

Cognitus

A Science Case for High Performance
Computing in the Nordic Region



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NordForsk Policy Paper 1 –2015

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Computing in the Nordic Region

NordForsk, 2015
Stensberggata 25
N-0170 Oslo
www.nordforsk.org
Org.nr. 971 274 255

Design: jnd.no
Cover Illustration: Eliro/Shutterstock
Printed by: 07 Group

ISSN 1504-8640



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A Science Case for High Performance Computing in the Nordic Region

NordForsk is an organisation under the Nordic Council of Ministers that works to promote cooperation in all fields of research and research-driven innovation when this adds value to activities being conducted in the Nordic region.

The Nordic e-Infrastructure Collaboration (NeIC) is an organisation that facilitates the development and operation of high-quality e-Infrastructure solutions in areas of joint Nordic interest. NeIC is a distributed organisation consisting of technical experts from academic high-performance computing centres across the Nordic countries. NeIC was established as an organisational unit under NordForsk in Oslo on 1 January 2012.

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Preface

High Performance Computing (HPC) is an increasingly more vital element in modern research, accelerating scientific progress and enabling scientists to do everything from creating more efficient wind turbines to understanding the human genome. Access to large-scale HPC resources is critical to ensuring the competitiveness of Nordic research.

In 2013 and 2014, the Nordic e-Infrastructure Collaboration (NeIC) conducted an evaluation of the Nordic High Performance Computing (NHPC) project and the Nordic use of PRACE (Partnership for Advanced Computing in Europe). In their conclusions, these evaluations put forth strong recommendations to develop the scientific case for Nordic HPC, identifying the researchers using HPC and mapping where and how they obtain access to these resources. The results could in turn be used to guide decisions on future Nordic HPC investment and participation in international projects. The Cognitus project was launched as a response to these recommendations. The idea was that optimizing access and availability to existing and upcoming HPC services for researchers and research groups across the Nordic countries would serve to increase the level of scientific excellence.

This report presents several recommendations and provides decision-makers in the Nordic countries with valuable insight that will help to promote more globally competitive Nordic HPC.

NordForsk works to enhance the quality, impact and cost efficiency of Nordic research infrastructure by facilitating expanded cross-border access to, and joint use of, existing research infrastructures in the Nordic region and globally and by supporting the establishment of new joint Nordic research infrastructures. We therefore welcome this report, support its recommendations, and hope they will spur the enhancement of Nordic collaboration in this highly important field.

We would like to thank Dr. Rob Pennington for his excellent work in conducting this study.

April 2015



Gunnel Gustafsson
Director of NordForsk



Gudmund Høst
Director of NeIC

Executive Summary

In 2013 and 2014, NeIC used external expert panels to evaluate two important aspects of the Nordic high performance computing (HPC) environment, the Gardar NHPC shared resource in Iceland and the use of or involvement with the PRACE project by researchers and e-infrastructure providers in the Nordic countries. The two evaluations made strong recommendations to develop the scientific case for Nordic HPC, which could then be used to inform and guide decisions in future Nordic HPC investment and participation in international projects. The NeIC Board tasked NeIC with coordinating this effort in June 2014 as **the Cognitus project**.

This study has used three approaches to obtain information about the science case for HPC in the Nordic region. The first was to obtain the generally available information in key topics associated with researchers' use of HPC in the Nordic countries, primarily using web searches and interactions with people knowledgeable about the topics in the region.

The second approach was to identify the researchers who were already large users of the HPC resources within each country and also of internationally available HPC systems. In addition, key people in each country who are responsible for the major resources were also identified. Two surveys were prepared asking essentially the same questions from the two different points of view, that of a researcher and that of a provider of resources to researchers. The survey effort was focused on building a picture of the research strengths within the Nordic region that have impacts and effects that reach beyond national borders and on what should be done to enable this research through Nordic HPC efforts.

The third approach was to conduct interviews using either videoconferencing or the telephone to discuss the survey and related topics with the survey recipients who were willing to participate, in many cases completing it as part of the call.

Research approaches that depend on computations have a long history in the Nordic region and have been strongly influenced by problems that are of direct societal relevance, such as weather and natural resources, as well as fundamental scientific and engineering questions. As a result, research programs have developed in a wide range of domains, at different scales and through a variety of mechanisms for support. This has led to a richness of approaches in a highly diverse set of local and national research environments within a geographic region that has also developed a very high level of formal and informal cooperation and collaboration.

The scientific research capabilities and strengths that this range of approaches has produced are significant and are world-class in a number of different areas. Nordic researchers have achieved scientific leadership through their individual efforts, institutional and university research programs and national and international research collaborations.

As the forefront of scientific research advances and new knowledge is discovered, the questions become more complex. As a result, researchers are driving in two significantly different directions. The first is to fully and deeply explore the fundamental problems that are their principal focus. This requires developing a significantly deeper understanding that may also be extremely tightly focused. The second is to understand the broader implications and applicability of their research and, inversely, to understand the implications of others' research results as they relate to their own endeavors. This simultaneous narrowing of focus and broadening of scope is leading to new larger collaborations as researchers explore the full scope of the problems that they are investigating.

These changes in research collaborations are deeply connected with changes in nature and scale of research infrastructures, ranging from the development of instrumentation through the dissemination and reuse of the data, publications and other results. Intrinsic in virtually all aspects of research infrastructure is the need to understand and incorporate digital techniques.

Findings and recommendations



Findings and recommendations

Finding #1: Research in the Nordic region that depends on computational capabilities is clearly internationally competitive. Continued investment in excellence in computational research and education on national scales is vital to continuing this success.

Recommendation #1: Funding for national programs must have a focus on the research priorities and needs that are defined in national science cases and scenarios.

Finding #2: Support for research excellence and collaborations must include an informed balance of computational and data resources, including training and support. There are very different levels of clarity or information about the scientific justification for the computational research infrastructure in the different countries.

Recommendation #2: At the national level, a clear set of science cases for computational and data research infrastructure in each country should be published and used to inform and guide the acquisition, support and coordination of the national computing and data resources. The national science cases should be periodically updated to reflect the changing research environment and topics.

Finding #3: Researchers in different research domains may rely on access to different sets of computational and data resources. Researchers in Universe Sciences rely significantly on PRACE Tier-0 resources and those in Chemistry and Materials Science rely on the respective national resources. Each of these are different strengths in the Nordic region.

Recommendation #3: The national science cases, along with other indicators and information, should be used to inform the continued development of the Nordic science case as part of the responsibilities of NeIC.

Finding #4: Support for computing and data research infrastructure capabilities that are competitive internationally will be critical to extending this success into the future. The current model of access to PRACE Tier-0 level resources being granted at no cost to Nordic researchers based solely on the merits of the research is likely to change in the near future.

Recommendation #4: The national focus and funding needs to be augmented with funding for an international program. This may be in the form of a joint Nordic involvement with PRACE, as it evolves, that can provide a coordinated Nordic Tier-0 level of capability. This should be considered to be a logical extension of national programs and appropriately incorporated into each national strategy. Ideally, this would include all of the Nordic countries but initiating it with a subset of the countries should be considered. The inclusion of a neutral broker in the form of NeIC would facilitate the openness and extensibility of the program in the future if not all of the countries are initially involved.

Finding #5: Collaborations are vital to national and international recognition and excellence for individual researchers, research groups and research-based organizations. They create new opportunities that leverage the investments within each country to deepen and extend knowledge networks, innovate technical capabilities and effectively address complex scientific problems, many of which are international in scope and have a high level of societal relevance.

Recommendation #5: The role of NeIC should be expanded to include identifying and, where feasible, initiating scientific and technical collaborations that reinforce those national science cases that cross international boundaries, including outside the Nordic region. Successful outcomes for these efforts cannot be assured but ideally the fruitful and productive collaborations will become part of the national science cases and be supported appropriately. NeIC should be recognized and supported in undertaking this aspect as it may entail some risks, just as the national programs assume risks associated with their research infrastructure.

Finding #6: Innovation and exploration are critical to fundamental and applied research. They need to be fostered through extended collaborations and coordination. The national approaches to supporting research infrastructure have different strengths that can be successfully built upon and, at several levels, coordinated in the Nordic region to enhance national research priorities and commitments as well as the capabilities available to the researchers.

Recommendation #6: The exchange of information, experiences, roadmaps and strategic priorities are important aspects of increasing innovation and exploration. This should be facilitated by NeIC through a mechanism similar to that developed for Recommendation #4. Such information should be publicly available whenever feasible.

Finding #7: Long timescales normally associated with extensive and ambitious research programs and shorter timescales associated with research projects need to be incorporated in the strategic planning for research infrastructures and for the implementations that grow out of that planning. High levels of uncertainty in funding can adversely affect research productivity, planning and directions.

Recommendation #7: The funding bodies in the Nordic countries need to work together to develop a set of guidelines for supporting the long-term programs that are needed for international computation and data research infrastructures as well as the collaborations that depend on them. The funding bodies must encourage and stimulate alignments between the national and international programs with clear recognition of the potential for synergies and excellence through the efforts of the national research and e-infrastructure programs.

Based on the aggregate of the previous findings and recommendations, there is one additional recommendation.

Recommendation #8: The information, roadmaps and guidelines developed as part of the previous recommendations must have a path for implementation to be effective. In particular, the national resource providers and NeIC should be equipped with funding and authority to carry out recommendation #4 for sustainable Nordic access to a Tier-0 class capability. NeIC could be instrumental in facilitating the development of such implementation plans.



Background

Researchers in all of the Nordic countries are making increasing use of local, national and international computing resources as part of their research routine. Each of the countries supports its national researchers and also cooperates through the Nordic e-Infrastructure Collaboration (NeIC), which is hosted by NordForsk. Over time, this has resulted in strong efforts to develop and share programs that enhance the national and regional capabilities in multiple science areas important to the Nordic region.

In particular, a Nordic computational science challenge should have many or all of the following characteristics:

- address a fundamental scientific question that is widely recognized as important and challenging to solve
- have international interest and relevance
- include Nordic researchers in scientifically significant roles
- require collaboration among research teams and communities
- be a long-term (multi-year) sustained effort with intermediate goals
- require large-scale infrastructure resources (HPC, storage, networks)

In 2013 and 2014, NeIC used external expert panels to evaluate two important aspects of the Nordic high performance computing (HPC) environment, including the Gardar NHPC shared resource in Iceland and the use of or involvement with the PRACE (Partnership for Advanced Computing in Europe) project by researchers and e-infrastructure providers in the Nordic countries. The two evaluations made strong recommendations to develop the scientific case for Nordic HPC, which could then be used to inform and guide decisions in future Nordic HPC investment and participation in international projects. The NeIC Board has tasked NeIC with coordinating this effort.

PRACE is an international not-for-profit association that includes Denmark, Finland, Norway, and Sweden. The goal of PRACE is to enhance European competitiveness for the benefit of society. This is accomplished through peer reviewed access to world-class tiered computing resources and services to researchers from all disciplines for the conduct of high-impact scientific discovery, engineering research and development.

Additional information about the use of PRACE by Nordic researchers was used along with a survey of HPC users to build up the picture of the science case for HPC in the Nordic region. The survey was intended to provide a high-level view of many different research projects and their future computational needs, particularly those that go beyond the computing and storage capabilities that researchers are currently using.

The survey was focused on building a picture of the research strengths within the Nordic region that have impacts and effects that reach beyond national borders and on what should be done to enable this research through Nordic HPC efforts.

All of the questions were intended to help develop a high-level characterization of the ways in which researchers use the computing and data systems. Estimates were requested, rather than detailed or exact statistics, to get this overview of how the systems are used.

In addition, there have been a number of studies on the science cases relating to computing and data research infrastructure. A subset is listed here for context and can provide additional useful information. The Swedish Science Cases for e-infrastructure is an excellent reference and is one example of an effective approach.

1. PRACE Scientific Case for HPC in Europe 2012-2020
<http://www.prace-ri.eu/prace-the-scientific-case-for-hpc/>
2. Nordic Computational Grand Challenge survey 2007
https://www.notur.no/sites/notur.no/files/publications/pdf/ncgc_survey_2007.pdf
3. Future Directions for NSF Advanced Computing Infrastructure to Support US Science and Engineering in 2017-2020: Interim Report (2014)
http://www.nap.edu/openbook.php?record_id=18972&page=R1
4. NSF ACCI Task Force Reports
<https://www.nsf.gov/cise/aci/taskforces/>
5. The scientific case for eInfrastructure in Norway (2010)
Published by the Norwegian Research Council
http://www.forskningsradet.no/en/Home_page/1177315753906
6. Swedish Science Cases for e-infrastructure (2014)
<https://publikationer.vr.se/en/product/swedish-science-cases-for-e-infrastructure-2/>

Approach

Due to the differences in the mechanisms to support research in each of the Nordic countries, the descriptions, impacts and extent of the effects are often in different standard formats or have different types of information. While this may at first glance seem to be a limitation on the ability to draw inferences and conclusions, it can be a deep strength of the region. This diversity in mechanisms allows the exploration of the range of effects that can be brought about by HPC and storage research infrastructure when it is available to researchers. Considered in another light, the lack of data or information on a specific topic within a given country does not necessarily lead to a similar lack of data in another country. This leads to a very rich and broad, though heterogeneous, range of information that is eminently usable and useful if considered carefully. Given the extensive levels of collaboration and the amount of information available in each country, it is likely that the result can be a unique set of data describing the science impact of HPC in the region.

The study has used three methods to obtain information about the science case for HPC in the Nordic region. The first was to obtain the generally available information in key topics associated with researchers' use of HPC in the Nordic countries, primarily using web searches and interactions with people knowledgeable about the topics in the region. Given the generally open approach to information in the Nordics (and Europe) around research projects and programs, this was an extremely useful part of the process.

The second method was to identify the researchers who were already large users of the HPC resources within each country and also of internationally available HPC systems. In addition, key people in each country who are responsible for the major computational research infrastructure resources were also identified. Two surveys were prepared asking essentially the same questions from the two different points of view, that of a researcher and that of a provider of resources to researchers. These individuals were emailed an appropriate survey to gather information on their research projects and the use of HPC.

The third method was to conduct interviews using either videoconferencing or the telephone to discuss the survey and related topics with the researcher, in some cases completing it as part of the call. This was relevant to providing context and more complete information about the importance of the topics for the researchers.



International projects and collaborations



International projects and collaborations

It is important to note the importance of looking at computational research projects in a larger context than just the Nordic region. For many topics, there are a very limited number of venues that allow for comparison of the competitiveness of research projects. Fortunately, the connection between research and high performance computing provides this to some extent through the PRACE, the US Department of Energy (DOE), Innovative and Novel Computational Impact on Theory and Experiment (INCITE) and US National Science Foundation (NSF) Petascale Computing Resource Allocations (PRAC) programs. Each of these programs is extremely competitive and each awards access to the resources only to the best research groups.

PRACE is the premier European high performance computing research infrastructure available to researchers. Regular access to PRACE Tier-0 resources is made available through a competitive call for proposals process that began in mid-2010 with the first call, under which nine of the 59 proposals submitted were granted access to Tier-0 resources.

The two programs in the US provide access to the leading-edge computational systems that are available for open scientific research through a peer reviewed process. More information is included in Appendices B and C.

PRACE and INCITE are open to international PIs and the PRAC program allows international co-investigators. The ability of a research team to successfully compete for access to these top-tier international resources is a reflection of the quality of the research and the competence of the research team to carry it out on the most advanced computing resources available.

The researchers in the Nordic region have demonstrated a notable level of success in such competitions, with a total of 49 projects, of which 32 have been led by Nordic researchers. The scientific impact of these world class projects extends to the collaborators, students and post-docs who are part of the projects. There are a total of 121 Nordic researchers who have been explicitly named as part of the awards.

In considering the researchers who have been successful in these international competitions, it is not obvious that there is a strong correlation with the major research projects on the national systems. This could be due to the limited time windows for identifying the major national users but it is also likely that some of the research problems are sufficiently different on the different scales of systems.

The successive, for Calls for Proposals 2–9 for Regular Access, from April 2011 through April 2014, resulted in 30 awards to teams led by researchers at Nordic institutions and an additional 13 that included Nordic researchers as part of the successful teams. The resources available through PRACE at the end of 2014 were:

- Curie (Bull Bullx cluster, CEA, France)
- Fermi (IBM Blue Gene/Q, CINECA, Italy)
- Hermit, (Cray XE6, HLRS, Germany)
- Juqueen (IBM Blue Gene/Q)
- Mare Nostrum (IBM System X iDataplex, BSC, Spain)
- SuperMUC (IBM System X iDataplex, LRZ, Germany)

Information on each of the calls is listed at <http://www.prace-ri.eu/closed-calls/> and the current resources are described at <http://www.prace-ri.eu/prace-resources/>

Appendix A contains detailed information on the PRACE awards that have been made that include Nordic researchers. It contains information from the PRACE website (<http://www.prace-ri.eu/>) on Regular Access awards for calls 1–9. The information in the appendix includes the title of the award, the list of PIs and collaborators, the abstract and the resources awarded.

Table 1 Awards to Nordic PI and co-PIs for PRACE Tier-o, DOE INCITE and NSF PRAC Projects

Area	PRACE Tier-0	DOE INCITE	NSF PRAC
BioChemistry, Bioinformatics and Life Sciences	6		
Chemical Sciences and Materials	6	5	
Earth System Sciences	3		
Engineering and Energy	5		
Fundamental Physics	7		
Mathematics and Computer Science	1		
Universe Sciences	15		1

Tables 1 summarizes the projects for the PRACE Tier-o awards that include Nordic researchers. There have been 329 PRACE Tier-o awards up through call 9 to researchers in all countries. Nordic PIs have led 30 projects and an additional 13 have involved Nordic researchers. There is a clear strength in the Nordic region in topics relating to Universe Sciences in the PRACE Tier-o competitions.

The 2014 Nordic PRACE study estimated the usage of the PRACE Tier-o resources over a two-year period (calls 2–7) to effectively amount to approximately 25% of a Tier-o system.

Table 2 PRACE Tier-o Awards for Calls 2–9 Biochemistry, Bioinformatics and Life Sciences

Name (call)	Title	Lead Organization (Countries)
Prof. Mattia Falconi (6th)	DNANANO Molecular dynamics simulation and experimental characterization of a DNA nanocage family.	University of Rome “Tor Vergata”
Prof. Ilpo Vattulainen (6th)	Unlocking the role of lipids in the activation mechanism of the Epidermal Growth Factor Receptor (LIPIDS-EGFR)	Tampere University of Technology
Prof Hannu Hakkinen (7th)	NANO-GOLD AT THE BIO-INTERFACE	University of Jyväskylä
Prof. Kresten Lindorff-Larsen (7th)	NMRFUNC	University of Copenhagen
Dr. Thomas Kjaergaard (8th)	Linear Scaling and Massively Parallel Coupled-Cluster Calculations on the Leucine Transporter within a DEC framework	Aarhus University
Ilpo Vattulainen (9th)	Lipidmodulation of the toll-like receptor TLR4	Tampere University of Technology

Table 3 PRACE Tier-o Awards for Calls 2–9 Chemical Sciences and Materials

Dr. Branislav Jansik (4th)	High-accuracy quantum mechanic models for extended molecular systems	Aarhus University Institute of Chemistry
Prof Hannu Häkkinen (5th)	Plasmonic ligand-stabilized gold nanoclusters	University of Jyväskylä
Emilio Artacho (9th)	Large-scale radiation damage cascades from first principles	CIC nanoGUNE
Martti Puska (9th)	EXCIST – Excited state charge transfer at the conjugated organic molecule – semiconductor interface	Aalto University School of Science
Prof. Enrico Bodo (8th)	Aminoacid anions in organic compounds: charting the boundary of room temperature ionic liquids	Univ. of Rome, “Sapienza”
Dr. Arkady Krasheninnikov (3rd)	Effects of irradiation on nanostructures from first principles simulations	University of Helsinki Department of Physics

Table 4 PRACE Awards for Calls 2–9 for Earth System Sciences

Dr. Colin Jones (4th)	HiResClim : High Resolution Climate Modelling	Swedish Meteorological and Hydrological Institute (SMHI)
Dr. Francisco Doblas-Reyes (7th)	HiResClim: High Resolution Ensemble Climate Modeling	Institut Catal de Cincies del Clima
Prof. Anatoly Belonoshko (8th)	EGOIST – Endogenic oil synthesis in the deep Earth interior: ab initio molecular dynamic simulation	The Royal Institute of Technology (KTH)

Table 5 PRACE Tier-o Awards Calls 2–9 Engineering and Energy

Prof. Xue-Song Bai (8th)	Direct numerical simulation of partially premixed combustion in internal combustion engine relevant conditions	Lund University
Prof. Arne Johansson (2nd)	REFIT - Rotation effects on flow instabilities and turbulence	KTH Department of Mechanics
Prof. Xue-Song Bai (4th)	Direct numerical simulation of reaction fronts in partially premixed charge compression ignition combustion: structures, dynamics	Lund University Department of Energy Sciences
Dr. Timo Kiviniemi (4th)	Full-f gyrokinetic simulation of edge pedestal in Textor	Aalto University School of Science
Dr. Simone Camarri (6th)	TRADELINBO Transition delay in Blasius-like boundary layers by passive control: complementary investigation and numerical support to an ongoing experimental activity	University of Pisa

Table 6 PRACE Tier-o Awards Calls 2–9 Fundamental Physics

Dr. Arnaud Beck (8th)	LEAC – Laserplasma Electron Acceleration for CILEX	CNRS
Prof. Claudio Pica (4th)	Strong interactions beyond QCD	University of Southern Denmark
Dr. Ari Hietanen (6th)	Simulating Dark Matter on the Lattice	University of Southern Denmark
Prof. Kari Rummukainen (6th)	CWIN - Mapping the conformal window	University of Helsinki
Constantia Alexandrou (9th)	Nucleon structure using lattice QCD simulations with physical pion mass	Univ. of Cyprus and the Cypress Institute
Claudio Pica (9th)	MCH - Minimal Composite Higgs	Univ. of Southern Denmark
Thomas Grismayer (9th)	Pair-dominated plasmas in ultra intense fields: from the laboratory to extreme astrophysical conditions	Instituto Superior Tecnico

Table 7 PRACE Tier-o Awards Calls 2–9 Mathematics and Computer Science

Prof. Johan Hoffman (8th)	FENICSHPC – High performance adaptive finite element methods for turbulent flow and multiphysics with applications to aerodynamics, aeroacoustics, biomedicine and geophysics	The Royal Institute of Technology (KTH)
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Table 8 PRACE Tier-o Awards Calls 2–9 Universe Sciences

Prof. Aake Nordlund (2nd)	Ab Initio Modeling of Solar Active Regions	University of Copenhagen Niels Bohr Institute
Prof. Mats Carlsson (3rd)	Physics of the Solar Chromosphere	University of Oslo Institute of Theoretical Astrophysics
Prof. Paolo Padoan (4th)	Extreme Star-Formation Modeling: From the Galactic Fountain to Single Stars in One Run	Catalan Institute for Research and Advanced Studies (ICREA) and University of Barcelona Institute of Cosmos Sciences (ICC)
Prof. Aake Nordlund (4th)	Ab Initio Modeling of Solar Active Regions	University of Copenhagen Niels Bohr Institute
Dr. Iljan Iliev (5th)	LocalUniverse - Our Neighbourhood in the Universe: From the First Stars to the Present Day	University of Sussex
Prof. Garrelt Mellema (5th)	Simulating the Epoch of Reionization for LOFAR	Stockholm University

Table 9 PRACE Tier-o Collaboration and Nordic Researchers

Dr. Minna Palmroth (5th)	Vlasiator: Global hybrid-Vlasov simulation for space weather	Finnish Meteorological Institute
Dr. Troels Haugboelle (6th)	StarLife - Protostars: From Molecular Clouds to Disc Microphysics	University of Copenhagen
Prof. Mats Carlsson (7th)	Physics of the Solar Chromosphere	University of Oslo
Dr. Troels Haugboelle (8th)	STARZOOM - Zooming in on Star Formation	University of Copenhagen
Dr. James Bolton (8th)	Rare structures in the Lyman alpha forest: bridging the gap between small and large scales.	Univ. of Nottingham
Dr. Petri Kapyla (8th)	SOLDYN: Simulations of SOLar DYNamo cycle and differential rotation	University of Helsinki
Prof. Giovanni Lapenta (8th)	Magnetic Reconnection in Three dimensional Turbulent Configurations	KU Leuven
Prof. Garrett Mellema (9th)	PRACE ₄ LOFAR	Stockholm University
Ilian Iliev (9th)	Multi-scale simulations of Cosmic Reionization	University of Sussex

PRACE Tier-o Collaborations

One of the important trends in working with complex research problems is the need for effective collaborations. This is necessary to more realistically address the problems, which often have a number of separate aspects or components that may cross domains or require specific skills or expertise. Table 9 can be viewed as a measure of where the collaborations take place, whether between colleagues in the same institution (column 4), within the same country (column 5), within the Nordic region (column 6) and between researchers in the Nordic region and other parts of the world (columns 7 and 8).

One possible inference to be drawn from the data in the table is that there is not a strong bias towards local collaborations, either in the same institution or the same country, even though these are often the easiest to initiate and maintain. In fact, of the 43 Tier-o projects with Nordic involvement shown in the table, 60% involve collaborations outside the Nordic region, split evenly between those led by Nordic PIs and those not led by Nordic PIs that include Nordic co-PIs. Given the competitive nature of the Tier-o process, this suggests that researchers are more focused on successful science projects regardless of locality and that Nordic researchers are perceived as valuable research partners. This may also be reflected in the collaborations that are shown in the DOE INCITE and NSF PRAC awards that include Nordic researchers.

Table 9 PRACE Tier-o Collaborations and Nordic Researchers

Call	Total number of Awards	Nordic PI	Nordic PI and All co-PIs at Same Institution	Nordic PI and All co-PIs in the Same Country	Nordic PI and Only Nordic co-PIs	Nordic PI and non- Nordic co-PIs	Non-Nordic PI and Nordic co-PIs
1	9	0	0	0	0	0	0
2	17	2	0	0	0	2	0
3	24	2	0	1	1	1	0
4	43	5	2	3	3	2	1
5	57	4	0	2	2	2	1
6	57	4	2	2	2	2	2
7	35	3	2	2	2	1	1
8	44	6	3	3	4	2	4
9	43	4	3	3	3	1	4
Total	329	30	12	16	17	13	13

DOE INCITE awards

The DOE INCITE program provides access to the leadership class DOE funded machines at Oak Ridge National Lab (ORNL) and Argonne National Lab (ANL). The process is highly competitive and includes a rigorous scientific and technical review of the proposed projects.

The Titan system at ORNL is a Cray XK7 system that combines general purpose computing cores with GPU accelerators, <https://www.olcf.ornl.gov/computing-resources/titan-cray-xk7/>
The Mira system at ANL is an IBM Blue Gene/Q system, <http://www.alcf.anl.gov/user-guides/mira-cetus-vesta>.

The information on DOE INCITE awards that include either a Nordic PI or co-PI is shown below. The period covered was from 2010–2015. DOE allows proposers from institutions outside the US to be project PIs and this is reflected in their statistics for 2015 which identify 11% of the 56 awarded projects as having non-US PIs. One of these awards, in Physical Chemistry, was to a PI in Denmark, who also had a 2014 award. The materials science projects in table 10 included researchers from the Technical University of Denmark as co-investigators.

The INCITE projects listed include the initial awards and the renewals of these awards for a total 35,000,000 processor hours on the IBM Blue Gene architecture for Materials Science and 72,000,000 processor hours on the Cray XK7 architecture for Physical Chemistry research. Detailed information on these projects is available in Appendix B.

Table 10 DOE INCITE Awards with a Nordic PI or co-PIs

Jeffrey Greeley	2010	Materials Science	Probing the Non-Scalable Nano Regime in Catalytic Nanoparticles with Electronic Structure Calculations	Argonne National Laboratory
Jeffrey Greeley	2011	Materials Science	Probing the Non-Scalable Nano Regime in Catalytic Nanoparticles with Electronic Structure Calculations	Argonne National Laboratory
Jeffrey Greeley	2012	Materials Science	Probing the Non-Scalable Nano Regime in Catalytic Nanoparticles with Electronic Structure Calculations	Argonne National Laboratory
Poul Jørgensen	2014	Physical Chemistry	Large-Scale Coupled-Cluster Calculations of Supramolecular Wires	Aarhus University
Poul Jørgensen	2015	Physical Chemistry	Large-Scale Coupled-Cluster Calculations of Supramolecular Wires	Aarhus University

NSF PRAC Projects on Blue Waters

Of the 29 PRAC awards listed as science teams on the Blue Waters system at NCSA at the University of Illinois, only two listed co-PIs who are not currently at US institutions. One of these two awards had two Nordic researchers included as co-PIs, one from Denmark and one from Norway. From information provided by the Blue Waters project office, a total of six Nordic researchers have Blue Waters accounts associated with this project which has 6,500,000 node hours for universe physics. Detailed information on the science project is available in Appendix C. The Blue Waters system is a Cray XE/XK hybrid machine and is described at <https://bluewaters.ncsa.illinois.edu/hardware-summary>

Table 11 NSF PRAC Award to the Project with Nordic co-PIs

Robert Stein	2012	University of Michigan	Ab Initio Models of Solar Activity	Universe Science
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PRACE Tier-1 Projects

The PRACE Tier-1 resources are national level systems that are made available by the individual countries for allocation and support of research projects through PRACE. These 23 systems are listed in Appendix G, which was sourced from the PRACE resources website, <http://www.prace-ri.eu/tier-1-resources/>

This arrangement enables researchers to access highly capable and well supported systems that may not be available to them through their own national allocations mechanisms, increasing the range of architectures that can be used to solve the computational problems. In addition, support structures and professional staff who are familiar with the national systems are available to researchers with Tier-1 awards. This can also be a strong mechanism for supporting international collaborations on national systems that might otherwise be inaccessible to such collaborations.

