Rapport thématique « Calcul et données »
Conseil Scientifique de l'IN2P3

1. Summary

This document tries to present the activities of IN2P3 teams working with High-Performance Computer in particle and nuclear theoretical physics. We review the research goals and the codes developed to achieve them. The quality of the science produced is unquestionable given the number of grant recipients identified. We highlight the current challenges with regards to the continuous development of numerical codes and algorithm required to run on the next generation machines. We review the institutional resources in term of equipment and human resources.

2. Scientific challenges

i. Particle physics

In 1904, after the discovery of the electron, Thomson suggested a very British model of the not yet discovered atom, the "plum pudding model", where electrons are surrounded by a volume of positive charge, like negatively charged plums embedded in a positively charged pudding. Improving on the observation of Rutherford, Geiger and Marsden observed the scattering at more than $90°$ of α particles impinging on thin gold films. In 1911, Rutherford's modeling of the Geiger-Marsden experiment proved the existence of the atomic nucleus. In 1932, Chadwick discovered the existence of the neutron, immediately recognized as one of the constituents of nuclei, suggested by Rutherford in its Bakerian lecture. A year later, Stern and his collaborators measured the anomalous magnetic moment of the proton, providing the first evidence that nucleons were more than just point-like Dirac particles. In 1967, a deep inelastic scattering experiment by Friedman, Kendall, and Taylor revealed point constituents originally called "partons" as parts of hadrons. The work on asymptotic freedom in 1973, by Politzer, Wilczek and Gross reframed the theory of strong interaction into Quantum Field Theory, which gave the final endorsement that Quantum Chromodynamics is the theory of the strong interaction. In 1974, Wilson formulated a version of QCD on a discrete spacetime lattice [1]. It was only years later that meaningful numerical simulation based on the Wilson formulation of QCD on a lattice (LQCD), provided the first color confinement potential. Unfortunately, QCD is highly non-perturbative at low-energy. For LQCD, this translates into the requirement of generating a large number of field configurations, computing the path integral with Monte Carlo sampling while running the lattice spacing $a \to 0$, in practice, a few tenth to hundredth of fm, to achieve sufficient accuracy at low-energy. LQCD is done in two parts, the first is to compute the gauge configurations, which is then use to evaluate the observable of interest.

The extraction of fundamental quantities in flavor physics experiments must be supported by theoretical calculations. A few relevant physical inputs can be computed with LQCD. The goal is to achieve a sufficiently high accuracy in the numerical computation, so that experimental results of LHCb, Belle-2, charmed meson factories, ATLAS, CMS, and lower-energy experiments like JLab, can be exploited in their full glory for the hunt for the Higgs coupling to the quarks sector, in particular $h \to c\bar{c}$ and the examination of the $\bar{b}c$ currents. A collateral consequence that comes for free, is to improve our understanding of the long-range dynamics of the strong interaction.

In the last decade, heavy ion collisions, for instance at RHIC, observed that high transverse momenta seem to be suppressed differently depending on the hadron species [2]. Proton-proton scattering is often used as the reference to obtain quantitative conclusions. This requires access to the full inelastic cross section, which is, evidently, an experimental challenge. Even so proton-proton scattering is not fully understood, modeling collision between light- to heavy-ions starting from a parton model in a single framework, is the only path to interpret data at CERN, AUGER and RHIC altogether. For heavy ion collisions, up to $200 + 200$ nucleons, the formation of a quark-gluon plasma should be included and the dynamics obtained by solving hydrodynamical equations.

ii. Nuclear physics

In recent years, the focus of low-energy nuclear physics has moved towards the extremes of the Segrè chart, i.e., to unstable proton- and neutron-rich as well as to super-heavy nuclei. These poorly known systems sometimes display unconventional phenomena that challenge our understanding and call for more systematic and predictive theoretical frameworks. In this context, theoretical approaches that start (solely) from the knowledge of basic interactions between nucleons have attracted considerable attention given their systematically improvable character and their capacity to thoroughly assess theoretical uncertainties. Such methods have undergone important progress in the last $10 - 15$ years and have proven successful in explaining and predicting the structure of nuclei from stable to very neutron-rich systems (e.g., [3]). These progresses are paired with the emergence of High-Performance Computing allowing scientists to efficiently use large-scale distributed-memory systems. Limited to very light nuclei only a decade ago, *ab initio* techniques are nowadays able to address the structure of medium-mass systems with more than 100 nucleons [4]. This progress goes hand in hand with the development of nuclear Effective Field Theory (EFT). Nuclear EFTs are constrained only by the symmetries of the Standard Model and encode the details of the nonperturbative QCD dynamics in a finite number of parameters at each order of its low-energy expansion. With proper power counting, EFT yields a renormalizable and thus model-independent derivation of nuclear interactions, which can be matched to lattice QCD results. The conjunction of *ab initio* methods (AIMs) and properly renormalizable EFTs will permit the field to go forward and to make new discoveries.

