Strategic plan for research for the Department of Astronomy and Theoretical Physics at Lund University 2014 – 2020

The research at the Department of Astronomy and Theoretical Physics revolves around the principal questions about the structure of reality, from the smallest particles to the largest astronomical objects and the structure of life itself. We hold a strong international position in these research areas and intend to strengthen it even more over the coming years.

Much of the success of our research stems from the presence of creative individuals working together to explore some of the most fundamental questions in natural science. It is therefore natural that several of our top priorities in our research plan for 2014–2020 focus on the hiring and retention of key personnel. In that respect our top priorities as a department during the period 2014-2020 include (in chronological order):

- Transiting the Computational Biology and Biological Physics (CBBP) group into a new era with new leadership (2014 – 2017).
- Replacing Prof. Dainis Dravins with an internal recruitment (2014 – 2017).
- Replacing Prof. Torbjörn Sjöstrand through a international recruitment (2018 – 2020).

Although our research areas are seemingly disparate, there is a very strong common denominator – scientific discovery using computers. This approach is becoming increasingly important also in other areas of science. We therefore aim to raise our profile in this area by:

- Developing the COMPUTE research school to a University wide resource connecting researchers across the faculties (2014 – 2017).

In addition, all our research areas are very successful in attracting assistant professors and similar, often funded through external high-profile grants, such as ERC starting grants. It is of the highest importance to the department to select and promote these individuals in a structured and clear way as they will form the next generation of permanent staff. This work will have a high priority within the timeframe of this strategic plan.

By recruiting, mentoring and maintaining our excellent staff, we will be able to take forward our extensive portfolio of research activity. Major research directions will include:

- Maximising our return on investment in the development of the Gaia satellite and its ground-based follow-up.
- Develop comprehensive multi-scale models and machine learning methods that take advantage of the ongoing revolution in experimental techniques in life sciences.
- Make predictions for and interpret results from a number of current and future particle physics experiments, notably at the LHC.
- Understand the formation and evolution of planetary systems and black holes.
- Taking advantage of MAX IV (2017 – 2020), and potentially developing research lines relevant for ESS.

1. Current status

a. Description of the department and its three major research areas

The Department of Astronomy and Theoretical Physics formed through a merger in 2010. The merger has been relatively smooth and it has brought several benefits, including the jointly run COMPUTE graduate school and better possibilities to find suitable candidates for roles such as head of department. The merger has also enhanced and extended our scientific interactions and broadened our teaching base. Research carried out in three main areas: Theoretical Particle Physics, Astronomy and Astrophysics, and Computational Biology and-Biological Physics (CBBP).

Theoretical Particle Physics Particle physics aims at exploring and increasing our understanding of the fundamental building blocks of nature and the forces that act between them. The expansion of our knowledge is taking place at three main frontiers: the energy frontier, the intensity frontier, and the cosmic frontier (using the classification of the US strategy for particle physics). The first frontier is represented by physics at high-energy accelerators, with the Large Hadron Collider (LHC) at CERN being the current flagship, but other future projects are also envisioned, such as the International Linear Collider (ILC) and a Future Circular Collider (FCC). The second relates to high-precision measurements, primarily at lower energies where several experiments are now about to start (like Belle-II and Muon g–2), but also in dedicated experiments at the LHC, notably LHCb. The third involves exploring major mysteries like the presence of dark matter and dark energy in the Universe.
The theoretical particle physics group at our department is actively involved in research at all three frontiers, with a high international visibility. For more than 35 years, starting with the Lund string fragmentation model, one of the main activities has been the modeling of high-energy particle collisions at accelerators such as the LHC. The resulting so-called event generator programs, notably Pythia, are used by essentially all high-energy physics experiments in the world as one of their key tools. We also perform high-precision calculations and develop tools for testing new theories at both the high-energy and the intensity frontiers, as well as develop scenarios for new physics with cosmic implications.
Particle theory research in Lund is of a phenomenological character, i.e. we stay in close contact with the experimental reality, making predictions for observables that can be measured, and testing the consequences of new theories by comparing with existing data, e.g., the Pythia generator was essential for the Higgs particle discovery in 2012. Notably the group has a very prominent international position, in relation to its size, in the exploration of the strong force, both at high and at low energies. This has resulted in outstanding citation rates, documented, e.g., in the RQ08 bibliometric study. The group activities have recently been complemented by studies of possible extensions to the current “Standard Model” of particle physics, especially relating to models with several Higgs particles, but also including astroparticle physics and cosmology. Scientific challenges here come both from traditional particle physics, such as the hierarchy problem, and from the observations of dark matter and dark energy.

