and whole suite of x-ray spectroscopy tools. Laser-heating studies, as well as Mössbauer and Raman spectroscopy studies will be carried out in high-pressure laboratories at Uppsala University.

Finally we will model the response of the outer gaseous layers to the strong stellar irradiation for "hot-Jupiter" type planets studying the stability of their atmospheres. This work will be based on the expertise of the Stellar Atmosphere group in collaboration with the IRFU group analyzing the data on the atmosphere of Titan.

The first 3 year period will be dedicated to perfecting the theoretical models which should reach adequate status by the time the 2nd generation of the VLTI instrumentation and the ALMA sub-millimeter telescope will become operational around 2011-2012. At this point priorities will probably shift to confronting model predictions with observations. To achieve such flexibility we include in the proposed budget one visiting professor position and two assistant professorships that can be re-filled correspondingly 1-2 times per year or once every 4 years. The two associate professorships will be used to bring in or keep the essential expertise in the fields of large-scale computer simulations (3D magneto-hydrodynamics) and interferometric observations and data analysis.

Besides the research outlined above, CASPS will also organize scientific meetings and schools related to our field. This activity will be coordinated with NORDITA that also has an extensive organizational experience. Another very important direction of work is spreading the information about planetary research to the general public. We plan to run a professional quality home page for CASPS and organize various public events. In this respect we will establish closer collaboration with the area of astrobiology represented by the graduate school of Astrobiology in Stockholm and by the Swedish Astrobiology network (<http://www.astrobiologi.se/swedish.html>). The coming International Year of Astronomy and the planned new planetarium in Uppsala will be very helpful in starting the outreach program.

5 National and international partners and networks

Our current research projects rely on wide international collaboration in order to achieve a proper balance between specialization and breadth. Here are our main partners working in the fields relevant to planetary research:

NORDITA has world leading expertise in 3D MHD simulations, dynamo, numerical methods and parallel computing. The PENCIL code³ developed by Axel Brandenburg is our main working tool in simulating outer layers of stars and the circumstellar medium. PENCIL is continuously evolving by efforts of the community using the code. We are involved in several of them, important for applications to protoplanetary disks, e.g. computing radiative energy transport, simulating interaction between gas and solids and implementing variable grid resolution. Axel Brandenburg is co-supervising the thesis work of Wladimir Lyra in Uppsala.

³<http://www.nordita.org/2005/software/pencil-code/>

Star formation group at Astronomy Department of the Stockholm University is actively pursuing two directions of interest to our project: theoretical models of accretion and outflows from young stellar objects as well as imaging and spectroscopy of these objects in the far infra-red. This group is also participating in the work of the Astrobiology school in Stockholm which is close to planetary research.

Onsala Space Observatory is leading Swedish efforts in radio astronomy. Onsala has unique expertise in sub-millimeter imaging and spectroscopy with APEX and is the competence center for the future observations with ALMA. Onsala is also actively participating in formulation of the space missions like DARWIN aimed at planet characterization.

MPIA Heidelberg is the leading European research center studying protoplanetary disks. In particular the group headed by Thomas Henning is doing HD simulations of disk dynamics, detailed non-grey radiative energy transport, disk chemistry and migration of chemical elements. Other important subjects include non-equilibrium dust formation and dust opacity, dynamics of solids and disk-planet interaction. This group is also leading observational efforts using VLTI and the construction of the ESO SPHERE instrument.

Geneva Observatory is leading the European efforts in the search for exoplanets. This group detected the first exoplanet around a solar-type star. Using a number of specially designed spectrometers and systematic surveys of nearby stars they discovered statistically significant number of objects covering a mass range from several jupiter-masses to a few earth-masses. The group has unique expertise in astronomical instrumentation and data analysis and in deriving characteristics of extrasolar planets for a wide range of physical parameters. We are working together with Geneva Observatory on building a full Stokes polarimeter for the HARPS spectrometer on the ESO 3.6m telescope on La Silla.

ESO provides access for the European astronomical community to the world's best observational facilities. Planetary research is very high on the ESO priority list and it is one of the main points of the science cases for the future instruments and telescopes like ALMA and the ELT. We are working together with ESO on the implementation of the HARPS spectropolarimetric option and on the ESPRESSO spectrometer for the VLT - a prototype of the high-resolution spectrometer for the ELT.