In spite of the rapid advances in AIMs, the more phenomenological Energy Density Functional (EDF) approach, which has a long-standing tradition in the French nuclear physics community, is the most versatile many-body method, thanks to its polynomial scaling in terms of nucleon constituents. EDF is the nuclear physics equivalent of density functional theory in quantum chemistry and in condensed matter. Nevertheless, there are fundamental differences in particular the lack of proper existence theorem such as Kohn and Sham theorem in condensed matter. Similarly, it is a standard tool for interpretation of nuclear data such as nuclear deformation, nuclear dynamics, response to an external probe etc... The affordable computational cost together with a reduced set of parameters tailoring the functional make it a prime tool for data-driven modeling and thus a potential target for IA inspired developments. EDFs currently remain the only microscopic method able to compute heavy and superheavy nuclei. The overarching goal of bridging AIMs and EFTs with EDF towards a common denominator still remains to be achieved.

On the reaction side, the need of reliable and predictive calculations where no data is available is even stronger. Precise, fundamental nuclear data is essential both for the sustainability of our civilization e.g., technological applications, and to our understanding of the universe. For instance, understanding the consequences of cataclysmic events in the cosmos such as the merger of two neutron stars leading to the synthesis of medium-to-heavy elements via the r-process requires an extensive set of accurate reaction rates at low-energy. Measuring those data in the laboratory is a considerable undertaking. Unfortunately, to-date, a faithful microscopic description of nuclear reactions (i.e., whose theoretical uncertainties are equivalent to those of measurements) remains an unfinished challenge. In short, advancing our understanding of the universe (and our technological level) requires precision results in nuclear physics, if possible measurable or otherwise calculated. Nevertheless, solving the scattering equation is a complex problem. The rapid increase, as a function of the energy, of the number of degrees of freedom in free space i.e., the number of reacting bodies in the outgoing channel, together with the dimensionality of the opened reaction channels, makes numerical techniques only applicable to the simplest systems. Those are either very-light nuclei or elastic collisions. Fortunately, AIMs for reactions is able to both provide a guideline for building the simplified approximate methods and make substantial contributions to evaluate key reaction rates in innovatory experimental projects such as at CERN (PUMA or GBAR experiments) and USDoC/NIST.

iii. Astrophysics

As of August 2017, observational astrophysics has entered a new era. Simultaneous observations of Gravitational Waves (GW170817), a γ-Ray Burst (GRB170817A) and the ensuing Astronomical Transient kilonova (AT2017gfo), were all associated with a binary merger of neutron stars (NS), which coined the new epoch of “multi-messenger observations” [5]. It was soon realized that the merger of Binary Neutron Stars (BNS) is not only an important source of GWs, but also has the potential to be a laboratory for studying properties of matter at densities and temperatures not accessible by terrestrial laboratories.

As cataclysmic events, at the origin of GWs, are the only looking glass for properties of dense matter, the accumulation of observations may lead to better our understanding of compact objects of the Universe, NS being a prototypical example. Due to the lack of direct measurements in the laboratory, there are many unknowns in the composition of dense nuclear matter [6]. The Equation of State (EoS) of matter is mostly inferred from the region of -or probed by- stable states of matter or through the observation of celestial bodies. The gap to be filled in order to reach densities of NS, leaves critical questions, which are yet unanswered:

- is the matter still largely composed of nucleons, as in the external region of the core?
- do new degrees of freedom appear, such as quarks?
- if so, what signatures in the GW and electro-magnetic signals would be made by hadronization during the BNS coalescence?

Recent studies on the survival time of supra-massive NS and the strength or frequency of the main mode of GW emission after the merger, have begun to provide the first steps forward e.g., [7]. Similarly, GW observations have shown their ability to globally constrain the EoS of dense matter ([8] among others). The prerequisites for using GW emission as a tool to probe dense EoS are i) to reach a better understanding of the multi-messenger emission and ii) to achieve an accurate modeling of the role of magnetic fields and its dynamic properties. So that, we can, in the future, expect GW observations to shed new light on the composition of the NS core and more generally on the nature of the phase transition(s) in dense matter. Therefore, it is timely to concentrate the current efforts towards modeling of dense matter and in General Relativity MagnetoHydroDynamic simulations.

