Theory and Computing

Nuclear theory is making major conceptual and computational advances that address the fundamental questions of the field. This concerns – on the one hand – the high-temperature and high-density behaviour of matter and, secondly, how hadrons and nuclei emerge from the strong dynamics of quantum chromodynamics (QCD). These are driven by discoveries such as the detection of perhaps the most exotic state of matter, the quark-gluon plasma, which is believed to have existed in the very first moments of the Universe. High-precision measurements of the quark structure of the nucleon are challenging existing theoretical understanding. Nuclear physicists have started to explore a completely unknown landscape of nuclei with extreme neutron-to-proton ratios using radioactive and short-lived ions, including rare and very neutron-rich isotopes. These rare nuclei lie at the heart of nucleosynthesis processes in the Universe.

As detailed throughout this document, nuclear theory plays a crucial role in shaping existing experimental programs in Europe and provides guidance to new initiatives in nuclear physics. Combining theory initiatives in a concerted effort is essential for optimal use of the available resources, in particular by providing platforms for scientific exchange and the training of the next generation of nuclear theorists. At the same time it is important to strengthen collaborations and accessibility in the area of high-performance computing (HPC). The following sections describe the coordinated European efforts in nuclear theory through the European Centre for Theoretical Studies in Nuclear Physics and Related Areas (ECT*) and the European and national compute infrastructure.

ECT*, Trento, Italy

The European Centre for Theoretical Studies in Nuclear Physics and Related Areas (ECT*) started operating in 1993 as a ‘bottom up’, community-driven initiative of the European nuclear physics community and has since developed into a very successful research center for nuclear physics in a broad sense. ECT* is unique and the only center of its kind in Europe. It is similar in scope and mission to the Institute for Nuclear Theory in Seattle (INT), USA, and collaborates with European Universities, Institutes and laboratories. It is an institutional member of NuPECC, the Associated Nuclear Physics Expert Committee of the European Science Foundation. With around 700 scientific visitors each year, from all over the world, spending from a week to several months at the Centre, ECT* has gained a high visibility. As stipulated in its statutes, ECT* assumes a coordinating function in the European and international scientific community by:

- conducting in-depth research on topical problems at the forefront of contemporary developments in theoretical nuclear physics

- fostering interdisciplinary contacts between nuclear physics and neighbouring fields such as particle physics, astrophysics, condensed matter physics, statistical and computational physics and the quantum physics of small systems

- encouraging talented young physicists by arranging for them to participate in the activities of the ECT*, by organizing training programs and establishing networks of active young researchers

- strengthening the interaction between theoretical and experimental physicists.

These goals are reached through international workshops and collaboration meetings, advanced doctoral training programs and schools, and research carried out by postdoctoral fellows and senior research associates as well as long term visitors. Cooperations exist with the Physics Department and the Center for Bose-Einstein Condensation (BEC) at the University of Trento and with the Interdisciplinary Laboratory for Computational Science (LISC) of the Bruno Kessler Foundation. There are presently cooperative agreements with other scientific institutions, in particular the ICTP in Trieste, the Extreme Matter Institute (EMMI) in Darmstadt, the Helmholtz International Center for FAIR, the JINR in Dubna, the research Center RIKEN, the National Astronomical Observatory of Japan, the ITP of the Chinese Academy of Science and the Asia Pacific Center for Theoretical Physics in Korea.

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With the emergence of a common European Research Area (ERA) and growing international cooperation, ECT* faces new opportunities and challenges. Significant European and global investments are made presently in accelerator centers and other experimental facilities. Their efficient utilization requires coordination and exchange of ideas – experiments stimulating theory and *vice versa*. Interdisciplinary contacts between the various subfields covered by ECT* and with related areas of physics and science is beneficial to all parties.

High-performance Computing in Europe

Computational Challenges in Nuclear Theory

Accompanying the experimental developments, qualitative changes in the theoretical understanding of strong-interaction (QCD) matter have taken place through significant improvement in numerical algorithms and high-performance computing. Lattice simulations of the QCD thermodynamics have entered the precision era, now providing stringent predictions of the equation of state near the quark-hadron transition for moderate baryon chemical potentials. Similarly, lattice studies of hadron structure and spectroscopy have led to major advances on a quantitative level. Lattice calculations of hadronic contributions to precision observables are indispensable for exploring the limits of the Standard Model. A combination of techniques has also provided links between lattice QCD calculations of nuclear few-body systems and ab initio methods for the solution of the nuclear many-body problem. Effective field theories rooted in QCD attempt at building a bridge through direct lattice simulations of the properties of light nuclei or to convert the results of lattice QCD into input Hamiltonians that can be used in ab initio many-body methods.

The theoretical tools have matured such that they begin to span the strong-interaction landscape from the elementary constituents, quarks and gluons, as the building blocks for the computation of hadrons and nuclei to the computation of the equation of state for infinite nuclear matter and neutron star matter. In all areas of theoretical nuclear physics algorithmic and computational advances thus hold promise for breakthroughs in predictive power including proper error estimates.