The available information on the Tier-1 awards is not directly comparable to the Tier-0 award information as it is not published with the same amount of detail as the Tier-0 awards. Of particular note is that in some cases, projects from researchers from countries without Tier-1 resources appear as external projects for a site with Tier-1 resources. It appears that Denmark is the Nordic country most affected by this. On the other hand, the PRACE project has published a number of reports on the support provided to the Tier-1 projects that are an excellent resource for understanding the level of expertise available to the scientific researchers.

The information available on the projects is summarized in Appendices D and E, along with references to a number of the relevant PRACE reports.

Table 12 includes the total numbers of proposals submitted for DECI-9 to DECI-12 from all countries as well as just those from the Nordic region. The success rate for Nordic proposals is significantly above the average. Appendix F includes information on the numbers of submissions by country.

Table 12 DECI Calls Projects Submitted and Awarded for DECI-9 to DECI-12

DECI Call	Total # of Proposals Submitted	Total # of Proposals Awarded	Proposals from the Nordic Region Submitted	Proposals from the Nordic Region Awarded
DECI-9	45	31	8	6
DECI-10	85	37	12	8
DECI-11	117	52	11	9
DECI-12	61		12	9

The information in Table 13 has been extracted from the Nordic PRACE report and includes information on the break down by country for the DECI projects awarded in the Nordic region.

Table 13 Tier-1 Awards to Nordic PIs by Country

Call	Denmark	Finland	Norway	Sweden
DECI-7	0	2	0	4
DECI-8	1	2	0	4
DECI-9	1	2	0	3
DECI-10	1	3	0	5
DECI-11	2	3	2	2



Socio-economic challenge projects/ Societally relevant projects in PRACE

One very interesting set of projects that have been supported for access to the PRACE Tier-o systems is generally associated with applications that are considered to be community codes. The codes were chosen because of their possible impact on associated research communities. In some cases, these codes were not considered to be necessarily well suited for the Tier-o architectures and the goal was to understand what was required for the code to be effective or whether this was feasible.

Fifteen projects were proposed and eight were approved to go forward, of which two were led by Nordic researchers. The projects included the following:

- Safe and Environmental-friendly energy production
- Rational drug design – Project leader Soon-Heum Ko (LiU)
- Rational drug design
- Sustainable food supply – Project leader Thomas Röblitz (UiO)
- Future aircraft transportation
- ‘Big data’ management and processing
- Understanding of climate change
- Natural environment protection

Two of the approved projects were led by researchers at Nordic institutions (LiU and UiO) and were successful at utilizing Tier-o resources. In one case, the LSDALTON code was evaluated for performance and in the other the use of workflows was evaluated in the context of biological data. Additional information is in Appendix H.



Surveys and Interviews

The survey was envisioned as providing a high-level view of many different research projects and their computational needs. The questions were intended to help develop a high-level characterization of the ways in which researchers use the computing and data systems. Estimates were requested, rather than detailed or exact statistics, to get an overview of how the systems are used.

Requests for information through a survey and a follow up call were sent out by email to 121 researchers and 17 HPC providers across the Nordic region. The list of researchers was compiled from multiple sources and included the Nordic PRACE Tier-0 principal investigators for Calls 2-9 (22), the Nordic Tier-1 PIs (35) from DECI-7 to DECI-12, major users provided by the HPC providers in the Nordic region (81) as well as others who were identified in further discussions with researchers and providers. There was some overlap in the different lists of researchers so the total number of researchers who were contacted is less than the sum of the groups of researchers. The total responses in Table 14 include researchers and providers who returned the survey, were interviewed for the survey or did both. The overall response rate was >30%.

Table 14 Survey Response Summary by Country

	DK	FI	IS	NO	SE	Totals
Surveys sent out	25	34	5	27	47	138
Total responses	9	8	5	14	13	45

The summarized responses to the questions by the researchers are included along with the survey in Appendix J. The ranges of responses had to be expressed in a form that was easily characterized and communicated rather than detailed and explicit, partially because the responses were estimates or descriptive. This approach is useful for the type of high-level view that this project was looking for.

To facilitate this, the responses were summarized and are included in parentheses after each question. A single number indicates that the response was positive or confirmation of the importance of this information or item. Two numbers in the parentheses indicate the numbers of positive and negative responses, respectively. Not every researcher answered every question so the totals are not equal to the total number of responders.

Table 15 includes a classification of the researchers’ responses by their field of research if that information was provided. The PRACE Tier-0 fields were used to bin the responses into an appropriate field as part of the analysis of the data. The most immediate difference is that the most commonly represented field is Chemical Sciences and Materials. This is generally consistent with the information in the surveys from the computational resource providers. This is an aspect that should be carefully considered in the future planning for Nordic computational and data resources as it may suggest that there may be a set of research interests or strengths that may not be fully addressed at a national level.

Table 15 Survey Responses by Research Area

Area	Survey Responses
BioChemistry, Bioinformatics and Life Sciences	4
Chemical Sciences and Materials	10
Earth System Sciences	2
Engineering and Energy	2
Fundamental Physics	3
Mathematics and Computer Science	2
Universe Sciences	4

This section will highlight some specific topics that should be considered in future planning for Nordic computational and data research infrastructure. The first is, as noted above, in comparing Table 15 and Table 1. Even though both types of resources are relatively general purpose, the populations of researchers who use them appear to be different. This can lead to high expectations and needs for support as was highlighted in the responses to Q9 in the survey. The responses reflected a consistent need for general support, training, code development and, to a lesser extent, domain support. This was also noted in the Nordic PRACE report as an important aspect of working with the PRACE environment.

In terms of important outcomes of the research process, papers, impact and students were rated as very important. These were closely followed by software and datasets. Software and datasets are becoming widely recognized as fundamental parts of research and this should be considered in future planning. The first set of priorities is, as one might anticipate, for an individual researcher. The second set may be considered to be important to collaborations and the effects of the research process that extend beyond a research group and often extend beyond national boundaries.

The second question was related to computing facilities and a majority of the researchers who responded have access to and use international facilities. A majority similarly expressed the view that the Nordic computing facilities compare favorably with those of their collaborators and competitors, which reflects well on the facilities and approaches to supporting computational research in the Nordic countries.

The third question related to the types of usage of the systems. The most common response was software development but this was also the response with a lower level of utilization, as might be expected. The highest level of utilization was for high-risk explorations of new possibilities followed by the exploration of parameter spaces, production of data products and evaluation of more complex problems all roughly equivalent. This may be indicative that the types of research usage are reasonably well balanced between the need to push the limits of the research possibilities as well as consistently provide results. The importance of software was also reflected in the responses to the question about user support.

The fourth question showed that the majority of the researchers depend on continuous long-term access for their research projects. Continuity is vital to research. Software may take a decade or more before it achieves a significant level of adoption and datasets can be a valuable long-term research resource.

The responses to the question on using the system for capability, capacity, combination, workflow, or time dependence modes showed that capability was the most common as well as the dominant usage mode at roughly 2X the use in capacity mode. This is an expected outcome of the surveying the users of HPC resources.

Tracking the different modes over time would be useful in detecting changes in usage patterns.

The primary use of the systems was for modeling or simulation, as might be expected, but a significant number of the researchers were also involved with data analysis or other data-related activities. It may be that the data analysis and workflow usage mode are linked and will evolve in time.

The responses to the question on the types of resources needed rated floating point performance, storage, memory and software as the highest needs. Given that this was a set of researchers selected for their use of high performance computing, the inclusion of storage and software as major priorities is important because it emphasizes the importance of these aspects.



The image shows a close-up, low-angle view of a server room. Numerous black cables hang down from the top, creating a complex, web-like pattern. In the background, rows of server racks are visible, each filled with glowing yellow lights that create a strong, warm glow. The perspective is looking upwards, emphasizing the height and density of the infrastructure.

Findings/observations

Findings/observations

The following are a set of observations from the process of gathering information for the report and from other work.

Researchers have a strong dependence on the research infrastructure that is available to them. Changes to the infrastructure will have effects on the research programs and researchers have a high level of competence in maximizing their research output in response to the changes but this is a limited level of flexibility.

In the global research environment, competitiveness is a vital requirement for researchers. As a result, collaborations are formed among the researchers based on competence regardless of location. Having access to computational resources can be a clear benefit in these collaborations and can enhance competence.

Application experts are a high-demand, scarce resource that have a large multiplier effect on scientific productivity, particularly for small research teams. Sharing such expertise through programs such as PRACE, has been highly beneficial.

Access to unique or different platforms that are not yet mainstream is often limited. An example is application accelerators, which are just beginning to become common after a long incubation period. There are possible strengths in finding ways to increase the amount of information and access to such new technologies, particularly since there are already some limited-scale efforts in the Nordics.

Continuity for research and applications is extremely important. Research careers and programs may span decades, building on previous work and collaborations to produce software, datasets and scientific results of high and lasting value.

Finding #1: Research in the Nordic region that depends on computational capabilities is clearly internationally competitive. Continued investment in excellence in computational research and education on national scales is vital to continuing this success.

Finding #2: Support for research excellence and collaborations must include an informed balance of computational and data resources, including training and support. There are very different levels of clarity or information about the scientific justification for the computational research infrastructure in the different countries.

Finding #3: Researchers in different research domains may rely on access to different sets of computational and data resources. Researchers in Universe Sciences rely significantly on PRACE Tier-0 resources and those in Chemistry and Materials Science rely on the respective national resources. Each of these are different strengths in the Nordic region.

Finding #4: Support for computing and data research infrastructure capabilities that are competitive internationally will be critical to extending this success into the future. The current model of access to PRACE Tier-0 level resources being granted at no cost to Nordic researchers based solely on the merits of the research is likely to change in the near future.

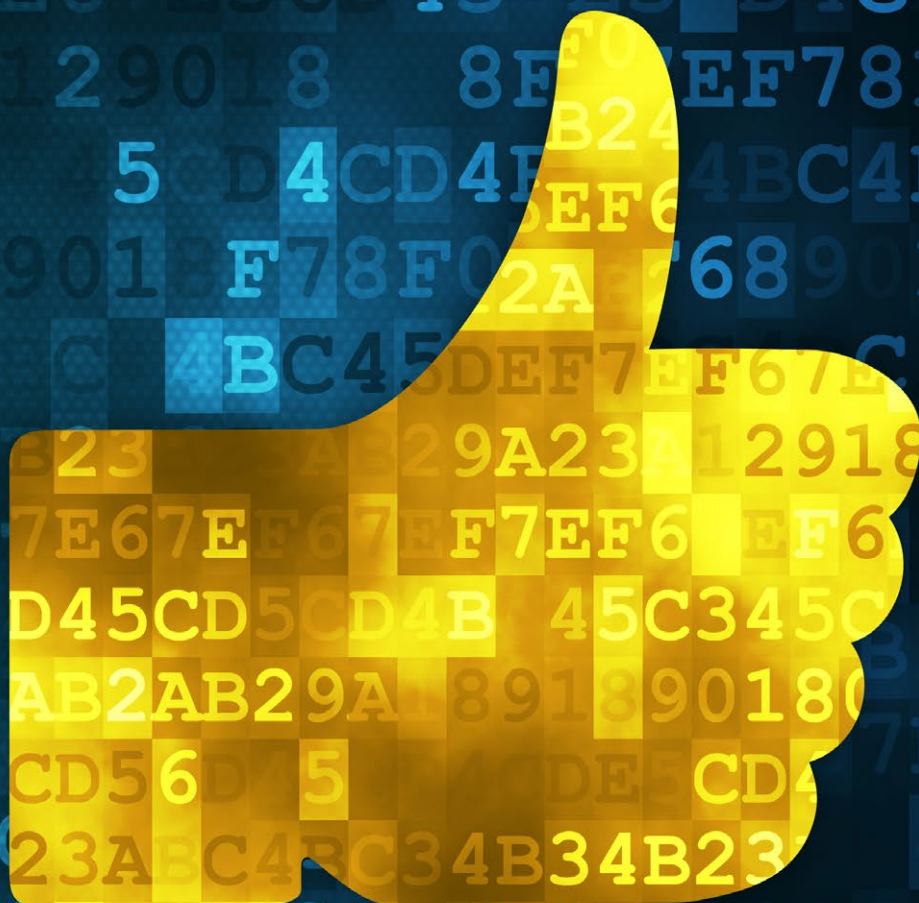
Finding #5: Collaborations are vital to national and international recognition and excellence for individual researchers, research groups and research-based organizations. They create new opportunities that leverage the investments within each country to deepen and extend knowledge networks, innovate technical capabilities and effectively address complex scientific problems, many of which are international in scope and have a high level of societal relevance.

Finding #6: Innovation and exploration are critical to fundamental and applied research and they need to be fostered through extended collaborations and coordination. The national approaches to supporting research infrastructure have different strengths that can be successfully built upon and, at several levels, coordinated in the Nordic region to enhance national research priorities and commitments as well as the capabilities available to the researchers.

Finding #7: Long timescales normally associated with extensive and ambitious research programs and shorter timescales associated with research projects need to be incorporated in the strategic planning for research infrastructures and for the implementations that grow out of that planning. High levels of uncertainty in funding can adversely affect research productivity, planning and directions.



Recommendations



Recommendations

The major challenge that needs to be considered is the appropriate set of actions that will support the wide range of research programs in the Nordic region, some of which will be incompatible. These recommendations have been formulated to help prioritize and guide some of the decisions on directions related to supporting Nordic science projects. They are intended to be taken as a whole but each recommendation may be considered for action separately.

There are two basic premises that underlie the recommendations. The first is that it is in the best interests of the researchers that there is a continued effort to gather and share information between the countries about research priorities, programs and needs. The second is that there is an understanding and continuing long-term commitment to the collaborations that already exist between the countries at multiple levels.

Recommendation #1: Funding for national programs must have a focus on the research priorities and needs that are defined in national science cases and scenarios.

Recommendation #2: At the national level, a clear set of science cases for computational and data research infrastructure in each country should be published and used to inform and guide the acquisition, support and coordination of the national computing and data resources. The national science cases should be periodically updated to reflect the changing research environment and topics.

Recommendation #3: The national science cases, along with other indicators and information, should be used to inform the continued development of the Nordic science case as part of the responsibilities of NeIC.

Recommendation #4: The national focus and funding needs to be augmented with funding for an international program. This may be in the form of a joint Nordic involvement with PRACE, as it evolves, that can provide a coordinated Nordic Tier-0 level of capability. This should be considered to be a logical extension of a national program and appropriately incorporated into each national strategy. Ideally, this would include all of the Nordic countries but initiating it with a subset of the countries should be considered. The inclusion of a neutral broker in the form of NeIC would facilitate the openness and extensibility of the program in the future if not all of the countries are initially involved.

Recommendation #5: The role of NeIC should be expanded to include identifying and, where feasible, initiating scientific and technical collaborations that reinforce those national science cases that cross international boundaries, including outside the Nordic region. Successful outcomes for these efforts cannot be assured but ideally the fruitful and productive collaborations will become part of the national science cases and be supported appropriately. NeIC should be recognized and supported in undertaking this as it may entail some risk, just as the national programs assume risks associated with their research infrastructure.

Recommendation #6: The exchange of information, experiences, roadmaps and strategic priorities are important aspects of increasing innovation and exploration. This should be facilitated by NeIC through a mechanism similar to that developed for Recommendation #4. Such information should be publicly available whenever feasible.

Recommendation #7: The funding bodies in the Nordic countries need to work together to develop a set of guidelines for supporting the long-term programs that are needed for international computation and data research infrastructures as well as the collaborations that depend on them. The funding bodies must encourage and stimulate alignments between the national and international programs with clear recognition of the potential for synergies and excellence through the efforts by the national research and e-infrastructure programs.

Based on the aggregate of the previous findings and recommendations, there is one additional recommendation.

Recommendation #8: The information, roadmaps and guidelines developed as part of the previous recommendations must have a path for implementation to be effective. In particular, the national resource providers and NeIC should be equipped with funding and authority to carry out recommendation #4 for sustainable Nordic access to a Tier-0 class capability. NeIC could be instrumental in facilitating the development of such implementation plans.

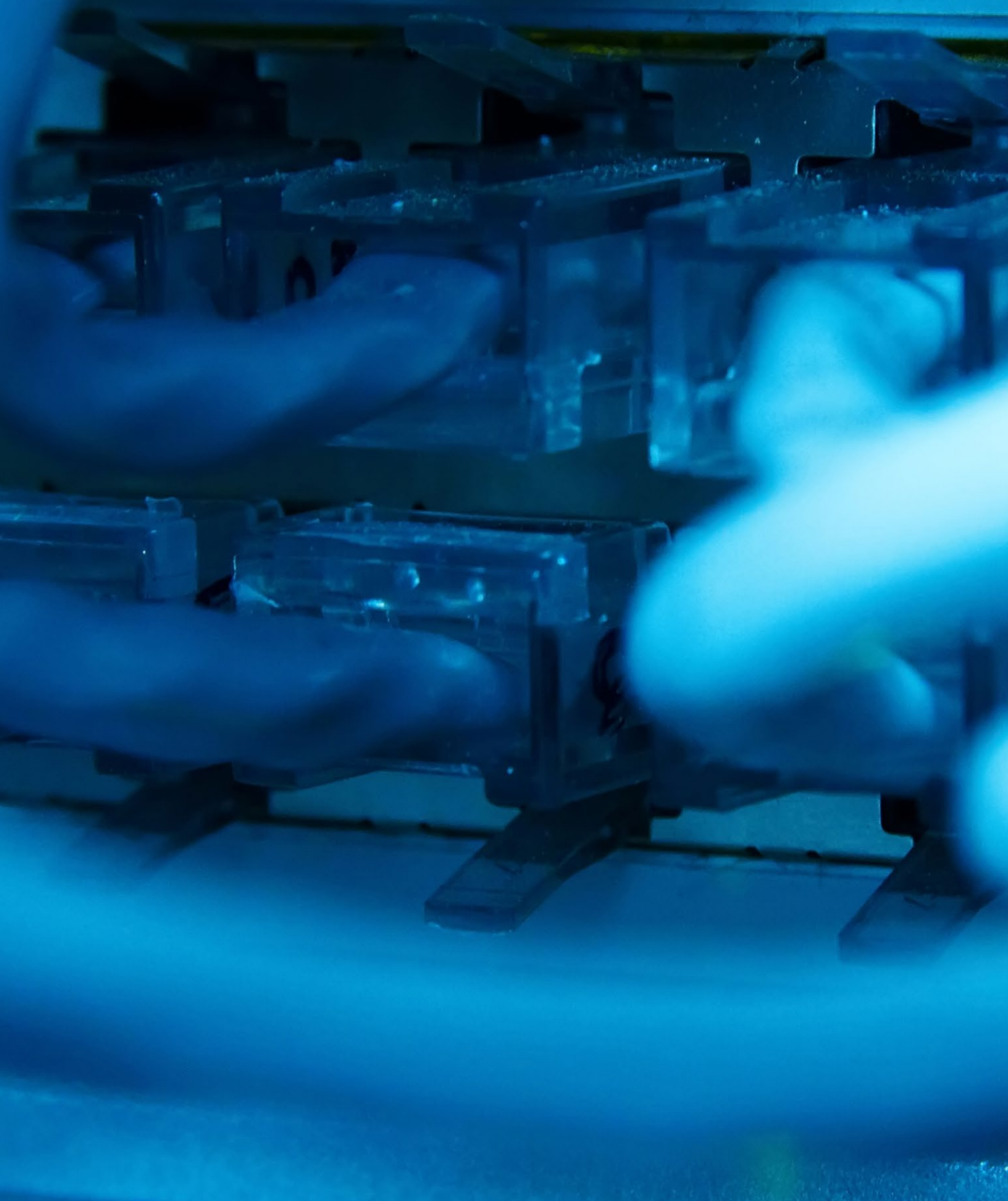
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Conclusions

The scientific research capabilities and strengths in the Nordic region are significant and are world-class in a number of different areas. Nordic researchers have achieved scientific leadership through their individual efforts, institutional and university research programs and national and international research collaborations.

The changes in research collaborations are deeply interconnected with changes in nature and scale of research infrastructures, ranging from the development of instrumentation through the dissemination and reuse of the data, publications and other results.

Researchers in all of the Nordic countries are making increasing use of local, national and international computing resources as part of their research routine. The types of use vary by domain, research project and time scales but they are all becoming increasingly dependent on the digital research infrastructure.

The opportunities for increasing the support of the science effort are significant but will require an increasing level of innovation, coordination, planning and support. This must be supported by the national programs through cooperation and support. In light of the history of continued collaboration despite the difference in approaches, this seems entirely possible and achievable.

Acknowledgements

Dr. Pennington was an external advisor to NeIC for the Cognitus project, which was created by NeIC in response to a request by the NeIC Board. This report was developed by Dr. Pennington with consultation and help from the NeIC staff, the computational research infrastructure providers in each of the five Nordic countries, the many researchers who took the time to respond to the survey and other requests for information as well as colleagues in other countries who shared their insights and experiences as this study was carried out

Appendices





Appendix A

PRACE Tier-o Awards

This appendix contains information from the PRACE website (<http://www.prace-ri.eu/>) on Regular Access awards for Call 1-9. The information includes the title of the award, the list of PIs and collaborators, the abstract, and the awarded resources. The projects have been grouped by the category of research.

1. BioChemistry, Bioinformatics and Life Sciences

- Molecular dynamics simulation and experimental characterization of a DNA nanocage family (Call 6)

Project leader: Mattia Falconi, University of Rome “Tor Vergata”, Italy

Collaborators: Cassio Alves, Universidade de Sao Paulo, Brazil; Cristiano L.P. de Oliveira, Universidade de Sao Paulo, Brazil; Birgitta R. Knudsen, Aarhus University, Denmark; Federico Iacovelli, University of Rome “Tor Vergata”, Italy

Abstract: Understanding and exploiting new, complex functional materials is intrinsically an interdisciplinary effort at the interface between physics, chemistry, biology, material science, and engineering. The unique self-recognition properties of DNA determined by the strict rules of Watson-Crick base pairing makes this material ideal for the creation of self-assembling, predesigned nanostructures in a bottom-up approach. The construction of such structures is one of the main focuses of the thriving area of DNA nanotechnology, where several assembly strategies have been employed to build increasingly complex three-dimensional DNA nanostructures. To achieve this goal it is necessary to estimate the thermodynamics of all possible pairings of DNA sequences and select the sequences so that the desired product is by far the most thermodynamically favorable one. Obviously, the complexity of doing so, even when designing rather simple structures involving more than a few DNA strands, by far exceeds the capacity of the human mind. Therefore, the design of DNA sequences for the construction of nanostructures must rely on sophisticated computational tools in order to rule out sequence combinations prone to form unwanted structures.

Common for all DNA nanostructures presented until date is that they rely at least to some extent on synthetic DNA oligonucleotides, which makes their construction rather expensive. This fact, taken together with some of the common analysis techniques, such as Small Angle X-ray Scattering (SAXS) and Cryo-Transmission Electron Microscopy (Cryo-TEM) requiring quite large amounts of material, pose a serious challenge to the validation of the structures. Thus, to counter such obstacles long-time atomistic simulations, which can predict the likelihood of successful assembly as well as structural properties of DNA nanostructures before experiments, are of great value.

Aim of this project is to address the fundamental challenges related to the development of new functionally structured materials based on DNA and to gain a deep understanding of the structure and dynamics of a series of planned nanostructures on multiple length and time scales. To accomplish this task, not achievable with the regular computing resources, we need the large computational facilities offered by the Tier-o Systems. In detail, an automatic procedure has been implemented to identify the best oligonucleotide sequences that will be assembled to form eight three-dimensional DNA cages, having different regular or irregular geometry. For each nanocage 400 ns of molecular dynamics simulation will be executed. After having screened the oligo sequences using simulative methods, some selected DNA nanocage structures will be experimentally assembled with the help of an extensive toolbox of DNA binding, cutting, ligating, or recombining enzymes, which may all prove valuable for synthesis, manipulation, or functionalization of DNA nanostructures. Finally, the structural-dynamical properties of the produced cages will be investigated.

using spectroscopic experimental techniques, such as SAXS and CryoTEM, in conjunction with extensive classical molecular dynamics simulation. The results obtained through the molecular dynamics simulations will help to improve the design and the stability of the studied DNA nanostructures.

Resource awarded: 7 million core hours on CURIE FN @ GENCI@CEA, France

• Unlocking the role of lipids in the activation mechanism of the Epidermal Growth Factor Receptor (LIPIDSEGFR) (Call 6)

Project leader: Ilpo Vattulainen, Tampere University of Technology, Finland

Collaborators: Karol Kaszuba, Tampere University of Technology, Finland; Adam Orlowski, Tampere University of Technology, Finland; Tomasz Rog, Tampere University of Technology, Finland

Abstract: Epidermal growth factor receptor (EGFR) is a membrane glycoprotein composed of an extracellular ligand binding domain, a single helical transmembrane segment, and an intracellular domain with kinase activity. It is considered as one of the most important membrane receptors, since a major fraction of drug development is targeted to EGFR, with an objective to alter its activity. This is largely due to the fact that EGFR-mediated signaling pathways regulate, e.g., cell proliferation and differentiation, which implies that uncontrolled activation of EGFR is often linked to emergence of diseases such as breast and lung tumors. In essence, EGFR is one of the important targets for cancer therapies.

Yet, despite about 40000 articles published about EGFR, the understanding of how it is activated and stimulated is still quite limited. There is clearly a need for new ideas to unravel how the function of EGFR is modulated by its environment.

In this project, we approach this issue from a new perspective using very recent findings that suggest the role of lipids to be important in regulating EGFR activity. For instance, depletion of cholesterol from plasma membranes has been shown to lead to hyperactivation of EGFR, whereas increasing cellular GM3 levels have been highlighted to inhibit its action. The recent biochemical observations raise an intriguing question as to how the conformational changes in EGFR are induced by the lipid environment surrounding the receptor. As unraveling this issue is very difficult through experiments, here we resort to extensive atomistic molecular dynamics simulations. Using this approach we consider the behavior of EGFR in different lipid environments that are chosen to match the compositions used in previous and ongoing biochemical studies. The research will be carried out in close collaboration with experimental partners, the focus being on the effect of GM3 on EGFR activation, and the objective being to unravel the inhibitory mechanism induced by GM3.

Resource awarded: 60.036 million core hours on HERMIT @ GCS@HLRS, Germany

• NMRFUNC (Call 7)

Project leader: LindorffLarsen, Kresten; University of Copenhagen, DENMARK

Collaborators: Kaare Teilum, University of Copenhagen, DENMARK; Francesco Luigi Gervasio, University College London, UNITED KINGDOM; Michele Vendruscolo, University of Cambridge, UNITED KINGDOM

Abstract: Proteins are biological macromolecules that play a central role in biology, biotechnology and medicine. The last 50 years in protein science have provided us with a plethora of atomic resolution structures of proteins that are not only stunningly beautiful, but have also provided crucial insight into the mechanisms by which proteins function. Proteins are, however, also dynamic molecules and recent years have seen an explosion in our ability to characterize protein motions using both computations and experiments. Importantly, we now know that the way a protein moves can have a large impact on the function of the protein, and that it is not just the structure but also the dynamics

of a protein that determines its function. Examples include how motions in enzymes aid in substrate binding and release, or in conformational changes that enable protein molecules to transduce signals in cells. From an experimental point of view, nuclear magnetic resonance (NMR) spectroscopy has emerged as the central most important technique that can be used to study protein dynamics. NMR spectroscopy has the unique ability to provide atomic level data that reports on the structure, dynamics and thermodynamics of the motions in proteins. A relatively recent development in NMR is the ability to study the structure and dynamics of larger proteins, and protein complexes. Another exciting area of development is in experimental studies of so-called intrinsically disordered proteins. These are proteins that display an unusually large amount of dynamics, and which do not attain a single well-defined structure in the cell. Simultaneous with these developments in experiments, the last few years have also seen important progress in our ability to use molecular dynamics simulations to study the structure and dynamics of proteins. This progress has been enabled in part by substantial improvements in both the quality and accuracy of the force fields used in simulations, and in methods that allow for increased sampling of the conformations of proteins. We suggest utilizing new computational methods that integrate the strengths of NMR spectroscopy and molecular dynamics simulations to study the structural dynamics of proteins. If successful, the results may provide new insights in many of the areas where protein dynamics affect function, including understanding biological systems and designing new, more selective drug molecules towards proteins or improved enzymes.

Resource awarded: 11,289,600 core hours on CURIE TN @ GENCI@CEA, France

• Linear Scaling and Massively Parallel CoupledCluster Calculations on the Leucine transporter within a DEC framework (Call 8)

Project leader: Dr Thomas Kjaergaard, Aarhus University, Denmark

Research field: Biochemistry, Bioinformatics and Life sciences

Collaborators: Janus Eriksen, Aarhus University, Denmark Patrick Ettenhuber, Aarhus University, Denmark Ida Hoeyvik, Aarhus University, Denmark Frank Jensen, Aarhus University, Denmark Poul Joergense, Aarhus University, Denmark Kasper Kristensen, Aarhus University, Denmark Birgit Schiøtt, Aarhus University, Denmark

Abstract: The project aims at using the DivideExpandConsolidate (DEC) strategy to extend the application range of accurate quantum chemical calculations by applying state of the art coupled-cluster methods, CCSD (coupledcluster with single and double excitations) and CCSD(T) (CCSD with an approximate treatment of triple excitations), to molecular systems with sizes beyond the scope of standard implementations, thereby impacting real-life applications.