3. Project

The age of truly effective parallel computer dates from the 90's to the late 2010s. The Message Passing Interface (MPI) standard was introduced in 1994. It opened the access to efficient memory-distributed computer systems rather than shared-memory systems based on vector processors, which suffered from memory contention. MPI allows for data interconnect via a network standard that features both very high throughput and very low latency. It is often completed by an implementation of shared-memory multiprocessing, which efficiently utilized the remaining available core computing-power, i.e., most of the computing power of a multi-core many-processor node. For the latter, the most commonly used standard is OpenMP, which was released in 2002. Most of the applications developed or used by the IN2P3 teams follow a hybrid MPI/OpenMP implementation of parallelism.

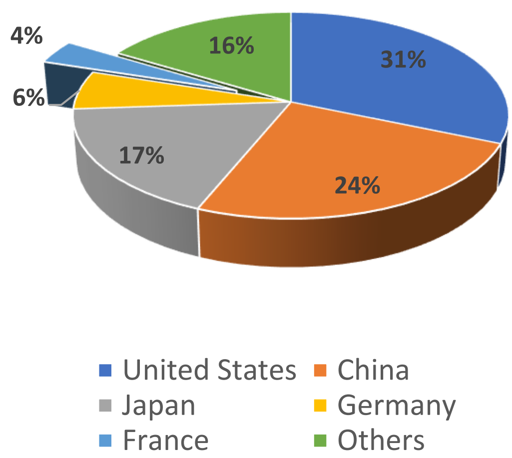

Figure 1: HPC countries by performance share.

The development of High-Performance Computing (HPC) is strongly correlated to international geopolitics. The main systems are hosted in either members of the G7 or in China, as illustrated in Figure 1. The national share on the world stage is $\sim 4\%$, in terms of peak performance, which is roughly constant since 2010. On the other hand, China has almost tripled its share of HPC systems from $\sim 9\%$ to $\sim 25\%$. These investments are directly benefiting fundamental science. More than half of systems officially labeled and opened to the public are accessible through calls for project to applicants performing fundamental research. However, in the last decade, HPC systems operated by private companies for weather prediction, mineral exploration, energy production or data science were commissioned. This highlights that HPC related technologies and applications are mature enough to leave the field of fundamental science applications. For institutes like IN2P3, this is an advantage in terms of the professional outlook for the PhD students trained to use and develop HPC applications but also poses a significant threat to the share of fundamental science on HPC systems.

The public infrastructure for numerical simulation was structured in 2005 with the creation of the GENCI, which was given the mandate to host Tier-1 computing systems for national users. At that time, CEA/TGCC, CNRS/IDRIS, MESRI/CINES and CNRS/IN2P3/CC were identified as large-scale computing centers. CCIN2P3 is not part of the GENCI due to his High Throughput Computing (HTC) paradigm focused on servicing computing needs of CERN experiments. In a nutshell, HTC aims at operating embarrassingly parallel long-running tasks. Five year later, the EU commission followed this footstep and established the Partnership for Advanced Computing in Europe (PRACE) to finance Tier-0 supercomputers and to open computing centers to transnational access. GENCI machines are subsidized in part ($\sim 50\%$) by the PRACE program and cpu.h allocations are shared accordingly.

However, the frontier between HTC and HPC with the Many-Task Computing (MTC) approach is no more a clear cut. MTC is a parallel implementation that is communication intensive, without resorting to MPI.

Codes

Nuclear structure

`MFDn` (many fermion dynamics), `GSM` (Gamow Shell Model) and `FUSIoN` codes solve the Schrödinger equation via expanding an ansatz in a many-body basis of Slater determinants constructed from tensorial product of harmonic oscillator (HO) wave function using arbitrary Hamiltonians.

`Ev8` is an open-source solver of the Hartree-Fock+BCS equation based on the Skyrme EDF on a 3D mesh. An extended version of this code solves the HFB equation for nuclei up to few hundred of nucleons. The `Esperance` code solves the Hill-Wheeler equation and performs symmetry restoration. This is the so-called multi-reference EDF, which allows to study the spectroscopy of heavy nuclei. `Esperance` uses constrained HFB solutions as input, for instance from `Ev8`.

Nuclear reactions

The `FUSIoN` code solves the scattering problem using the resonating group method and computed the scattering observable via the R-matrix method.

At IPHC the scattering solutions of the Merkuriev-Faddeev equations is obtained in configuration space. The results obtained are exact.

QGP

`EPOS` is a consistent quantum mechanical multiple scattering approach based on partons and strings. Cross sections and particle production are calculated consistently. Nuclear effects related to Cronin transverse momentum broadening, parton saturation, and screening are included in EPO. High density effects leading to collective behavior in heavy ion collisions are also taken into account.