Astronomy and Astrophysics Astronomy is concerned with exploring the constituents of Universe from its largest scales, such as the cosmic microwave background, to scales more readily comprehended by humans, such as exoplanets and asteroids. As outlined in the European ASTRONET Science Vision Report, major frontiers in astronomical research today lie in broadly four areas: extreme astrophysics (black holes, supernovae and gamma-ray bursts); the formation and evolution of galaxies; the origin and fate of stars and planetary systems; and advancing astronomy through studies of our own Solar System. Research in Astrophysics at Lund University encompasses all four thematic areas, through a coherent study of the constituents of our own Milky Way, using a combination of theory, observation, and programmatic work for space missions. The group plays a leading role in the recently launched ESA Gaia satellite mission which will measure with exquisite precision the positions and motions of one billion celestial objects. The Gaia data will inform us about how the Milky Way has been built up over time and it will find some ten thousand planetary systems around other stars. It will also detect potentially dangerous near-Earth objects. Astronomers in Lund are actively involved in programmes for the processing and science exploitation of Gaia data, and for the acquisition of complementary data from ground-based telescopes (e.g., Gaia-ESO Survey). Theoretical work concerns exoplanet systems, the growth of black holes, and the progenitors of the brightest explosions in the Universe (supernovae and gamma-ray bursts). Observational as well as theoretical work benefits from the participation in the development of next-generation instrumentation (e.g., CTA, PLATO, and 4MOST) and working on measuring astrophysically interesting atomic data in the Edlén laboratory. Active development of methods is occurring across all research areas, such as the development of new techniques to determine a star's temperature and methods to study the formation and subsequent stability of planetary systems. Astronomy research is an inherently international activity and astronomers at Lund University are no exception. In connection with RQ08, we found that we published with authors at over one hundred institutions worldwide. This figure has scarcely diminished.

Computational Biology and Biological Physics (CBBP) The research within CBBP spans several frontiers, where a range of biological problems are tackled using a common platform of theoretical and computational methods. We apply quantitative methods to solve some of the most important problems in medicine for the benefit of society. The research is conducted in close collaboration with experimental groups in biology and medicine. In RQ08, CBBP was rated as "outstanding". Four main research directions are pursued – systems biology, biomolecular physics, machine learning for medical diagnosis, and bio-nano physics.
In systems biological research mathematical models of dynamics in plants are constructed. By combining experiments and models, often integrating genetic, molecular and physical data, we quantitatively characterize the dynamics to reveal fundamental design principles. We focus on stem cell development and organ formation in three dimensions, plant-pathogen interactions and circadian rhythms. One topic in biomolecular physics is efficient and proper characterization of the vast conformational space sampled by macromolecules such as proteins. Here we are in particular working on applications including protein folding, binding and aggregation. A particular focus is on intrinsically disordered proteins and their roles in disease-linked aggregation and cell regulation.
By combining information from gene data, clinical data and disease history we develop machine learning methods for medical diagnosis and prediction of disease progression. Applications include risk assessment for heart transplantations, recurrence analysis of breast cancer patients and early prediction of Alzheimer's disease. Bio-nano physics operates in the borderland between nanophysics and biology. By computational and analytical methods, we develop a framework for fast genome identification based on nano-channel experiments, and model protein diffusion to understand gene regulation at the nano-scale.

b. Staff, postdocs and student numbers

In total the department employs 9 professors, 6 lecturers, 7 researchers, XXXX postdocs, and 28 PhD students. These numbers are relatively similar to those for RQ08.