For this purpose, we will consider neurotransmitter sodium symporters, which are membrane proteins responsible for regulating the level of neurotransmitter signaling. They are the main target for psycho stimulants, antidepressants, and medications against e.g., anxiety, obesity, and addictive drugs. No high-resolution structures of these mammalian proteins are yet available, but the structure of a bacterial homologue, the leucine transporter (LeuT), was published in 2005. It has been speculated that the binding of two ligand molecules are required to activate the transport mechanism, and two possible binding sites have indeed been identified in LeuT by crystallography, binding assays, and molecular dynamics simulations. We propose to use this system as a target for the DECCSD and DECCSD(T) methods, where we aim at calculating benchmark binding energies for the binding of one and two leucine ligands to a model of the LeuT protein.

The DECCSD and DECCSD(T) methods have been implemented using the technology we previously have used for DEC second order Møller-Plesset perturbation theory (MP2) calculations. For DECCP2 we have shown that our implementation exhibits both strong and weak scaling. We want to show similar scalings for DECCSD and DECCSD(T) implementations by investigating increasingly larger stacks of benzene rings and cytosine nucleotides. These calculations will allow us to probe if stacking can be described by pairwise interactions between units, or whether cooperative binding effects are important. The DECCSD(T) interaction energies will also be compared to those from commonly used

force fields that have been parameterized using pairwise interactions, and thereby probe the accuracy of force field methods, which are currently used routinely to estimate noncovalent binding affinities. Our investigation may in this way provide information for improving these empirical models.

Resource Awarded: 40,000,000 core hours on CURIE TN @ GENCI@CEA, France

• Lipid-modulation of the toll-like receptor TLR4 (Call 9)

Project leader: Ilpo Vattulainen, Tampere University of Technology, Finland

Research field: Biochemistry, Bioinformatics and Life sciences

Collaborators: Moutusi Manna, Tampere University of Technology, Finland Edouard Mobarak, Tampere University of Technology, Finland Tomasz Rog, Tampere University of Technology, Finland

Abstract: Toll-like receptors (TLRs) constitute a class of membrane proteins that are part of the innate or non-specific immunological system. Meanwhile, ligands for TLRs are pathogens like bacterial lipids, lipoproteins, and bacterial fragments. After recognition of specific ligands, TLRs trigger signaling cascades resulting in the generation of pro-inflammatory and antimicrobial responses. As TLRs are involved in numerous illnesses and pathologies such as infectious and auto-immunological diseases, atherosclerosis, and cancer, TLRs are potential targets for drugs, highlighting their importance in health. This is also stressed by the fact that the ligands of TLRs are used in cancer therapy and often added to vaccines in order to increase their efficiency. Yet, the mechanistic understanding of their effects are not known. In this study, we will perform large-scale atomistic molecular dynamics simulations of the active dimer complex of TLR4 (encoded by the TLR4 gene) embedded in a lipid bilayer to understand how specific glycolipids affect the TLR4 conformation and dynamics. We further unravel the role of each component in these interactions resulting in the activation of the protein. The studies are bridged to experiments and have potential for a high impact on pharmacological applications of TLR4.

Resource Awarded: 21000000 core hours on HERMIT

2. Chemistry and Materials

• Effects of irradiation on nanostructures from first principles simulations (Call 3)

Project leader: Arkady Krashennikov, University of Helsinki, Finland

Collaborators: Jussi Enkovaara, CSC, Finland / Jani Kotakoski, University of Helsinki, Finland / Ari Ojanperä, Aalto University, Finland

Abstract: Recent experiments on ion and electron bombardment of nanostructures demonstrate that irradiation can have beneficial effects on such targets and that electron or ion beams can serve as tools to change the morphology and tailor mechanical, electronic and even magnetic properties of various nanostructured materials. It is also evident from the data obtained so far that the conventional theory of defect production in bulk materials does not work at the nanoscale, or it requires considerable modifications. In this project we will use first principles atomistic computer simulations to model interaction of energetic ions and electrons with nanostructures. Such an approach assumes that the only information on the target available is the types of atoms it consists of, then a quantum mechanical approach to the coupled electron-ion system is used to calculate the material structure, properties and time evolution. Although several approximations are used and many-body problem is considerably simplified, this approach makes it possible to simulate the behavior of the system with a high accuracy (which is achieved at high computation cost, though) and without any materials-specific adjustable parameter. In practice, by using time-dependent and static density functional theory implemented in a

computer code GPAW, we will simulate impacts of highenergy ions onto nanostructures with the aim of estimating the amount of kinetic energy of the projectile deposited into the target and the number of defects produced by the impact. With regard to the systems, we focus our research on very important nanostructures such as graphene and boron nitride sheets, which have similar atomic structure but different electronic properties (semimetal and widegap semiconductor). This should make it possible to understand from first principles the deposition of projectile kinetic energy into electronic degrees of freedom for systems with different electronic structures and its conversion into defects. We will also simulate interaction of energetic electrons with these nanostructures and calculate probabilities for defect production and for irradiationinduced transformations. Armed with the knowledge on basic transformations, we then model evolution of graphene with grain boundaries under electron irradiation. We will also calculate the electronic structure of graphene sheets with grain boundaries and other defects. Based on the knowledge obtained for graphene and boronnitride sheets, we will extrapolate our findings to other nanosystems and assess irradiation as a means for tailoring the electronic properties of nanostructures.

Resource awarded: 10 000 000 corehours at CURIE Thin Node partition, GENCI@CEA

3. Chemical Sciences and Materials

• Highaccuracy quantum mechanic models for extended molecular systems (Call 4)

Project leader: Branislav Jansik, Aarhus University – Institute of Chemistry, Denmark

Collaborators: Kasper Kristensen, Aarhus University – Institute of Chemistry, Denmark/ IdaMarie Hoyvik, Aarhus University – Institute of Chemistry, Denmark/ Patrick Ettenhuber, Aarhus University – Institute of Chemistry, Denmark/ Poul Jorgensen, Aarhus University – Institute of Chemistry, Denmark

Abstract: Many years of theoretical research together with the ongoing revolution in computer technology have made coupled cluster (CC) calculations the stateoftheart method for small molecules. The CC calculations are able to provide highly accurate molecular energies, nuclear forces, and all parameters needed for describing the interaction of a molecule with its surroundings, including perturbing fields. Molecular properties, such as harmonic frequencies, excitation energies nuclear shieldings, frequencydependent polarizabilities and hyperpolarizabilities and a plethora of molecular spectra, are all within reach.

Standard CC wave function calculations are expressed in the canonical HartreeFock (HF) basis, which is a highly delocalized basis. However, the main task of the correlated calculation is to describe shortrange electronelectron interactions, which is a very local phenomenon. The discord in description of a local phenomenon using a nonlocal basis inherently leads to a scaling wall, e.g., the seventh power scaling of CCSD(T) calculations, rendering this highly accurate method limited to small molecules only.

The computational scaling of existing CC methods represents a roadblock to progress. One challenge of the 21st century is to remove this roadblock. The ultimate goal is to obtain CC methods that scale linearly with system size, or even better, where calculations for small and large molecular systems have the same wall time, provided a sufficient number of processors is available.

The key to progress in CC applicability is to express the CC wave function in a basis of local HF orbitals and exploit the inherently short-range physics of electron correlation. In a breakthrough, we have recently shown how such a local HF basis may be obtained and shown how to take advantage of the local nature of electron correlation to obtain a linearly scaling CC formulation. We denote the new method DECCC (DivideExpand Consolidate Coupled Cluster).

Using DECCC approach, the CC calculation may be split into number of calculations on small fragments of the molecular orbital space, while retaining both full control of the error in the total energy and the blackbox character of the traditional CC methodology. Each of the fragment calculations can be carried

out independently, making the method embarrassingly parallel. The number of these calculations scales linearly with molecule size. DECCC is entirely on par with standard CC except its scaling is linear with respect to molecule size and therefore DECCC is suitable for applications on large molecules

The success of the DECCC approach will open a new era of accurate quantum calculations on large molecular systems such as nanoparticles and proteins. It holds potential to accelerate research, not only in chemistry and physics, but in molecular science in general.

Resource awarded: 3.000.000 core hours on CURIE FN (GENCI@CEA, France)

• Plasmonic ligandstabilized gold nanoclusters (Call 5)

Project leader: Hannu Häkkinen, University of Jyväskylä, Finland

Collaborators: Sami Malola, University of Jyväskylä, Finland | Ville Mäkinen, University of Jyväskylä, Finland | Jussi Enkovaara, CSC – the Finnish IT Center for Science, Finland

Abstract: Stabilizing gold nanoparticles by thiolate ligand molecules is a wellknown synthetic route to produce airstable, electrochemically and thermally stable cluster compounds with tunable sizes and properties in the nanometer scale. These cluster compounds constitute a class of very interesting novel nanomaterials that have been employed in a wide range of studies in molecular biology, inorganic chemistry, surface science and materials science with a wide range of potential applications in sitespecific bioconjugate labelling, drug delivery and medical therapy, functionalisation of gold surfaces for sensing, molecular recognition and molecular electronics and nanoparticle catalysis. A detailed understanding of the emergence of collective excitations in metallic nanostructures has been an open challenge in solid-state chemistry and physics. Through the computational studies of ligandstabilized gold nanoclusters that are defined “to the molecular precision”, i.e, by exact composition and structure, this project aims at breakthroughs in microscopic understanding of the “birth of a plasmon” in nanoscale noble metal clusters. This is of a wide scientific interest, since it will answer fundamental questions pertaining to transformation of nanoscale matter and nanoparticles from “molecular” to “metallic” regime with the concomitant change of optical response of the electrons from discrete transitions to collective behavior. Plasmonics is a rapidly developing field of (nano)optics with wideranging applications, consequently, finding out the fundamental limits to the miniaturization bears an obvious technical significance as well.

Resource awarded: 18,358.272 corehours on Hermit (GAUSS@HLRS, Germany)

• NANOGOLD AT THE BIOINTERFACE (Call 7)

Project leader: Hakkinen, Hannu; University of Jyväskylä, Finland

Collaborators: Xi Chen, University of Jyväskylä, Finland; Lars Gell, University of Jyväskylä, Finland; Lauri Lehtovaara, University of Jyväskylä, Finland; Sami Malola, University of Jyväskylä, Finland

Abstract: In this project, large-scale quantum chemical and molecular dynamics simulations are employed to investigate binding of 1 – 3 nm diameter functionalized gold nanoclusters to viruses. Information about binding mechanisms and effects of clusters on the dynamics and stability of viruses is of utmost importance in order to understand mechanisms of virus uncoating (release of the viral genome via opening of the virus capsid) and may help development of stabilized viruses to be used in novel vaccines against viral diseases.

Resource awarded: 43,171,840 core hours on HERMIT @ GCS@HLRS, Germany

- **Aminoacid anions in organic compounds: charting the boundary of room temperature ionic liquids (Call 8)**

Project leader: Dr. Enrico Bodo, University of Rome “Sapienza”, Italy

Research field: Chemistry

Collaborators: Antonio Benedetto, University College Dublin (UCD), Ireland Lorenzo Gontrani, CNR, Italy Pietro Ballone, NTNU Norwegian University of Science and Technology, Norway

Abstract: Ionic liquids (ILs) are salts made by complex, sterically mismatched molecular ions which possess a low melting point owing to the fact that the electrostatic interactions are weakened and lattice formation frustrated by geometric effects. In contrast to traditional organic solvents, ILs possess negligible flammability and volatility and represent a new class of “green” solvents that are inherently safer and more environmentally friendly than conventional solvents. Their use as solvents in chemical processes is in line with the topics covered in the Horizon 2020, as the development of green and sustainable procedures is one of its objectives.

The combination of amino acids in their deprotonated and thus anionic form with choline and phosphocholine cations gives origin to a novel and potentially important class of organic ionic liquids. Preliminary results have revealed intriguing structural motives as well as regular patterns in the properties that could guide the experimental investigation of these compounds. Analysis of the abinitio data highlights that proton transfer in these liquids may be possible to such an extent that was not possible with other ionic liquids (including protic ones).

The main focus of this project is a theoretical description of a series of liquids composed by amino-acid anions (alanine [Ala], serine [Ser], cysteine [Cys], valine [Val], phenylalanine [Phe], aspartic acid [Asp], asparagine [Asn], and histidine [His]) combined with choline and phosphocoline cations. The description of the bulk phase will be performed using CarParrinello molecular dynamics (CPMD) in order to unravel their nanoscopic structure and the mechanisms of possible proton transfer processes that can affect their macroscopic properties and their use as new solvents with tunable ionicity. The transfer of a proton between the Choline cation to the aminoacid anion has the net result of neutralizing the ionic couple involved. Ideally, we can imagine that a collective, complete transfer of protons from the cations to the anions in the liquid phase could lead to a transition from an ionic liquid to a traditional polar liquid. This kind of chemical transition may be triggered by temperature pressure changes or by mixing different compounds. This study has the potential of opening an unexpected and advantageous route to the synthesis, characterization and design of new, unconventional materials whose chemical/solvation properties can be tuned upon changes of their molecular structure. In particular one could be able to control the degree of autoionization and ultimately the solvation properties of a fluid by engineering the right molecular structure.

Given the time limitation of abinitio approaches, a variety of constrained simulations will be used to investigate free energy barriers opposing proton transfer events, entering the definition of kinetic models used to extend the simulation results to time scales inaccessible to abinitio methods. The first quality check of the computation will be provided by a comparison of the liquid structure with Xray diffraction experiments that are currently under development at the PI institution. Additional checks will be provided by comparison with the results of conductivity measurements, dielectric spectroscopy and neutron scattering experiments that are being planned.

Resource Awarded: 8,166,667 core hours on CURIE TN @ GENCI@CEA, France

- Large-scale radiation damage cascades from first principles (Call 9)

Project leader: Emilio Artacho, CIC nanoGUNE, Spain

Research field: Chemistry

Collaborators: Fabiano Corsetti, CIC nanoGUNE, Spain Kai Nordlund, University of Helsinki, Finland

Abstract: Cascade dynamics in bulk materials from ion irradiation give rise to complex processes that disrupt the crystalline structure over large regions. Characterising and understanding such processes has long been recognized as a significant challenge in materials science, as well as being of great practical importance, especially in the nuclear industry. Although collision cascades have until now been studied with empirical classical potentials, due to the large length and time scales involved, electronic structure methods offer the possibility of much greater accuracy and true ab initio predictive power. To this end, we use density-functional theory with the SIESTA code to simulate a number of collision cascades in silicon entirely from first principles, using a large system size of more than four thousand atoms and a total simulation time of forty picoseconds.

Resource Awarded: 36000000 core hours on HERMIT

- EXCIST – Excited state charge transfer at the conjugated organic molecule – semiconductor interface (Call 9)

Project leader: Martti Puska, Aalto University School of Science, Finland

Research field: Chemistry

Collaborators: Kari Laasonen, Aalto University, Finland Olga Syzgantseva, Aalto University, Finland

Abstract: The current project aims the understanding of physical factors, governing the interfacial excited state charge transfer (CT) between conjugated organic molecules and a semiconductor surface. For this purpose, we follow the electron and coupled electron-ion dynamics via ab initio simulations. Recent efficient implementations of the Ehrenfest Dynamics (ED) approach and the Real-Time Time-Dependent Density Functional Theory (RT-TDDFT) into the GPAW program have opened a way of such simulations for systems, containing hundreds of atoms. The objective of this project is to apply the above techniques to analyse the factors, affecting the electron injection rate at the organic dye – semiconductor interface. Among the factors to be investigated are: the role of the ionic dynamics in CT, the impact of the anchoring mode, the influence of surface characteristics and the initial excitation. The results of this work will help us to elucidate the CT- mechanisms on the molecular level and can be generalized and applied to a broader range of semiconductor – organic molecule interfaces, facilitating the optimal design of novel materials.

Resource Awarded: 92160 core hours on CURIE, 5923840 core hours CURIE TN

4. Earth System Sciences

• HiResClim: High Resolution Climate Modelling (Call 5)

Project leader: Colin Jones, Swedish Meteorological and Hydrological Institute (SMHI), Sweden

Collaborators: Laurent Terray, CERFACS, France | Sophie Valcke, CERFACS, France | Eric Maisonnave, CERFACS, France | Christophe Cassou, CERFACS, France | Klaus Wyser, Swedish Meteorological and Hydrological Institute (SMHI), Sweden | Uwe Fladrich, Swedish Meteorological and Hydrological Institute (SMHI), Sweden | Muhammad Asif, Catalan Institute of Climate Sciences, Spain | Domingo Manubens, Catalan Institute of Climate Sciences, Spain | Francisco DoblasReyes, Catalan Institute of Climate Sciences, Spain | Chandan Basu, Linkoping University, Sweden | Torgny Faxen, Linkoping University, Sweden | Wilco Hazeleger, Royal Netherlands Meteorological Institute (KNMI), Netherlands | Richard Bintanja, Royal Netherlands Meteorological Institute (KNMI), Netherlands | Camiel Severijns, Royal Netherlands Meteorological Institute (KNMI), Netherlands

Abstract: HiResClim aims to make major advances in the science of climate change modelling. This will be achieved by addressing the dual requirements of; increased climate model resolution and increased number of ensemble realizations of future climate conditions for a range of plausible socioeconomic development pathways. Increased model resolution aims to deliver a significant improvement in our ability to simulate key modes of climate and weather variability and thereby provide reliable estimates of future changes in this variability. A large ensemble approach acknowledges the inherent uncertainty in estimating longterm changes in climate, particularly in phenomena that are highly variable and, of which, changes in the occurrence of the rare but intense events are those impacting society and nature most strongly. To provide credible risk assessment statistics on future change in phenomena such as; extratropical and tropical cyclones, heatwaves, droughts and flood events, the combination of high climate model resolution and a large ensemble approach is unavoidable. In HiResClim we attack both of these requirements in a balanced approach, which, as well as being the most efficient way to utilise the most advanced HPC systems of today, is also the only path to providing more robust and actionable estimates of future climate change.

Resource awarded: 38.000.000 corehours on MareNostrum (BSC, Spain)

• HiResClim: High Resolution Ensemble Climate Modeling (Call 7)

Project leader: DoblasReyes, Francisco; Institut Catal de Cincies del Clima, Spain

Collaborators: Muhammad Asif, Institut Catal de Cincies del Clima, Spain; Domingo Manubens, Institut Catal de Cincies del Clima, SPAIN; Eric Maisonnave, CERFACS, France; Laurent Terray, CERFACS, France; Sophie Valcke, CERFACS, France; Wilco Hazeleger, Royal Netherlands Meteorological Institute (KNMI), Netherlands; Camiel Severijns, Royal Netherlands Meteorological Institute (KNMI), Netherlands; Uwe Fladrich, Swedish Meteorological and Hydrological Institute (SMHI), Sweden; Colin Jones, Swedish Meteorological and Hydrological Institute (SMHI), Sweden; Klaus Wyser, Swedish Meteorological and Hydrological Institute (SMHI), Sweden

Abstract: HiResClim aims to make major advances in the science of estimating climate change and formulating climate predictions. This will be achieved by addressing the dual requirements of increased climate model resolution and increased number of ensemble realizations of future climate conditions over a range of time scales and for a set of plausible socioeconomic development pathways. Increased model resolution aims to deliver a significant improvement in our ability to simulate key modes of climate and weather variability and, thereby, provide reliable estimates of future changes in this variability. The multimodel ensemble approach acknowledges the inherent uncertainty in estimating changes in climate over seasonal to centennial time scales, particularly in phenomena that are highly variable and, of which, changes in the occurrence of the rare but intense events are those impacting society and nature most strongly. To provide credible risk assessment in phenomena such as extra-tropical and tropical cyclones, heat waves, droughts and flood events to inform climate adaptation and climate services, the combination of high climate model resolution and a multimodel ensemble

approach is unavoidable. In HiResClim we attack both of these requirements using a seamless multi model climate modelling approach, which, as well as being the most efficient way to utilise the most advanced HPC systems of today and improve the realism of climate simulations, is also the only path to providing robust and actionable estimates of climate changes. The requirements of the project were defined considering the two stateoftheart coupled model used, ECEarth and ARPEGEMO HR.

Resource awarded: 50,440,000 core hours on MareNostrum @ BSC, Spain

- **EGOIST – Endogenic oil synthesis in the deep Earth interior: ab initio molecular dynamic simulation (Call 8)**

Project leader: Prof. Anatoly Belonoshko, The Royal Institute of Technology (KTH), Sweden

Research field: Earth System Sciences

Collaborators: Pavel Gavryushkin, V.S. Sobolev Institute of Geology and Mineralogy, Siberian Branch, RAS, Russian Federation Konstantin Litasov, V.S. Sobolev Institute of Geology and Mineralogy, Siberian Branch, RAS, Russian Federation Tymofiy Lukinov, The Royal Institute of Technology (KTH), Sweden

Abstract: Physics and chemistry of COH fluids at high pressures and temperatures of Earth interior is important in several applications. First, the thermodynamics of these fluids is needed to describe properties of the Earth interior which, in turn, might be important for predicting seismic events. Second, estimating the balance of CO₂ between atmosphere and Earth interior is impossible without detailed knowledge of thermodynamics of COH fluids. Third, there are indications from experiment that chemical reactions in COH fluids at high P and T might lead to a synthesis of hydrocarbons and heavy alkanes, providing a possibility for formation of oil deposits at the relevant depth. Experimental difficulties in studying COH fluids at high PT are numerous – for example, diffusion of H₂ is one of them.

Therefore, a theoretical approach is a valuable asset in these studies. Presently, we can compute phase and chemical equilibrium using density functional theory and molecular dynamics. When combined together, they represent a powerful tool. We shall study various components in COH system, systematically collecting data on their equations of state to use for computing, in turn, their Gibbs free energy. Minimization of the Gibbs free energy allows to determine chemical composition at equilibrium as soon as thermodynamics of all possible components is available. DFT based MD is similar in a way to a high PT experiment, yet without experimental problems. While theoretical approach has its own limitations, they are well known and understood. Thus, we expect that the acquired knowledge of thermodynamics, phase and chemical equilibrium in COH system will be highly reliable. In a way, our simulations are similar to a real experiment – we shall place a certain composition into an experimental box and apply certain pressure and temperature. That will allow us to observe the chemical composition that forms in the 'experimental' chamber. We expect to observe chemical reactions that lead to formation of hydrocarbons and alkanes and describe the range of pressures, temperatures and compositions where these reactions occur. This, in turn, might enable an educated search for the regions in the Earth interior that might contain the products of this reaction. As a spinoff, the acquired knowledge will help us to solve the problem of excessive CO₂ as well as to understand the interior of icy planets and satellites of giant planets.

Resource Awarded: 50,000,000 core hours on MareNostrum @ BSC, Spain

5. Engineering and Energy

- REFIT – Rotation effects on flow instabilities and turbulence (Call 2)

Project leader: Arne Johansson, KTH Department of Mechanics, Sweden

Collaborators: Dr. Geert Brethouwer, KTH Stockholm, Sweden / Prof. Dan Henningson, KTH Stockholm, Sweden / Prof. Rebecca Lingwood, University of Cambridge, United Kingdom / Prof. Martin Oberlack, Technische Universität Darmstadt, Germany / Dr. Philipp Schlatter, KTH Stockholm, Sweden

Abstract: Flows in gas turbines, turbo machinery, pumps, compressors, cyclone separators and other industrial apparatus are often rotating or swirling. They are also usually turbulent since flow rates and thus Reynolds numbers are generally large, meaning that the fluid motions fluctuate in a chaotic and irregular manner in space and time. The induced Coriolis force on the fluid or gas, also occurring when there is a flow over wings, turbine blades and other curved surfaces, causes many intriguing and complex physical phenomena. Coriolis forces, for example, can damp as well as enhance the turbulent fluctuations and influence the mean flow rate. Capturing such effects in engineering turbulence models has so far proved to be elusive and in order to improve and validate those models high quality data of rotating turbulent flows are badly needed. Experiments on rotating flows are inherently complicated since it usually requires turning of equipment. A viable and potentially very accurate alternative is direct numerical simulation (DNS) whereby the whole spatial and temporal range of turbulent scales are resolved without invoking models. Rotating channel flow is particularly relevant from a fundamental and engineering perspective. Recent DNSs in our group have revealed interesting phenomena in channel flows at high rotation rates; turbulence is then damped near both channel walls and the flow can become partly or completely laminar leading to huge flow rate changes at a constant pressure drop. Moreover, preliminary DNS uncovered an instability not observed previously in rotating wallbounded flows. This instability caused large fluctuations in the turbulence intensity and wall shear stresses in a periodiclike manner. Although previous DNSs of rotating channel flow have produced invaluable information, they were restricted to low Reynolds numbers, Re , since the range of scales that needs to be resolved and thus the computational costs of DNS increase dramatically with Re . The results of those previous DNS cannot simply be extrapolated to industrial flows with a commonly much higher Reynolds number. However, with the resources provided by the PRACE project we are able to perform simulations of rotating turbulent flows at a much higher Reynolds number. Proper simulations of the periodiclike instabilities at high rotation rates and high Re will require especially massive computational resources. The aim of the proposed project is therefore to perform DNS of rotating turbulent channel flow at an order of magnitude higher friction Reynolds number than previously performed DNS. In particular, the goal is to carry out the first wellresolved DNS of the periodiclike instabilities occurring at high rotation rates since they can potentially have an important impact in industrial applications. Those new large-scale DNS can help to address unresolved questions about rotation, swirl and streamline curvature effects in industrial flows. The computed high Reynolds number DNS data are also vital in order to develop and validate engineering models for turbulent flows with rotation, swirl or streamline curvature in industrial applications and to study instabilities in rotating flows. The DNS data will therefore be made available to the wider scientific community.

Computer system: JUGENE, GAUSS/FZJ Resource awarded: 46 000 000 corehours

- **Direct numerical simulation of reaction fronts in partially premixed charge compression ignition combustion: structures, dynamics (Call 4)**

Project leader: XueSong Bai, Lund University, Sweden

Collaborators: Yu Rixin, Lund University, Sweden/ Henning Carlsson, Lund University, Sweden/ Fan Zhang, Lund University, Sweden/ Rickard Solsjo, Lund University, Sweden

Abstract: Recent public concerns on global warming due to emissions of the green house gas CO₂, as well as emission of pollutants (soot, NO_x, CO, and unburned hydrocarbons) from fossil fuel combustion, have called for development of improved internal combustion (IC) engines that have high engine efficiency, low emissions of pollutants, and friendly to carbon neutral renewable fuels (e.g. biofuels). The European and world engine industry and research community have spent great effort in developing clean combustion engines using the concept of fuellean mixture and low temperature combustion which offers great potential in reducing NO_x (due to low temperature) and soot and unburned hydrocarbon (due to excessive air), and meanwhile achieving high engine efficiency. One example is the wellknown homogeneous charge compression ignition (HCCI) combustion engine, which operates with excessive air in the cylinder, and produces simultaneously low soot and NO_x. However, HCCI combustion is found to be very sensitive to the flow and mixture conditions prior to the onset of auto-ignition. As a result, HCCI engine is rather difficult to control. At high load (with high temperature and high pressure) engine knock may occur with pressure waves in the cylinder interacting with the reaction fronts, causing excessive noise and even mechanical damage. At low load (with lower temperature and pressure) high level emissions of CO and unburned hydrocarbon may occur, which lowers the fuel economy and pollutes the environment. Recently, it has been demonstrated experimentally that with partially premixed charge compression ignition (PCCI) which can be attained by using multiple injections of fuel at different piston positions, smoother combustion can be achieved by managing the local fuel/air ratio (thereby the ignition delay time) in an overall lean charge.

There are several technical barriers in applying the PCCI concept to practical engines running with overall fuel lean mixture, low temperature combustion. For example, it is not known what the optimized partially premixed charge is for a desirable ignition, while at the same time maintaining low emissions. The main difficulty lies in the nonlinear behavior of the dominating phenomena and the interaction among them (e.g. chemistry and turbulence). To develop an applicable PCCI technology for IC engine industry, improved understanding of the multiple scale physical and chemical process is necessary. Further, there is a need to develop computational models for simulating the process for the design where a large number of control parameters are to be investigated.

The goals of this project are to achieve improved understanding of the physical and chemical processes in overall fuellean PCCI processes, and to generate reliable database for validating simulation models for analysis of the class of combustion problems. This shall lead to development of new strategies to achieve controllable low temperature combustion IC engines, while maintaining high efficiency and low levels of emissions (soot, NO_x, CO and unburned hydrocarbons). Direct numerical simulation (DNS) approach that employs detailed chemistry and transport properties will be employed.

Resource awarded: 20.000.000 core hours on CURIE TN (GENCI@CEA, France)

- Full-f gyrokinetic simulation of edge pedestal in Textor (Call 4)

Project leader: Timo Kiviniemi, Aalto University – School of Science, Finland

Collaborators: Jukka Heikkinen VTT, Finland

Abstract: Although research on magnetically confined fusion experiments already started several decades ago, perfectly controlled nuclear fusion has not yet been achieved. A major obstacle is that the transport of the fuel particles perpendicular to the magnetic field lines cannot be predicted by only neoclassical transport theory. Turbulence induced transport, a still unsolved problem in physics in general, has been attributed to be the main reason. It is causing fuel particles to drift from the magnetic field lines, disturbing the plasma confinement and thereby the fusion process. Turbulence induced transport is a transport regime characterized by chaotic properties. The ELMFIRE code, developed at Aalto University in Finland investigates this regime with a so called first principal computer model, which tracks individual particles. The code solves the coupled problem of Boltzmann's gas kinetic equation for the total particle distribution function and Maxwell's equations in a complex magnetic field, providing information on the complex interplay between the magnetic field, the electric field and the particle trajectories.

In the present proposal, the Elmfire code will be used to study turbulence and plasma rotation in the low and high confinement regimes of Textor. The steady state experimental profiles are obtained in the simulation by the balance of a heating model, particle/energy transport, radiation losses and energy transported to the limiter surface. The turbulence levels in the two regimes will be compared to the experimentally 'silent stage' in the inter ELM period. Furthermore the contribution of the phase velocity and the ExB back ground flow to the poloidal rotation of density fluctuations will be analyzed and investigations into decorrelation rates and probability distribution function of the turbulent fluctuations will be performed. The radial structure of the rotation shear and the radial electric field will be compared to the experimental obtained values.