LQCD

The openQCD package includes some of the most advanced simulation techniques for performing LQCD. In its latest version, the lattice theories supported are:

- 4-dimensional hypercubic lattice with even sizes $N_0\ x\ N_1\ x\ N_2\ x\ N_3$ under the following conditions: open, Schrödinger functional (SF), open-SF or periodic boundary in the time direction and periodic boundary in the space directions;
- $SU(3)$ gauge group, plaquette plus rectangle gauge action ;
- $\mathcal{O}(a)$-improved Wilson quarks in the fundamental representation. Supported quark multiplets are pure gauge, two-flavour theory, $2+1$ and $2+1+1$ flavour QCD, twisted mass doublets and theories with many doublets.

tmLQCD is an open-source software providing a set of tools to be used in lattice QCD simulations. It provides a (P)HMC implementation of Wilson twisted mass fermions and inverter for different versions of the Dirac operator.

Nissa is an open-source set of $SU(3)$ algorithm.

Astrophysics

The Italian team from the university of Trento published the new code named Spritz in summer 2020. It is one of the few codes in the world able to perform a full GRMHD simulation in 3D cartesian coordinate on a dynamical spacetime. It includes a composition and temperature dependent EoS for the description of neutron matter, as well as neutrino emission and reabsorption. It combines a robust approach for the computation of the vector potential for the evolution of the magnetic field with the use of a zero temperature EoS. It can work with any EoS, expressed as an array, via the EOS Omni library provided by Einstein Toolkit. IN2P3 team is not directly contributing to the development of this code.

4. Planning and progress

Porting to GPU towards exascale computing

GPU are soon to be ubiquitous in all HPC facilities. Programming on GPU is not a simple task, which required, in the past, to use a new interface like CUDA or OpenCL. This drawback is partially lifted with the introduction of OpenACC, which allows to annotate already existing code written in legacy languages. So far, almost none of the code used by IN2P3 teams are GPU enabled either with CUDA implementation or OpenACC.

Nevertheless, GPU are the path forward to reach the exascale frontier in HPC. This is due to the very advantageous ratio of bit operations to energy consumption of GPU. The speedup factor from standard many-core CPU to GPU is one-to-two orders of magnitude. This is quite significant for any HPC application. To efficiently use GPU, one should make sure that algorithm exploits the single instruction multiple data paradigm. In general, this is not trivial to achieve. Specific problems such as sparse linear algebra are not suitable for GPU unless significant time is spent to rewrite the algorithm. There are other drawbacks for using GPU such as the rate to write on GPU memory and their limited size. This may severely constrain how to port applications on GPU.

IN2P3 teams in particle and nuclear theoretical physics have contributed to the bottom-up writing of the French proposal for procuring an exascale machine within the PRACE program. Both core disciplines of IN2P3 will strongly benefit from the obtention of this type of machine. In both cases, either the accuracy of computation will be unprecedented or the range of applicability will be boosted to uncharted regions. For instance, in nuclear physics access to that type of computing power may directly feed on-demand experimental needs for data interpretation, speeding the discipline towards consistent EFT determined from data or LQCD, or allow for data-driven models. This will be a change of paradigm for many tools. To be able to port codes to GPU and to reach exascale computing, there is vast gap to be filled between our current capabilities (in term of HR) and what is needed to reach the goal of efficient tools for experimental physics.

5. State-of-the-art

All the scientific projects, which were reported for the redaction of this manuscript, produce high-end scientific results published in peered-review refereed journals, most of them being edited by the American Physical Society association. Additionally, as is reported in Tableau 1, 70% of staff scientists belong to either an IN2P3 or an ANR project, while 50% are part of a team requesting Tier-1 computing time at the GENCI. In addition, all the reported HPC projects have foreign collaborators (or the team members themselves) with an access to a computing center abroad (USA, Canada, Belgium, Italy, China etc…). We note that IN2P3, ANR or GENCI grants are reviewed, with the latter two being independent from the IN2P3 institute. All in all, these demonstrate the high quality of the research performed in the institute though the use of an HPC platforms.