Since RQ08, we have been successful in recruiting junior faculty funded by individual grants, including KVA fellowships, grants from the Swedish research council (VR), ERC starting grants and grants from Knut and Alice Wallenberg (KAW) foundation.

c. External funding (compared to RQ08)

At the time of RQ08 we had a total of about 5.5 MSEK in external funding (for the then two different departments). Today our grant income is less, about 2.7 MSEK. The large discrepancy can be traced to two things – a very large grant from SSF and in astronomy some large funding for studies of telescope design (a research area that has since then been discontinued) from Vinnova . If we instead break this down into grants from our more regular funding lines we find that our grant income from the Swedish National Space Board has increased from 1.4 MSEK to 2.9 MSEK and our income from the Swedish Research Council has increased as well, from 7.7 MSEK to 10.2 MSEK.

d. Production – PhDs, publications, and patents (compared to RQ08)

Compared to RQ08 our productivity in terms of research papers remains roughly the same (Note – in the material from the faculty there seems to be a drop between 2011 and 2012 in our output of research papers. This is clearly erroneous and can likely be traced back to incorrect labelling of papers in the database for the earlier years. This pattern shows up for several departments). Since 2008 we have examined 19 PhD dissertations. Patents – see below.

e. Collaborations within Lund University

For the whole Department the creation of the COMPUTE research school is seen as key to re-enforcing and expanding already existing networks within the Science Faculty as well as creating new collaborations within Lund University. COMPUTE is lead by members of our Department and spans some thirteen research groups across the entire Science Faculty.

CBBP remains a "hub" for several collaborations within Lund University, in part reflecting the fact that computational biology is becoming increasingly important in life sciences. Since RQ08 we have doubled such collaborations. Current projects include a project on soil carbon sequestration (with microbial ecology), the PlantLink competence centre (Lund University and SLU Alnarp), and a project on early diagnosis of Alzheimer's disease (with clinical memory research). We also have collaborations with oncology, immunotechnology (through the excellence centre Create Health), clinical physiology, experimental medical science, bio-physical chemistry (through the research school in pharmaceutical sciences, FLÄK) and the nano-meter structure consortium. Within particle physics our prime collaborators remains the experimental particle physicists. In astronomy we have expanded our Lund collaborations since RQ08. This has taken place through a program on astrobiology at the Pufendorf Institute, and ongoing collaborations with geologists. Cooperation with the laser centre continues.

f. National and international collaborations

We have large networks external to Lund University and these networks have expanded since RQ8. This expansion, in part, is because we have been very successful in recruiting new staff from outside Lund who bring new networks with them to the benefit of the whole research environment and further strengthening our good international visibility.

In particle physics the collaboration with the phenomenology group in Uppsala has expanded appreciably, with several joint publications, and the good contacts with their hadron physics experimental group has continued. We have very strong international ties, notably with CERN, where we go regularly, and we co-publish in various transnational collaborations.

In studies of the Milky Way our astronomers have consolidated their position in several large observational projects. Apart from Gaia, we play a leading role in the Gaia-ESO Survey (involving 400 European astronomers, including close collaborators in Uppsala) and in the 4MOST project where one of us is project (also with Uppsala). In theoretical astrophysics we continue to work with our international network of collaborators over a broad range of problems and we are active developers of the open source hydrodynamics code *Pencil Code*.

Most of the research within CBBP is conducted in close collaboration with experimentalists. An example at the national level is the KAW project ShapeSystems (with groups in Umeå and Linköping). Our research in medical applications is done mainly with national collaborators, whereas many of our collaborators are international (e.g., EMBL in Heidelberg, University of Cambridge, Caltech, MIT, Peking University).

Groups of our research staff are members of the EU Marie Curie network MCnetITN and the EU integrating activity Hadron Physics 3 and we have led one EU funded ITN and participated in another (ELSA and GREAT-ITN, respectively, both in astronomy).

g. Collaboration with industry

Mattias Ohlsson (CBBP) provides R&D expertise for diagnostic software used in medicine at Exini Diagnostics AB, Lund (http://exini.com/). He also, together with Carsten Peterson, works with Immunovia AB, Lund (http://www.immunovia.se/). This company specialises in developing tools to use biomarker signatures for diagnosis and prediction of human disease.

h. Infrastructure investments

Through a grant from KAW we are helping to build the next generation of infrastructure for Milky-Way research (4MOST) and the Gaia satellite itself forms part of the European astronomical infrastructure. We have successfully sought grant money to purchase the computer hardware necessary for our theoretical astrophysics research. The atomic astrophysics group have continued to maintain and develop its in-house instrumentation.

