Computing Properties of Hot and Dense Nuclear Matter from Quantum Chromodynamic

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

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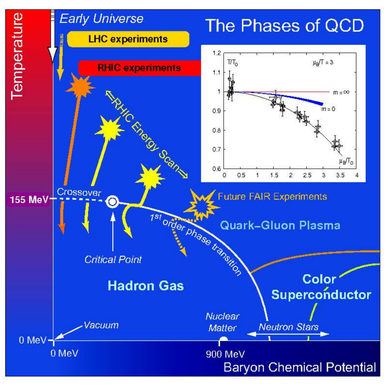
Abstract: Under conditions of extreme temperature or densities the constituents of protons and neutrons, quarks and gluons, get liberated and form a new, largely unexplored state of matter. Numerical calculations based on lattice regularized Quantum Chromodynamics (QCD) allow to study the transition from the hadronic phase to the quark gluon plasma phase. They provide input to the interpretation of large experimental programs at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory and the Large Hadron Collider (LHC) at CERN, Switzerland. In the poster, we describe recent successes at understanding the properties of hot and dense matter from lattice QCD, and future questions that will be addressed through our SciDAC activities. In particular, we describe the computational challenges, and the likely impact of the resulting calculations on current and future experiments.

Thermodynamics of Strongly Interacting Matter

At low temperatures and densities ordinary hadrons are the prevailing degrees of freedom that determine the properties of nuclear matter. However, under extreme conditions of high temperature or of high density (or both) this is expected to change. The theory of strong interactions (Quantum Chromo Dynamics (QCD)) predicts that a phase transition or crossover occurs that separates the low



temperature/density regime of ordinary hadronic matter from a high temperature/density region where quarks and gluons, the basic constituents of QCD, become the most relevant degrees of freedom.

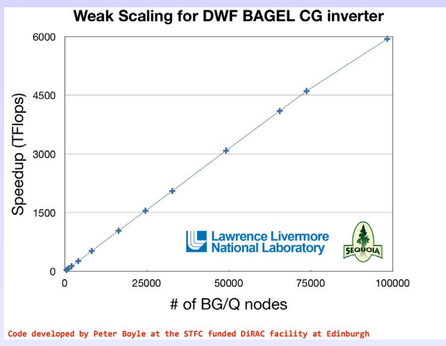
Deriving detailed predictions for the properties of matter at high temperature and density directly from QCD is paramount in shaping our understanding of nuclear matter in general, as well as for understanding the evolution of the early universe. Large experimental programs at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven, USA, and the Large Hadron Collider (LHC) in Geneva, Switzerland, exist which explore the properties of matter at high temperature and/or density, with the aim of mapping the boundaries between different phases of strongly interacting matter, and determining quantitatively the properties of matter in this domain. This is illustrated in the phase diagram displayed to the left. In an inset it also shows results from a lattice QCD calculation of the transition line (blue band) as well as a collection of experimental data on the temperature and baryon chemical potential values at which hadrons are formed (freeze-out) in heavy ion experiments.

Lattice QCD

Lattice QCD (LQCD) provides us the necessary non-perturbative, parameter free theoretical calculations of properties of hot and dense matter starting from the first principle QCD Lagrangian. LQCD is an alternative regularization scheme for QCD suitable for large scale numerical simulations. In this formulations the four-dimensional Euclidean space-time is discretized, fermions are introduced as site variables and the gluons are introduced as $SU(3)$ matrices residing on the links between the sites. The QCD path integral is then represented as an ordinary integral over all these site and link variables. This large dimensional integral, about 72M dimensional integral for a modest 32^4 lattice, is then numerically evaluated using the Hybrid Monte Carlo (HMC) technique. The HMC algorithm consists of two steps— a Molecular Dynamics evolution and a subsequent accept-reject step to implement the Monte-Carlo important sampling. Using the HMC algorithm many gluonic field configurations are generated. Various observable operators are measured on each gluonic field configuration and subsequent averaging is performed by measuring over many such gluonic field configurations to obtain observable quantities. The most computationally costly part for both the HMC gluon field generation and the measurements of observables involves the inversion of a large, sparse matrix representing the fermionic variables collectively. Thus a major part of the LQCD software developments are focused on developments/optimizations of fermion matrix inverters for the BlueGene/Q type and the GPU based supercomputers.