6. Resources

i. Technical and financial resources

CCIN2P3

The institute is operating the CCIN2P3, a national computing facility for the support of CERN experiments. CCIN2P3 is a Tier-1 facility for grid infrastructures such as EGI and WLCG, servicing HTC and cloud computing applications. The facility offers a large array of service for IN2P3 labs also providing long-term storage of experiments and, at the fringes, for theoretical simulations. Additionally, a batch system operates about 350 computing nodes available to all users belonging to a project (either experimental or theoretical). Among them 16 nodes are reserved for HPC applications requiring InfiniBand grade interconnects. Usage per parallel paradigm is reported in Figure 2. As expected, HPC only represents 1% of the total. This is rather in line with a cluster usage limited to a small number of users. However, threaded partitions are also used by the HPC teams. While we do not have fine coarse statistics, we note that threaded applications consumed 34% of the CCIN2P3 computing time. This partition is used by HPC users for pre- or post-processing as well as pre-

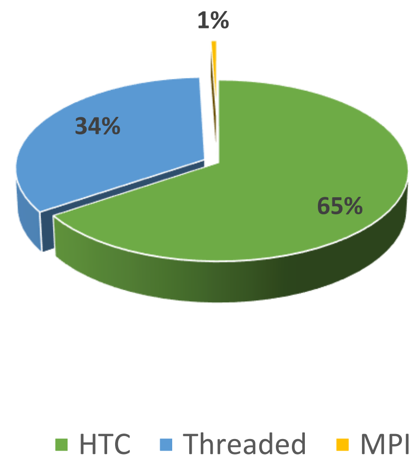

Figure 2: Share of CCIN2P3 per paradigm.

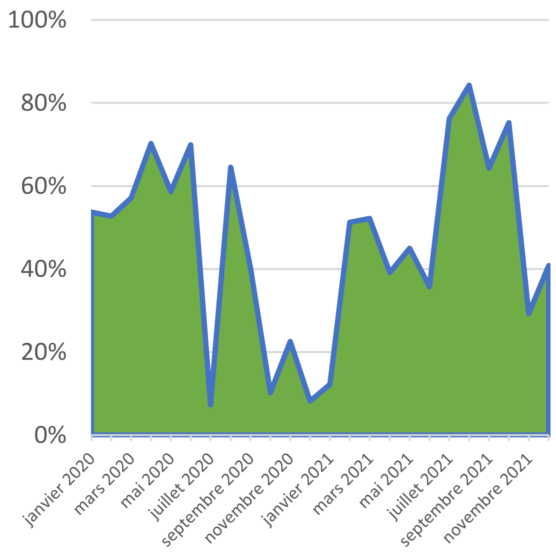

Figure 3: MPI/HPC partition usage.

deployment on Tier-1 machines. On Figure 3, we show the time-resolved usage of the HPC partition of the CCIN2P3 over the last four years. As noted above, the figure clearly illustrates the prototypical HPC paradigm with period of intense workload alternating with underuse. Interestingly, we can very clearly picture the effect of the COVID pandemic on the employment of the partition. A deep in usage can be seen one year after the burst of the COVID, and it seems that the average usage is not fully recovering since then. All of the above large fluctuations may be tracked back to the small number of permanent or fixed-term staff working in the field. GENCI computer centers or mesocenter are able to offset peaks and valleys effects through pooling of resources among many users.

However, we must emphasize that a persistent access to mesocenter computing -typically a few hundred of nodes- either for the preparation of GENCI project, or pre- or post-processing of a large-scale run, or simply recurring small-scale calculations, is instrumental for the success of applications reported in this report. For instance, all the GENCI projects reported here, were first tested, benchmarked and their parallel scaling evaluated using CCIN2P3 resources. 66% of them have ongoing use of CCIN2P3 for pre- or/and post-processing. And, at last, trivially parallel codes can run on CCIN2P3 HTC -High Throughput Computing, which includes single-node threaded jobs- or HPC partitions effortlessly using in the worst-case scenario MPI-enable python wrapper, and therefore do not require access to Tier-1 infrastructure. Henceforth, it is essential to acknowledge the need **for routine access to a mesocenter** by theoreticians in IN2P3 laboratories. In the recent years, there was a rollout of regional mesocenters hosted by universities, under the patronage of the GENCI. However, these facilities are not accessible at an institutional level and may (often) requires ad-hoc **financial participation at a laboratory level**, which given the scale of the theoretician teams in IN2P3 cannot be justified as a recurring laboratory expense. As a conclusion, the HPC capability of the **CCIN2P3** seems to be a **cost-efficient** institute-wide **capability** for supporting theoretical calculations that in turn increase the value of the institute experimental projects.