2. Visions for 2014 – 2017

a. Evolution of research

Theoretical Particle Physics Particle physics is in a harvest period after the LHC start-up, and further progress can be expected from a variety of other experiments. We believe that we have an excellent team for playing an active role in such topical research, not least given our renewal since RQ08. Typical questions we will study include: How can the precision of perturbative QCD predictions be increased? How can the borderline between perturbative and non-perturbative phenomena be understood better, both for proton and heavy ion collisions? How can low-energy effective theories be used more efficiently to probe properties both within and beyond the standard model (BSM)? What scenarios for BSM physics do have a realistic chance of being observed, and how? What are the prospects to discover further Higgs states? What is the connection between Dark Matter, Dark Energy and ordinary particle physics? As part of the 2013 European Strategy for Particle Physics, new studies are beginning on CERN flagship projects beyond the LHC, such as e+e- linear colliders or an even larger hadron collider. We intend to be fully involved in such studies, in various aspects of phenomenology and in event generator development to meet the new challenges.

Astronomy and Astrophysics With the successful launch of the Gaia satellite, we are entering the first phase of the mission, with a first data releases scheduled to arrive in 2016. Over its entire mission the Gaia data will measure the positions and motions of one billion objects. Its impact will be transformative: ranging from a radical increase in knowledge of near-Earth objects to the understanding of how the Milky Way has been built up over the last thirteen billion years. In Lund our work will have the common focus of the formation and evolution of the Milky Way and its constituents, including exoplanet systems. We will play a leading role in the ground-based observations crucial for the full exploitation of the Gaia mission. We will seek to recruit researchers in atomic astrophysics through the Marie Sklodowska-Curie programme and other visiting fellowships. Work within theoretical astrophysics will be developed both within extreme astrophysics, where we will work with observers of transient events such as supernovae and gamma-ray bursts to understand their observed distribution around their host galaxies. In exoplanet research we will consider the formation of Jupiter-mass planets and the mechanisms responsible for sometimes placing them very close to their host stars.

CBBP In systems biology the main focus will be to increase quantitative understanding of stem cell regulation, cellular polarity, circadian clocks and carbon sequestration, ranging from sub cellular to tissue scales. Novel branches will be to investigate variation in development and complex multi-species interactions, and to connect mechanics and morphogenesis. Within the biomolecular physics research, a central theme will be to characterize processes like protein folding, aggregation and binding under cell-like conditions. Current simulations and experiments typically pertain to more or less idealized test tube conditions. Likely to be particularly environment-sensitive are intrinsically disordered proteins, a subclass overrepresented among regulatory and disease-linked proteins. The overall trend toward personalized medicine makes machine learning methods increasingly important as a powerful tool for, e.g., survival and high-throughput analyses In this area focus will be on will be developing machine learning methods for survival analysis and antibody protein arrays, in close collaboration with researchers in medical science. Our research in bio-nano physics will work along three major research directions. First, DNA bar coding, where theoretical methods will be developed to link fluorescence profiles to DNA sequence. Second, the target finding of regulatory proteins to specific DNA sites will be modelled. Third, the spread of infectious diseases will be modelled, using data on disease properties and human interactions, e.g., from air traffic data.

b. Impact of the research

We live in very exciting times in both particle physics and astronomy where new breakthroughs may well change and challenge our understanding of the Universe in radical ways. Researchers at Lund take an active part in these fundamental. Examples include the exploration beyond the standard model of particle physics. Here we foresee possibilities to start breaking in to new areas with very high rewards but also high risk. The exploration of the Milky Way with the new tools provided by Gaia and massive ground-based spectroscopic follow-up will reveal if this benchmark galaxy actually fits our understanding of galaxy formation and evolution (e.g., how is the dark matter distributed?) leading, potentially, to fundamental revisions of our place in the Universe.
To enable this research it is important to maintain the continued development of event generators (e.g., Pythia in particle physics) and the astrometric solution for Gaia (astronomy).
With an ongoing revolution in experimental techniques, life sciences are at a stage where theoretical and computational modelling is becoming increasingly important. This area is attracting major attention across the world. CBBP is well positioned in this growing field, with an established and expanding network of collaborations with research groups in medicine and biology. We will remain at the forefront of unravelling the interplay between molecular interactions and cell mechanics in development, and the molecular mechanisms of protein misfolding diseases and regulatory cellular processes. Our research in high-throughput proteomics and fast sequencing will benefit the area of personalized medicine.