Resource awarded: 30.000.000 core hours on SuperMUC (GCS@LRZ, Germany)

- TRADELINBO Transition delay in Blasiuslike boundary layers by passive control: complementary investigation and numerical support to an ongoing experimental activity (Call 6)

Project leader: Simone Camarri, University of Pisa, Italy

Collaborators: Alessandro Talamelli, Alma Mater Studiorum, Universit di Bologna, Italy; Franco Auteri, Politecnico di Milano, Italy; Flavio Giannetti, Universita' degli Studi di Salerno, Italy; Andre a Fani, University of Pisa, Italy; Alessandro Mariotti, University of Pisa, Italy; Maria Vittoria Salvetti, University of Pisa, Italy; Jens Fransson, Royal Institute of Technology (KTH), Sweden;

Abstract: The main objective of the present project is to provide a numerical support and integration to the experiments of the ERC project AFRODITE (FP7 reference number: 258339). Both projects focus on the investigation of a method to delay transition to turbulence in Blasiuslike boundary layers, i.e. the region of the flow adjacent to a flat plate. Transition delay implies a friction drag reduction, which is mainly caused by the turbulent portion of the boundary layer. Thus, the direct implication of transition delay is a drag reduction for aerodynamic bodies, for which the friction drag is an important contribution on the overall drag. The project is divided in two subsequent parts. The first is aimed at validating the DNS setup against the experiments. Once validated, the DNS will be used in the subsequent stage of the work to (i) complete the information available from the experiments on the proposed transition control and (ii) to explore and select potentially interesting alternative configurations for future experiments.

If the project will be successful, we plan to obtain as an output the following points:

1. A part showing the accuracy assessment of the proposed Direct Numerical Simulation (DNS) setup against the experiments of the AFRODITE project. This validation is carried out on three points: (a) validation of the steady flow, (b) validation of the flow with TollmienSchlichting waves superposed and (c) validation of the simulation of transition. The three points are subsequent also in terms of difficulty of the DNS involved.
2. A part showing how results from (1) has contributed to add information concerning the transition delay mechanism.
3. A part showing set of alternative configurations for the transition control devices, to be tested in future experiments and which could lead, in future, even to a patent.
4. A part dedicated to the investigation of global instabilities in the wake past a set of bluff roughness elements.

Resource awarded: 15 million core hours on FERMI @ CINECA, Italy

• Direct numerical simulation of partially premixed combustion in internal combustion engine relevant conditions (Call 8)

Project leader: Prof. XueSong Bai, Lund University, Sweden

Research field: Engineering

Collaborators: Henning Carlsson, Lund University, Sweden Vivianne Holmen, Lund University, Sweden Siyuan Hu, Lund University, Sweden Rickard Solsjo, Lund University, Sweden, Rixin Yu, Lund University, Sweden

Abstract: In the past decade, the European and world engine industry and research community have spent a great effort in developing clean combustion engines using the concept of fuellean mixture and low temperature combustion which offers great potential in reducing NO_x (due to low temperature), soot and unburned hydrocarbon (due to excessive air), and meanwhile achieving high engine efficiency. One example is the well known homogeneous charge compression ignition (HCCI) combustion engine, which operates with excessive air in the cylinder, and produces simultaneously low soot and NO_x. However, HCCI combustion is found to be very sensitive to the flow and mixture conditions prior to the onset of autoignition. As a result, HCCI engine is rather difficult to control. At high load (with high temperature and high pressure) engine knock may occur with pressure waves in the cylinder interacting with the reaction fronts, leading to excessive noise and even damage on the cylinder and piston surface. At low load (with lower temperature and pressure) high level emissions of CO and unburned hydrocarbons may occur, which lowers the fuel efficiency and pollutes the environment. Recently, it has been demonstrated experimentally that with partially premixed charge compression ignition, also known as partially premixed combustion (PPC), smoother combustion can be achieved by managing the local fuel/air ratio (thereby the ignition delay time) in an overall lean charge.

There are several technical barriers in applying the PPC concept to practical engines running with overall fuel lean mixture, low temperature combustion. For example, it is not known what the optimized partially premixed charge is for a desirable ignition, while at the same time maintaining low emissions. The main difficulty lies in the nonlinear behavior of the dominating phenomena and the interaction among them (e.g. chemistry and turbulence). To develop an applicable PPC technology for IC engine industry, improved understanding of the multiple scale physical and chemical process is necessary. Further, there is a need to develop computational models for simulating the process for the design where a large number of control parameters are to be investigated.

The goals of this project are to achieve improved understanding of the physical and chemical processes in overall fuellean PPC processes, and to generate reliable database for validating simulation models for analysis of the class of combustion problems. This shall lead to development of new strategies to achieve controllable low temperature combustion IC engines, while maintaining high efficiency and

low levels of emissions (soot, NO_x, CO and unburned hydrocarbons). Direct numerical simulation (DNS) approach that employs detailed chemistry and transport properties will be used to study the mechanisms responsible for the onset of auto ignition, and the structures and dynamics of the reaction front propagation in PPC conditions.

Resource Awarded: 26,000,000 core hours on SuperMUC @ GCS@LRZ, Germany;

6. Fundamental Physics

• LEAC – Laserplasma Electron Acceleration for CILEX (Call 8)

Project leader: Dr Arnaud Beck, CNRS, FRANCE

Research field: Fundamental Constituents of Matter

Collaborators: Jacob Trier Fredriksen, University of Copenhagen, DENMARK, Arnd Specka, CNRS, FRANCE

Abstract: CILEX (Centre Interdisciplinaire Lumiere Extreme) is the Interdisciplinary Center on EXtreme Light. This facility located in the Paris area will host the APOLLON10P laser, which will deliver pulses eventually as short as 15 fs at a still unreached instantaneous power of eventually 10PW. CILEX also hosts the associated experimental infrastructures, which will offer the possibility to achieve scientific breakthroughs in various domains (electron and ion acceleration, X ray generation, highfield science). In particular, Laboratoire Leprince Ringuet at Ecole Polytechnique, France, and Niels Bohr institute at the university of Copenhagen, Denmark, are collaborating on the laserplasma acceleration of electrons. In this domain, the scientific goal of CILEX is twofold: explore laser wakefield acceleration at the highest possible powers, and realize a two stages acceleration experiment. CILEX operation will start in 2015 and be open to the international community shortly afterwards.

The first objective of the simulation campaign is to finalize the design of the dedicated experimental area of the CILEX facility and identify optimal laser and plasma parameters in terms of electron beams and Xray sources quality for the initial campaign of acceleration experiments. Numerical simulations will provide guidance in the choice of several crucial design parameters.

The second objective is to evaluate the spectrum and phasespace of the generated relativistic electrons and photons so that instruments with proper detection ranges can be designed before the first laser shots. A well targeted detection range allows for a higher resolution so the overall quality of a large amount of experimental data will be impacted.

Finally, the numerical simulations will help to gain insight into the physics at play in these new regimes and will prove invaluable to help prepare the analysis of the experimental data produced by this future worldleader laser facility. These results will be published in international journals, and will be relevant to the scientific program of existing or upcoming shortpulse, petawattclass laser facilities such as Texas Petawatt Laser (USA) or Berkley Lab Laser Accelerator (USA). It is also an important step towards even more ambitious future experiments on the ELIBeamlines project in Europe.

To do so, two PIC codes are going to be used. First, CalderCirc, a robust and well demonstrated reduced code that will allow a quick exploration. And then, PhotonPlasma, a very modern, fully 3D, code running in a hybrid openMP – MPI mode, to get accurate, quantitative results in the regions of interest previously highlighted by CalderCirc.

PhotonPlasma has already proven an excellent scalability on IBM Blue Gene/Q using the JUQUEEN system. It uses an original high order explicit scheme with filtering, specifically designed for laser propagation in a plasma. The heaviest 3D runs of our campaign will be run on the same architecture provided by the Fermi system.

CalderCirc is MPI only, has a small memory footprint and is optimized for intel processors. CILEX cases have already been run with it on Curie's thin nodes successfully for one million cpu hours previously granted by GENCI.

Resource Awarded: 80,000,000 core hours on FERMI @ CINECA, Italy; 2,500,000 core hours on CURIE TN @ GENCI@CEA, France

• Strong interactions beyond QCD (Call 4)

Project leader: Claudio Pica, CP3Origins, University of Southern Denmark – IMADA, Denmark

Collaborators: Francesco Sannino, CP3Origins, University of Southern Denmark, Denmark/ Luigi Del Debbio, University of Edinburgh, UK/ Biagio Lucini, Swansea University, UK/ Antonio Rago, University of Plymouth, UK/ Agostino Patella, CERN, Switzerland/ Stefan Sint, Trinity College Dublin, Ireland

Abstract: The Strong Nuclear Force, described by the theory of Quantum Chromodynamics (QCD), is one of the three fundamental forces of Nature contained in the Standard Model (SM) of particle physics. QCD is responsible for binding the quarks together to form nuclei and for the origin of about 90% of the mass of all ordinary matter.

Recently people started to realize that new strong interactions could contain the key to understand the new physics beyond the SM, which may soon be discovered by the Large Hadron Collider experiments at CERN. These new kinds of strong interactions are, in fact, becoming rapidly more relevant and popular in the scientific community.

Nonetheless, so far QCD is the only strong interaction, which has been studied in great detail. We have acquired a precise quantitative understanding of QCD thanks to Lattice simulations during the last 30 years. QCD dynamics is however not suitable for beyond SM physics.

It is only in the last few years that reliable Lattice simulations of new strong forces have started. In particular it was demonstrated that a particular model, known as Minimal Walking Technicolor (MWT), has a dynamics which is fundamentally different from QCD, namely it is infrared (IR) conformal. Models such as MWT could indeed be the starting point to build novel extensions of the SM which satisfy the experimental constraints. Much however remains to be done to understand MWT in detail.

With this project we aim to push our initial investigation of MWT to a new level of accuracy. We aim to understand, in a precise quantitative way, some of the most important aspects of the novel dynamics of MWT: the running of its couplings and its critical behavior in the IR. Such knowledge is not only fundamentally interesting from a theoretical perspective, but also extremely relevant for building new models based on the novel dynamics.

Achieving the level of accuracy we aim for requires the large computational resources available to PRACE. Local resources available to members of the team in the UK and Denmark will also be used for this project, to complement the larger numerical simulations performed at PRACE facilities.

Resource awarded: 22.133.333 core hours on FERMI (CINECA, Italy)

• Simulating Dark Matter on the Lattice (Call 6)

Project leader: Ari Hietanen, University of Southern Denmark, Denmark

Collaborators: Claudio Pica, University of Southern Denmark, Denmark; Francesco Sannino, University of Southern Denmark, Denmark; Ulrik Sondergaard, University of Southern Denmark, Denmark

Abstract: Most of the matter in the universe is in the form of dark matter. It does not emit or absorb light, and its existence has only been observed from its gravitational effect on the visible matter. However, little is known about the elementary constituents of dark matter, and the study of those, is one of the most topical problems in experimental and theoretical particle physics. In this project, we study a model where a dark matter candidate is a composite particle, which dynamics is described by yet to be found technicolor interactions. The particle would be many ways similar to a proton, except it does not have a charge, and only interacts weakly with the visible matter. In addition, we will study if a light Higgs particle could emerge from the Technicolor theory. Because the theory includes strong dynamics, no analytic solution to them is known, and large scale lattice calculations are the only first principle method known to gain knowledge about the model.

Resource awarded: 7.3 million core hours on MareNostrum @ BSC, Spain

• CWIN – Mapping the conformal window (Call 6)

Project leader: Kari Rummukainen, University of Helsinki, Finland

Collaborators: Marco Panero, Helsinki Institute of Physics, Finland; David Weir, Helsinki Institute of Physics, Finland; Tuomas Karavirta, Jyväskylä University, Finland; Kimmo Tuominen, Jyväskylä University, Finland; Anne Mykkinen, University of Helsinki, Finland; Teemu Rantalaiho, University of Helsinki, Finland; Jarno Rantaharju, Riken advanced institute for computational science, Japan

Abstract: The LHC particle accelerator at CERN, together with other upcoming experiments and astrophysical observations, is on the course of completing our picture of the Standard Model of particle physics in the near future. Even more exciting are the hints that these experiments may open the window on new physics, physics beyond the Standard Model. At the same time, modern numerical lattice simulation methods of quantum fieldtheories have matured to very precise and reliable calculational tools, as shown by the remarkable success of lattice QCD simulations.

In this project we apply simulation methods to a novel direction: we study theories which are conformal or almost conformal at long distances. This means that the long distance physics becomes scale invariant. Conformal theories are ingredients for a candidate theory for new physics possibly found at LHC, technicolor. Technicolor is among the most popular extensions of the Standard Model. The physics is strongly interacting; thus, nonperturbative lattice simulations are needed to study it.

We study two candidate theories for conformal or almost conformal physics: SU(2) gauge field theory with either six fundamental representation fermions or two adjoint representation fermions. The initial lattice studies of these theories started a few years ago in a flurry of activity, including by our group. However, definite results are still lacking. In this project we aim at precision results of the two theories under study, using large volumes and statistics enabled by PRACE and highly developed simulation methods and tools.

Resource awarded: 50 million core hours on FERMI @ CINECA, Italy

• Nucleon structure using lattice QCD simulations with physical pion mass (Call 9)

Project leader: Constantia Alexandrou, University of Cyprus and The Cyprus Institute, Cyprus

Research field: Fundamental Physics

Collaborators: Giannis Koutsou, The Cyprus Institute, Cyprus Karl Jansen, DESY, Germany Marc Wagner, Goethe University Frankfurt am Main, Germany Vincent Drach, Odense University, Denmark Roberto Frezzotti, Università di Roma Tor Vergata, Italy Giancarlo Rossi, Università di Roma Tor Vergata, Italy Chris Micahel, University of Liverpool, United Kingdom

Abstract: Fundamental properties of the nucleon, which makes the bulk of the visible matter in our universe are computed with focus on quantities that probe physics beyond the standard model. We use ab initio simulations of the fundamental theory of the strong interactions Quantum Chromodynamics (QCD) formulated in terms of quarks and gluons. The novelty of this project is that it uses simulations with physical values of the quark masses and recently developed methods to compute disconnected quark loop contributions. Using noise reduction techniques we aim at reaching unprecedented accuracy in the calculation of fundamental quantities such as the nucleon axial charge, the spin carried by the quarks in the proton and the charge radius as well as observables that probe beyond the standard model such as the neutron electric dipole moment, the nucleon sigma-terms and the charge and tensor charges. The project is part of the European Twisted Mass Collaboration, a consortium of more than 50 physicists from eight European countries. Approximately 20 PhD students and postdoctoral fellows are involved in these complex computations at the forefront of scientific computing.

Resource Awarded: 65000 core hours on CURIE H, 25300000 core hours on FERMI, 13800000 core hours on SUPERMUC

• MCH – Minimal Composite Higgs (Call 9)

Project leader: Claudio Pica, CP3-Origins, University of Southern Denmark, Denmark Research field: Fundamental Physics

Collaborators: Rudy Arthur, CP3-Origins, University of Southern Denmark, Denmark Michele Della Morte, CP3-Origins, University of Southern Denmark, Denmark Vincent Drach, CP3-Origins, University of Southern Denmark, Denmark Martin Hansen, CP3-Origins, University of Southern Denmark, Denmark Ari Hietanen, CP3-Origins, University of Southern Denmark, Denmark Tuomas Karavirta, CP3-Origins, University of Southern Denmark, Denmark Francesco Sannino, CP3-Origins, University of Southern Denmark, Denmark

Abstract: The historical discovery of a new boson by the Large Hadron Collider (LHC) experiments at CERN, which has very rapidly led to the Nobel prize in physics to F. Englert and P. Higgs, has been the culmination of a journey lasted more than fifty years and it has opened a new era for high-energy physics. We are now left with the crucial question of the nature of the new boson: is this newly discovered particle the Standard Model “Higgs boson” or it is something different? Is the new boson a fundamental particle or it is a composite state? Several extensions of the Standard Model exist in which the new boson is not elementary but instead made of something else. In this project we will investigate this possibility. Our project focuses on the minimal realisation of two popular proposals in which the Higgs boson is a composite state: Technicolor and the so-called “composite Higgs” models. In Technicolor, the Higgs is a (light) scalar state, equivalent to the $\rho(770)$ — also known as the sigma resonance — in QCD. The Higgs-like state can be light due to the non-perturbative dynamics of the model and, in addition, because of the back-reaction of the Electroweak sector on the new Technicolor sector. In the second class of theories, the “composite Higgs” models, the Higgs-like state is the equivalent of pions in QCD, and it is light due to spontaneous breaking of a global symmetry. Recently the simplest realisation of a model, which can be used for both the above proposal, has been explicitly constructed. This model is based on the $SU(2)$ gauge theory with 2 Dirac fermions in the fundamental representation. This model in isolation features spontaneous chiral symmetry breaking with 5 Goldstone bosons, 3 of which are needed to give mass to the Electroweak gauge bosons. An Higgs-like state is present in the model which, depending on how the model is embedded in the SM Electroweak sector, can be either the Technicolor scalar state or the extra Goldstone bosons or a mix of these two possibilities.

Resource Awarded: 7500000 core hours on MARE NOSTRUM

- **Pair-dominated plasmas in ultra intense fields: from the laboratory to extreme astrophysical conditions (Call 9)**

Project leader: Thomas Grismayer, GoLP/IPFN – Instituto Superior Tecnico, Portugal

Research field: Fundamental Physics

Collaborators: Ricardo Fonseca, GoLP/IPFN – Instituto Superior Tecnico, Portugal Joana Martins, GoLP/IPFN – Instituto Superior Tecnico, Portugal Luis Silva, GoLP/IPFN – Instituto Superior Tecnico, Portugal Marija Vranic, GoLP/IPFN – Instituto Superior Tecnico, Portugal Mattias Marklund, Chalmers University, Sweden Warren Mori, UCLA, United States

Abstract: Can we generate relativistic electron-positron (e^-e^+) pair plasmas in the laboratory using intense lasers, that mimic extreme astrophysical scenario? What is the role of collective effects in relativistic pair plasmas and what are their radiation signatures? These are prominent scientific questions where the physics of plasmas is intrinsically connected with quantum electrodynamics effects. This proposal aims to exploit the unique computing facilities provided by PRACE to address these exciting challenges by leveraging on the recently pioneered advances on ab initio simulations of quantum electrodynamics (QED) effects in plasmas with particle-in-cell (PIC) simulations. The main scientific route to address some of these outstanding challenges consists in exploring in the laboratory pair-dominated plasmas under the presence of ultra-intense fields and mimicking astrophysical scenarios resorting to the unprecedented power of future laser facilities. The intensity of the ultra-intense lasers of the Extreme Light Infrastructure (ELI) now under construction will provide transient fields whose magnitudes approach those assumed to be present in pulsars. This unique combination of parameters opened by the interaction of ultra-intense lasers provides a platform to study the dynamics of pair-dominated plasmas and promises to unveil some mysteries associated to a physics that is yet to be explored. The first goal of this research project is to predict the optimal laser parameters and configurations for the design of future experiments related to pair creation. The interaction of multiple lasers of ultra-high intensity leads to the development of pair cascades, forming eventually a pair-plasma approaching the critical density with large number of hard photons. The second objective is to investigate astrophysical scenarios such as the magnetosphere of pulsars where pair creation is believed to play a crucial role. For instance the pair plasma density inferred from the radiation of pulsars is found to be 1000 times bigger than the one given by standard force-free models that do not take into account pair creation. It is necessary to include such effects in a self-consistent manner in order to recover the observational results in simulations. Another key goal of this proposal is to investigate the radiation signatures in the Compton Regime, a regime not accessible with standard electromagnetic methods. We are here taking advantage from the fact that the QED-PIC code emits photons corresponding to the radiation of the particles in the presence of intense fields. The relevant temporal and spatial scales associated with these scenarios are very disparate. In addition, the microphysics that rules pair-dominated plasmas and photon emission is non-linear and stochastic and the associated collective phenomena very complex. Thus, full-scale, massively parallel kinetic particle-in-cell simulations are critical to address the challenges outlined in this proposal. This research proposal will take advantage of the available outstanding numerical and visualization frameworks in our group, and from the use of new advanced QED-PIC algorithms in order to model quantum regime of pair-plasma physics in various scenarios. The unique computational infrastructures provided by PRACE will be critical to explore some of the most fundamental physics questions at the forefront of science identified in this proposal.

Resource Awarded: 25000000 core hours on SUPERMUC

7. Mathematics and Computer Science

- FENICSHPC – High performance adaptive finite element methods for turbulent flow and multiphysics with applications to aerodynamics, aeroacoustics, biomedicine and biophysics (Call 8)

Project leader: Dr Johan Hoffman, KTH Royal Institute of Technology, Sweden

Research field: Mathematics and Computer Sciences

Collaborators: Cem Degirmenci, KTH Royal Institute of Technology, Sweden Johan Jansson, KTH Royal Institute of Technology, Sweden Niclas Jansson, KTH Royal Institute of Technology, Sweden Aurelien Larcher, KTH Royal Institute of Technology, Sweden

Abstract: This project concerns the development of parallel computational methods for solving turbulent fluid flow problems with focus on industrial applications, such as the aerodynamics of a full aircraft at realistic flight conditions, the sound generated by the turbulent flow past the aircraft during landing and takeoff, the blood flow inside a human heart and geophysical flows. The massive computational cost for resolving all turbulent scales in such problems makes Direct Numerical Simulation of the underlying Navier-Stokes equations impossible. Instead, various approaches based on partial resolution of the flow have been developed, such as Reynolds Averaged Navier-Stokes equations or Large Eddy simulation (LES). For these methods new questions arise: what is the accuracy of the approximation, how fine scales have to be resolved, and what are the proper boundary conditions? To answer such questions, a number of challenges have to be addressed simultaneously in the fields of fluid mechanics, mathematics, numerical analysis and HPC.

The main focus of the research at The Computational Technology Laboratory (CTL) is the development of high performance, parallel, adaptive algorithms for FEM modeling of turbulent flows and multiphysics, including fluid structure interaction and aeroacoustics. The adaptive finite element method G2 has been developed over the past 10 years for time-resolved simulations of turbulent flows and it works as an implicit LES method with a residual-based subgrid model that accounts for the unresolved scales. With mesh adaptivity based on “a posteriori” error estimates, efficient parallelization, and the use of unstructured meshes, G2 constitutes a powerful tool in Computational Fluid Dynamics, which can be used to solve time dependent problems efficiently. Of particular interest is the error estimation framework of G2 and, currently, we work to extend the framework to include uncertainty quantification of data and modeling parameters. Within our group, there are a number of projects in various applications areas, where the new adaptive algorithms are being used and developed.

These areas include aerodynamics, aeroacoustics, biomedicine, geophysics and FSI. In the past 3 years, we have obtained significant results in the development of G2. These include: the implementation of a hybrid MPI+PGAS linear algebra backend, which enhanced the performance of the code for larger core counts as compared to the previous MPI implementation; the successful computation of the flow past an extremely complex nose landing gear geometry and the flow past a high lift device, both as contributions to the second workshop on Benchmark problems for Airframe Noise Computations, BANCII, proposed and developed by NASA. For the following year, we plan to follow up these contributions with more detailed, larger computations. In 2013 we were granted the EU FP7 project: “Extensive UNified-domain SimulatiON of the human voice” (EUNISON) for the simulation of the human voice based on our framework. We have also successfully participated in a NASA/Boeing challenge/workshop on simulation of a full aircraft (HiLiftPW2), and we are invited to submit a paper to the AIAA SciTech 2014 conference based on our results. Our adaptive results were specifically highlighted in the summary by the organizers.

Resource Awarded: 10,000,000 core hours on HERMIT @ GCS@HLRS, Germany; 10,000,000 core hours on SuperMUC @ GCS@LRZ, Germany;

8. Universe Sciences

• Ab Initio Modeling of Solar Active Regions (Call 2)

Project leader: Aake Nordlund, University of Copenhagen, Denmark

Collaborators: Mrs Gisela Baumann, University of Copenhagen Copenhagen, Denmark / Dr Remo Collet, Max Planck Institute for Astrophysics Garching (Munich), Germany / Dr Damian Fabbian, Instituto de Astrofísica de Canarias La Laguna (Tenerife), Spain / Dr Klaus Galsgaard, University of Copenhagen Copenhagen, Denmark / Dr Troels Haugboelle, University of Copenhagen Copenhagen, Denmark / Dr David MacTaggart, University of Copenhagen, Denmark / Prof. Fernando MorenoInsertis, Instituto de Astrofísica de Canarias La Laguna (Tenerife), Spain / Dr. Roald Schnerr, Royal Swedish Academy of Sciences Stockholm, Sweden / Dr Jacob Trier Frederiksen, University of Copenhagen, Denmark

Abstract: The Sun is a fascinating astrophysical object, given its proximity and relevance to us, and the intricate physics of its readily observable surface layers, which provide a unique and comprehensive test bench for nonthermal astro and plasma physics. Studies of the Sun's atmosphere and heliosphere thus help us understand basic physical processes, and are also of direct importance for understanding the environment in which the Earth moves and the perturbations to which its magnetosphere is subjected (space weather). The overarching scientific aim of this research is to understand the dynamics of solar active regions – sunspots and their neighborhoods – and their interaction with the subsurface solar convection zone and the overlying solar corona, on scales that range from less than 10 km to about 50,000 km, using both 3D MHD simulations and 3 D relativistic charged particle (particle-in-cell code) simulations. These simulations will be coupled in an unprecedented way, such as to bridge more than a factor of 5,000 in scales of structure and dynamics of Solar active regions. Right now Europe has a unique opportunity for progress in this area, thanks to access to PetaFlop computing and a new generation of computational tools. For the first time ever, this will allow ab initio modeling of non-thermal processes in a complex and very well observed astrophysical setting; one where a unique combination of spatial, temporal, and wavelength resolution is available from observations. The results from the proposed project will be compared directly with observations from the current space borne observatories SDO (Solar Dynamics Observatory) and RHESSI (Reuven Ramaty High Energy Solar Spectroscopic Imager). Predictions can also be made for the future IRIS (Interface Region Imaging Spectrograph) satellite observatory. European scientists have a heavy involvement in all of these three satellite observatories. The project uses mainly two wellproven MPI codes that parallelize well to tens of thousands of cores; a staggered mesh magnetohydrodynamics code (the Copenhagen Stagger Code), and the PhotonPlasma Code – a relativistic particle-in-cell (PIC) code with modular provisions for particle-particle interactions (Coulomb collisions, Bremsstrahlung, Compton scattering, etc.), which also has builtin facilities for online computation of nonthermal radiation diagnostics.

Computer system: JUGENE, GAUSS/FZJ Resource awarded: 60 000 000 corehours

• Physics of the Solar Chromosphere (Call 3)

Project leader: Mats Carlsson, University of Oslo, Norway

Collaborators: Boris Gudiksen, Viggo Hansteen, University of Oslo, Norway / Jorrit Leenaarts, Utrecht University, The Netherlands

Abstract: This project aims at a breakthrough in our understanding of the solar chromosphere by developing sophisticated radiationmagnetohydrodynamic simulations.

The enigmatic chromosphere is the transition between the solar surface and the eruptive outer solar atmosphere. The chromosphere harbours and constrains the mass and energy loading processes that define the heating of the corona, the acceleration and the composition of the solar wind, and the energetics and triggering of solar outbursts (filament eruptions, flares, coronal mass ejections) that govern nearEarth space weather and affect mankind's technological environment.

Smallscale MHD processes play a pivotal role in defining the intricate fine structure and enormous dynamics of the chromosphere, controlling a reservoir of mass and energy much in excess of what

is sent up into the corona. This project targets the intrinsic physics of the chromosphere in order to understand its mass and energy budgets and transfer mechanisms. Elucidating these is a principal quest of solar physics, a necessary step towards better spaceweather prediction, and of interest to general astrophysics using the Sun as a close up RosettaStone star and to plasma physics using the Sun and heliosphere as a nearby laboratory.

Our group is worldleading in modelling the solar atmosphere as one system; from the convection zone where the motions feed energy into the magnetic field and all the way to the corona where the release of magnetic energy is more or less violent. The computational challenge is both in simplifying the complex physics without losing the main properties and in treating a large enough volume to encompass the large chromospheric structures with enough resolution to capture the dynamics of the system. We have developed a massively parallel code, called Bifrost, to tackle this challenge. The resulting simulations are very timeconsuming but crucial for the understanding of the magnetic outer atmosphere of the Sun.

Resource awarded: 21 760 000 corehours at HERMIT, GCS@HLRS Initio

• Modeling of Solar Active Regions (Call 4)

Project leader: Aake Nordlund, University of Copenhagen – Niels Bohr Institute, Denmark

Collaborators: Klaus Galsgaard, University of Copenhagen, Denmark/ Troels Haugboelle, University of Copenhagen, Denmark/ Jacob Trier Frederiksen, University of Copenhagen, Denmark/ Remo Collet, University of Copenhagen, Denmark/ Gisela Baumann, University of Copenhagen, Denmark/ Damian Fabbian, Instituto de Astrofísica de Canarias, Spain/ Fernando MorenoInsertis, Instituto de Astrofísica de Canarias, Spain/ Robert Stein, Michigan State University, USA

Abstract: The Sun is a fascinating astrophysical object, given its proximity and relevance to us, and the intricate physics of its readily observable surface layers, which provide a unique and comprehensive test bench for nonthermal astro and plasmaphysics. Studies of the Sun's atmosphere and heliosphere thus help us understand basic physical processes, and are also of direct importance for understanding the environment in which the Earth moves and the perturbations to which its magnetosphere is subjected (space weather).

