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Physique Nucléaire et Astrophysique Nucléaire

Addressed aspects

1) Quantum computing. State of the art and applications
2) How artificial intelligence can boost nuclear theory? Neural network

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1) Quantum computing. State of the art and applications

Quantum simulations for many-body physics in condensed matter, chemistry, atomic physics, and nuclear physics may potentially bring us to address so-called ‘Grand Challenge’ problems, that is problems that cannot be addressed using classical computation. Quantum computing may provide the possibility to work with Hilbert space dimensionalities that are exponentially larger than those accessible with classical computers. A few algorithms for quantum computation were designed during the last two decades and first calculations for simple systems became feasible.
In this context, there is presently a lot of excitement among physicists, chemists, engineers and computer scientists. Companies such as Google, Amazon, IBM, Microsoft, and Rigetti are driving this and software is presently publicly available (for example cloud access is possible). First proofs of principle calculations were performed in chemistry and very recently in nuclear physics. For instance, the first real-world solved problem was carried out for the H2 molecule on two qubits [1] followed by a calculation on BeH2 on six qubits [2]. Along the same line, in nuclear physics, first calculation was performed for the deuteron [3] followed by application to heavier systems [4]. A variety of emerging technologies are now available or under development like small trapped-ion systems, cold-atom systems, annealing devices as well as superconducting quantum devices. These new hardware progress give the opportunity to perform pioneering calculations on quantum computers. In this context, intensive efforts are now devoted, especially in the US laboratories [5], to explore the potentialities of quantum computers for nuclear physics, particle physics and astrophysical problems. In recent years, a number of progress were recently made in this context [6-8] preparing future applications in nuclear physics and QCD.

Overall, this field is experiencing a new boost on a global scale. Programming on prototypes of quantum computers remains today a challenge in particular concerning adapted algorithms and the control of the quantum noise inherent to these types of computation. It seems timely to investigate whether the domains covered by the IN2P3 institute both at the informatics and/or fundamental research levels can benefit from these recent advances.

The quantum technology is clearly a disruptive technology with a high risk/high gain balance. Among the current challenges that are not specific to our fields but that should be addressed to progress in the next decade are:

a) Quantum Computing is now at the NISQ (Noisy Intermediate-Scale Quantum) era meaning that the noise in quantum gates is limiting the size of quantum circuits that can be executed reliably. This implies that applications of quantum computing todays should account for the inherent noise and quantum computers limited capabilities.

b) The quantum coherence that is the basis of quantum computers is destroyed due to coupling to environment on a rather short time-scale. This considerably reduce the type of quantum circuits one can perform quantum circuits one can send to a real quantum computer. For this reason, hybrid technologies where specific operations are sent back and forth between quantum computer/classical computers are now developed. The use of quantum computers in the IN2P3 fields in the near future requires to adapt to these constraints.

c) Progress in the field will also necessitate to understand, control and eventually take advantage of the physics of quantum systems in a noise environment. Specific efforts should be made to progress on the understanding and description of quantum many-body systems treated with a set of Qubits coupled to one or several destructive environments.

d) On a longer term prospective, beyond the NISQ era, one should anticipate the technology improvement and question the possibility to address complex theory problems that could not be made today on classical computers. To quote some of the problem, we mention ab-initio theories in nuclear physics or lattice QCD. This implies that novel algorithms adapted to the technology used in the quantum computer should be proposed and developed. In general, specific problems under interest should be completely rethink.

e) Besides the targeted goal in theoretical physics, many experimental, engineering or informatics branches of IN2P3 can potentially benefit from the quantum computing technologies using progress in quantum circuits, quantum annealing and/or quantum sensing. Each of these branches might require in the near future a specific survey to estimate the new opportunities. Particle recognition of particles in particle physics detectors is one of recent illustrations where this possibility has been seriously considered.

To give some illustrations of what is presently done in France outside IN2P3, the Paris Center for Quantum Computing (PCQC) was created in Paris, including computer scientists, physicists (mainly on quantum optics and cryptography), and mathematicians. Several GDRs exist, for instance the GDR IQFA (Quantum Information: Foundations and Applications) at the interface between the INP and INSIS institutes of CNRS. In 2018, an ERC synergy grant was attributed to INAC (CEA), CEA-LETI and the Insitut Néel (CNRS) in Grenoble (Qucube project) for the construction of a quantum processor with at least a hundred of physical qubits with silicon quantum technology.

To start a wide-ranging reflection on this within IN2P3, a meeting was organized in Orsay in December 2019: 'Journées Thématiques IN2P3 – Quantum Computing: state of the art and applications' (https://indico.in2p3.fr/event/19917/). The goal of this meeting was to invite experts in the field of quantum computing to present to non-expert scientists and engineers the state of the art in this area of research.

Such a reflection should be pursued within a short- and long-range reflection on activities in which IN2P3 could be involved in the following years.