c. Consequences for the rest of society

Particle physics and astronomy are about understanding the Universe we live in and the fundamental laws that govern it, with important philosophical implications. It is not about changing society as such, although by-products of basic science often have done just that.
With an aging population and increasing health care costs, computerized clinical decision support will play an increasing role. Our machine learning group is involved in both preclinical and clinical research, including the development of decision support systems for, heart transplantations. Work on modelling plant growth will open up for new strategies, e.g., in biofuel production. Understanding of misfolding diseases, such as Alzheimer's and Parkinson's, through biomolecular modelling is key to develop rational therapies.
We train our masters and PhD students in basic science. Skills learnt through their research and training are applicable to many fields. Our former PhD and masters students make use of their training in a broad range of professions addressing some of the biggest challenges in society, including storage of nuclear waste and the next generation of medical technologies.
The general public have an enormous interest in astronomy as well as in the smallest constituents of the Universe. In satisfying the public's curiosity we also promote the study of our subjects through various outreach activities, such as the masterclass in particle physics. The department is responsible for the running and upkeep of the faculty of science's planetarium. Last year some 9000 people visited the 540 shows given at the Planetarium. Of these, 3400 visitors came from schools in Skåne.

d. Inventions and patents

While our efforts mainly focus on basic science, they have lead to algorithmic inventions being patented (Mattias Ohlsson in CBBP).

e. New infrastructure

We aim to consolidate and further develop interactions between scientists in different fields using computers as a major tool by our development of the COMPUTE research school. By combining groups spanning a very broad range of research areas, COMPUTE has a high potential to develop significant interdisciplinary research at Lund University. Thus continued

support in fundamental sciences will have an impact across a much broader range of subjects. COMPUTE also forms a natural complement to LUNARC. The services provided by LUNARC in terms of high-performance computing and support suits our needs very well and is used extensively by many groups in the department. It is important to us that this facility stays competitive through regular hardware upgrades.
MAX IV will be important for work related to structural biology as well as to the atomic data work carried out in the Edlén laboratory. Continued participation in the development of the next generation of astronomical infrastructure, such as 4MOST, CTA, and PLATO, is crucial.

3. Visions for 2018 – 2020

a. Research directions, trends, and research areas
Theoretical Particle Physics Particle physics phenomenology will remain our focus. After the restart of LHC in 2015 new results are expected, both in terms of higher precision measurements of the Higgs particle properties and new major discoveries. Our continued development of event generators means that we will retain a major role. We will also contribute to new tools for phenomenology, precision calculations and proposals for BSM physics. Besides the LHC, we will also continue to study physics at a number of running and planned experiments, at the energy and intensity frontiers.
In addition, some kind of breakthrough should be expected in dark matter searches. This may lead the whole particle physics field into new paths. New major experiments would be proposed, even ESS may play a role. The Lund group has the breadth of knowledge and experience to support some of the necessary preparatory work. There are also concrete ideas to study the neutron electric dipole moment at the ESS. We already have expertise both in the new physics that would be the searched-for signal and in the hadronic parts that constitute the background. Nevertheless, it would be sensible to further strengthen our expertise in this area.

Astronomy and Astrophysics We will continue the work started in the previous period and we have several aims. Consolidation of our role as a leader of exoplanet research, with the aim to having strengthened the ties with geology as well as participating in the upcoming ESA PLATO mission. Our involvement in 4MOST and Gaia will start to focus on the science exploitation phase in this period. This will be a prime time for Galactic research and it will be important to have solicited additional resources such that we are able to make the most of our significant inside knowledge in these projects. It will be an exciting time with many new discoveries and the potential to build deeper ties with modellers and theorists in this field. Within extreme astrophysics, we will study the contribution of compact binaries to the population of transient events found in all-sky surveys and consider the growth of the supermassive black holes found in the nuclei of galaxies such as our own Milky Way.