The overarching scientific aim of this proposal is to produce the first ab initio models of the dynamics of solar active regions – sunspots and their neighborhoods – and their interaction with the subsurface solar convection zone and the overlying solar corona, on scales that range from 10 km to 50,000 km, using both 3D MHD simulations and 3D relativistic charged particle (particlein-cell code) simulations. The interaction of magnetic flux emerging through the solar surface with the overlying coronal magnetic field creates violent events – solar flares – where charged particles are accelerated to relativistic energies, and with the combination of MHD simulations that can model the large scale dynamics and charged particle simulations that can model the non thermal particle acceleration we can study both the cause and the effects of these violent events.

This project was initiated with a grant from the 2nd PRACE call and produced already in the first 6 months of JUGENE access outstanding results, which are now in the process of being published (for details see the separately emailed progress report). The results from this project are being compared with observations from the current satellite observatories SDO (Solar Dynamics Observatory) and RHESSI (Reuven Ramaty High Energy Solar Spectroscopic Imager). Predictions are also being made for the future IRIS (Interface Region Imaging Spectrograph) satellite observatory. European scientists have a heavy involvement in all of these three satellite observatories, and the PI of the current proposal is a collaborator on the SDO and IRIS missions.

The project uses mainly two wellproven MPIcodes that parallelize well to hundreds of thousands of cores; a staggered mesh magnetohydrodynamics code (the Copenhagen Stagger Code), and the PhotonPlasma Code – a relativistic particlein-cell (PIC) code with modular provisions for particleparticle interactions (Coulomb collisions, Compton scattering, etc.), which also has builtin facilities for high cadence particle tracing, and on line computation of nonthermal radiation diagnostics.

Resource awarded: 45.000.000 core hours on JUGENE (GCS@Jülich, Germany)

- **StarFormation Modeling:**
From the Galactic Fountain to Single Stars in One Run (Call 4)

Project leader: Paolo Padoan, Catalan Institute for Research and Advanced Studies (ICREA) and University of Barcelona – Institute of Cosmos Sciences (ICC), Spain

Collaborators: PerAke Nordlund, University of Copenhagen, Denmark/ Christian Brinch, University of Copenhagen, Denmark/ Jes Kristian Joergensen, University of Copenhagen, Denmark/ Troels Haugboelle, University of Copenhagen, Denmark/ Remo Collet, University of Copenhagen, Denmark/ Mika Juvela, University of Helsinki, Finland/ Sami Dib, Imperial College, London, UK/ Eugenio Schisano, Istituto Nazionale di Astrofisica, Italy/ Sergio Molinari, Istituto Nazionale di Astrofisica, Italy

Abstract: The process of star formation is crucial to cosmology and astrophysics. The first massive stars may have been responsible for reionizing the Universe. Stars also provide a dominant energy source to the interstellar medium (ISM) of galaxies and control their chemical enrichment. Because of the complexity of this process, involving the mutual interaction of magnetic fields, gravity and supersonic turbulence, no complete theory or numerical model of star formation is available to date. Further progress in this field requires a new class of numerical simulations that can address both the main physical processes and the huge range of scales involved. These challenging simulations are timely because of the wealth of new observational data from ongoing international campaigns with Planck, Herschel, and ALMA, in which our team is involved.

The objective of this PRACE proposal is to study star formation as a multiscale process, using simulations with an unprecedented dynamic range (seven orders of magnitude in linear scale).

The ISM goes through a complex life cycle known as the Galactic fountain: Massive stars explode as SNe, sending hot gas out of the disk into the halo, where it cools, condenses, and then falls down on the disk again. Because of computational limitations, current star formation simulations are based on unphysical initial conditions and artificial driving forces that can only mimic this energy injection from largescale processes. We propose to overcome these limitations using numerical simulations of unprecedented size and complexity, which can resolve the collapse of individual protostellar cores while simultaneously modelling the Galactic fountain. We are already carrying out the largest star formation simulations to date, thanks to a series of large allocations on the NASA/Ames Pleiades system, awarded to the PI of this proposal. These simulations cover a range of scales from 100 AU to 100 pc. Using the European supercomputing resources provided by this PRACE call, we propose to jump to the next level reaching 10 kpc, where we can simulate the whole Galactic fountain, while retaining the ability of resolving the formation and evolution of every individual star in the volume. These simulations are now possible, thanks to the specific combination of our unique OpenMP/MPI hybrid version of the public adaptivemeshrefinement code Ramses and the largenode supercomputers accessible in this PRACE call. Over the last year we have added several new physics modules to Ramses, and we have improved its performance on many levels, particularly through the development of a new hybrid version. We have proved excellent scalability and performance of our hybrid version of Ramses, up to 2,048 nodes (24,576 cores) on Pleiades, demonstrating that we are able to carry out our extreme simulations running on the whole Hermit machine.

Resource awarded: 16.875.000 core hours on SuperMUC (GCS@LRZ, Germany)

• LocalUniverse – Our Neighbourhood in the Universe: From the First Stars to the Present Day (Call 5)

Project leader: Ilian Iliev, University of Sussex, United Kingdom

Collaborators: Stefan Gottloeber, LeibnizInstitut fuer Astrophysik Potsdam (AIP), Germany | Steffen Hess, LeibnizInstitut fuer Astrophysik Potsdam (AIP), Germany | Noam Libeskind, LeibnizInstitut fuer Astrophysik Potsdam (AIP), Germany | Gustavo Yepes, Universidad Autónoma de Madrid, Spain | Alexander Knebe, Universidad Autónoma de Madrid, Spain | Daniel Severino, Universidad Autónoma de Madrid, Spain | Peter Thomas, University of Sussex, United Kingdom | William Watson, University of Sussex, United Kingdom | Aurel Schneider, University of Sussex, United Kingdom | Garrelt Mellema, Stockholm University, Sweden | Kyungjin Ahn, Chosun University, Republic of Korea | Paul Shapiro, The University of Texas at Austin, United States | Yi Mao, The University of Texas at Austin, United States | Mia Bovill, The University of Texas at Austin, United States | Anson D'Aloisio The University of Texas at Austin, United States | Yehuda Hoffman, Hebrew University of Jerusalem, Israel | Pierre Ocvirk, Strasbourg University, France | Dominique Aubert, Strasbourg University, France

Abstract: Reionization is believed to be the outcome of the release of ionizing radiation by early galaxies. Due to the complex nature of the reionization process it is best studied through numerical simulations. Such simulations present considerable challenges. The tiny galaxies which are the dominant contributors of ionizing radiation must be resolved in volumes large enough to derive their numbers and clustering properties correctly. The ionization fronts expanding from these galaxies into the surrounding neutral medium must then be tracked with a 3D radiative transfer method. The combination of these requirements makes this problem a formidable computational task. The Epoch of Reionization leaves imprints on the smallest galaxies that can still be observed today in the nearby universe. This 'Near-Field Cosmology' therefore holds clues to the history of reionization and is a subject of great current interest. Our local volume is by far the best-studied patch in the Universe, with a wealth of data available. Reionization will have left useful fossil records (e.g. abundance of satellites; numbers and radial distribution of globular clusters and metal-poor stars) in the properties of our neighbourhood which will help us use local observations to understand the young universe. In this project we propose to perform several beyond-current-state-of-the-art constrained simulations of the local cosmic structures and their reionization. Our main goals are: 1) simulate the complete star formation and galaxy formation history of our local volume, from the very First Stars to the present day; 2) derive the complete reionization history of the Local Group with focus on internal (by own sources) vs. external (by nearby proto-clusters) scenarios and their observable consequences; 3) model in detail the effects of reionization on the number, distribution and star formation histories of the Local Group satellite galaxies and globular clusters; and 4) Cosmic archaeology: find the expected distribution of the surviving low-mass metal-free stars by tracking their parent halos to the present day. Our simulations will be the first ever to achieve these goals, resulting in significant breakthroughs in our understanding of the young Universe, unavailable by any other means. Achieving this will require performing one of the largest cosmological N-body simulation ever attempted, with about 550 billion (5.5×10^{11}) particles. This will be based on a constrained realisation of the Gaussian field of initial density perturbations. This technique allows imposing available observational data as constraints on the initial conditions and thereby yielding large-scale structures which closely mimic the actual nearby universe. In particular, constrained simulations reproduce the key structures of the local cosmic web of structures like the Local Group, Virgo and Coma clusters with sizes and relative positions which closely resemble the actual ones. We will then use a radiative transfer simulation to follow the reionization of this volume. This will allow us to study the "memories" of reionization remaining in our Local Group, for comparison with observations. We will then follow this up with semi-analytical modelling of the formation of galaxies in our volume through cosmic time.

Resource awarded: 26.000.000 core-hours on SuperMUC (GAUSS@LRZ, Germany)

• Simulating the Epoch of Reionization for LOFAR (Call 5)

Project leader: Garrelt Mellema, Stockholm University, Sweden

Collaborators: Ilian Iliev, University of Sussex, United Kingdom | William Watson, University of Sussex, United Kingdom | Saleem Zaroubi, University of Groningen, Netherlands | Alexandros Papageorgiou, University of Groningen, Netherlands | Hannes Jensen, Stockholm University, Sweden | KaiYan Lee, Stockholm University, Sweden

Abstract: Reionization is believed to be the outcome of the release of ionizing radiation by early galaxies. Due to the complex nature of the reionization process it is best studied through numerical simulations. Such simulations present considerable challenges related to the large dynamic range required and the necessity to perform fast and accurate radiative transfer calculations. The tiny galaxies which are the dominant contributors of ionizing radiation must be resolved in volumes large enough to derive their numbers and clustering properties correctly, as both of these strongly impact the corresponding observational signatures. The ionization fronts expanding from all these millions of galaxies into the surrounding neutral medium must then be tracked with a 3D radiative transfer method which includes the solution of nonequilibrium chemical rate equations. The combination of these requirements makes this problem a formidable computational task. We propose to perform several simulations with the main goal to simulate, for the very first time the full, very large volume of the Epoch of Reionization (EoR) survey of the European radio interferometer array LOFAR, while at the same time including all essential types of ionizing sources, from normal galaxies to QSOs. The structure formation data will be provided by Nbody simulation of early structure formation with 8192^3 (550 billion) particles and 500/h Mpc volume. This combination of large volume and high resolution will allow us to study the multiscale reionization process, including effects which are either spatially very rare (e.g. luminous QSO sources, bright Lymanalpha lineemitters) or for which the characteristic length scales are large (e.g. Xray sources of photoionization and heating; the soft UV that radiatively pumps the 21cm line by Lymanalpha scattering; the H₂ dissociating UV background). This structure formation simulation will be used in the LOFAR Epoch of Reionization Key Science Project to construct a large library of reionization simulations on nonPRACE facilities and will be essential in the interpretation of the LOFAR observations. On Curie we will use the structure formation results to perform a reionization simulation which will address the likely stochastic nature of the sources of reionization, an aspect that to date has not been explored. We will also study the effects from the early rise of the inhomogeneous Xray background. The forming early galaxies, and the stars and accreting black holes within them emit copious amounts of radiation in all spectral bands, which in turn affects future star and galaxy formation. There are multiple channels for such feedback which need to be taken into account, an important one of which are the subtle, but farreaching effects of Xrays which strongly modulate the redshifted 21cm emission and absorption signals at early times.

Resource awarded: 3.000.000 corehours on Curie FN, and 19.000.000 corehours on Curie TN (GENCI@CEA, France)

• Vlasiator: Global hybrid Vlasov simulation for space weather (Call 5)

Project leader: Minna Palmroth, Finnish Meteorological Institute, Finland

Collaborators: Sebastian von Althaus, Finnish Meteorological Institute, Finland | Ilja Honkonen, Finnish Meteorological Institute, Finland | Yann Kempf, Finnish Meteorological Institute, Finland | Sanni Hoilijoki, Finnish Meteorological Institute, Finland | Dmitry Pokhotelov, Finnish Meteorological Institute, Finland | Arto Sandroos, Finnish Meteorological Institute, Finland | Hannu Koskinen, University of Helsinki, Finland

Abstract: The constant blow of solar wind builds the richest reachable plasma laboratory with spatial and temporal scales not attainable in terrestrial laboratories. Plasma phenomena within the near-Earth space (magnetosphere) create space weather, referring to harmful effects that can endanger technological systems or human life in space. Space weather predictions are mostly at an empirical stage, while future forecasts are based on numerical simulations of the coupled solar wind-magnetosphere-ionosphere system. Current large-scale space weather simulations are based on the simple magnetohydrodynamic (MHD) theory assuming that plasma is a fluid. Accurate characterization of the physics of space weather needs to be based on the plasma kinetic theory including multi-component plasmas. Finnish Meteorological Institute is developing a 6-dimensional Vlasov theory-based simulation called Vlasiator, in a Starting Grant project by the European Research Council. In Vlasiator, ions are distribution functions, while electrons are MHD fluid, enabling a self-consistent global plasma simulation that can describe multi-component and multi-temperature plasmas to resolve non-MHD processes that currently cannot be self-consistently described by the existing global plasma simulations. The novelty is that by modeling ions as distribution functions the outcome will be numerically noiseless, although six-dimensional, as the 3-dimensional ordinary space contains a 3-dimensional phase space for ions. Vlasiator includes advanced high-performance computing techniques available from load balancing to highly scalable grids to allow massively parallel computations. Local and global tests show that the simulation is physically and technically mature to be tested in a massively parallel setup. In this project, we focus on one of the main questions in space physics concerning energy circulation from the solar wind to the magnetosphere. We investigate 1) the shocked plasmas surrounding the magnetosphere (the magnetosheath) aiming to provide a better description of the bow shock and foreshock region than from earlier simulation efforts and 2) the processes enabling energy and mass transfer to the magnetosphere (reconnection).

1) We reproduce the detailed global structures and the time dependence of the magnetosheath in 3-dimensional phase space. Information derived from the full distribution function and its moments have never been obtained from a noiseless self-consistent simulation, and therefore we will be able to give new invaluable evidence in interpreting magnetosheath waves and particle acceleration, shock structure, and feedbacks to the magnetosphere. 2) We investigate the magnetosheath and magnetopause as influenced by reconnection between the solar wind and terrestrial magnetic fields, and quantitatively assess the influence of ion kinetics to the dynamics of reconnection. With the first self-consistent approach including ion kinetics, we are able to investigate consequences of reconnection in a global setup including realistic solar wind boundary conditions. The recent major interest towards space weather is manifested as a race towards world's first accurate space weather model. Vlasiator is a unique code with recently enabled capacity to investigate the proposed issues. The physics will address the most critical topics in space weather. The proposing team is one of the leading space simulation groups in the world and given the chance will be able to answer the challenge.

Resource awarded: 30.000.000 core-hours on Hermit (GAUSS@HLRS, Germany)

• StarLife – Protostars: From Molecular Clouds to Disc Microphysics (Call 6)

Project leader: Troels Haugboelle, University of Copenhagen, Denmark

Collaborators: Christian Brinch, University of Copenhagen, Denmark; Soeren Frimann, University of Copenhagen, Denmark; Aake Nordlund, University of Copenhagen, Denmark; Jacob Trier Fredriksen, University of Copenhagen, Denmark; Remo Collet, University of Copenhagen, Denmark; Colin McNally, University of Copenhagen, Denmark; Gareth Murphy, University of Copenhagen, Denmark; Martin Pessah, University of Copenhagen, Denmark; Paolo Padoan, University of Barcelona, Spain

Abstract: Understanding the physical processes that determine the rate at which gravitating bodies accrete mass and radiate energy is vital for unraveling the formation, evolution, and fate of almost every type of object in the Universe. This is particularly true in the context of star formation, where there is an intricate interplay between largescale environmental factors, which regulate the supply of mass and angular momentum for the ensemble of forming stars, and smallscale plasma physics processes, which control the ultimate rate at which energy is dissipated. These two fundamental processes operate over a wide range of spatial and temporal scales and it is thus impossible to study all of them at once in a single numerical simulation. This proposal addresses this limitation by employing two code families, which have been specifically developed to deal with the challenges at each end of the associated physical scales. The assembled team has a broad combination of scientific and technical expertise, and is focused on bridging the gap between molecular cloud scales, which determine the initial and boundary conditions for protostellar disc accretion, and the microphysics scales, which determine the ultimate fate of the accretion energy.

Herschel and ALMA are revolutionizing observational star formation, resolving for the first time the intricate structure of filaments that feed the stellar envelopes. Interpreting the observations will require modeling large statistical samples of protostars at high enough resolution, so that they can be used as synthetic templates for interpreting real observations. We will perform groundbreaking global simulations that will follow the formation and evolution of a thousand protostellar systems down to the opacity limit, with resolved discs and outflows embedded in a large scale model of a molecular cloud. We will employ sophisticated post processing techniques to build a large database with more than a hundred thousand synthetic images of the protostars from different viewpoints, evolutionary stages, and wavelengths, which can be used for nonparametric modeling and interpretation of observations of protostars, in particular from ALMA.

The simulations will also provide an unprecedented global view of the formation of protostellar discs, in the presence of selfconsistently evolved ‘external’ magnetic fields. Previous disc studies have used idealized initial conditions and relied on the fluidMHD framework, which breaks down at the very low levels of ionization in cold discs, and at the very low densities in disc coronae. The details of how magnetic fields reconnect and energy is dissipated in protostellar discs is of fundamental importance, and needs to be understood on solid physical grounds by going beyond the fluid regime. We will carry out the first ever 3D particlein-cell simulation that follows the magnetorotational instability and its non-linear evolution to saturation. By selfconsistently calculating the neutralionelectron interactions, as well as the photon spectrum emitted by accelerated charged particles, we will be able to compute both the thermal energy dissipation and the emergent nonthermal spectrum from first principles. This will open up a completely new window into one of the most important instabilities in modern astrophysics.

Resource awarded: 75 million core hours on JUQUEEN @ GCS@Jülich, Germany

• Physics of the Solar Chromosphere (Call 7)

Project leader: Carlsson, Mats; University of Oslo, Norway

Collaborators: Boris Gudiksen, University of Oslo, Norway; Viggo Hansteen, University of Oslo, Norway

Abstract: This project aims at a breakthrough in our understanding of the solar chromosphere by developing sophisticated radiationmagnetohydrodynamic simulations in order to interpret observations from the upcoming NASA SMEX mission Interface Region Imaging Spectrograph (IRIS).

The enigmatic chromosphere is the transition between the solar surface and the eruptive outer solar atmosphere. The chromosphere harbours and constrains the mass and energy loading processes that define the heating of the corona, the acceleration and the composition of the solar wind, and the energetics and triggering of solar outbursts (filament eruptions, flares, coronal mass ejections) that govern nearEarth space weather and affect mankind's technological environment.

Smallscale MHD processes play a pivotal role in defining the intricate fine structure and enormous dynamics of the chromosphere, controlling a reservoir of mass and energy much in excess of what is sent up into the corona. This project targets the intrinsic physics of the chromosphere in order to understand its mass and energy budgets and transfer mechanisms. Elucidating these is a principal quest of solar physics, a necessary step towards better spaceweather prediction, and of interest to general astrophysics using the Sun as a close up RosettaStone star and to plasma physics using the Sun and heliosphere as a nearby laboratory.

Our group is worldleading in modelling the solar atmosphere as one system; from the convection zone where the motions feed energy into the magnetic field and all the way to the corona where the release of magnetic energy is more or less violent. The computational challenge is both in simplifying the complex physics without losing the main properties and in treating a large enough volume to encompass the large chromospheric structures with enough resolution to capture the dynamics of the system. We have developed a massively parallel code, called Bifrost, to tackle this challenge. The resulting simulations are very timeconsuming but crucial for the understanding of the magnetic outer atmosphere of the Sun.

Resource awarded: 34,560,000 core hours on SuperMUC @ GCS@LRZ, Germany

• SOLDYN: Simulations of SOLar DYnamo cycle and differential rotation (Call 8)

Project leader: Dr Petri Kapyla, University of Helsinki, Finland

Research field: Universe Sciences

Collaborators: Joern Warnecke, Max Planck Institute for Solar System Research, Germany Maarit Mantere, Aalto University, Finland Elizabeth Cole, University of Helsinki, Finland Axel Brandenburg, NORDITA, Sweden

Abstract: The Sun exhibits magnetic activity at various spatial and temporal scales. The best known example is the 11year sunspot cycle which is related to the 22year periodicity of the Sun's magnetic field. The sunspots, and thus solar magnetic activity, have some robust systematic features: in the beginning of the cycle sunspots appear at latitudes around 40 degrees. As the cycle progresses these belts of activity move towards the equator. The sign of the magnetic field changes from one cycle to the next and the large-scale field remains approximately antisymmetric with respect to the equator. This cycle has been studied using direct observations for four centuries. Furthermore, proxy data from tree rings and Greenland ice cores has revealed that the cycle has persisted through millennia. The period and amplitude of activity change from cycle to cycle and there are even periods of several decades in the modern era when the activity has been very low. Since it is unlikely that the primordial field of the hydrogen gas that formed the Sun billions of years ago could have survived to the present day, the solar magnetic field is considered to be continuously replenished by some dynamo mechanism. The cycle also manifests itself in the occurrence of space weather events, where a huge amount of energy is released in violent eruptions on the Sun. These events can have huge impacts on human kind due to power grid failures, high radiation doses in particular on polar flights and high risk on spacecraft outside the Earth's magnetosphere.

We study the solar dynamo and magnetic eruptions by performing two sets of highresolution global numerical simulations of the turbulent convection zone with or without a simplified corona above. The results of the study are likely to help in understanding what is causing solar activity and how magnetic eruptions are initiated.

Resource Awarded: 32,352,064 core hours on HERMIT @ GCS@HLRS, Germany;

- **STARZOOM – Zooming in on Star Formation (Call 8)**

Project leader: Dr Troels Haugboelle, University of Copenhagen, Denmark

Research field: Universe Sciences

Collaborators: Christian Brinch, University of Copenhagen, Denmark Soeren Frimann, University of Copenhagen, Denmark Jes Kristian Joergensen, University of Copenhagen, Denmark Aake Nordlund, University of Copenhagen, Denmark Oliver Lothar Gressel, University of Copenhagen, Denmark Colin McNally, University of Copenhagen, Denmark Gareth Murphy, University of Copenhagen, Denmark Martin Pessah, University of Copenhagen, Denmark Paolo Padoan, University of Barcelona, Spain

Abstract: Newborn stars, surrounded by centrifugally supported discs of gas and dust, reside in the central regions of hot cores, which are embedded in colder, extended envelopes. Above the discs and close to the star, outflows are launched in the form of winds and jets. These systems exist for a few million years during and after the birth of the star. In the early stages of this process, the envelope collapses under its own gravity, and a disc is quickly formed. By removing excess angular momentum and potential energy, this accretion disc functions as a conduit, which allows most of the gas and dust to either accrete onto the star or be lost in the outflows, while leaving a small fraction of the mass in the form of planets. Detailed modelling of the properties of protostellar systems is thus a prerequisite for understanding planet formation. Because of the small scale of the inner protoplanetary disc, relative to the distance of even the nearest star forming regions, very few detailed – spatially resolved – observations have been available in the past. The Herschel satellite and the new submillimeter facility ALMA are revolutionizing observational star formation. In particular, ALMA is currently providing many new observations of protostellar systems, and a more complex picture is emerging with e.g. warped discs containing intricate structures, such as largescale dust devils, and many signs of newborn planets perturbing the gas and dust.

Unravelling the physical processes at play is crucially important and requires modelling, and understanding, an intricate interplay between largescale environmental factors, which regulate the supply of mass, angular momentum, and magnetic flux to the forming stars, and smallscale processes close to the star, which control the evolution and dynamics in the inner part of the envelope and protoplanetary disc. This proposal will encompass these disparate scales using extremely deep adaptive mesh refinement simulations, reaching a factor of a billion in linear resolution compared to the outer scales of the simulated domain. These unprecedented capabilities are complemented by a unique approach that we have developed to provide boundary conditions by embedding our model in to some of the largest models ever made of star forming regions.

Using the CURIE supercomputer we will perform, for the first time ever, a systematic study that bridges the gap between molecular cloud scales, where magnetic fields are anchored and the initial and boundary conditions for protostellar accretion are set, and the much smaller disc and jet scales, which determine the ultimate evolution of protostellar systems. Because of the unique combination of methods and resources, this study will have a major impact in our global understanding of how stars and planets form.

Resource Awarded: 4,000,000 core hours on CURIE FN @ GENCI@CEA, France; 6,000,000 core hours on CURIE TN @ GENCI@CEA, France;

- **Rare structures in the Lymanalpha forest: bridging the gap between small and large scales. (Call 8)**

Project leader: Dr James Bolton, University of Nottingham, United Kingdom

Research field: Universe Sciences

Collaborators: John Regan, University of Helsinki, Finland Matteo Viel, INAF, Italy Martin Haehnelt, University of Cambridge, United Kingdom Ewald Puchwein, University of Cambridge, United Kingdom Debora Sijacki, University of Cambridge, United Kingdom Avery Meiksin, University of Edinburgh, United Kingdom Frazer Pearce, University of Nottingham, United Kingdom

Abstract: The intergalactic medium (IGM) is the rarefied material which spans the vast distances between galaxies in the Universe. The IGM therefore straddles the interface between studies of galaxy formation and the evolution of large scale structure, and its observable properties are closely intertwined with both processes. One of the key observational probes of the IGM is the Lymanalpha forest of hydrogen absorption lines observed in the spectra of distant quasars. Careful comparison between detailed hydrodynamical simulations of the Lymanalpha forest and high resolution, high signal-to-noise echelle spectra have yielded valuable insights into how cold dark matter is, the epoch of reionisation and the interplay between galaxies and gas in the early Universe. A key limitation of the existing numerical models, however, is their narrow dynamic range. This translates into rather small simulation volumes due to the requirement of resolving the Jeans scale in the IGM. Highly resolved simulations are essential for quantitative comparison to the available high-quality, high resolution observational data. Large scale variations and rare objects, such as massive dark matter haloes and deep voids, are therefore not well captured in existing Lymanalpha forest simulations. This significantly limits the utility of these models when confronted with observational data, and requires large corrections to be applied to the simulation results. This PRACE project aims to alleviate these issues, by bridging the important gap between small and large scales with a suite of the highest resolution Lyman-alpha forest simulations performed to date within large volumes.

Resource Awarded: 15,000,000 core hours on CURIE TN @ GENCI@CEA, France;

• Magnetic Reconnection in Threedimensional Turbulent Configurations (Call 8)

Project leader: Prof Giovanni Lapenta, KU Leuven, Belgium

Research field: Universe Sciences

Collaborators: Jorge Amaya, KU Leuven, Belgium Emanuele Cazzola, KU Leuven, Belgium Jan Deca, KU Leuven, Belgium Maria Elena Innocenti, KU Leuven, Belgium Evan Alexander Johnson, KU Leuven, Belgium Koen Kemel, KU Leuven, Belgium Vyacheslav Olshevsky, KU Leuven, Belgium Lorenzo Siddi, KU Leuven, Belgium Andrey Divin, Uppsala University, Sweden

Abstract: We aim at modeling of the most striking process in astrophysical plasma: magnetic reconnection. Magnetic reconnection is believed to be the only way the magnetic field energy is released to particles. In this fundamental process, magnetic field lines of opposite polarity are brought together and fused into a new magnetic configuration. The end effect of reconnection is conversion of magnetic energy to kinetic energy of the particles and a corresponding increase in thermal energy and flow velocity of the plasma. Because of its kinetic nature, magnetic reconnection in space plasmas could be thoroughly described and understood only by means of computer modeling. Of particular interest to the physicists now is the threedimensional (3D) volumetric, random reconnection that might be happening in numerous nullpoints and smallscale current sheets in the highly turbulent interstellar environment.

We will conduct numerous threedimensional simulations of such reconnection, which will allow us to answer the three important questions:

1. What agents are important for energy dissipation in the complex null-point configurations that are luckily present in interstellar plasma: the X-type null-points, or null-lines?
2. What are the signatures of such reconnection (waves, particle jets, non-thermal particle spectra, etc.), that could be determined by spacecraft and in laboratory devices?
3. What are the properties of turbulent reconnection and how those compare to magnetohydrodynamic (MHD) turbulence?