GENCI

The GENCI is the national agency that aims at coordinating both national or supra-national (EU level) HPC platforms in France. Deployment of HPC infrastructures is backed up by the expertise of CEA/TGCC, CNRS/IDRIS and MESRI/CINES, which are responsible for on-site management, technical support and training to users. Machine access is granted via bi-annual call for projects. Proposals are reviewed by a committee of experts that checks the following topics:

CT 1. Environment;
CT 2. Non-reactive flows;

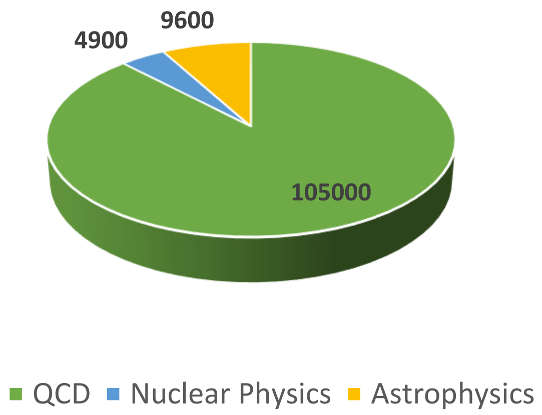

Figure 4: Resources requested at GENCI by topics (kcpu.h).

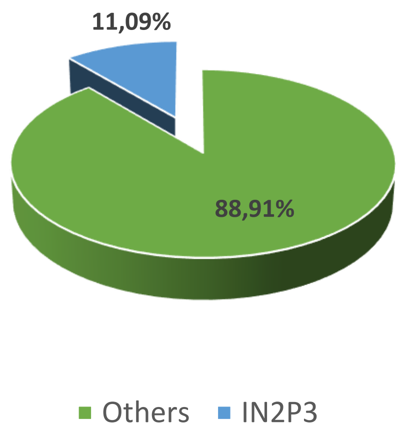

Figure 5: IN2P3 share of national resources.

CT 3. Reactive and multiphase flows;
CT 4. Biology and health;
CT 5. Astrophysics and Geophysics;
CT 6. Theoretical and plasma physics;
CT 7. Computer science, algorithms and mathematics;
CT 8. Molecular modeling applied to biology;
CT 9. Quantum Chemistry and Molecular Modeling;
CT 10. Physical chemistry and material properties;
CT 11. Artificial intelligence and transverse applications of computing.

They are responsible for a fair-share allocation of about 1Ma cpu.h nationwide. Roughly the same amount of computer power is provided by the GENCI to PRACE users that is Tier-0 computing time requested at the EU level by larger collaborations than hosted at IN2P3. Principal investigators of the institute submit theoretical proposals in CT 5&6. The share of computing time granted as a function of the fundamental science themes presented in Section 2 is shown in Figure 4. It is apparent that lattice QCD consumes more than 80% of the cpu.h requested by the institute, which is inherent to the nature of the Monte Carlo simulation requested for generating configurations. The rest of the requests are shared between nuclear physics (33% of the $\sim 20\%$ leftovers) and nuclear astrophysics simulations (66%). These statistics are roughly in line with last review of CT 6 that reports 80% share for LQCD and a growing number of third-party requests for theoretical simulation. In Figure 5, we present the total computing time requested by the institute to the GENCI. It shows that a solid 10% of the national resources for HPC are requested for performing scientific computation for supporting theoretical developments of IN2P3. This is quite significant and, if translated to cash would correspond to **1.56 M€** (using the 1.23 cent per cpu.h as reported in the GENCI year review). We can conclude that an efficient use of **resources external to the institute** is made through theoretical applications of HPC.

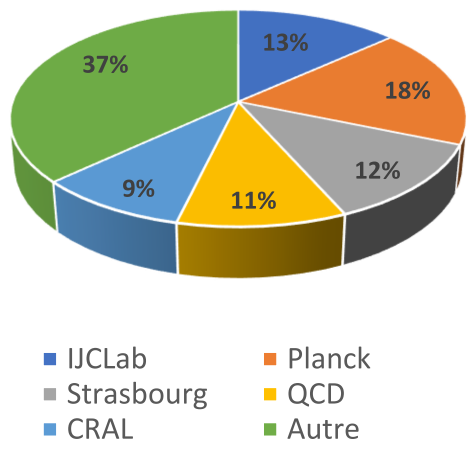

Figure 6: CCIN2P3 HPC per laboratory and projects.

ii. Human resources

Tableau 1 shows IN2P3 personnel that have self-reported working on scientific projects involving HPC calculations. We have identified their area of expertise at a higher resolution than the challenges reported in section 2 (nuclear, astrophysics, particle physics) and the HPC centers where they are users. Almost all of the staff report having access to CCIN2P3 in addition to a medium- to large-scale HPC facility. We have identified $\sim 70\%$ belongs to either an IN2P3 or an ANR project. They are geographically and uniformly spread among all the laboratories of the institute. There is no laboratory that dominate in terms of permanent staff. Conversely, in Figure 6 we report the CCIN2P3 usage per project/laboratory for the HPC partition. It is also evident from the data, that no laboratory or project identifies as a key user of the resources. This is of course different for the GENCI data due to the LQCD computing load. The figure shows a clear correlation with the location of the staff; however, we can pinpoint that the lack of dedicated CCIN2P3 projects for theoreticians prevents accurate reporting.

