A LQCD spin-off: sub-minute high performance Monte Carlo calculations for accelerator physics, radiotherapy and nuclear medicine

Research Project / Research Group Description:
QCD is the theory of the strong interactions that glue together quarks inside hadrons. Is it a confining theory? This is one of the fundamental questions. K. Wilson invented Lattice QCD (LQCD) to understand asymptotic freedom and the confinement of QCD from first principles.

Since the number of degrees of freedom is very large, Monte Carlo (MC) methods and massively parallel computers are mandatory. Most of our quantitative results of LQCD are based on such numerical studies. But our expertise in LQCD and MC simulations can also be used to model and analyze radiation transport for accelerator physics and radiation therapy (RT) applications, which is a widely used form of tumor control based on the application of ionizing radiation. An essential requirement for successful RT is that absorbed dose distributions (ADD) delivered to the tumor will be maximized while absorbed dose to organ at risk will be minimized in such a way that complications will be reduced and rate of cure will be increased. Therefore, an accurate theoretical calculation of ADD is crucial. MC methods are able, in principle, to predict radiation-matter interactions exactly and therefore to obtain ADD in any arbitrary material.

PENELOPE [1] is a general-purpose, versatile and thorough MC code for simulation of coupled electron-photon transport in arbitrary materials and geometries. It incorporates a detailed material library and complex geometries can be modeled using quadric surfaces and/or voxelized volumes. PENELOPE incorporates physical models based on the most reliable information currently available from 50 eV to 1GeV.

The main factor restricting the MC precision is its inherent statistical uncertainty, which can be reduced providing enough computational time and facilities are used. This has severe limitation on its application in real-time clinical practice since performance time needs to be reduced from the multi-hour timescale usually required in realistic clinical cases for state-of-the-art MC codes to the order of tenths of a second. The present project proposal aims to address such important problem in RT by improving the speed of the computational algorithms forming part of PENELOPE. The results of this project will allow performing fast and accurate calculations of the ADD in RT.
[1] J. Baró et al, Nucl. Instr. and Meth. B 100, 31–46 (1995).

Job position description:
Monte Carlo simulations are the gold standard for modeling and analyzing radiation transport through matter. They try to mimic nature by following multiple particle trajectories across an absorber material using the laws of physics. PENELOPE [1], developed at the University of Barcelona, is a well-tested MC code for the simulation of electrons, positrons, and photons in arbitrary materials and geometries. PENELOPE's core is made of a set of FORTRAN subroutines and a rather comprehensive programming knowledge is required before starting a simulation. It is important to mention that the physics library included in the 2001 version of PENELOPE was included in the Geant4 distribution as an optional physical library to address a more

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precise treatment of electromagnetic showers and interactions at low-energy (keV scale). It was also recommended for simulations were the atomic effects (fluorescence x-rays, Doppler broadening, etc.) and low-energy positrons were relevant.

Specific Aims
This project aims to address the following milestones:
Translation. In order to fully use PENELOPE in clinical situations making use of modern techniques based on massively parallel GPU (Graphics Processor Units) and Intel Xeon Phi coprocessors, it is imperative to abandon FORTRAN and translate this software into more modern languages, like C++ ANSI. This is fundamental to apply parallelization techniques and address memory occupation issues.

Benchmarking. Once such computing work has been done a full battery of benchmarking tests has to be undertaken to reproduce as many scenarios as possible in an energy range as large as possible. This will include both theoretical and clinical cases already analyzed by the Medical Physics Group of the University of Valencia.

Optimization. Once the new code is fully tested the algorithms will require to be optimize, probably even reprogrammed in such a way that both the full parallelization capabilities and parallelization performance of GPUs and Xeon Phi coprocessors can be used.

Skills required
Knowledge of C++ ANSI is an indispensible requirement for this project.
Fortran knowledge is also recommended.
A good working knowledge on radiation physics.

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