Resource Awarded: 25,000,000 core hours on SuperMUC @ GCS@LRZ, Germany

• Multi-scale simulations of Cosmic Reionization (Call 9)

Project leader: Ilian Iliev, University of Sussex, United Kingdom

Research field: Universe Sciences

Collaborators: Romain Teyssier, University of Zurich, Switzerland Dominique Aubert, Observatoire Astronomique de Strasbourg, France Pierre Ocvirk, Observatoire Astronomique de Strasbourg, France Kyungjin Ahn, Chosun University, Korea, Republic of Karl Joakim Rosdahl, Leiden University, Netherland Garrelt Mellema, Stockholm University, Sweden Keri Dixon, University of Sussex, United Kingdom David Sullivan, University of Sussex, United Kingdom Peter Thomas, University of Sussex, United Kingdom Jun-Hwan Choi, The University of Texas at Austin, United States Anson D'Aloisio, The University of Texas at Austin, United States Hyunbae Park, The University of Texas at Austin, United States Paul Shapiro, The University of Texas at Austin, United States

Abstract: The first billion years of cosmic evolution are one of the last largely uncharted territories in astrophysics. During this key period the cosmic web of structures we see today first started taking shape and the very first stars and galaxies formed. The radiation from these first galaxies started the process of cosmic reionization, which eventually ionized and heated the entire universe, in which state it remains today. This process had profound effects on the formation of cosmic structures and has left a lasting impression on them. This reionization process is inherently multi-scale. It is generally believed to be driven by stellar radiation from low-mass galaxies, which cluster on large scales and collectively create very large ionized patches whose eventual overlap completes the process. The star formation inside such galaxies is strongly affected by complex radiative and hydrodynamic feedback effects, including ionizing and non-ionizing UV radiation, shock waves, gas cooling and heating, stellar winds and enrichment by heavy elements. Understanding the nature of the first galaxies and how they affect the progress, properties and duration of the cosmic reionization requires detailed modelling of these complex interactions. The aim of this project is to combine a unique set of simulations of cosmic reionization covering the full range of relevant scales, from very small, sub-galactic scales, for studying the detailed physics of radiative feedback, all the way to very large cosmological volumes at which the direct observations will be done. These simulations will be based on several state-of-the-art numerical tools, discussed in the sections below, including Adaptive Mesh Refinement (AMR) techniques for achieving very large dynamic range in radiative hydrodynamics calculations (RAMSES-RT code), GPU-based acceleration for radiative hydrodynamics (RAMSES-CUDATON), and a massively-parallel, highly numerically efficient radiative transfer method for accurate modelling at large scales (C2-Ray). We will complement the numerical simulations with semi-analytical galaxy formation modelling to explore the large parameter space available, to improve the treatment of reionizing sources in large-scale radiative transfer simulations as well as to derive detailed observational features of the first galaxies in different observational bands. The questions we will address are: 1) how do the radiative feedback from the First Stars hosted in cosmological minihaloes and dwarf galaxies affect the formation of early structures and subsequent star formation?; 2) how much does high-redshift galaxy formation differ from the one at the present day? What are the observational signatures of the first galaxies? 3) how important is the recently pointed out effect of local modulation of the star formation in minihaloes due to differential supersonic drift velocities between baryons and dark matter?; 4) how does the metal enrichment and the transition from Pop III (metal-free) to Pop II stars occur locally and how is this reflected in the metallicity distribution of the observed dwarf galaxies and globular clusters? and 5) How are these feedback effects imprinted on large-scale observational features?

Resource Awarded: 500000 core hours on CURIE FN, 150000 core hours on CURIE H, 13000000 core hours on CURIE TN, 8000000 core hours on MARE NOSTRUM

• PRACE₄LOFAR (Call 8)

Project leader: Garrelt Mellema, Stockholm University, Sweden

Research field: Universe Sciences

Collaborators: Kyungjin Ahn, Chosun University, Korea, Republic of Fabian Krause, University of Groningen, Netherlands Saleem Zaroubi, University of Groningen, Netherlands Hannes Jensen, Stockholm University, Sweden Kai Yan Lee, Stockholm University, Sweden Suman Majumdar, Stockholm University, Sweden Keri Dixon, University of Sussex, United Kingdom Ilian Iliev, University of Sussex, United Kingdom Chaichalit Srisawat, University of Sussex, United Kingdom David Sullivan, University of Sussex, United Kingdom

Abstract: Cosmic reionization is the process that took place 12 billion years ago when the first generations of stars and galaxies formed in the Universe. Ionizing radiation produced by stars and more extreme objects such as black holes, escaped from the galaxies and spread through the medium in between the galaxies. This process transformed this medium from entirely neutral to entirely ionized, which it has remained ever since. Reionization is at the forefront of modern cosmological research. Within the next few years we expect to transform our knowledge about this period through the detection of the redshifted 21cm radio signal from neutral hydrogen during reionization. The European radio interferometer array LOFAR is best placed to make this discovery. However, the discovery of the signal alone will need interpretation in terms of the properties and distribution of the galaxies that caused reionization. This PRACE proposal forms part of the efforts of the LOFAR-EoR Key Science Project and will provide the basic data needed to interpret the observations. We will perform several simulations with the main goal to simulate, for the very first time the full, very large volume of the Epoch of Reionization (EoR) survey of LOFAR, while at the same time including all essential types of ionizing sources, first stars, normal galaxies and QSOs. The structure formation data will be provided by an N-body simulation of early structure formation with 6912^3 (330 billion) particles and 500/h Mpc volume. This combination of large volume and high resolution will allow us to study the multi-scale reionization process, including effects which are either spatially very rare (e.g. luminous QSO sources) or for which the characteristic length scales are large (e.g. X-ray sources of photoionization and heating; the soft UV that radiatively pumps the 21-cm line by Lyman-alpha scattering; the H₂-dissociating UV background). We will complement the results from this simulation with results of smaller volumes, which allow us to include the effects of structures not resolved in this very large volume. This structure formation simulation will be used in the LOFAR Epoch of Reionization Key Science Project to construct a large library of reionization simulations on non-PRACE facilities on which the interpretation of the LOFAR observations will be based. As part of this proposal we will use the structure formation results to perform reionization simulations, which will address the likely stochastic nature of the sources of reionization, an aspect that to date has not been explored. We will also study the effects from the early rise of the inhomogeneous X-ray background and how much of this background is due to the first stars. The forming early galaxies, and the stars and accreting black holes within them emit copious amounts of radiation in all spectral bands, which in turn affects future star and galaxy formation. There are multiple channels for such feedback, which need to be taken into account, an important one of which are the subtle, but far-reaching effects of X-rays which strongly modulate the redshifted 21-cm emission and absorption signals at early times.

Resource Awarded: 19000000 core hours on CURIE TN

Appendix B

DOE INCITE Awards That Include Nordic Researchers

This appendix includes information on DOE INCITE awards that include either a Nordic PI or co-PI. The period covered was from 2010-2015. DOE allows proposers from institutions outside the US to be project PIs and this is reflected in their statistics for 2015 which identify 11% of the 56 awarded projects as having non-US PIs.

The information on awards provided in this appendix is extracted from the DOE INCITE factsheets that are available online at: <http://www.doeleadershipcomputing.org/incite-awards/>

Information on the DOE INCITE program is available at:
<http://www.doeleadershipcomputing.org/incite-program/>

Information on the DOE Titan system at Oak Ridge National Laboratory is available at
<https://www.olcf.ornl.gov/computing-resources/titan-cray-xk7/>

Information on the DOE Mira system at Argonne National Laboratory is available at:
<http://www.alcf.anl.gov/user-guides/mira-cetus-vesta>

2010 DOE INCITE Award / Type: New

• Title: Probing the Non-Scalable Nano Regime in Catalytic Nanoparticles with Electronic Structure Calculations

Principal Investigator: Jeffrey Greeley, Argonne National Laboratory

Co-Investigators: Thomas Bligaard, Technical University of Denmark
Jens Jørgen Mortensen, Technical University of Denmark
Jens Nørskov, Technical University of Denmark
Kristian Thygesen, Technical University of Denmark

Scientific Discipline: Materials Science: Nanoscience

INCITE Allocation: 10,000,000 processor hours

Site: Argonne National Laboratory

Machine (Allocation): IBM Blue Gene/P (10,000,000 processor hours)

Research Summary: The profoundly new physical and chemical phenomena that arise at length scales intermediate between those of isolated molecules and bulk materials have been the subject of an explosion in nanoscience research in the past decade. These novel properties, which cannot be understood by simple extrapolation of either molecular or bulk properties into the nano regime (hence “non-scalable”), have been exploited for applications ranging from high-strength carbon nanotubes to highly active catalytic materials. In spite of these powerful and important developments, however, fundamental understanding of how nanoscale objects differ from their smaller or larger cousins (molecules and bulk materials, respectively) has been lacking. The only means of performing reliable electronic structure analyses of nanosystems is to perform explicit electronic structure calculations of these nanometer-sized objects, calculations that have been prohibitively costly to date.

In this work, we will combine novel, highly parallelizable electronic structure (Density Functional Theory) codes with the hardware available through the INCITE program to provide unprecedented insights into the evolution of the electronic and chemical properties of metal particles across the nanoscale regime. This analysis will, firstly, determine the critical size at which nanoparticles of various geometries become truly metallic (bulk-like) in their electronic structures; this is a fundamental,

unresolved question in nanoscience. Additionally, by coupling this electronic analysis to related calculations of the surface catalytic properties of platinum and gold nanoparticles, we will answer the longstanding question of whether changes in nanoparticles' electronic properties with size can account for the remarkably high catalytic activities that have been experimentally observed in nanoparticles with diameters of 2-4 nm.

Taken together, our combined electronic and catalytic analyses will provide novel physical insights into the nano regime and, as such, will open up significant new possibilities for the manipulation and selection of nanoparticles for groundbreaking technological applications.

2011 DOE INCITE Award / Type: Renewal

• Title: Probing the Non-Scalable Nano Regime in Catalytic Nanoparticles with Electronic Structure Calculations

Principal Investigator: Jeffrey Greeley, Argonne National Laboratory

Co-Investigators: Thomas Bligaard, Technical University of Denmark

Jens Jørgen Mortensen, Technical University of Denmark

Jens Nørskov, Technical University of Denmark

Nichols Romero, Argonne National Laboratory

Kristian Thygesen, Technical University of Denmark

Scientific Discipline: Materials Science: Nanoscience

INCITE Allocation: 15,000,000 processor hours

Site: Argonne National Laboratory

Machine (Allocation): IBM Blue Gene/P (15,000,000 processor hours)

Research Summary: The project's work for 2011 will continue fundamental studies of the size-dependent properties of metal nanoparticles in the non-scalable nano regime. This size range, in which nanoparticles' properties change in a manner that cannot be extrapolated from less computationally demanding bulk or single-crystal surface calculations, is known to exhibit rapid, size-dependent property changes for a variety of applications. To understand variations in electronic and catalytic properties in this regime, it is essential to perform accurate first-principles calculations.

These calculations, which will ultimately assist in the design of enhanced nanocatalysts, are the continuing focus of this proposal. Researchers will continue to make use of GPAW, their highly scalable, $O(N^3)$, real space, and grid-based Density Functional Theory (DFT) code, for nanocatalytic modeling efforts. To date, they have determined changes in key thermodynamic parameters relevant to the oxidation of carbon monoxide, a classic reaction in heterogeneous catalysis, on gold (Au) nanoparticles ranging in size from 13 to 1415 atoms. Building upon these results, and taking advantage of code improvements from the past year, the project will determine correlations between these thermodynamic properties and corresponding kinetic properties on Au nanoparticles; such relationships have been established on bulk-like single crystal metal surfaces, but never in the non-scalable nano regime. In addition, researchers intend to extend their analyses from Au, a noble metal with a full, 10-electron, d-band, to platinum (Pt) and rhodium (Rh), two catalytically relevant metals with partially filled d-bands which are known, in many cases, to exhibit properties substantially different from those of gold.

The net result of these new studies will be a comprehensive, first principles-based picture of how the catalytic and electronic properties of a diverse array of metal nanoparticles, including Au, Pt, and Rh, evolve from those of molecular-like metal clusters to those of bulk-like metallic surfaces. Such understanding can only be obtained through a combination of accurate electronic structure calculations and the resources available through the INCITE program.

2012 DOE INCITE Award / Type: Renewal

• Title: Probing the Non-Scalable Nano Regime in Catalytic Nanoparticles with Electronic Structure Calculations

Scientific Discipline: Materials Science: Nanoscience

INCITE Allocation: 10,000,000 processor hours

Site: Argonne National Laboratory

Machine (Allocation): IBM Blue Gene/P (10,000,000 processor hours)

Research Summary: The project's work for 2012 will continue fundamental studies of the size-dependent properties of metal nanoparticles in the nonscalable nano regime. This size range, in which nanoparticles' properties change in a manner that cannot be extrapolated from less computationally demanding bulk or single crystal surface calculations, is known to exhibit rapid, size-dependent property changes for a variety of applications. To understand variations in electronic and catalytic properties in this regime, it is essential to perform accurate first-principles calculations.

These calculations, which will ultimately assist in the design of enhanced nanocatalysts, are the continuing focus of this proposal. Researchers will continue to make use of GPAW, their highly scalable, $O(N^3)$, real space, and grid-based Density Functional Theory (DFT) code, for nanocatalytic modeling efforts. To date, they have determined changes in key thermodynamic parameters relevant to the oxidation of carbon monoxide, a classic reaction in heterogeneous catalysis, on gold (Au) nanoparticles ranging in size from 13 to 1,415 atoms. In addition, they have established that the size-dependent trends for Pt differ from Au particles in significant ways and are analyzing the electronic structure of Pt systems to understand these results.

Building upon the analyses from last year, they will introduce both stoichiometric and reduced TiO_2 oxide supports into their calculations. These supports can have a significant impact on metal nanoparticles' catalytic properties, but limitations in computational resources have prevented researchers from understanding the detailed effect of these supports. The net result of these new studies will be a comprehensive, first principles-based picture of how the catalytic and electronic properties of oxide-supported metal nanoparticles evolve from the properties of molecular-like metal clusters to those of bulk-like metal surfaces.

2014 DOE INCITE Award / Type: New

• Title: "Large-Scale Coupled-Cluster Calculations of Supramolecular Wires"

Principal Investigator: Poul Jorgensen, Aarhus University

Co-Investigators: Jacek Jakowski, The University of Tennessee,
Kasper Kristensen, Aarhus University,
Bobby Sumpter, Oak Ridge National Laboratory

Scientific Discipline: Chemistry: Physical

INCITE Allocation: Oak Ridge National Laboratory Cray XK7 (24,000,000 processor hours)

Research Summary: Researchers are developing noncommercial open-source software for electronic structure calculations by extending the application range of coupled-cluster wave function methods to large molecular systems. Applications will be performed on a new class of organogelators generated from self-assembly of 1-aza-adamantanetetriones (AATs) into 1D molecular wires.

Quantum mechanics is the key to understanding the molecular world of chemistry and other related molecular sciences. In particular, the electronic Schrödinger equation has to be solved to describe the electronic structure of a molecular system. Two different strategies have been used for obtaining

approximate solutions to the Schrödinger equation: wave-function-based methods and density functional theory. The coupled-cluster model is the state-of-the-art wave function method and has been used to compute energy levels, structures, and various molecular properties for small molecular systems to an accuracy challenging that of experimental results. The proposed coupled-cluster scheme will extend the application range of accurate quantum chemical calculations into new territory. Researchers will use it to study a new class of molecules, the AATs, for which the use of coupled-cluster methods may turn out to be particularly useful. AATs efficiently self-assemble into ordered nanostructures, and their electronic and physical properties can be experimentally tuned. They are therefore promising model materials, and in their 1D self-assembled supramolecular wire form, they have potential applications in the fields of molecular electronics and optoelectronics.

2015 DOE INCITE Award / Type: Renewal

• Title: Large-scale Coupled-Cluster Calculations of Supramolecular Wires

Principal Investigator: Poul Jørgensen, Aarhus University

Co-Investigators: Jacek Jakowski, Oak Ridge National Laboratory
Kasper Kristensen, Aarhus University,
Bobby Sumpter, Oak Ridge National Laboratory

Scientific Discipline: Chemistry: Physical

INCITE Allocation: Site: Oak Ridge National Laboratory Cray XK7 (48,000,000 processor hours)

Research Summary: Electronic structure calculations of a wide range of molecular properties today are an integrated part of many branches of molecular sciences. The coupled-cluster (CC) model is the state-of-the-art wave function method, and, for small molecular systems, various molecular properties have been computed to an accuracy challenging experimental results. However, the application range of CC methods so far has been limited to small molecular systems because of their computational scaling with system size. For this reason, density functional theory (DFT) has developed into a workhorse for large-scale applications. The major drawback of DFT calculations is that they generally do not possess the accuracy and the predictive power of the CC methods.

We are developing non-commercial open source software for electronic structure calculations by extending the application range of coupled-cluster wave function methods to large molecular systems. Applications will be performed on a new class of organogelators generated from self-assembly of 1-azadamantanetriones (AATs) into one-dimensional molecular wires.

The goal of this project is twofold: we wish to develop a stable, massively parallel CC program to make available free to the general user, and we want to apply it to the AAT class of supramolecular wires. The computational method for achieving these goals is the divide–expand–consolidate (DEC) scheme—where the inherent locality of electron correlation effects is used to formulate CC calculations in a linear-scaling and massively parallel manner.

The outlook for the proposed development is immense. Today, quantum mechanical calculations on large molecular systems are routinely carried out using DFT. The reliability of these calculations is severely limited. With the DEC development, CC methods may also be applied to large molecular systems with the same rigorous error control as for small molecules. This proposal is a huge step in this direction, which, in a larger perspective, will transform the field of electronic structure calculations for large molecules from being largely a tool for rationalizing observed phenomena to becoming truly predictive.

Appendix C

NSF PRAC Award

NSF Blue Water projects

Of the 29 PRAC awards listed as science teams, only two listed co-PIs who are not currently at US institutions. (<https://bluewaters.ncsa.illinois.edu/science-teams>). One of the two awards had two Nordic researchers included as co-PIs as shown below. From information provided by the Blue Waters project office, a total of six Nordic researchers have Blue Waters accounts associated with this project, which has 6,500,000 node hours for the project.

The Blue Waters system is a Cray XE/XK hybrid machine and is described at <https://bluewaters.ncsa.illinois.edu/hardware-summary> and the NSF PRAC program information is at http://www.nsf.gov/funding/pgm_summ.jsp?pims_id=503224&org=OCI&from=home.

Projects information is from <https://bluewaters.ncsa.illinois.edu/> under “About/Science Teams”.

2012: NSF Blue Waters PRAC awards

- Title: “Ab Initio Models of Solar Activity”

Principal Investigator: Robert F. Stein, Michigan State University

co-PIs: William Abbett, Bart De Pontieu, Mats Carlsson, Aake Nordlund

Blue Waters Allocation: 6,500,000 node hours

The goal of this project is to understand how internal solar magneto-convection powers the Sun’s activity, and how that activity heats the chromosphere and corona and accelerates charged particles to relativistic energies. The research team uses three-dimensional, compressible, finite difference, magneto-hydrodynamic (MHD) codes to solve the equations for mass, momentum and internal energy in conservative form plus the induction equation for the magnetic field. They use a particle-in-cell plasma code to calculate charged particle acceleration and radiation in regions of reconnecting magnetic fields.

Appendix D

PRACE Tier-1 DECI 7-8 Awards

Information on the DECI-7 and DECI-8 programs was obtained from the PRACE website (<http://www.prace-ri.eu/>) under DECI Tier-1 Access Awarded Projects.

DECI 7th Call

Physics and Astrophysics

- Project Name: Planck-LFI

Principal Investigator: Hannu Kurki-Suonio

Research area: Cosmology, Astrophysics

Abstract: Planck is a European Space Agency satellite mission, whose task is to map the structure of the cosmic microwave background (CMB) in unprecedented detail, surpassing the accuracy of previous missions, like the NASA WMAP. The cosmic microwave background is radiation from the Big Bang, and it shows us the structure of the early universe. Planck will constrain cosmological models and examine the birth of large-scale structure in the universe. It is thought that this structure originates from quantum fluctuations in the very early universe during a period of accelerated expansion called inflation, but Planck results are needed for a better understanding of this. The main scientific results expected from Planck are cosmological, but as a by-product, Planck will also yield all-sky maps of all the major sources of microwave to far-infrared emission, opening a broad expanse of other astrophysical topics to scrutiny. Planck was launched in May 2009, and the final results from the mission will be published in early 2014. Planck carries two instruments, the Low-Frequency Instrument (LFI) and the High-Frequency Instrument (HFI), utilizing different technologies. It is important to map the sky at many frequencies to be able to separate the cosmic microwave background from the astrophysical foreground radiation. Two Planck data processing centres (DPCs) have been set up, one for each instrument, but the most resource-intensive tasks need to be done on supercomputers. Because of the weakness of the signal and the high accuracy desired, Planck data analysis is a complicated task, requiring sophisticated statistical methods to separate out the signal from instrument noise and systematic effects. Simulation work will dominate the computational load of Planck data analysis. Analysis pipelines will indeed be predominantly run on simulated rather than real data since Planck analysis codes either require simulations for self-calibration and validation of results, or depend critically on simulations for the results themselves. The objective of this application is to carry out two resource-intensive tasks that are needed as part of Planck LFI data analysis: 1) timeline-to-map Monte Carlo simulation of Planck data: thousands of realizations of instrument noise and hundreds of realizations of cosmic microwave background signal; also simulations of astrophysical foreground radiation signal; the analysis of this data in parallel to the analysis of the real data from the sky 2) cosmological parameter estimation for a number of cosmological models, in particular those related to multi-field inflation.

Biology, Biosciences and Biophysics

- **Project Name:** SIVE-2

Principal Investigator: Prof. Erik Lindahl

Research area: Biosciences: molecular dynamics simulation of viral entry

Abstract: Membrane fusion, the process by which neuronal exocytosis and infection by enveloped viruses occur, has been notoriously difficult to characterize at a molecular level. Part of the problem is that the underlying reaction that fusion proteins catalyze is not fully understood. The development of robust predictive models for the mechanism of lipid membrane fusion and its catalysis by viral fusion proteins will greatly aid in the understanding of the underlying physical process and how to effectively target it with antiviral agents. We have developing high-performance simulation methods to analyze membrane fusion. In our work thus far, we have simulated vesicle fusion at atomic resolution, yielding novel insight into structure and mechanism of fusion intermediates. We are now extending these simulations to generate high-fidelity models of fusion in a experimental model systems, and predict the catalytic mechanism of influenza fusion proteins. We particularly plan to examine how influenza-catalyzed fusion is similar to or differs from protein-free fusion. Simulations are performed using the Gromacs software package that we and our collaborators develop, one of the fastest in the world.

- **Project Name:** TanGrin

Principal Investigator: Vesa Hytonen

Research area: Computational Biophysics

Abstract: Cells are typically friendly and outgoing, meaning that they enjoy social situations and in particular communication. One of the means by which they do so is receptor molecules embedded in cell membranes. These receptors take part in communication between a cell and its outside world, thereby connecting the cell to its environment. One of the key proteins doing this is integrin. It mediates attachment between a cell and the tissues around it, and it also plays an important role in cell signaling by which it regulates functions and properties of cells such as their migration and shape. Meanwhile, integrins are also central components in cancer metastasis, and different tumor types have been reported to have altered numbers of the ir specific integrins. Understanding of the function as well as signaling pathways of the integrins would therefore pave way to finding better treatments for a number of diseases. To understand proteins function, one has to clarify how it is activated. Here, we focus on two appealing aspects related to this matter. First, talin is known as a key protein that binds directly to integrin and is involved in its activation process. Second, experimental studies have reported that patches close to the integrin-binding site in talin appear to interact with acidic phospholipids in a cell membrane. Given the importance of talin in integrin activation and the possibly significant role of specific lipids in this process, it is exciting that the details of these lipid-protein interactions are not known. In this project, we will use atomistic molecular dynamics simulations to consider the complex comprised of integrin and the integrin-bound talin interacting with lipids in a membrane. Our main objective is to unravel how the conformation of the integrin-bound talin depends on its interactions with lipids. More concretely, does talin interact with specific lipids, and what are the most central interaction mechanisms driving conformational changes of talin? Through these considerations our aim is to better understand the cellular adhesion process overall, and in this spirit contribute for future applications for better health.

Project Name: MUSIC

Principal Investigator: Dr. Mikael Djurfeldt

Research field: Computational Neuroscience

Abstract: MUSIC (<http://software.incf.org/software/music>) is an API specification that allows for run-time exchange of data between parallel applications in a cluster environment. A pilot implementation was released 2009. MUSIC is designed specifically for interconnecting large scale neuronal network simulators, either with each-other or with other tools. In this project, we will benchmark MUSIC and test its scalability up to hundreds of thousands of cores. The primary objective of MUSIC is to support multi-simulations where each participating application itself is a parallel simulator with the capacity to produce and/or consume massive amounts of data. Applications publish named MUSIC input and output ports. A specification file lists the applications participating in a multi-simulation and also specifies how ports are connected. The current version of the API supports transfer of time-stamped events, multi-dimensional time series and text messages. The API encourages modularity in that an application does not need to have knowledge about the multi-simulation in which it participates. Large scale neuronal network models and simulations have become important tools in the study of the brain and the mind. Such models work as platforms for integrating knowledge from many sources of data. They help to elucidate how information processing occurs in the healthy brain, while perturbations to the models can provide insights into the mechanistic causes of diseases such as Parkinson's disease, drug addiction and epilepsy. A better understanding of neuronal processing may also contribute to computer science and engineering by suggesting novel algorithms and architectures for fault tolerant and energy efficient computing. Simulations of increasingly larger network models are rapidly developing. In principle, we have, already today, the computational capability to simulate significant fractions of the mammalian cortex. Neuronal network models have been formulated for a great diversity of different simulation tools. The reuse of such models is hampered by the lack of interoperability due to the multitude of languages and simulators used. Also, reimplementation of one model in other software is in practice both time consuming and error prone. Interoperability can be facilitated in several ways. One approach is to provide a model specification in some standardized format which can be understood by many simulation tools. Another approach is to allow different simulation tools to communicate data on-line. The MUSIC project was initiated by the INCF (International Neuroinformatics Coordinating Facility; <http://www.incf.org>) as a result of the 1st INCF Workshop on Large Scale Modeling of the Nervous System in order to support on-line communication between neuronal simulators and address the interoperability and reusability problems. In this PRACE project we will test the limits of MUSIC scalability and make the software ready for use in projects such as the Human Brain Project (candidate for the EU FET Flagship initiative).

Chemistry

- **Project Name:** CASiMIR

Principal Investigator: Dr. Patrick Jockel

Research area: Atmospheric Chemistry

Abstract: The project “Chemistry of the Atmosphere Simulated with an Earth System Model for the Interpretation of Satellite based Remote sensing observations (CASiMIR)” aims at an improved understanding of the physical and chemical processes, which determine the chemical state of the Earth atmosphere. Particular regions of interest are the polar upper troposphere and stratosphere. Here, the occurrence of polar stratospheric clouds (PSCs) and the heterogeneous chemistry (e.g., chlorine activation) on their particle surfaces are important processes responsible for the spring-time ozone depletion (Antarctic ozone-hole). Despite their importance, these processes are still not understood in detail. New data from satellite based remote sensing instruments promise additional insight in comparison to simulations with state-of-the-art atmospheric chemistry models, which represent the current knowledge about the underlying processes. A direct comparison of observations from satellite with results from model simulations, in particular of short-term and (in time and space) highly variable phenomena, such as PSCs, is, however, not straightforward. The ECHAM/MESSy Atmospheric Chemistry (EMAC) general circulation model has therefore been equipped with a new diagnostic capability: For instruments on sun-synchronous orbiters, the highest possible model data coverage, suitable for point-to-point comparison between satellite observations and model results, is achieved at the lowest possible output storage requirements. This new technique is applied in a series of EMAC model simulations for process studies revealing and assessing the gaps in the current understanding of the chemistry and dynamics in the polar upper troposphere and stratosphere. The simulations include sensitivity studies on the PSC forming process and a simulation with a finer model grid-resolution to optimally represent the horizontal gradients of short-lived, highly variable constituents. The results of the analyses will feed back to the further model development. The project, as detailed process study with a model of high complexity, is ambitious in terms of computational requirements and in particular in terms of data intensity, pushing the usage of resources, which are only available in a computational grid like PRACE, to the limits

Materials Science

- **Project Name:** DiSMuN (Diffusion and spectroscopical properties of multicomponent nitrides)

Principal Investigator: Prof. Igor Abrikosov

Research area: Materials science

Abstract: Hard protective coatings applied on the cutting tools are crucial for all types of metal cutting and drilling in contemporary industry. The better the coating, the more efficient is the industrial production process. Multicomponent nitrides, such as TiAlN and CrAlN, are the backbone materials used for these coatings and the fundamental understanding of their properties are crucial for a further materials development. In this project we aim at investigating the diffusion processes and spectroscopic properties of multicomponent nitrides using the most fundamental quantum mechanical equations of physics. Since the mixed systems form disordered solid solutions when grown as thin films the stochastic distribution of e. g. Ti and Al atoms in the crystals must be carefully considered which adds a huge complexity and computational challenge to our project. To investigate atomic diffusion in these materials we will use electronic structure codes to calculate the energy barriers needed to be overcome by diffusing species, both inside bulk materials and on top of crystal surfaces. The different local chemical environments in the solid solutions will be studied using a large number of parallel calculations of different paths inside, and on top of, alloy supercells. In order to accurately interpret experimental spectroscopical measurements of nanostructured multicomponent nitrides we will apply

state-of-the-art modeling scheme for these properties: the Bethe-Salpeter equation. In this methodology the intricate quantum mechanics of the spectroscopical process is modelled far more accurately than with standard density functional theory methods. Using a clever parallel procedure these difficult equations will be solved to give a solid ground in the understanding of the nanostructure of multicomponent nitrides in collaboration with experimental work.

- **Project Name: SPIESM (SPIESM : Seasonal prediction improvement with an Earth System Model)**

Principal Investigator: Prof. Francisco Doblas-Reyes

Research field: Earth Sciences and Environment

Abstract: This project contributes to the “Reducing Uncertainty in global Climate Simulations using a Seamless climate prediction system (RUCSS)” project funded by the Spanish Science and Investigation Ministry. In RUCSS we aim at testing the seamless approach (Palmer et al., 2008) for climate modelling with the EC-Earth Earth System Model (ESM) to constrain the sources of uncertainty in both short-term climate prediction and climate-change projections by increasing the understanding of the climate system. In this project, detailed analysis of climate simulations with different time horizons will be carried out using similar metrics to better understand the development of the systematic errors in EC-Earth with the hope of reducing the risk of overconfidence in both climate predictions and long-term projections. Among the processes that will be investigated are the water vapour feedback in the extratropics, the climate variability at the surface of the tropical Pacific and the extraordinary summer warming and drying observed and foreseen over Southern Europe. The basic premise of the seamless approach is that there are fundamental physical processes in common to both seasonal and decadal forecast, as well as climate-change time scales. If essentially the same ESM using a similar ensemble system can be validated both probabilistically and from a physical point of view on time scales where validation data exist, that is, on daily, seasonal and decadal time scales, then users will have the possibility of a) modifying the probabilistic estimates of regional climate-change, b) gaining insight into the ESM limitations to reduce the systematic error and c) improve the realism of the unavoidable physical parameterizations used in dynamical models. The seamless approach makes no distinctions about the relevance of particular processes in an ESM as a function of the time scale of the target problem, the correct representation of all physical processes affecting all types of climate simulations. This initiative is both innovative and ambitious. A limited number of seasonal forecasting research and operational groups already exists in Europe (EUROSIP, an operational system to which the UK Met Office, Météo-France and the European Centre for Medium-Range Weather Forecasts contribute; Stockdale et al., 2009), Canada (with the multi-model operational system run by Environment Canada; Derome et al., 2001), USA (the National Centers of Environmental Prediction, NCEP, with their Climate Forecast System; Saha et al., 2006), Australia (the Australian Bureau of Meteorology runs the POAMA system; Wang et al., 2008), and Korea (the Asia-Pacific Climate Community, APCC gathers quasioperational multi-model seasonal forecast information; Wang et al., 2008). At the same time, a great interest in climate modelling has risen in Europe and some skill in seasonal predictions of summer temperature has been found over Southern Europe, as well as for other regions where there are European interests (e.g. South America and areas of Africa).