Project	Personnel	Laboratory	HPC Center	Topic
IN2P3 project ENFIA	Nadya Smirnova	IP2iB	Mesocentre MCIA	*Ab initio*
				Nuclear structure
IN2P3 project BRIDGE	Guillaume Hupin	IJCLab	GENCI	*Ab initio*
ANR NECTAR			CC-IN2P3	Nuclear reactions
ANR NEWFUN	Michael Bender	IP2I	CC-IN2P3	Nuclear structure
	Karim Bennaceur		In-house cluster	
IN2P3 project PUMA	Rimantas Lazauskas	IPHC	GENCI	*Ab initio*
			CC-IN2P3	Nuclear reactions
IN2P3 project Speedy Charmonia	Benoît Blossier	IJCLab	PRACE	Lattice QCD
				Non-perturbative QCD
ANR LatHiggs			GENCI	
NC	Mariane Mangin-Brinet	LPCS		Nucleon structure and spectroscopy
IN2P3 project Flavour Probes	Vincent Morénas	LP-Clermont	CC-IN2P3	
				Flavor physics
NC	Marek Ploszajczak	GANIL	In-house cluster	Nuclear structure
NC	Hubert Hansen	IP2I	GENCI	Dense nuclear/QCD
	Jérôme Margueron		CC-IN2P3	Neutron stars
EPOSHQ	Klaus Werner	Subatech	CC-IN2P3	Quark-gluon plasma
	Jörg Aichelin			
	Pol-Bernard Gossiaux			HE nuclei-nuclei collisions
	Marlène Nahrgang			

Tableau 1: IN2P3 personnel self-reporting using HPC for theoretical particle and nuclear physics calculations.

All of IN2P3 staff reported above are part of international collaborations for developing HPC application. This has the advantage of sharing the efforts with foreign partners and, by this means, of a cquiring out-of-institute expertise. We also have to report that many of the scientists trained in France are hired abroad making a net loss of capabilities. The table also pinpoints the lack of institute wide policy on the topic, with the exception of LQCD for which IN2P3 personnel is geographically distributed. Last, the evolution of the workforce closely follows the CNRS 01/02 recruitments of nuclear/particle/astrophysics theoreticians, for which we have seen an increase in the last year but that did not turn into a renewal for the teams using HPC.

While the data are only partial, we show on **Erreur ! Source du renvoi introuvable.** students currently enrolled in a PhD program for a project using HPC. Data are self-reported. Yet, we can see that we are almost reaching a one-to-one ratio between permanent staff and PhD students. This is often the case in theory teams, however for the present case this means that students are not turned away by PhD project that involves large-scale computing skills. This is also a positive take away for the future of the discipline since many young scientists are being trained to use HPC as a tool for theory to support experimental programs.

7. Technical achievement

There are identified needs for institutional support in term of both postdocs, permanent scientists and "ingénieurs de recherche" dedicated to the development of HPC codes. This was clearly reported by the community in the document on the initiative of the GENCI that will serve as a basis to submit an application to the EU for hosting an exascale machine. This concerns either porting code towards GPU architecture, which is time consuming due to the specificity of vector machines and their memory congestion that requires fine tuning, or to support the developments, rewriting or new HPC applications within international collaborations.

We were reported that interconnection to/from GENCI machines (more specifically CEA/TGCC) to computer center abroad is very tedious to establish specifically for the transfer of large data files. The lack of a policy in this regard poses a significant threat to both efficient collaborative work and, for scientists outside the IN2P3 topics, may impede urgent decision making in the event of disasters.

The advent of exascale computing which is roughly an increase of one to two orders of magnitude in computational power, will revolutionize our usage of HPC applications. We will roughly be able to achieve ten times our current capability or increase five to ten-fold the accuracy of the modeling or simulations. Therefore, having support from teams of theoreticians, which have both access to HPC centers and are developing HPC tools, will be a competitive step for experimentalists whose goals are to publish new results backed-up by theory in high-impact journals. International competition is already underway. The need for human resources should not be underestimated.

