From Quantum computing to Machine Learning

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Nov 29, 2017

Strategic importance

This letter states our intent to submit a proposal for **two FISP PhD fellowships** at the Department of Physics of the University of Oslo.

The aim is to lay the foundation for the development of new activities in Computational Science and Physics at the University of Oslo, with a strong focus on computational technologies for the future, from quantum computing to machine learning.

The proposed activities are expected to lead to an application for a future center of excellence (The Norwegian SFF program) in Computational Physics and Science application, where focus on new computational approaches for studying complex systems will play a central role.

Quantum Computing and Machine Learning are two of the most promising approaches for studying complex physical systems where several length and energy scales are involved. Traditional many-particle methods, either quantum mechanical or classical ones, face huge dimensionality problems when applied to studies of

Synergies and impact. Based on the above arguments, the long-term perspective for this application is to lay the foundation for a new center of excellence in research, where Computational Science and Physics play a central role. Since the problems to be addressed are complex multiscale scientific problems, the center will, by the very nature of the problems, be multidisciplinary.

Furthermore, this activity will have strong educational outcomes and is expected to be tightly linked with the newly established center of excellence in education, the **Center for Computing in Science Education** (CCSE). This center aims at developing a novel research program on assessment methods in science educations, with large implications for the way research in science education is conducted. Machine Learning will play a central role there as well when analyzing large data sets, providing us thereby with a truly quantitative approach to science education. We expect thus that the two PhD fellows involved with this project will benefit from cross-fertilizations and synergies with the activity at the CCSE and viceversa.

The present proposal will also lay the foundation, in close

Background and previous experience

This research is strongly rooted in the activities of the award winning Computational Physics group at the Department of Physics. Since 2003, close to 70 students have finalized their Master of Science theses, and approximately half of these students have continued with PhD studies. These highly qualified candidates testify to a strong and robust educational environment. We have presently several excellent PhD candidates who are finalizing or will finalize their Master of Science theses. Many of these candidates have applied and developed Machine Learning methods to solve complex and interacting many-particle systems. These activities have a strong overlap with the research programs of the two principal investigators (Hjorth-Jensen and Malthe-Soerenssen). We foresee also strong links with the CCSE.

The two PIs have a long-standing experience in developing and applying algorithms for quantum mechanical and molecular dynamics simulations of many interacting particles, with applications spanning from dense subatomic matter to the physics of complex materials.

Research Program

The research program will focus on two main topics:

- **Quantum Computing** for studies of quantum mechanical systems with many particles (PhD 1). The focus is on
  - Subatomic matter
  - Atomic and molecular physics, with applications to Materials Science and Life Science
- **Machine Learning** focusing on the training of potentials for Molecular dynamics studies of large numbers of interacting particles (PhD 2), with applications to systems in
  - Condensed Matter Physics,
  - Materials Science and
  - Life Science

Another possible project which links the two main topics is to use Machine Learning algorithms to study quantum mechanical systems. Here one can think of using restricted Boltzmann machines and supervised learning to improve and optimize correlations in classical quantum mechanical many-body methods. A further approach is to use supervised learning to optimize density functionals. Density Functional theory is widely used to described

Why Multiscale Science? The aim of a program on multiscale physics is to develop a first principle approach to systems of relevance for a variety of fields, from materials science to nano-technology and biological systems and even atomic nuclei and stars. Common to all these systems is that they entail a truly multiscale physics program that involves a proper understanding of the links between the various scales, starting from quantum-mechanical first principle studies of atoms, molecules and eventually other spatially confined systems to Density functional theories and finally microscopically derived potentials to be used in molecular dynamics calculations. Such a program involves insights and collaborations across disciplines in order to foster progress.

The computations required for accurate modeling and simulation of large-scale systems with microscopic resolution involve a hierarchy of levels of theory: quantum mechanics (QM) to determine the electronic states; force fields to average the electronics states and to obtain atom based forces (FF), molecular dynamics (MD) based on such an FF; mesoscale or coarse grain descriptions that average or homogenize atomic motions; and finally continuum level descriptions. By basing computations on first principles QM it is

From Quantum Computing to Machine Learning. Enabling simulations of large-scale many-body systems is a long-standing problem in scientific computing. Quantum many-body interactions define the structure of the universe, from nucleons and nuclei, to atoms, molecules, and even stars. Since the discovery of quantum mechanics, a lot of progress has been made in understanding the dynamics of certain many-body systems. While some of our insight comes from a small set of analytically solvable models, numerical simulations have become a mainstay in our understanding of many-body dynamics. The progress in numerical simulations has accelerated in the last few decades with the advent of modern high performance computing (HPC) and clever developments in classical simulation algorithms such as, quantum Monte Carlo,large-scale diagonalization approaches, Coupled-Cluster theory and other renormalization schemes. Despite the monumental advances, classical simulation techniques are reaching fundamental limits in terms of the size of the quantum systems that can be processed. Fortunately, the disruptive new field of quantum simulations has emerged, promising to enable simulations far beyond those which are classically tractable. In particular, scientific applications