From Quantum computing to Machine Learning

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Strategic importance

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.

1. 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, **Computing Across the Disciplines**, where focus on new computational approaches for studying complex systems will play a central role
2. Establish an educational Marie-Curie training program on Computational Science and Physics
3. Strong links with the newly established center of excellence in education, Center for Computing in Science Education

Multiscale Science

The aim of our research 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.

Mulitscale challenges in Subatomic Physics

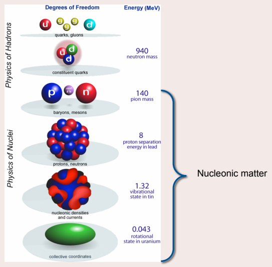

Figure: The many scales pose a severe challenge to first principle descriptions of nuclear systems.

Why Quantum Computing and Machine Learning

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.
The IBM Quantum Experience allows you now to test real quantum computing systems.

Challenges to Traditional Many-Particle Methods

Traditional many-particle methods, either quantum mechanical or classical ones, face huge dimensionality problems when applied to studies of systems with many interacting particles.
To be able to define properly effective potentials for realistic molecular dynamics simulations of billions or more particles, requires both precise quantum mechanical studies as well as algorithms that allow for parametrizations and simplifications of quantum mechanical results. Quantum Computing offers now an interesting avenue, together with traditional algorithms, for studying complex quantum mechanical systems.

More Challenges to Traditional Many-Particle Methods

Machine Learning allows us to parametrize these results in terms of classical interactions. These interactions are in turn suitable for large scale molecular dynamics simulations of complicated systems spanning from subatomic physics to materials science and life science.

Machine Learning plays nowadays a central role in the analysis of large data sets in order to extract information about complicated correlations. This information is often difficult to obtain with traditional methods.

1. Developing activities in these frontier computational technologies is thus of strategic importance for our capability to address future science problems.
2. The problems we target satisfy the dual criteria of being integral to the fundamental understanding of complex physical systems and also compelling a major conceptual advance in method or theory with broad applications to other science fields.

Long-term perspective, synergies and impact.

- The long-term perspective for this application is to lay the foundation for a new center of excellence in research **Computing Across the Disciplines**
- Strong educational outcomes with tight links with the newly established center of excellence in education, the **Center for Computing in Science Education** (CCSE).
- Establishment of an educational Marie-Curie training program on Computational Science and Physics, with a strong focus on the above research topics.
- This project will enable several research collaborations in fields like Materials Science, Condensed Matter Physics, Subatomic Physics and Life Science.

Background and previous experience

- This research is strongly rooted in the activities of the award winning Computational Physics group at the Department of Physics.
- We have presently several (6) excellent PhD candidates who are finalizing or have finalized their Master of Science theses. Many of these candidates have applied and developed Machine Learning methods to solve complex and interacting many-particle systems. We have presently 27 MSc students.
- 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 and life science.
- The proposal will also benefit from extensive collaborations with leading Universities and Laboratories in Northern America (Oak Ridge National Laboratory, Michigan State University and University of Washington).

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, in particular properties of dense 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

A Machine Learning approach to Science Education, as represented by the CCSE, offers a link for further synergies and testbeds of algorithms from Machine Learning.