Compute Infrastructure

Most of the advances in modern nuclear theory have become and continue to be possible through major investments in the European compute infrastructure. In the following the computational landscape from which the nuclear theory community benefits is described. The largest national HPC resources are briefly described and examples of other national facilities are given. The coordination of the national infrastructures through the "Partnership for Advanced Computing in Europe" (PRACE) is outlined. Comments are also made on perspectives and future challenges for HPC in Europe as far as they are relevant for Nuclear Theory.

National HPC resources

France

The main organization for high-performance computing in academic areas in France is GENCI (Grand Equipment National de Calcul Intensif). The French national computing resources, made available by GENCI for the scientific communities, are installed and operated in three computing centers: the Très Grand Centre de calcul du CEA (TGCC) at Bruyères-le-Châtel near Paris, the Institut du développement et des ressources en informatique scientifique (Idris) of CNRS at Orsay near Paris and the Centre informatique national de l'enseignement supérieur (Cines) at Montpellier. In particular TGCC is an HPC infrastructure, hosting Petascale supercomputers. This supercomputing center has been planned to host the first French Tier-0 machine *Curie*, with a peak performance of 1.75 Pflop/s and 15 PB in disk storage. It is funded by GENCI for the PRACE Research Infrastructure (to be discussed below) and the next generation of Computing Center for Research and Technology (CCRT).

Germany

In Germany, the "Gauss Centre for Supercomputing" (GCS) is the leading Tier-0 centre in Europe. GCS is the alliance of the three Tier-1 national supercomputing centres, the High Performance Computing Center Stuttgart (HLRS), the Jülich Supercomputing Centre (JSC), and Leibniz Supercomputing Centre, Garching near Munich (LRZ). A CRAY XC40 (*Hazel Hen*)-system is installed at the HLRS, with a peak performance of 7.42 Pflop/s. It has 965 TB of main memory and a total of 11 PB of storage capacity. JSC provides access to the IBM Blue Gene/Q system *JUQUEEN* with a peak performance of 5.9 Pflop/s. The main memory amounts to 448 TB. In addition, the JSC hosts the general-purpose cluster *JURECA* with a peak performance of more than 2.2 Pflop/s and 281 TB of main memory. Both systems share 20 PB of common disk storage. The third GCS HPC system *SuperMUC* is located at the LRZ in Garching. The installation consists of two IBM/Lenovo clusters, delivering a peak performance of 3.2 and 3.6 Pflop/s respectively. The main memory is 340 TB and the system provides about 20 PB of hard disk space. A successor for *JUQUEEN* with a target peak performance of about 50 Pflop/s will be installed at JSC in several stages, starting in 2018.

Italy

The main organization for high performance computing in academic areas in Italy is CINECA . CINECA is a non-profit Consortium, made up of 70 Italian universities and 5 institutions and is another Large Scale Facility in Europe. It is a PRACE Tier-0 site featuring the system *Marconi*. The *Marconi* system has two different partitions: The first partition *(Marconi-A1*) has a peak performance of 2 Pflop/s and the system provides 17 PB of hard disk space. The second partition *(Marconi-A2*), which will become available at the end of 2016, is based on a many-core architecture and the peak performance will be boosted to approximately 13 Pflop/s. In the middle of 2017 the first partition will be replaced by a new one reaching a total computational power in excess of 20 Pflop/s. The second CINECA system is the Tier-1 IBM cluster system *Galileo*, which went into operation in 2016 and provides a peak performance of about 1Pflop/s and 1TB of disk space.

Spain

Academic HPC computing in Spain is organized through the network RES („Red Española de Supercomputación“). RES is an alliance of 12 academic institutions and their supercomputers and is coordinated by the Barcelona Supercomputing Centre (BSC). One of these machines, *MareNostrum*, located at BSC is the Spanish Tier-0 system offered under PRACE. *MareNostrum*, is an IBM installation and currently consists of 48,896 cores. This amounts to a peak speed of roughly 1Pflop/s and a main memory is 104,6 TB. The system provides 2 PB of disk storage.

Switzerland

The *Piz Daint* supercomputer is the flagship HPC system of the "Swiss National Supercomputing Centre" (CSCS) in Lugano. Having been installed in 2016, it is a Cray XC50 system with a total of 206,720 compute cores amounting to a peak performance of nearly 16 Pflop/s. It currently ranks number 8 in the Top500 list (Nov. 2016). The total system's memory is about 195 TB.

United Kingdom

In the UK computational nuclear theory is part of DiRAC (Distributed Research utilising Advanced Computing), the integrated supercomputing facility for theoretical modelling and HPC-based research in particle physics, nuclear physics, astronomy and cosmology. Academic users have access to a total of five installations, including clusters (based in Cambridge, Durham and Leicester) and a BlueGene/Q facility (based in Edinburgh), with a combined performance of 2 Pflop/s and a storage capacity of 4 PB. DiRAC is funded via the national Science and Technology Facilities Council (STFC), which covers nuclear physics besides particle physics and astronomy. Succession to the current facilities is being planned and expected to arrive during 2017.