JILA/CASA (Boulder CO) has extensive expertise in space-born optical and ground-based radio observations and data analysis. Our current collaboration covers detection of convection on supergiants and classification of planet-forming regions based on radio spectral energy distributions measured with APEX. This collaboration will intensify when ALMA becomes operational.

6 Organizational structure and activity plan

Several components of expertise, infrastructure and an established collaborative network needed for realization of our proposal are present in Uppsala already today. The Department of Astronomy and Space Physics, the Uppsala division of the Swedish Space Physics Institute, the Condensed Matter Theory group and the Department of Geosciences will form the core of the CASPS. CASPS organizational structure will follow the Guidelines for organizing interdisciplinary centers adopted by Uppsala University. The top coordinating structure will be the board with representation of all departments involved plus the Swedish Space Physics Institute (IRFU) and NORDITA. Because education will be part of the activities the board will include student representatives.

To ensure an efficient start of both the scientific and organizational activities, we plan a kick-off workshop with representatives from all local departments and selected external collaborators. The currently semi-regular seminars will become a weekly event where common projects and related science will be discussed in detail. The visitor programme will be announced within the first few months and we aim at organizing a first PhD school together with NORDITA within the first year of operation.

7 Project requirements

CASPS is more than a direct continuation of our on-going research. In fact, we expect the largest progress in the subject to come from the interaction between fields. Thus we consider the proposed project as an excellent way of renewing our scientific activities and establishing much closer collaboration between partners. At the same time the existing senior researchers involved in CASPS have obligations in completing the on-going projects. We also have a number of people on temporary positions that could play an instrumental role for the project on longer time scales. Therefore, our highest priority is with funding for dedicated manpower. A visiting professor position will attract people with the highest level of competence. The two associate professor positions (forskarna) will be used to select young scientists interested in building up CASPS, capable of taking scientific leadership and providing functional interfaces between fields in such a multi-disciplinary project. The two assistant professorships (forskarassistenten) will allow us to recruit young talented scientists early in their carrier with additional flexibility that will allow adjusting specializations as the project progresses. Considering that we are bringing four different disciplines together this number of new positions is really the necessary minimum.

Our extensive collaboration requires adequate travel resources which are next on our priority list.

As a university department we should not miss the opportunity to use such a major research initiative for education. The subject is very attractive for undergraduate students of all grades and we plan to get students involved in the research process at an early stage. We also plan on organizing summer schools for PhD students inviting

the best candidates internationally.

The project provides an excellent opportunity for outreach activities which is vital for increasing public awareness and support of natural sciences in Sweden, as well as inspiring youngsters to pursue careers in science. The topic itself - how stars and planets are formed - appeals to most people since it directly describes the earliest history of the Solar System, the formation of Earth and hence the prerequisite of our existence. Graphic visualizations of numerical computer models of e.g. molecular cloud collapse or planetary growth by agglomeration are powerful tools of catching public attention and transfer knowledge. A forum for such shows and educational efforts is the Planetarium envisioned at the Ångström Laboratory, representing Saturn in the "Swedish Solar System". Serious efforts in these directions require investments. We envisage to apply for resources to construct the planetarium external foundation(s) while a part-time manpower to coordinate the outreach activities is included in this application.

A significant part of our research plan consists of computer simulations. For that we need to have adequate departmental and individual computing resources. Departmental computing facilities are needed for code development and testing: two important components not supported by the SNIC infrastructure (today a typical waiting time for starting a 16 CPU job on any of the 6 largest Swedish supercomputers is over one week). The need for such resources is explicitly stated in the KoF report. We plan to apply for central computing and storage facilities from the Alice and Knut Wallenberg foundation; however, the cost of individual computing equipment is included in this application.

Summing up, the required resources can be divided in 7 categories:

1. Research manpower (1 visiting professor position, 2 associate professors, 2 assistant professors, 2-3 PhD students).
2. Joint research activity in form of workshops and conferences.
3. Education in the form of schools for master and PhD students.
4. Travel for visiting network partners, presenting results at international meetings and observations.
5. Outreach activities including a professional web site, events for schools and the general public, public lectures and planetarium programs.
6. Upgrade of individual computing equipment (some desktops and laptops).
7. Shared computing facilities consisting of a computing server and a storage server for which we will apply for additional funds from the Knut and Alice Wallenberg foundation.