CBBP Computational biology is a growing and rapidly evolving field. One clear trend in medicine is toward individualized treatment. In this development, machine-learning methods provide an indispensable tool. A grand challenge likely to attract more and more attention is comprehensive and realistic modelling of whole cells. Steps in this direction are being taken, but this research is still at a very early stage. Current systems biology and molecular approaches represent opposite extremes in terms of spatial and temporal scales. Advances toward creating virtual cell models require synergistic multi-scale methods to bridge this gap in scales. CBBP has the capability to play an important role in this development. For this, it is crucial that we continue to have a broad profile in our research topics.

b. Consequences of such research
Given the long time scales involved in particle physics experiments, the research done in Lund will continue to play an essential role in the exploration of particle physics. New breakthroughs may open a new chapter in our understanding of particle physics and the structure of

the Universe alike. Even so, the basic tools and calculations done by the group will stay central to future developments of the field. In astronomy, a new understanding of the Milky Way as a galaxy will pave the way for a deeper understanding of galaxy formation and evolution across the Universe and might also have implications for our understanding of the nature of dark matter. The search for habitable Earths outside the solar system will continue. Our theoretical work on the formation and evolution of exoplanet systems and supermassive black holes will enable us to stay at the forefront of these developments.

Physical modelling of cells would enable a quantitative and systematic understanding of biological systems, and especially the interplay between cellular processes. For example, it would provide the possibility for predicting the effects of biomolecules and potential drug candidates on an entire cell, instead of focusing on single targets at a time.

c. Preconditions for such research

Under item b. we described each of our three research areas separately. However, for success in any of them the same preconditions apply – for significant impact it is important to retain a broad research profile, yet with clear focuses. As our research is driven by the curiosity of individual researchers keeping the size of the research groups above a critical level will remain a high priority. For this it is very essential to keep a stable base of permanent staff, complemented with postdocs and PhD students. These must be sought via external grants. If these are not successful, our means to have a large impact in our research areas diminishes. Therefore, apart from actively seeking funding opportunities an eye must always be kept on focusing the research such that the individual research groups remain above a critical size.

By 2017 all four currently permanent senior researchers in theoretical particle physics will be older than 50. Therefore the top priority is to transition current junior faculty into permanent positions. Prof. Torbjörn Sjöstrand will retire in 2019. It is imperative to recruit a successor, possibly but not necessarily within the same field. In order to continue activity with the highly successful Pythia event generator, which has been the most used event generator in particle physics over the last 30 years. Here a directed international recruitment may be important.

Prof. Dainis Dravins will retire prior to 2017. We will seek to replace him internally from amongst our younger members of academic staff. Prof. Lennart Lindegren will also retire. He has played a world-leading role in astrometric space missions. We wish to maintain Lund's leading role in this area. This would be enabled by the recruitment of new academic staff working in fields at the interface of observational studies and theoretical work on dynamical evolution within the Galaxy. Re-opening Lennart Lindegren’s position might be a means to achieving both of these goals.

For the long-term success of all our research areas it is a high priority to actively mentor and promote our young scientists who will form the basis of our next generation of permanent staff. For some of them, notably those working in the expanding research areas covered by CBBP, there is an urgent need to look into the transition to permanent staff.

d. Possible innovations

It is possible that the research in computational support for medicine will lead to some innovations, e.g., in the area of clinical decision support.

e. Strong research environments at Lund University

If ESS should come to have an important role to play for particle physics, then Lund University should take the lead in building up a strong group that, as part of a bigger international collaboration, can carry out the relevant experiments. Our group in theoretical particle physics should then also be further extended in this direction, to provide theory support. Alternatively, research in astroparticle physics and cosmology could gain in importance, and a new such research environment could emerge, encompassing members from astronomy and experimental and theoretical particle physics.

There are several strong research environments involving astronomers in Lund, while astronomy itself forms a coherent research unit working within the common goal of understanding the formation and evolution of our Galaxy and its constituents.

Computational biology collaborates tightly with experimental groups through LU research environments such as Create Health and PlantlLink. The motivation for building ESS is in part its potential in life sciences, and to realize this potential computational modelling will be instrumental. Here CBBP will play a natural role.