Appendix A:. List of abstracts of the "Demande d'Attribution de Ressources Informatiques" (DARI) submitted to the GENCI.

i. GENCI project 0502271

La prise de données en physique des saveurs par les expériences s'accompagne nécessairement d'un travail théorique soutenu car l'extraction des quantités fondamentales s'effectue après une mise en commun des résultats expérimentaux et des prédictions théoriques. Celles-ci peuvent être délicates à faire à cause des effets de l'interaction forte, omniprésents dans les processus auxquels nous nous intéressons. Tandis que la formulation théorique exacte (QCD) décrit l'interaction entre les constituants élémentaires (les quarks et les gluons), l'expérience n'accède qu'aux états libres de ces constituants. La dynamique de ces états lies (mésons et baryons) est décrite par la QCD non-perturbative. A ce jour, la seule méthode qui nous permette de résoudre les effets non-perturbatifs d'une théorie des champs non-abélienne, à partir de principes théoriques premiers, est la méthode des simulations numériques

ii. GENCI project 0506006

Scattering experiment is the most important experimental technique in the quantum physics. Analysis of the experimental results strongly relies on the scattering theory. We are interested in a rigorous ab initio description of the nonrelativistic scattering processes. This domain of research has three major goals: provide accurate solutions for the physical phenomena test the knowledge of the interactions between the elementary particles and provide a guideline for building the simplified approximate methods. Because of a rapid rise in the complexity of the scattering process (number of degrees of freedom as well as possible reaction channels), the rigorous techniques are applicable only to the simplest systems, containing only a few particles. For a long time, rigorous solution of the scattering problem has been limited to the systems made of up to four particles. Few years ago, we have for the first time obtained rigorous solutions for collision process in a system made of five nucleons. We consider different facets of the aforementioned problem by beginning with the formal aspects of the scattering theory, then development of the efficient numerical techniques and approximations, finally realistic applications providing predictions for the realistic physical systems. Our domain of application includes nuclear, atomic as well as some exotic molecular systems. We participate actively, by providing theoretical expertise, in the innovatory experimental projects at CERN (PUMA, GBAR) and NIST (parity violating neutron spin rotation).

iii. GENCI project TMP20541

La nouvelle ère de l'astrophysique multi-messagers a commencé avec la première observation d'ondes gravitationnelles (Gravitational Waves, GW) et de contreparties électromagnétiques (signaux EM), comme les sursauts de rayons gamma (SRG), provenant de fusions d'étoiles à neutrons binaires (Binary Neutron Star, BNS). Elle nécessite la maîtrise de la relativité générale (RG) dans son régime fort, des processus dynamiques sous champs magnétiques forts et la connaissance ultime des propriétés de la matière dense. En rassemblant des experts mondiaux dans ces différents domaines, notre collaboration internationale vise à étudier les questions fondamentales de la matière dense en couplant des simulations magnétohydrodynamiques (MHD) en relativité générale (General Relativity MagnetoHydroDynamics, GRMHD) au métamodèle pour la matière nucléaire récemment développé et étendu pour inclure la température finie, la clusterisation nucléaire (matière inhomogène dans l'écorce) et diverses transitions vers des états exotiques dans la matière dense (transition de phase du premier ordre, crossover quarkyonique, etc). Les ressources demandées nous permettront d'aborder la question des multi-messagers (GW, SRG, neutrinos) produits par la coalescence de BNS et décrits par les simulations GRMHD et dans quelle mesure ces signaux fournissent des informations sur les propriétés de la matière dense, par exemple, des phases exotiques. Les premières explorations 1 de cette question ont conduit à des conclusions différentes, provenant des différentes transitions de phase qui ont été explorées, comme les auteurs l'ont eux-mêmes souligné. Dans l'étude proposée, nous prévoyons d'explorer différents types de transitions de phase, plus prononcées que celles qui ont étés étudiées jusqu'à présent tout en s'assurant qu'elles sont compatibles avec les connaissances actuelles. De cette façon, nous fournirons une compréhension plus large du rôle des transitions de phase. De plus, nous serons les premiers à implémenter des champs magnétiques et à analyser leur rôle dans la compréhension globale des transitions de phase.

iv. GENCI project 0513012

The present project pertains to low-energy nuclear theory, and more specifically to the microscopic description of atomic nuclei both from an *ab initio* perspective and via energy density functional methods. Its main objectives are:

1. To perform systematic calculations of nuclear structure and reactions with state-of-the heart *ab initio* techniques;
2. To develop new numerical methods that aim at the description of deformed medium-mass nuclei in an *ab initio* fashion, thus extending the current domain of applicability of *ab initio* calculations;
3. To apply the energy density functional approach to cases of high experimental interest.

The overall long-term goal is to achieve a global first-principles description of the nuclear chart with associated theoretical errors.

Appendix B:. Bibliography

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