Ireland

In Ireland, there is the national centre for high-performance computing – ICHEC. Via the supercomputer *Fionn* - with a compute capacity of roughly 140Tflop/s - it provides access through peer-reviewed applications.

In addition to the major Tier-0 facilities there are a number of national supercomputing resources, largely dedicated to nuclear theory, as for instance QPACE2 in Regensburg, QPACE3 at the Jülich Supercomputing Centre, MOGON in Mainz, HPC WALES in Wales and the LOEWE CSC in Frankfurt.

High-performance Computing at the European level

At the European level the use of compute infrastructures is coordinated through PRACE. PRACE currently has 25 member countries: Austria, Belgium, Bulgaria, Cyprus, Czech Republic, Denmark, Finland, France, Germany, Greece, Hungary, Ireland, Israel, Italy, The Netherlands, Norway, Poland, Portugal, Slovakia, Slovenia, Spain, Sweden, Switzerland, Turkey and the United Kingdom. PRACE realizes its mission by offering world-class computing and data management resources and services by coordinating access to national Tier-0 HPC facilities through a peer review process.

The computer systems and their operations, accessible through PRACE, are provided by five PRACE members (BSC in Spain, CINECA in Italy, SNCS in Switzerland, GCS in Germany and GENCI in France). The HPC centers managed by PRACE provide in total about 46 Pflop/s distributed among the 5 major institutions. PRACE distributes about 2 billion processor hours per year for fundamental research.

Over the entire period of its operation until October 2016 PRACE has distributed about 15% of the resources to fundamental physics. This only considers the resources provided by the four initial partners (France, Germany, Italy, Spain). PRACE phase II is now starting, with an additional participation of Switzerland. Among the PRACE computing systems the Swiss Supercomputer *Piz Daint* currently is the most powerful installation. About 1/3 of its compute resources are distributed through PRACE. The allocation rules are slightly changing and might affect the distribution of resources.

In addition, PRACE, in cooperation with the European data infrastructure project EUDAT, manages DECI - the Distributed European Supercomputer Initiative, which provides European Tier-1 access to architectures such as CrayXC30/Cray XC40, Intel clusters with various processor and memory configurations and hybrid systems made available from Cyprus, Czech Republic, Finland, Greece, Hungary, Ireland, Italy, Norway, Poland, Spain, Sweden, the Netherlands and the United Kingdom.

Concerning the future of HPC at the European level, PRACE is heavily involved in the future strategy for European Exascale computing.

International Competitiveness and Perspectives

Worldwide, China currently takes the lead in HPC with the two largest installations reaching a peak performance of 125 Pflop/s (Sunaway TaihuLight at the National Supercomputing Center in Wuxi) and 33.9 Pflop/s (Tianhe-2 at the National Supercomputing Center in in Guangzhou). These installations are, however, of limited use for theoretical physics calculations. In the USA the largest installation, Titan at Oak Ridge National Laboratory, Sequoia at Lawrence Livermore National Laboratory, Cori at NERSC and Mira at Argonne National Laboratory are listed as number 3, 4, 5 and 9 in the top 500 list. They provide in total a peak performance of 85 Pflop/s. A large fraction of these resources is made available to the theoretical physics community through national programs such as INCITE and the ASCR Leadership Computing Challenge (ALCC). Together these programs distributed almost 10 billion core processor hours in 2016. About 10% of this is available to research in nuclear physics. In Japan the two largest installations are listed as number 6 and 7 in the top 500 list. The newest installation, Oakforest-PACS, started to operate in December 2016 and reaches a peak performance of 25 Pflop/s.

Planning of future HPC installations is recognized as being of strategic importance for all international players. Roadmaps towards Exascale computing facilities and planning for next generation installations are underway in Europe as well as in the USA and Asia. All major computing centers organized in PRACE plan for new installations for the next years that will reach a peak performance in the 10-30 Pflop/s range. Major steps towards Exascale performance are expected to be taken early in the 2020's, enhancing today's computing power in a single installation by more than a factor 50. In the USA, current plans are to have an Exascale computer in operation in 2021-23. Such HPC systems are likely to utilize hundreds of thousands of nodes equipped with novel CPUs perhaps emerging from the current GPU and multi-core GPU lines. Presumably one will find machines with a heterogeneous computing environment. This will lead to an even more complex compute environment and users will face major challenges for software development that can utilize these machines efficiently. In the USA, this problem has been faced since some time with a unique funding line for a software development program. The program Scientific Discovery through Advanced Computing (SciDAC) supports the development of optimized software for HPC systems. There is a unique funding line for applications in Nuclear physics that has the goal ''to enable and support research on current high-profile computationally intensive topics in theoretical nuclear physics of direct relevance to the experimental research programs at existing or approved NP facilities''. A counterpart of such an initiative, specifically devoted of Nuclear physics, does not exist in Europe but would be highly beneficial in particular in view of the even more complex compute infrastructure the community will get access to in the near future. Being ready to exploit such upcoming machines efficiently in an early stage will be mandatory for staying competitive in this rapidly evolving field of research opportunities.