DECI 8th Call

Astro Sciences

- **Project Name:** PLANETESIM

Principal Investigator: Dr. Anders Johansen, Lund University, Sweden

DECI granted Core hours: 6200054

Abstract: The planets of the solar system and the exoplanets – planets that orbit stars other than the sun – are a fascinating research area. Fuelled by new detection methods that find more and more planets around other stars, satellite missions to other planets, moons and asteroids in our solar system, and the ever growing power of supercomputers, planet research is in rapid development and enjoys lots of interest from the broad public. The field is closely tied with the perhaps most fundamental question of all: how common is life in the universe? – a question pursued by astronomers, geologists, biologists, physicists and chemists in concert.

Planets form in discs of gas and dust orbiting young stars as dust and ice particles collide and grow to ever larger bodies. An important stage in the planet formation process is the formation of km-scale planetesimals. Planetesimals are building blocks of both terrestrial planets like the Earth and of the solid cores of gas giant planets such as Jupiter. A fundamental problem is that cm-sized pebbles do not stick when they collide. Supercomputer simulations performed by members of our group have identified a surprising phenomenon that allows growth from pebbles to planetesimals: pebble-sized particles concentrate in dense filaments that protect them from gas drag, in a process related to why bicycle riders and migrating geese travel in groups. The densities of pebbles gets so high that gravity takes over and leads to gravitational collapse to form planetesimals.

The aim of this research project is to use high-resolution computer simulations to understand the birth sizes of planetesimals. The asteroid belt between Mars and Jupiter and the Kuiper belt beyond Neptune are examples of planetesimal belts left over from the planet formation process. The largest asteroids and Kuiper belt objects have sizes that are similar to the largest planetesimals that form in the computer simulations, but an important feature of both these populations is that the size distribution of the planetesimals show a break around 50 km in radius. This has been dubbed the missing intermediate-sized planetesimals problem.

Previously we have in our computer simulations only been able to form the largest planetesimals (with radii of 150-1500 km) from overdense filaments of pebbles. Small planetesimals form from small-scale particle overdensities and hence it requires very high-resolution simulations to model their formation. Modelling planetesimal formation at much higher resolution than previously, using PRACE supercomputers, we will investigate the size distribution of planetesimals down to 30 km in radius and compare to the observed size distributions of asteroids and Kuiper belt objects. We will also monitor the fraction of newly born planetesimals that are in binaries and compare to the binary fraction of the Kuiper belt. This will give us insight into the dominant physical processes that govern planetesimal formation and hence give constraints on how efficiently planetesimals grow to form planets.

Biosciences

- **Project Name:** CYTODYN

Principal Investigator: Tomasz Rog, Tampere University of Technology, Finland

DECI granted Core hours: 4200000

Abstract: The cytochrome (cyt) bc₁ is an electron transfer complex situated on either the inner mitochondrial membrane of eukaryotes, or the plasma membrane of bacteria. It is an important redox carrier of the multi phase electron transport chain that up keeps major part of our body's energy metabolism. The reaction mechanism of cyt bc₁ complex, also referred to as the Qcycle transfers

electrons to the cyt b subunit to generate a proton gradient across the mitochondrial membrane. During one cycle two hydrogens move into the mitochondrial matrix or negative (N) side and four protons move into the positive (P) side or the inter membrane space, or periplasmic side, in prokaryotes. Ultimately, the hydrogens pushed against the electrochemical gradient flow back to the mitochondrial matrix; the influx is coupled to generate adenosine triphosphate (ATP) molecules by ATP synthase. In spite of its importance, the detailed mechanism of the proton and electron transfer in cyt complexes has remained unknown. This is mainly due to limitations of the current experimental techniques. The main sources of knowledge about cytochrome are studies of mutants that allow one to determine the importance of each residue. However, all these studies are indirect, and the proposed views have been debated. In this study we will perform molecular dynamics simulation studies of the cyt bc₁ complex in explicit lipid bilayer, at physiological salt concentration. The main task of this study will be to calculate the free energy of substrate binding, and to elucidate substrate bonding modes.

• Project Name: Photoreception

Principal Investigator: Lars H. Andersen, Anastasia Bochenkova, Aarhus University, Denmark

DECI granted Core hours: 10500000

Abstract: The project is aimed at studying photoactive proteins at the atomic level. Photoactive proteins are widespread in nature and enable the signal transduction in biological photoreceptors triggered by the absorption of a photon with a particular wavelength. Opsin proteins containing a protonated Schiff-base retinal chromophore are perhaps the best known as they provide vision in vertebrates. We propose to use the PRACE infrastructure for the computationally demanding modeling of photophysical and photochemical properties of chromophores of these proteins at different levels: isolated chromophore units, then the well-defined atomic-scale interactions within the hosting protein medium, and finally, whole proteins. One of the highlight goals is to understand the catalytic role played by proteins in the ultrafast excited-state reaction dynamics of biological photoreceptors and in the self-regulation of their photo-physical properties. Ultimately, this will lead to an understanding of both wavelength tuning and efficiency of the primary steps in vision. State-of-the-art electronic structure methods and their large-scale parallel implementations within our original Firefly package, being one of the fastest and the most efficient quantum chemistry packages available today, will be used to track the excited-state evolution of photoactive proteins and their de-excitation pathways through intersection regions of electronic states. Our new extended approach to multistate multiconfiguration quasi-degenerate perturbation theory XMCQDPT2 approved in a number of applications surpasses known methods both methodologically and computationally. The invariance of the new theory makes it unique on the world scale and especially attractive for the purposes of our project. The results of this project will include highly accurate predictions of photoabsorption and emission line shapes of the bare chromophores and photoactive proteins, structures of the minimum energy conical intersections and topographies around them, quantum yields of primary photoinduced reactions and excited-state lifetimes. Importantly, the project proposed is a joint theoretical and experimental endeavor. As a new initiative on the world-scale, we aim at studying the ultrafast excited-state dynamics in biological systems in vacuum. The fs pump-probe experiments will be carried out to determine, for the first time, the intrinsic response time of the isolated retinal in the protonated Schiff-base form. The project will provide new standards for light-induced protein dynamics and will provide new insight in the molecular basis of vision. It will rely on modern laser-technology and ion-storage techniques which are available in the research group at Aarhus University. Our strategy is to combine expertise of the theoretical team in the field of the state-of-the-art quantum methods with the leadership of Aarhus University when it comes to laser-action spectroscopy techniques for studying the biomolecular ions in the gas phase. We firmly believe that our new joint initiative will open an avenue for the future ground-breaking research in a very broad and highly interdisciplinary field of science, which combines physics, chemistry and biology.

Earth Sciences

Project Name: PARAMETER

Principal Investigator: Heikki Järvinen, Finnish Meteorological Institute, Finland

DECI granted Core hours: 4200000

Abstract: Modern society is profoundly reliant on numerical simulation models. More powerful computers and better understanding of underlying science has led to increasingly complex simulation tools. It is of utmost importance that the simulation results that are used as a basis for decision making are accompanied by uncertainty estimates, or probabilities of the outcomes. Thus users can decide on the level of risk they are prepared to take, depending on their vulnerabilities, and take appropriate action.

Practically all discrete numerical simulation models contain closure schemes where some unresolved quantities are expressed via specified parameters rather than being explicitly modelled. The PARAMETER project aims at applying advanced parameter estimation techniques (i) to quantify the modelling uncertainty related to these model parameters, and (ii) to tune the predictive skill of the models by means of algorithmic model parameter estimation. Specifically, the PARAMETER project will focus on tuning the predictive skill of numerical weather prediction models, based on the methods published recently by the research team.

The scientific research behind the methods to be applied in the DECI project PARAMETER is funded by the NOVAC project of the Computational Science Research Programme of the Academy of Finland, the Nessling foundation, the EU/FP7 project EMBRACE (www.embrace-project.eu), and the Academy of Finland Centre of Excellence in Inverse Problems.

Engineering

• **Project Name:** PIPETURB

Principal Investigator: Dr. Philipp Schlatter, KTH – Royal Institute of Technology, Sweden

DECI granted Core hours: 6250000

Abstract: The flow of fluids in pipes with circular cross-sections is frequently encountered in a variety of environmental, technical and even biological applications. Typical examples of pipe flows can be found in urban drainage systems, transport of natural gas or oil in the energy sector, or the flow of blood in veins and arteries. Accordingly, the understanding of flow physics in pipes has a direct and substantial impact on everyday life and an adequate knowledge of such flow problem will help in finding scientific methods to reduce drag and the like. The Navier-Stokes equations govern the dynamics of turbulent flows. This set of equations, when properly non-dimensionalized, includes the Reynolds numbers (Re) as the main characterization. Re is by far the most important non-dimensional number in fluid mechanics, and can be considered as a measure for the “speed” of the flow inside the pipe. Turbulence is a characteristic state of flows with sufficiently high speeds, or high Reynolds numbers. Most fluid flows observed in nature are indeed turbulent. Of particular importance in flows delimited by solid walls is the near-wall region in which a large fraction of the drag stems from velocity fluctuations in a thin boundary layer adjacent to surfaces. Near-wall turbulence structures in wall-bounded shear flows primarily scale in terms of the so-called viscous length scale, which might be very small as Re is increased. However, according to recent experimental studies, very large-scale motions with lengths of $5R$ up to $20R$ are found in fully developed turbulent pipe flow (R being the radius). These structures, being strongest in the outer region, even extend throughout the layer and even leave their footprint quite close to the wall. These large-scale structures are very energetic and active. Large-scale motions thus play an important role in the dynamics of turbulent pipe flows. The aim is to study fully developed high-Reynolds number turbulent pipe flow through direct numerical simulations (DNS). DNS attempts to resolve all relevant scales of the turbulent flow. These will be carried out using the massively parallel

DNS code available at KTH Mechanics, nek5000, which is based on an accurate and efficient spectral-element discretization. Pipe flow is the case which is easiest realisable in experiments. However, due to numerical difficulties related to the cylindrical coordinates and the corresponding numerical singularity arising along the symmetry line, it is the only canonical flow case that has not yet been thoroughly studied using DNS, as opposed to plane channels and boundary layers. The proposed work will be a complement to both the ongoing simulations of high-Reynolds number turbulent boundary layers and channels, but also relevant in conjunction with the forthcoming experimental studies of high-Reynolds number turbulent pipe flow within the CICLoPE project (CICLoPE consists of a 120 m long pipe with diameter 0.9m, situated near Bologna/Italy). To obtain a database for turbulent pipe flow that is well validated with both experiments and other simulations is very timely. Therefore, we intend to use this present DECI project to complement our simulations at lower Reynolds numbers with dataset pertaining to higher Re. Specifically, we would like to be able to present data in the range of $Re_T=180$ to 1000, all obtained in a long pipe employing the same high resolution. Such data will be valuable not only to increase our knowledge of generic wall turbulence, but will also allow for the development of better models of turbulence for industrial applications.

Materials Science

• Project Name: CANONS

Principal Investigator: Dr. Pär Olsson, KTH Royal Institute of Technology, Sweden

DECI granted Core hours: 3125000

Abstract: For future generation nuclear power plants, fission or fusion based, the need for improved fuels and structural materials is crucial. The use of nuclear power is associated with several major problems: the handling of the long-lived radioactive waste, the limited resources of U-235 and the safety and integrity of the structural materials. These issues are addressed by the development of advanced reactor types, GenIV reactors, in which Am and Pu are transmuted, thereby decreasing the effective half-life of the waste, and at the same time fissile fuel is generated from natural uranium (U-238). This is achieved by the use of non-moderated (fast) neutrons in the fission process, and so-called fast reactors have been used on an experimental scale for decades. A fundamental challenge connected to the use of fast neutrons is the damage induced in various parts of the reactor. Well known effects are hardening, embrittlement and swelling of the fuel and of internal parts such as cladding, spacers, tubes, and of the reactor vessel. Much effort has been put into experimental studies and modeling of radiation damage since its discovery about 50 years ago. The atomistic mechanisms behind hardening and swelling in metals and alloys are today well understood, although predictive modeling is difficult to achieve because of the complexity of these processes. In contrast, the fundamental mechanisms of radiation damage in typical fuel matrices, like uranium-oxide or, more importantly, in innovative fuels like metal-nitride matrices, are not well understood. In the current project, we will use first-principles electronic structure calculations to study the structural and thermal properties of radiation induced defects in ceramic fuels, and their interaction with transmutation gas atoms like He and Xe. We will also use first principles molecular dynamics to study the fundamental mechanisms of defect formation in ceramic crystals. Clearly, the investigation of how intense neutron radiation affects these fuels must be based on experiments. However, theoretical modeling, e.g., atomistic simulations may provide a firmer footing for the interpretation of such experiments, and in that sense plays, and will play, a very important role in the development of future advanced fuels. We are involved in two EU projects, in which experiments and modeling are essential parts.

For the modelling of the structural materials, special focus will be devoted to modelling the behaviour under irradiation of Oxide Dispersion Strengthened (ODS) steels. This new class of nano-structured materials has shown good resistance to radiation effects. However, these novel materials have not, and cannot, be tested in real life for timescales corresponding to the lifetime of a reactor. Therefore, we here propose to model the ageing and degradation of the mechanical properties of the ODS steels and other nano-structured materials. The modelling will be based on existing experimental data and on

first principles quantum mechanical calculations, feeding these data into higher scale models, such as kinetic Monte-Carlo, where the long-term evolution of the alloy microstructure can be simulated. The most compute intensive part of this project consists of the first principles calculations. The ODS and nano-structured materials have been shown in many studies to have a very good response to neutron irradiation. Especially the irradiation induced swelling and creep are minimal. However, these studies have all been performed for short time spans where the nano-clusters have no time to disintegrate and diffuse into the matrix or to grain boundaries or other sinks. Therefore, it is of critical importance to evaluate what will happen over longer times. The stability, under irradiation, of these nano-clusters can be assessed using a multi-scale modelling approach.

The largest computational load of these two efforts will be to perform first principles calculations using the VASP code, which has been optimized on numerous architectures, including Cray XE6. For future generation nuclear power plants, fission or fusion based, the need for improved fuels and structural materials is crucial. The use of nuclear power is associated with several major problems: the handling of the long-lived radioactive waste, the limited resources of U-235 and the safety and integrity of the structural materials. These issues are addressed by the development of advanced reactor types, GenIV reactors, in which Am and Pu are transmuted, thereby decreasing the effective half-life of the waste, and at the same time fissile fuel is generated from natural uranium (U-238). This is achieved by the use of non-moderated (fast) neutrons in the fission process, and so called fast reactors have been used on an experimental scale for decades. A fundamental challenge connected to the use of fast neutrons is the damage induced in various parts of the reactor. Well known effects are hardening, embrittlement and swelling of the fuel and of internal parts such as cladding, spacers, tubes, and of the reactor vessel. Much effort has been put into experimental studies and modeling of radiation damage since its discovery about 50 years ago. The atomistic mechanisms behind hardening and swelling in metals and alloys are today well understood, although predictive modeling is difficult to achieve because of the complexity of these processes. In contrast, the fundamental mechanisms of radiation damage in typical fuel matrices, like uranium-oxide or, more importantly, in innovative fuels like metal-nitride matrices, are not well understood. In the current project, we will use first-principles electronic structure calculations to study the structural and thermal properties of radiation induced defects in ceramic fuels, and their interaction with transmutation gas atoms like He and Xe. We will also use first principles molecular dynamics to study the fundamental mechanisms of defect formation in ceramic crystals. Clearly, the investigation of how intense neutron radiation affects these fuels must be based on experiments. However, theoretical modeling, e.g., atomistic simulations may provide a firmer footing for the interpretation of such experiments, and in that sense plays, and will play, a very important role in the development of future advanced fuels. We are involved in two EU projects, in which experiments and modeling are essential parts.

For the modelling of the structural materials, special focus will be devoted to modelling the behaviour under irradiation of Oxide Dispersion Strengthened (ODS) steels. This new class of nano-structured materials has shown good resistance to radiation effects. However, these novel materials have not, and cannot, be tested in real life for timescales corresponding to the lifetime of a reactor. Therefore, we here propose to model the ageing and degradation of the mechanical properties of the ODS steels and other nano-structured materials. The modelling will be based on existing experimental data and on first principles quantum mechanical calculations, feeding these data into higher scale models, such as kinetic Monte-Carlo, where the long-term evolution of the alloy microstructure can be simulated. The most compute intensive part of this project consists of the first principles calculations. The ODS and nano-structured materials have been shown in many studies to have a very good response to neutron irradiation. Especially the irradiation induced swelling and creep are minimal. However, these studies have all been performed for short time spans where the nano-clusters have no time to disintegrate and diffuse into the matrix or to grain boundaries or other sinks. Therefore, it is of critical importance to evaluate what will happen over longer times. The stability, under irradiation, of these nano-clusters can be assessed using a multi-scale modelling approach.

The largest computational load of these two efforts will be to perform first principles calculations using the VASP code, which has been optimized on numerous architectures, including Cray XE6.

- **Project Name: MBIOMARK**

Principal Investigator: Dr. Zilvinas Rinkevicius, KTH Royal Institute of Technology, Sweden

DECI granted Core hours: 1875000

Abstract: Alzheimer's disease is one of the most prominent cause of the acquired dementia in elderly patients and it affects around 35.6 million people worldwide. In Sweden among the 160 thousands with dementia around 45% have been diagnosed with Alzheimer's disease. The Alzheimer's disease have the profound impact on the patients and their families and the overall impact of this disease on the whole society is expected to increase in the future with the population aging in Europe. Early diagnostics of the Alzheimer's disease is essential for efficient treatment of this disease and efficient screening of the people within risk groups. Unfortunately, currently options for clinical diagnostics of early stages of the Alzheimer's disease is very limited and development of novel clinical imaging techniques are highly desirable. Present research project aims to address this problem and focuses on the development of the electron paramagnetic resonance imaging technique, which is promising methodology for in vivo imaging of early damage to brain tissue cause by Alzheimer's disease. Within this project we aim to develop novel fluorescent spin labels, which are employed as the contrast agents in the electron paramagnetic resonance imaging, using the state of the art molecular modeling tools.

Appendix E

PRACE Tier-1 DECI 9-12 Awards

The information in these tables was extracted from the PRACE-3IP PRACE Third Implementation Phase Project D7.2.1 Final Report on Applications Enabling, dated 23.06.2014. Additional descriptive information on the projects was extracted from:

- PRACE Third Implementation Phase Project, D2.6, Report on the DECI Call, dated 24.3.2014
- Final PRACE-2IP PRACE Second Implementation Phase Project D7.2.2 Final Report on Technical Support for DECI Projects, dated 22.08.2013,
- The SNIC website on successful PRACE applications, <http://www.snic.vr.se/apply-for-resources/prace-succesful-swedish-applications>
- The Notur projects website, <https://www.notur.no/projects/2014.1>
- PRACE-2IP, PRACE Second Implementation Phase Project, D2.3, Second Annual Report of WP2, Final, dated 22.8.13
- Overview of all HLRB-Projects: <http://www.lrz.de/projekte/hlrb-projects/list.html>

DECI-9 Project List

• Project Acronym: NMRCONF

Home site: CSC

Allocation: 2,080,000 CSCS Research area: Biology, Bioinformatics, and Biophysics

NMRCONF - This project uses Gromacs-PLUMED simulations and NMR spectroscopy to describe conformational changes in proteins.

• Project Acronym: CompSym

CSC home site

Allocation: 5,600,000 CSCS

CompSym - This project uses the Gromacs simulation software to study interaction of drug delivery liposomes with opsonin proteins

• Project Acronym: Planck-LFI2

Research area: Astrophysics, Cosmology

Allocation: 7,000,000 CSC

Planck-LFI2 - Planck is a mission of the European Space Agency (ESA) to map the anisotropies of the cosmic microwave background with the highest accuracy ever achieved. Computational resources for this work were provided through this DECI project.

Table 16 DECI-9 Nordic Projects

PRACE Site (home)	Project name	PRACE Site (exec)	Machine(s)
CSC	NMRCONF	CSCS	Rosa (XT5 CSCS)
	CompSym	CSCS	Rosa (XT5 CSCS)
	Planck-LFI2	CSC	Sisu (Sandy Bridge@2.6) Louhi XT (XT5 DC@2.3)
PDC	CoStAFuM	RZG	Hydra (Sandy Bridge@2.6)
	DifVib	EPCC	ICE-Advance (BGQ)
		PDC	Lindgren (XE6 12C@2.1)
	HydFoEn	UHEM	Karadeniz (Intel Nehalem@2.93)

• Project Title: CoStAFuM
(Computational Studies of Advanced Functional Materials)

Principal Investigator: Prof. Olle Eriksson, Uppsala University

Research area: Materials Science

Allocation: 9 687 608 standard DECI hours (NTNU, Norway; RZG, Germany)

CoStAFuM - Computational Studies of Advanced Functional Materials (CoStAFuM) deals with state-of-the-art computational materials science methods applied to advanced functional materials. The project aims to study the (i) correlated electron system, (ii) graphene and molecular-interface systems, (iii) lattice dynamics and (iv) core shell structures and nanoparticles.

These topics will be studied by ab initio density functional theory based methods implemented in codes like VASP and SIESTA.

• Project Title: DifVib (Diffusion in multicomponent nitrides and vibrational thermodynamics from first-principles)

Principal Investigator: Prof. Igor Abrikosov, Linköping University

Research area: Materials Science

Allocation: 6 250 000 standard DECI hours (SNIC/PDC, Sweden; EPCC, UK)

DifVib: For some applications, in-house codes such as SCAILD for lattice dynamics and Rspt for dynamical mean field theory will be used. Transition metal nitrides (TMN), such as TiN and ZrN, are important technological materials owing to their outstanding mechanical, electrical, and corrosive-resistant properties, in combination with applicability in industrial-scale thin film deposition systems. In continuation of the DECI-7 project DiSMuN this project conducts again pioneering theoretical work on the diffusion of adatoms on different crystal surfaces of TiAlN and aims to study aspects of diffusion in nitrides, focusing on TiAlN, ZrAlN and HfAlN. To investigate atomic diffusion in these materials electronic structure codes are used to calculate the energy barriers needed to be overcome by diffusing species, both inside bulk materials and on top of crystal surfaces.

In a second part of the project related to Earth's core structure the project targets completely disordered alloy phases of Fe-Ni and Fe-Ni-Si using special quasirandom structure method in first-principles simulation. This method is based on a new technique developed to study vibrational thermodynamics from first-principles at high pressure and high temperatures.

Although the technique is developed from the theoretical point of view, the code of realization is yet to be finished and the enabling help of PRACE experts is needed in order to obtain greater scalability in parallelization of the applied codes.

• **Project Title:** HydFoEn
(Hydrogen storage materials for energy applications) Cancelled

Principal Investigator: Prof. Rajeev Ahuja, Uppsala University

Research area: Materials Science

Allocation: 2 501 125 standard DECI hours (UHEM, Turkey)

HydFoEn - Our energy-hungry world has become increasingly depending on new methods to store and convert energy for new, environmentally friendly modes of transportation and electrical energy generation as well as for portable electronics. Hydrogen would be ideal as a synthetic fuel for transport vehicles because it is lightweight, highly abundant and its oxidation product (water) is environmentally benign. However, the storage of hydrogen remains a problem and hinders the highly desirable development in this direction.

The project on hydrogen storage materials for energy applications deals with studying the interaction of hydrogen with novel materials having multiple length scales such as clusters, nano-particles, nano-tubes, multi-layers, and crystalline bulk. The materials include light metal hydrides such as alkali-alanates and boro-hydrides and Metal organic frameworks. Due to the lightweight of these materials, the gravimetric density of hydrogen is higher than that in the inter-metallic hydrides. Although these materials are regarded as potential candidates for a new generation of hydrogen storage materials and are critical to a new hydrogen economy, very little fundamental understanding is available about the nature and strength of hydrogen bonding, the influence of catalysts on the uptake and release of hydrogen and the effect of nanostructuring on the thermodynamics of hydrogen.

This project aims at providing this fundamental understanding by carrying out first principles calculations based on density functional theory.

DECI-10 Project List

Table 17 DECI-10 Nordic Projects

PRACE Site (home)	Project name	PRACE Site (exec)	Machine(s)
CSC	CONVDYN13	RZG	Hydra (Sandy Bridge@2.6)
	HIV1-GSL	EPCC	HeCToR XE6 (XE6 16C@2.3) Archer (Sandy Bridge@2.6)
	HyVaMPI	UIO	Abel (Sandy Bridge@2.6)
	NANODROPS	EPCC	HeCToR XE6 (XE6 16C@2.3) Archer (Sandy Bridge@2.6)
PDC	DNSTF	EPCC	HeCToR XE6 (XE6 16C@2.3) Archer (Sandy Bridge@2.6)
	LipoSim	PDC	Lindgren (XE6 12C@2.1)
	MEGAREACT	UIO	Abel (Sandy Bridge@2.6)
	PLANETESIM-2	FZJ	JuRoPA (Intel Nehalem@2.93)

- **Project Acronym:** CONVDYN13

Home site: CSC

Research area:

Allocation: 5,419,008, RZG

CONVDYN13 - This project uses the Pencil software to study convection driven dynamos in rapidly rotating late-type stars. An example of such a star is the Sun during its first billion years.

- **Project Acronym:** HIV1-GSL

Principal Investigator:

Research area:

Allocation: 7,000,000, EPCC

HIV1-GSL - This project uses the Gromacs software to study functional roles of glycosphingolipids in modulating entry of human immunodeficiency virus type 1 (HIV-1) into host cell. In addition to the role of glycosphingolipids as facilitators of HIV infection, some of them can act as a natural resistance factor for HIV prevention.

- **Project Acronym:** HyVaMPI

Principal Investigator:

Research area:

Allocation: 3,500,000, UIO

HyVaMPI - This project uses a novel plasma code, Vlasiator, to study plasma dynamics in the Earth's space environment. The aim is too facilitate the future numerical forecast of space weather, which affect spacecraft and space-based technological solutions for positioning and communications.

- **Project Acronym:** NANODROPS

Principal Investigator:

Research area:

Allocation: 10,141,200, EPCC

NANODROPS - This project uses molecular dynamics (Gromacs software) and dissipative particle dynamics (own DPD code) to study the interaction of triglycerides and nanoparticles with lipid biomembranes.

- **Project Title: DNSTF**
(Direct numerical simulation of finite size fibres in turbulent flow)

Principal Investigator: Prof. Gustav Amberg, KTH - Royal Institute of Technology

Research area: Mechanical Engineering, Fluid Mechanics

Allocation: 8 437 500 standard DECI hours (EPCC, UK)

DNSTF - The goal of this project is to adapt a numerical model of the dynamical behaviour of finite size fibres in high Reynolds number, turbulent flow. The chosen approach is to start from direct numerical simulations for both turbulent flow and to resolve the flow around individual fibres. The turbulent flow is modelled by an entropy lattice Boltzmann method and the interaction between fibres and carrier fluid is modelled through an external boundary force method (EBF). Direct contact and lubrication force models for fibre-fibre interactions and fibre-wall interaction are taken into account to allow for a full four-way interaction. This model will allow to study the influence of wall effects and interaction effects on turbulent flow.

- **Project Title: LipoSim (Large scale simulations of liposomes as drug carriers)**

Principal Investigator: Prof. Leif A. Eriksson, University of Gothenburg

Research area: Materials Science (Drug Design)

Allocation: 8 750 000 standard DECI hours (PDC, Sweden)

LipoSim - This project employs massively parallel computations in order to simulate drug delivery from a drug-loaded liposomes into a cellular plasma membrane. The use of PRACE facilities enables us to understand at a detailed atomic level, how different lipid mixtures, drug concentrations and sizes of the liposome or micelle based carriers influence the ability of these to actually bring the drug molecules to their intended targets. We focus in this landmark study on different compounds aimed for cancer therapy, with the aim to thereby have established a system to be used in the study of a wide range of other compounds in the future, in order to better optimize conditions for their usage in connection with lipid vesicles for drug delivery. Deeper insight into these processes will also allow researchers to design new molecules that better dissolve into and transfer between liposome and cell, or that are able to diffuse out of the liposome as response to small variations in the local environment.

- **Project Title: MEGAREACT (Metal catalysed gasification reactions)**

Principal Investigator: Prof. Kim Bolton, University of Borås

Research area: Materials Science

Allocation: 750 000 standard DECI hours (UiO, Norway)

MEGAREACT - Gasification, the conversion of carbonaceous material to a gaseous product with an employable heating value, is one of the most important and effective production methods of energy carriers employed toward sustainable development. Making use of quantum mechanics simulation tools, mechanisms of reactions during the metal catalysed gasification process are investigated. In particular, this project aims to obtain reactant and transition state energies and frequencies that are used to obtain the reaction barriers and Arrhenius pre-exponentials of the elementary reactions on a transition metal catalyst surface. These data will subsequently be used in kinetic modelling of the entire reaction. The first reaction that will be studied is the water gas shift (WGS) reaction, which is important in almost all gasification reactions.