References:

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2) How artificial intelligence can boost nuclear theory? Neural network

In the last decade, the field of machine learning have skyrocketed, encouraged by the successful new disruptive kinds of neural networks to data processing, e.g. image recognition. On the other hand, and despite the progress in high performance computing, nuclear theorists are still stumbling on the many-body problem for which sufficient accuracy and efficient algorithms must be achieved and devised, respectively. Why algorithm made to process data based on statistical analysis would matter in nuclear theory? It turns out that the dimensionality of the many-body problem is combinatorial and its solution (or partial solution) is, so far, designed by human brains and based on the scientist intuition of his/her representation of the physical system, which may be bias and partial. For instance, since Elliott's SU(3) model representation theory has been used in nuclear physics to adapt the many-body Hilbert space to the symmetries of the nuclear problem. The superiority of the method is shown in Figure 1 where the dimensionality of the problem can be severely shrunk. This example is a prototypical task that is concerned with weighting and sorting out vast data sets, and can be automatized, learned and improved by algorithms. Note that this intermediate step towards the solution of the Schrödinger equation does not carry any physics information henceforth it is not where the physicist inputs are the more relevant. Thus, developing new algorithms for the many-body problem based on weak artificial intelligence (AI) may revolutionized the field by removing the unnecessary preconditioning of the problem by the physicist. This question is no restricted to pure algorithmic concern but also extend to the development of new many-body method based on neural network. For instance, this is closely scrutinized by the many-body theory community of quantum chemistry and condensed matter. In fact, a first step in this direction have been achieved by solving spin lattice systems.

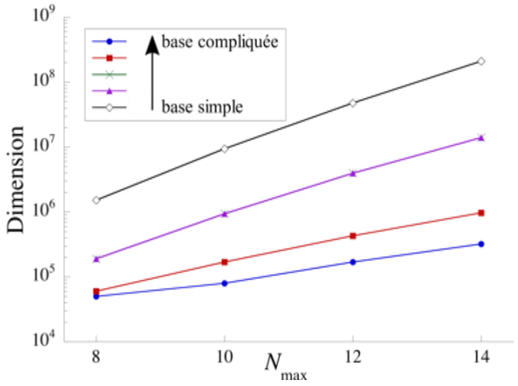

Figure 1: Typical dimension of the nuclear problem with 6 nucleons. Adapted from T. Dytrych at al. CPC 207, 202-210 (2016).

Unfortunately, in the low-energy nuclear community this potential has barely been considered. The few applications originate from North America and are restricted to fairly simple tasks such as 1D or 2D extrapolation of many-body truncation. An overarching goal for the community could consist in assessing the potential of AI and developing innovative solutions based on neural networks to solve quantum many body problems that are out of reach with traditional techniques.

In a nutshell, the main questions to be addressed are:

1. Can we develop innovative solutions based on neural networks to solve quantum many body problems that are out of reach with traditional techniques? A few ideas that could be considered are:
    a. Can we use neural networks to learn traditional many-body techniques i.e. as a metamodel which would allow computation at a cheap cost? This would strongly benefit experimental applications with the strong limitation that it is bound by the validity of the current structure models used in the learning set. It clearly stands as a first step.
    b. In the standard many-body toolchain, a number of processes require linear algebra in close connection with image processing, e.g. derivation of a soft nuclear interaction for configuration interaction methods like similarity renormalization group technique or Okubo-Lee-Suzuky method. Are these methods learnable by AI and could they be replaced by feedforward neural network? can we use generative adversarial network to reduce the contribution of induced operators of higher rank?

   c. Can we fully learn a nuclear interaction in momentum or harmonic oscillator spaces? Can we then use it as a traditional shell model interaction - meaning fit the input parameters of the nuclear interaction within the many-body model space truncation? Can we extract from mean-field (Khon-Sham) potentials the corresponding renormalized bare interaction parameters, for instance the chiral c_i, d_i ... constants in the case of chiral pionful(less) effective field interaction, using the same neural network? In other word can we reverse engineered the in-medium renormalization of the nuclear interaction?
   d. Can we use AI to systematically truncate the many-body space thus lifting the current computation limitation? Can established new many-body method based on neural network and reduce the computation of the many-body Schrodinger solution to polynomial time?
2. What nuclear phenomenology and properties can be learned by an AI and how is this information encoded into the AI internal representation? Can we infer unknown properties of nuclei from the AI internal representation of the physics? Can we finally make predictive nuclear models? Can we find new physics in region of the nuclear chart that is believed to be well known and tabulated?

A scientific program dedicated to this topic will allow physicists to characterize the value of neural networks to solve complex quantum problems. If the expected results are achieved, we will be in the unique situation where a major technological roadblock between basic research and its applications has been lifted. Finally, the progress made will have a significant transversal impact, particularly in the fields of quantum chemistry and atomic physics, which encounter the same type of problem.