Computing Properties of Hadrons, Nuclei and Nuclear Matter from Quantum Chromodynamics

SciDAC-3 Scientific Computation Application Partnership project

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A fundamental quest of modern science is the exploration of matter in all its possible forms. The overarching mission of theoretical Nuclear Physics is to establish a framework with which to perform high-precision calculations, with quantifiable uncertainties, of the properties and interactions of nuclear matter under a broad range of conditions, including those beyond the reach of laboratory experiment. Since the 1970's, quantum chromodynamics (QCD), a non-Abelian quantum gauge field theory constructed in terms of quarks and gluons, has been established as the theory of the strong interactions which, along with the electroweak interactions, is responsible for all nuclear phenomena. However, many aspects of nuclear physics are dictated by the regime of QCD in which its defining feature – asymptotic freedom – is concealed by confinement and by the structure of its vacuum. The numerical technique of Lattice QCD enables ab initio QCD calculations of strong interaction quantities in this regime.

Software and Algorithmic Developments

This project will undertake the algorithmic and software development needed to enable the nuclear physics lattice QCD community to make optimal use of forthcoming leadership-class and dedicated hardware to address key problems in nuclear physics, and to prepare for the exploitation of future computational resources in the exascale era.

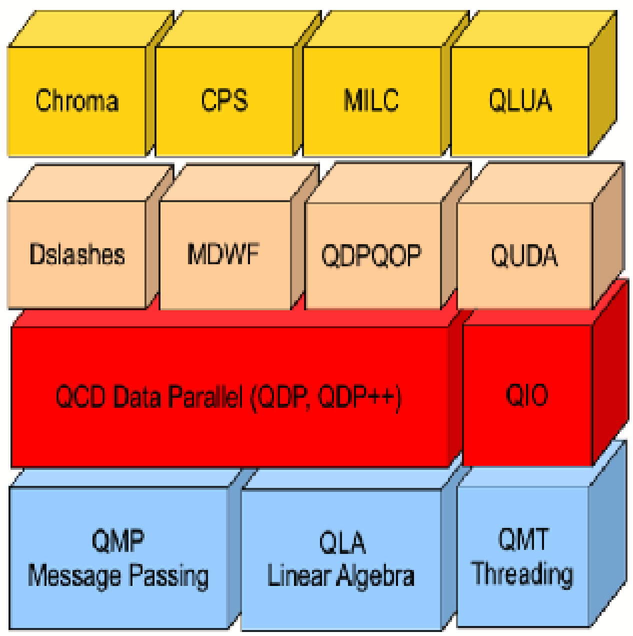

Figure 1: SciDAC Layers and the software module structure (http://www.usqcd.org/usqcd–software)

The project will further develop and optimize simulation software for lattice QCD calculations on leadership class computers, including those with heterogeneous architectures. The participating teams will improve and extend software libraries (Chroma, CPS, MILC, QLUA) by providing interfaces for heterogeneous computing environments and through the optimization of gauge field evolution algorithms and sparse matrix inverters. The former includes the development of new multi-time scale integrators and the latter will focus on the development of new multi-grid and domain decomposition inverters for several QCD fermion discretization schemes. The project furthermore will develop a domain specific language for lattice QCD computations which will enable the generation of highly optimized code within the ROSE compiler framework.

Collaborations and links to SciDAC Institutes

Work on algorithms will be performed in cooperation with the FastMATH SciDAC institute, while work on compiler will be carried out in cooperation with SUPER. The optimization of software for specific compute platforms will be coordinated with development teams of hardware manufactures at IBM, INTEL and NVIDIA.

The software development performed by this project is coordinated with that of the Scidac-3 project "Strongly-Coupled Field Theories at the Intensity and Energy Frontiers". Both projects are part of the software development effort of the USQCD Collaboration, which consists of nearly all of the high energy and nuclear physicists in the United States working on the numerical study of lattice gauge theories. All software developments will be made publicly available through the USQCD collaboration WEB page (http://www.usqcd.org).