- **Project Title:** PLANETESIM-2 (Towards an initial mass function of planetesimals)

Principal Investigator: Dr. Anders Johansen, Lund University

Research area: Astro Science

Allocation: 7 500 000 standard DECI hours (GCS/FZJ, Germany)

PLANET-SIM2 - The aim of this research project is to use high-resolution computer simulations to understand the birth sizes of planetesimals. The asteroid belt between Mars and Jupiter and the Kuiper belt beyond Neptune are examples of planetesimal belts left over from the planet formation process. The largest asteroids and Kuiper belt objects have sizes that are similar to the largest planetesimals that form in the computer simulations, but an important feature of both these populations is that the size distribution of the planetesimals show a break around 50 km in radius. This has been dubbed the missing intermediate-sized planetesimals problem.

This project is a follow-up to the corresponding DECI-8 project and will push the resolution up to 512^3 which will allow us to determine the initial mass function of planetesimals down to 30 km in radius and thus to compare critically to the observed properties of the Kuiper belt and the asteroid belt.

DECI-11 Project List

Table 18 DECI-11 Nordic Projects

PRACE Site (home)	Project name	PRACE Site (exec)	Machine(s)
CSC	DyNet	PSNC	Chimera (Intel Westmere EX@2.67)
	EERSC	RZG	Hydra (Sandy Bridge@2.6)
	gklocsoc	PDC	Lindgren (XE6 12C@2.1)
	Planck-LFI3	CSC	Sisu (Sandy Bridge@2.6)
	Syndecan	EPCC	Archer (Sandy Bridge@2.6)
PDC	FLOCS	EPCC	Archer (Sandy Bridge@2.6)
	GSTP	FZJ	JuRoPA (Intel Nehalem@2.93)
UIO	N-MILIB	UIO	Abel (Sandy Bridge@2.6)
	WeSearch	UIO	o (no results)

• Project Title: Network analysis of protein dynamics

Home Site: CSC

Research area: Biology, Bioinformatics, and Biophysics

Allocation: DyNet -

• Project Title: EERSC

Home Site: CSC

Research area: Astrophysics, Cosmology

PI has been a collaborator on a successful Tier-o awards

• Project Title: Syndecan

Home Site: CSC

Research area: Biology, Bioinformatics, and Biophysics

• Project Title: Gklocsoc

Home Site: - CSC

Research area: Engineering and Energy

• Project Title: FLOCS - Fully Localised Edge States in Boundary Layers

Principal Investigator: Dr. Philipp Schlatter, KTH - Royal Institute of Technology

Research area: Mechanical Engineering

Allocation: 12 500 000 standard DECI hours on Archer (EPCC, UK)

PI has been a collaborator on a successful PRACE Tier-o award.

- **Project Title:** GSTP - Global Gyrokinetic simulation of tokamak plasmas

Principal Investigator: Prof. Hans Nordman, Chalmers University of Technology

Research area: Plasma and Particle physics

Allocation: 5 000 000 standard DECI hours on JuRoPA (GCS/FZJ, Germany)

- **Project Title:** 11 N-MILiB

Principal Investigator: Helmer Fjellvåg, KI, UiO, Oslo

The main objective of the present research plan is to benefit from computational resources in order to identify and characterize new and promising materials for important future technologies with the help of state-of-the-art density-functional calculations - and thereby gain insight in inherent structure-property relationships. In this way, theory and modeling will act as major tool for feedback and enhanced interaction between prediction, synthesis, and understanding of physical properties of materials. The charge-discharge characteristics of the negative electrode can be widely altered depending on the kind and composition of alloys used. Extensive experimental research and development work has been conducted to improve the electrode materials where theoretical approach will be helpful to save money and needless experiment. Therefore we will search new compounds for electrode materials. Nanoscale modeling will be used to find critical particle size where the Li-transport might be different from that of bulk materials. In addition to that we are planning to investigate how the energetics is changing upon Li-ion migration in electrodes as well as electrolytes.

- **Project Title:** WeSearch

Principal Investigator: Stephan Oepen, UiO, Oslo

Language Technology (LT) is an interdisciplinary sub-field between computer science and linguistics that aims to enable computers to 'make sense' of human language, for example to extract structured information from unstructured text, to determine the sentiment of a product review, to translate from one language into another, or to organize and retrieve Internet content on the basis of abstract meaning, rather than just keywords. Several language technology tools have matured to a point that facilitates the in-depth analysis of relatively large amounts of running text. The Deep Linguistic Processing with HPSG Initiative (DELPH-IN; <http://www.delph-in.net>) is a multi-continent collaborative network maintaining an open-source repository of analysis tools for a variety of languages. The Language Technology Group (LTG) at the University of Oslo (UiO) has pioneered the adaptation and scaling up of DELPH-IN technologies for HPC utilization and through this work maintains a semantically analyzed version of the full English Wikipedia (about 900 million tokens in some 55 million sentences), i.e. the result of applying the DELPH-IN semantic parsing stack to the unstructured text of Wikipedia, to obtain structured, logical-form representations of meaning that facilitate a range of downstream applications. This community resource is an enabling technology for follow-up research, for example in the discovery of linguistic examples and in large-scale machine learning approaches to the syntactic and semantic structure of language. The proposed project will contribute to keep the Wikipedia semantic network up-to-date, as well as allow the application of semantic parsing to substantially larger text collections, so-called User-Generated Content (UGC).

DECI-12 Project List

Table 19 DECI-12 Nordic Projects

PRACE Site (home)	Project name	PRACE Site (exec)	Machine(s)
CSC	ALLOTRANS	EPCC	Archer (Sandy Bridge@2.6)
	complexIdyn	PDC	Lindgren (XE6 12C@2.1)
	PlanckLFI4	CSC	Sisu (Sandy Bridge@2.6)
PDC	DNSTF2	CSC	Sisu (Sandy Bridge@2.6)
	EXODUS	CASTORC	Cy-Tera (Cy-Tera)
		CYFRONET	Zeus BigMem (AMD 6276@2.3)
	FENICS	PDC	Lindgren (XE6 12C@2.1)
	MicroMagNum	ICHEC	Fionn-thin (Fionn- thin)
	ParaWEM	EPCC	Archer (Sandy Bridge@2.6)
		PDC	Lindgren (XE6 12C@2.1)
	VFEH	EPCC	Archer (Sandy Bridge@2.6)

• **Project title:** ALLOTRANS

Principal Investigator:

Research area: Biology, Bioinformatics, and Biophysics

Allocation:

• **Project Title:** PlanckLFI4

Principal Investigator: Hannu Kurki-Suonio

Research area: Astrophysics, Cosmology,

Allocation: PlanckLFI4 – see also the DECI-9 award.

• **Project Title:** FENICS

Principal Investigator: Prof. Johan Hoffman, KTH - Royal Institute of Technology and Vattenfall

Research area: Mechanical Engineering

Allocation: 1 250 000 standard DECI hours (PDC, Sweden)

• **Project Title:** DNSTF2

Principal Investigator: Prof. Gustav Amberg, KTH - Royal Institute of Technology

Research area: Mechanical Engineering, Fluid Dynamics

Allocation: 6 250 000 standard DECI hours (CSC, Finland)

- **Project Title:** ParaWEM

Principal Investigator: Prof. Gunilla Efraimsson, KTH - Royal Institute of Technology

Research area: Aerodynamics

Allocation: 3 750 000 standard DECI hours (EPCC, UK)

- **Project Title:** VFEH

Principal Investigator: Prof. Deliang Chen, University of Gothenburg

Research area: Earth Science

Allocation: 500 000 standard DECI hours (EPCC, UK)

- **Project Title:** EXODUS

Principal Investigator: Dr. Biplab Sanyal, Uppsala University

Research area: Materials Science

Allocation: 3 750 000 standard DECI hours (Cyfronet, Poland; Castorc, Cyprus)

Appendix F

PRACE DECI-9 to DECI-12 Proposals by Country

This information is primarily from the following two sources.

- PRACE-2IP, PRACE Second Implementation Phase Project, D2.3, Second Annual Report of WP2, Final, dated 22.8.13.
- PRACE Third Implementation Phase Project, D2.6, Report on the DECI Call, dated 24.3.2014.

The tables list the numbers of proposals submitted and projects awarded for each call for the DECI projects for DECI-9 through DECI-12. Full information on DECI-12 is not available.

DECI-9 Projects by country of origin			DECI-10 Projects by country of origin		
Country of PI	Proposals	Projects	Country of PI	Proposals	Projects
Argentina	1	1	Austria	1	0
Bulgaria	1	1	Belgium	5	1
Czech Republic	2	2	Czech Republic	1	1
Denmark	1	1	Denmark	1	1
Finland	2	2	Finland	4	3
France	5	4	France	1	0
Germany	6	4	Germany	8	5
Greece	2	1	Greece	7	0
India	0	0	Ireland	3	3
Ireland	3	3	Italy	12	2
Italy	3	3	Poland	1	1
Japan	0	0	Portugal	3	2
Norway	0	0	Spain	11	2
Portugal	2	1	Sweden	7	5
Slovak Republic	0	0	Switzerland	1	0
Spain	5	2	Netherlands	3	2
Sweden	5	3	Turkey	2	2
Switzerland	3	1	UK	14	7
Netherlands	0	0	Totals	85	37
Turkey	2	1			
UK	2	1			
USA	0	0			
Total	45	31			

DECI-11 Proposals submitted		
Country of PI	Number of PIs	Projects
Austria	4	
Belgium	5	
Croatia	1	
Czech Republic	3	
Denmark	4	2
Finland	3	3
France	5	
Germany	15	
Greece	6	
Hungary	2	
Iran	2	
Ireland	3	
Israel	3	
Italy	7	
Netherlands	2	
Norway	2	2
Poland	5	
Portugal	1	
Serbia	1	
Spain	10	
Sweden	2	2
Switzerland	3	
Turkey	4	
UK	24	
Total	117	52

DECI-12 Proposals submitted		
Country of PI	Number of PIs	Projects
Belgium	2	
Germany	1	
Denmark	2	1
Estonia	1	
Spain	2	
Finland	4	3
UK	16	
Greece	5	
Italy	16	
Netherlands	4	
Portugal	1	
Sweden	5	5
Turkey	2	
Total	61	

Appendix G

PRACE Tier-1 Resources

This resources table has been extracted from the PRACE resources website, <http://www.prace-ri.eu/tier-1-resources/>, last updated on Thursday 4 October 2012. It illustrates the range of systems available to researchers through DECI.

DECI site	Machine name	System type	chip	Clock speed (GHz)	no. nodes	no. cores	peak perfor- mance (Tflops)	Total memory (TB)	Memory per node (GB)	GPU cards
Bulgaria (NCSA)	EA"ECNIS"	IBM BG/P	PowerPC 450	0.85	2096	8192	27	4	2	
Czech Repulic (VSB-TUO)	Anselm	Bull Bullx B510 and B515 Cluster	Intel Sandy Bridge-EP, Inter-connect: Infini-band QDR / Fat Tree	2.4 (180 nodes) and 2.3 (27 nodes)	207	3312	66	13.2		23 nVIDIA Tesla M2090, 4 Intel Xeon Phi P5110
Finland (CSC)	Sisu	Cray XC30	Intel Sandy Bridge	2.6	736	11776	244.9	23.552	32	
France (CINES)	Jade	SGI ICE EX8200	Intel Quad-Core E5472/ X5560	3/2.8	1,536/ 1,344	12,228/ 10,752	267.88	90	30/32	
France (IDRIS)	Babel	IBM BG/P	PowerPC 450	0.85	10240	40960	139	20	2	
Germany (Jülich Super-computing Centre)	JuRoPA	Intel cluster	Intel Xeon X5570	2.93	2208	17664	207	51.75	24	
Germany (RZG)	Genius	IMB BG/P	PowerPC 450	0.85	4096	16384	54	8	2	
Germany (RZG)		Intel iData-Plex Linux Cluster	Intel Sandy Bridge	2.6	610	9760	200	40	64	
Ireland (Irish Centre for High-End Computing (ICHEC))	Fionn	SGI ICE X cluster	Intel Xeon E5-2695 v2, 12 core	2.4	320	7680	147.5	30	64	32 Nvidia K20 + 32 Intel Xeon Phi 5110
Italy (CINECA)	PLX	Intel iData-Plex Linux Cluster	Intel West- mere	2.4	274	3288	293	13	48	548 nVIDIA Tesla M2070/ M2070Q
Norway (SIGMA)	Abel	MegWare cluster	Intel Sandy Bridge	2.6	632	10112	260			

DECI site	Machine name	System type	chip	Clock speed (GHz)	no. nodes	no. cores	peak perfor- mance (Tflops)	Total memory (TB)	Memory per node (GB)	GPU cards
Poland (WCSS)	Supernova	cluster	Intel Westmere-EP	2.67	404	4848	51.58	9.5	24	
Poland (PSNC)	chimera	SGI UV1000	Intel Xeon E7-8837	2.66	1	2048	21.8	16	16000	
Poland (PSNC)	cane	cluster AMD&GPU	AMD Opteron™ 6234	2.4	227	5448	224.3	10.64	48	334 NVIDIA TeslaM2050
Poland (ICM)	boreasz	IBM Power 775 (Power7)	IBM Power7	3.83	76	2432	74.5	9.73	128	
Poland (Cyfronet)	Zeus-gpgpu	cluster Intel & GPGPU	Intel Xeon X5670/E5645	2.4/2.93	44	528	136.8	3.6	72-96	48 M2050/160 M2090
Spain (BSC)	MinoTauro	Bull Cuda Linux cluster	Intel Xeon E5649	2.53	126	1512	182	3.072	24	256 nVIDIA Tesla M2090
Sweden (PDC-Center for High Performance Computing)	Lindgren	Cray XE6	AMD Opteron 12-core “Magny-Cours”	2.1	1516	36384	305	47.38	32	
Switzerland (CSCS)	Monte Rosa	Cray XE6	AMD Opteron 16-core Interlagos	2.1	1496	47872	402	46	32	
The Netherlands (SARA)	Huygens	IBM pSeries 575	Power 6	4.7	108	3456	65	15.75	128-256	
Turkey (UYBHM)	Karadeniz	HP Nehalem cluster	Intel Xeon 5550	2.66	32	256	2.5	0.75	3	
UK (EPCC)	HECToR	Cray XE6	AMD Opteron 16-core Interlagos	2.3	2816	90112	829.03	90	32	
UK (ICE-CSE)	ICE Advance	IBM BG/Q	PowerPC A2	1.6	6144	98304	1250	96	1	

Appendix H

Socio-economic challenge projects/Societally relevant projects in PRACE

The information in this appendix is based on the following PRACE report:

PRACE-3IP PRACE Third Phase Implementation Project D7.1.1 Applications Addressing Major Socio-economic Challenges, version: 1.0 Author(s): Maciej Szpindler, ICM, Marcin Zielinski, SURFsara Date: 25.05.2013

The socio-economic challenge projects that have been supported for access to the PRACE Tier-0 systems are generally associated with applications that are considered to be community codes. The codes were chosen because of their possible impact on associated research communities. In some cases, these codes were not considered to be necessarily well suited for the Tier-0 architectures and the goal was to understand what was required for the code to be effective or if that was feasible.

There were 15 projects proposed and 8 were approved to go forward. The projects included the following:

- Safe and Environmental-friendly energy production – STFC
- Rational drug design – Project leader Soon-Heum Ko (LiU)
- Rational drug design – NCSA
- Sustainable food supply – Thomas Röblitz (UiO)
- Future aircraft transportation – Peter Stadelmeyer (JKU), Tomáš Karásek (VSB)
- ‘Big data’ management and processing – Cevdet Aykanat (BILKENT)
- Understanding of climate change – CASTORC
- Natural environment protection – SURFSARA, CINECA

Two of the approved projects were led by researchers at Nordic institutions (LiU and UiO) and were successful at utilizing Tier-0 resources. In one case, the LSDALTON code was evaluated for performance and in the other the use of workflows was evaluated in the context of biological data.

Detailed information on the efforts of the two Nordic led projects is available in two publications:

Enabling Large-Molecule Simulations of Biological Interest through LSDALTON’s DFT Method. Soon-Heum Ko (LiU), <http://www.prace-ri.eu/IMG/pdf/wp169.pdf>

Scaling of Biological Data Workflows to Large HPC Systems - A Case Study in Marine Genomics - T. Röblitz (UiO), <http://www.prace-ri.eu/IMG/pdf/wp171.pdf>

Appendix I

HPC Provider Survey

Survey for the Nordic Science Case for HPC Computing and Storage Providers

Researchers in all of the Nordic countries are making increasing use of local, national and international computing resources as part of their research routine. Each of the countries supports their national researchers and also cooperates through the Nordic e-Infrastructure Collaboration (NeIC), which is part of NordForsk. Over time, this has resulted in strong efforts to develop and share programs that enhance the national and regional capabilities in multiple science areas.

In 2013 and 2014, NeIC used external expert panels to evaluate two important aspects of the Nordic high performance computing (HPC) environment, including the Gardar NHPC shared resource in Iceland and the use or involvement with the PRACE project by researchers and e-infrastructure providers in the Nordic countries. The two evaluations made strong recommendations to develop the scientific case for Nordic HPC, which could then be used to inform and guide decisions in future Nordic HPC investment and participation in international projects. The NeIC Board has tasked NeIC with preparing a plan for this effort.

As part of this process, we are surveying researchers and other stakeholders to help draw out an understanding of the strengths across research domains and the region. The survey is intended to provide a high level view of many different research projects and their future computational needs, particularly those that go beyond the computing and storage capabilities that researchers are currently using.

The survey is focused on building a picture of the research strengths within the Nordic region that have impacts and effects that reach beyond national borders and on what should be done to enable this research through Nordic HPC efforts.

For all the questions are intended to help develop a high-level characterization of the ways in which the computing and data systems are useful to researchers. We are requesting reasonable approximations or estimates rather than detailed or exact statistics to get this overview of how the systems are used.

1/ Basic questions about the research projects that are on your computing and data systems:

- What areas of science are you supporting (here we use the PRACE domains)? Please break the usage of the computing and data system down roughly along these divisions in %:
- Biochemistry, bioinformatics and life sciences
- Chemical sciences and materials
- Earth system sciences
- Engineering and energy
- Fundamental physics
- Mathematics and computer sciences
- Universe sciences
- Other
- What are the implications and impact of the research you are supporting?
- Do you see the research areas changing in the future in terms of the usage in each area? If so, how do you think it will change and why?
- What types of collaborations are you working with in support of the research projects? Are they entirely within the Nordic region? Do they extend beyond the Nordic region? If so, what aspects are strengths within the Nordic region?
- Do you expect collaborative projects to become more common to support the research programs? If yes, who are your likely potential future partners and where are they located?
- What are the most important outcomes of the research on your systems?
- Scientific domain impact
- Research papers
- Software and tools
- Datasets
- Instruments and systems
- Student education and training
- Industrial or commercial application
- Other:_____

2/ General computing research infrastructure questions

- a) Do you work with any of the national or international computing or other research infrastructure facilities, such as those in ESFRI?
- b) How do the computing research infrastructure facilities that you provide in the Nordic region compare with those in other parts of the world?
- c) Are there aspects that you provide at the facilities in the Nordic region that are unique or hard to duplicate?
- d) What would be the best or most suitable computing or storage facilities for you to provide for your researchers? What makes them better or more suitable?
- e) Do you anticipate that the researcher's needs for computing, storage or e-infrastructure systems will change over the next five years? What would be driving the change?
- f) In the next five years, could they effectively use larger computing or storage systems? Would this change the types of problems that they work on? How much larger and when would the systems need to be? What about after five years?

3/ What do the researchers use the computing or storage systems for?

Can you roughly estimate the % for each?

Some uses serve multiple purposes so the total may be >100%.

- a) Software development, testing, optimization, and verification of correctness and reproducibility
- b) Mapping or exploring the ranges for models or parameter spaces
- c) High risk explorations of new possibilities
- d) Production of data products or other expected outcomes
- e) Evaluation of successively larger or more complex problems that are system size limited
- f) (Partial) re-runs due to past problems with the infrastructure
- g) Other uses: _____

4/ How would you describe the way in which the researchers need to use the system to be most effective for their research programs?

Can you estimate (roughly) the % for each?

- a) Continuous or very frequent use as part of the normal research routine
- b) Sporadic use only when needed to address some aspect of the work
- c) Short term projects or goals that may take a few months to finish
- d) Long term projects that can span years
- e) High intensity use of as much of the system resources as soon as possible
- f) Low intensity use that is routine in terms of size or time to solution
- g) Some other method of using the system?

5/ Which of these modes of using the system does their research mainly depend on? Can you estimate (roughly) the % for each?

- a) Capability – large scale highly parallel, large aggregate memory or data intensive computer codes
- b) Capacity – serial or small scale parallel, aggregate memory or data intensive computer codes
- c) Combination – concurrent execution of parallel computer codes to explore a parameter space or range of similar inputs to create an ensemble of results
- d) Workflow – sequential execution of serial or parallel computer codes
- e) Time dependent – externally time constrained computer codes
- f) Interactive – computer codes that require personal interaction during their execution
- g) Batch – computer codes that do not require personal interaction during their execution
- h) Any other ways in which you are using computing and data resources?

6/ How would you characterize the researchers' computer code(s)? Can you estimate (roughly) the % for each?

- a) Experimental data management
- b) Observational data management
- c) Modeling
- d) Simulation
- e) Data analysis
- f) Verification
- g) Visualization
- h) Other types of code?

7/ What type of data do they generally work with? Can you estimate (roughly) the % for each?

- a) Observational
- b) Experimental
- c) Simulation
- d) Images
- e) Text or unformatted data
- f) Other

8/ What types of resources do they need for their research?
Can you estimate (roughly) the % for each?

- a) General processing, floating point
- b) General processing, non-floating point (integer, text, image)
- c) Use of accelerator hardware (GPUs, FPGAs, MIC, other)
- d) Storage and I/O requirements
- e) Memory size and bandwidth requirements
- f) Low latency interconnect
- g) Software or tools
- h) Security for sensitive data
- i) Local or remote access
- j) Other
- k) Do not know

9/ What types of user support do you provide?

- a) General assistance
- b) Training, workshops and documentations
- c) Computer application code development tools, porting, tuning, optimization, or code review
- d) Domain related expertise, algorithms, software packages and tools

10/ Is there anything that you would like to add to the response that would be helpful in understanding the role of the computing and data needs or benefits. in your research?

Appendix J

Researcher Survey

The survey was developed and sent out to researchers who were identified as large users of the HPC resources within each country and also for internationally available HPC systems.

The list of researchers was compiled from multiple sources and included the Nordic PRACE Tier-0 principal investigators for Calls 2-9 (22), the Nordic Tier-1 PIs (35) from DECI-7 to DECI-12, major users provided by the HPC providers in the Nordic region (81) as well as others who were identified in further discussions with researchers and providers. There was some overlap in the different lists of researchers so the total number of researchers who were contacted is less than the sum of the groups of researchers.

The survey was envisioned as providing a high level view of many different research projects and their computational needs. The questions were intended to help develop a high level characterization of the ways in which researchers use the computing and data systems. Estimates were requested rather than detailed or exact statistics to get this overview of how the systems are used.

This resulted in ranges of responses that had to be expressed in a form that was easily characterized and communicated rather than detailed and explicit. This is useful for the type of high-level view that this project was looking for, particularly those aspects that might either confirm what could be considered to be common expectations or identify new aspects.

To facilitate this, the responses were summarized and are included in parentheses after each question. A single number indicates that the response was positive or confirmation of the importance of this information or item. Two numbers in the parentheses indicate the numbers of positive and negative responses, respectively. Not every researcher answered every question so the totals are not equal to the total number of responders.

Survey for the Nordic Science Case for HPC

Researchers in all of the Nordic countries are making increasing use of local, national and international computing resources as part of their research routine. Each of the countries supports their national researchers and also cooperates through the Nordic e-Infrastructure Collaboration (NeIC), which is part of NordForsk. Over time, this has resulted in strong efforts to develop and share programs that enhance the national and regional capabilities in multiple science areas.

In 2013 and 2014, NeIC used external expert panels to evaluate two important aspects of the Nordic high performance computing (HPC) environment, including the Gardar NHPC shared resource in Iceland and the use or involvement with the PRACE project by researchers and e-infrastructure providers in the Nordic countries. The two evaluations made strong recommendations to develop the scientific case for Nordic HPC, which could then be used to inform and guide decisions in future Nordic HPC investment and participation in international projects. The NeIC Board has tasked NeIC with preparing a plan for this effort.

As part of this process, we are surveying researchers and other stakeholders to help draw out an understanding of the strengths across research domains and the region. The survey is intended to provide a high level view of many different research projects and their future computational needs, particularly those that go beyond the computing and storage capabilities that researchers are currently using.

The survey is focused on building a picture of the research strengths within the Nordic region that have impacts and effects that reach beyond national borders and on what should be done to enable this research through Nordic HPC efforts.

1/ Basic questions about your research:

- a) What area of science are you are working in and what are the most challenging scientific questions or problems that you would like to work on in the future?
- b) What are the implications and impact of the research you are conducting?
- c) Do you see your research area changing in the future? If so, how do you think it will change and why?
- d) What collaborations are you working with as part of your research projects?
- e) Do you expect collaborative research projects to become more common in your field?
- f) What are the most important outcomes of your research?
 - 1) Scientific domain impact (25)
 - 2) Research papers (29)
 - 3) Software and tools 18)
 - 4) Datasets (14)
 - 5) Instruments and systems (2)
 - 6) Student education and training (22)
 - 7) Industrial or commercial application (13)
 - 8) Other (2)

2/ General computing research infrastructure questions

- a) Do you depend on any of the national or international computing or other research infrastructure facilities, such as PRACE? (20/9)
- b) How do the computing research infrastructure facilities that you use in the Nordic region compare with those of your collaborators or competitors in other parts of the world? (21/8)
- c) Are there aspects that you use or need from the facilities in the Nordic region or from facilities outside the region that are unique or hard to duplicate? (1/0)
- d) What would be the best or most suitable computing or storage facilities for you to use for your research? What makes them better or more suitable?
- e) Do you anticipate that your needs for computing, storage or e-infrastructure systems will change over in the next 5 years? What would be driving the change? (28/3)
- f) In the next 5 years, could you effectively use larger computing or storage systems? Would this change the types of problems that you can work on? How much larger and when would you need this? What about after 5 years?

3/ What do you use the large national or international computing or storage systems for? Can you estimate the % for each (aggregating to 100%)?

- a) Software development, testing and verification (27)
- b) Mapping or exploring the ranges for models or parameter spaces (23)
- c) High risk explorations of new possibilities (21)
- d) Production of data products or other expected outcomes (18)
- e) Evaluation of successively larger or more complex problems that are system size limited (18)
- f) Other uses? (7)

4/ How would you describe the way in which you need to use the system to be most effective for your research programs? Can you estimate the % for each?

- a) Continuous or very frequent use as part of the normal research routine (24)
- b) Sporadic use only when needed to address some aspect of the work (8)
- c) Short term projects or goals that may take a few months to finish (12)
- d) Long term projects that can span years (16)
- e) High intensity use of as much of the system resources as soon as possible (9)
- f) Low intensity use that is routine in terms of size or time to solution (5)
- g) Some other method of using the system? (1)

5/ Which of these modes of using the system does your research mainly depend on? Can you estimate the % for each?

- a) Capability – large scale highly parallel, large aggregate memory or data intensive computer codes (21)
- b) Capacity – serial or small scale parallel, aggregate memory or data intensive computer codes (18)
- c) Combination – concurrent execution of parallel computer codes to explore a parameter space or range of similar inputs to create an ensemble of results (13)
- d) Workflow – sequential execution of serial or parallel computer codes (10)
- e) Time dependent – externally time constrained computer codes (3)
- f) Interactive – computer codes that require personal interaction during their execution (8)
- g) Batch – computer codes that do not require personal interaction during their execution (18)
- h) Any other ways in which you are using computing and data resources? (2)

6/ How would you characterize your computer code(s)?

- a) Experimental data management (1)
- b) Observational data management (2)
- c) Modeling (18)
- d) Simulation (27)
- e) Data analysis (15)
- f) Verification (4)
- g) Visualization (7)
- h) Other types of code?

7/ What type of data do you generally work with?

- a) Observational (7)
- b) Experimental (3)
- c) Simulation (29)
- d) Images (5)
- e) Text or unformatted data (4)
- f) Other (0)

8/ What types of resources do you need for your research?

- a) General processing, floating point (27)
- b) General processing, non-floating point (integer, text, image) (3)
- c) Use of accelerator hardware (GPUs, FPGAs, MIC, other) (6)
- d) Storage and I/O requirements (23)
- e) Memory size and bandwidth requirements (21)
- f) Low latency interconnect (15)
- g) Software or tools (20)
- h) Security for sensitive data (2)
- i) Local or remote access (13)
- j) Other (0)
- k) Do not know

9/ What types of user support do you rely on?

- a) General assistance (21)
- b) Training, workshops and documentations (13)
- c) Computer application code development tools, porting, tuning, optimization (16)
- d) Domain related expertise, algorithms, software packages and tools (10)

Cognitus Project

This report has been prepared for the Nordic e-Infrastructure Collaboration (NeIC) Board to facilitate future decisions in the Nordic region in the area of high performance computing and related topics. An external expert, Dr. Robert Pennington, Deputy Director of the National Center for Supercomputing Applications at the University of Illinois Urbana-Champaign was engaged as a special advisor to NeIC for the project. He consulted with Nordic researchers, Nordic HPC systems staff, NeIC staff, as well as other researchers who have been engaged in similar activities in other countries.