Optimizing DWF software for BlueGene/Q

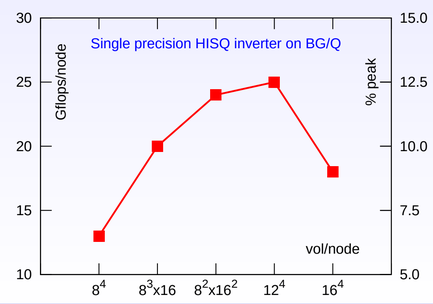
Domain Wall Fermion (DWF) is one of the very few fermion formulations within LQCD which possesses exact chiral symmetry even for a non-zero value of the lattice spacing. A few Lattice gauge theorists from UK and USQCD participated in the design of BlueGene/Q, which allowed a timely development of optimized Domain Wall Fermion (DWF), Mobius and Wilson inverters. Peter Boyle, Edinburgh University, developed most of the assembly generator library (BAGEL) optimized for BlueGene/Q, and also DWF inverters written with assemblies generated from BAGEL (BFM). Both BAGEL and BFM are publicly available at http://www2.ph.ed.ac.uk/ paboyle/bagel/ Bagel.html. DWF inverter in BFM achieves up to 66 GFlops/s per node in single precision and 47 GFlops/s in double precision. The DWF inverter in BFM achieves up to 66 GFlops/s per node in single precision, 47 GFlops/s in double precision. It has been run on up to 96 racks of BlueGene/Q at Sequoia, achieving 5.94 PFlops/s so far on a single job. A weak scaling performance plot for the DWF inverter on Sequoia is shown in the right column.

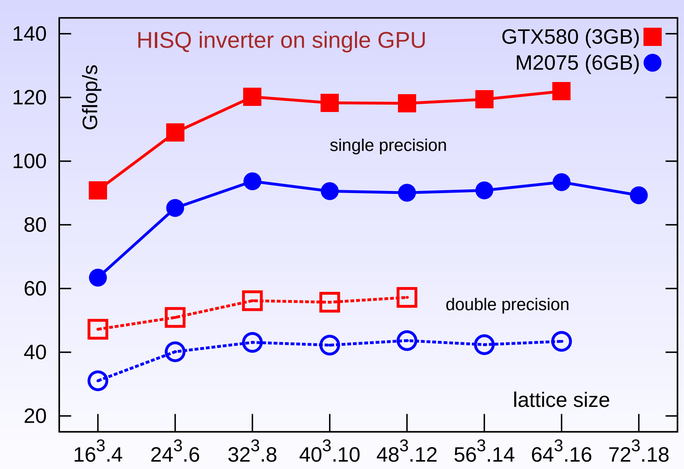


Routines in BFM are integrated into the Columbia Physics System(CPS) (http://qcdoc.phys.columbia.edu/cps.html), which has been used for DWF evolution and the measurement of thermodynamic observables by the HotQCD collaboration at Sequoia. CPS is built on USQCD SciDAC libraries such as QMP and QIO to benefit collectively from the USQCD SciDAC activities. To overcome Amdhal's law, a significant amount of work is done in CPS to make all the rest of routines needed for ensemble generation fully threaded and optimized, using OpenMP or pthread. Further optimization is planned for measurement routines.

Optimizing HISQ software for BlueGene/Q

Highly Improved Staggered Fermions (HISQ) is another fermion formulation which is extensively used for the study of the properties of hot and dense matter. For the HISQ fermions freely available software is developed by the MILC collaboration as part of the SciDAC project. This code can be linked together with SciDAC libraries that include architecture-dependent optimizations. Critical parts of the MILC code that rely on the SciDAC libraries are the conjugate gradient, gauge and fermion force as well as link fattening routines. Several layers of the SciDAC stack, namely, QMP, QIO, QLA, QDP and QOPQDP provide this functionality, with the highest level interface residing in the QOPQDP library. BlueGene/Q optimization enters at the level of communication, QMP, and also in the internal loops and data structures, mainly QDP. This optimization relies on IBM SPI and also multi-threading technology. QMP and QDP libraries optimized for BlueGene/Q are being currently developed at the Argonne Leadership Computing Facility utilizing the Mira supercomputer. Some preliminary performance results for the HISQ inverter on Mira is shown in the figure below.



Finite Density QCD on GPUs

LQCD computations at non-zero (baryonic) density demand a different type computing strategy involving the measurement of fermionic observables which requires a large number of inversions of the fermion matrix. For each gluonic field configuration one requires about 25000 inversions of the fermionic matrix. Due to this high computational cost such computations are at present limited to relatively smaller lattice sizes. Thus this type of computations are ideally suited to be performed utilizing GPU based supercomputers. Due to the modest memory requirements of the relatively smaller lattices it is possible to perform a matrix inversion using a single GPU, completely eliminating the bottleneck of GPU-GPU communications. Moreover, since many sets of such inversions can be performed independently and simultaneously with the use of many independent GPUs, this type of computations is ideally scalable on supercomputers based on thousands of GPUs such as the Titan at the Oak Ridge National Laboratory. Thus the main software development for this type of computations involve developments and optimizations of single GPU fermion matrix inverter for various GPU architectures. The figure on the right shows the performance of the single GPU HISQ inverter for the two different NVIDIA Fermi generation GPU architectures. This software suite is developed by the lattice gauge theory group of Bielefeld University, Germany, in collaboration with the lattice gauge theory group of the Brookhaven National Laboratory. Parallel to this software development there is also a large scale on-going effort by the USQCD collaboration in the direction of developments of multi-GPU software for large scale GPU based supercomputers. In order to utilize the potential of such architectures one requires codes that can simultaneously use the GPUs as well as the CPUs. Such software developments are in the pipeline.