Continuing progress on a lattice QCD software infrastructure

Bálint Joó on behalf of the USQCD Collaboration
Thomas Jefferson National Laboratory, Newport News, VA 23606, USA
E-mail: bjoo@jlab.org

Abstract. We report on the progress of the software effort in the QCD application area of SciDAC. In particular, we discuss how the software developed under SciDAC enabled the aggressive exploitation of leadership computers, and we report on progress in the area of QCD software for multi-core architectures.

1. Introduction
Large-scale numerical lattice quantum chromodynamics (QCD) simulation programs require extensive software infrastructure [1]. In this contribution we report on some advances in the SciDAC-supported software work in the USQCD national program [2] during the past year. Details about the scientific results from numerical QCD simulations can be found in [3].

Considerable effort was invested this past year in preparation for using the leadership computing facility at Argonne and Oak Ridge national laboratories. We have also carried out investigations into the efficient use of multicore architectures for QCD. Our data sharing efforts have progressed, and we continue to extend and refine standards within our collaboration and worldwide. This article is organized as follows. In Section 2 we present some highlights of our exploitation of leadership computing resources. We report on our threading research in section 3. We discuss data sharing in section 4 and briefly consider other activities in section 5.

2. Exploiting leadership facilities for QCD
During the last year, all of our large community codes have been successfully ported to leadership systems of interest. In particular, the Chroma [4] and MIMD Lattice Collaboration [5] (MILC) codes have been deployed on the Cray XT, Blue Gene/P, and recent cluster hardware, while the Columbia Physics System (CPS) [6] has been ported to the Blue Gene/P. Considerable effort has been invested in the optimization of high-performance components for these architectures.

We show in the left half of figure 1 the performance of the MDWF solver on the BlueGene/P at Argonne. MDWF is an optimized domain wall fermion (DWF) conjugate gradients inverter package, developed at MIT [7], which incorporates several DWF operator variants. One can see that the single-precision solver achieves 800 Mflops/core (about 25% of peak). The solver performance is roughly constant over a variety of volumes, indicating strong scaling, and the recursive data ordering on node results in effective use of cache for the larger problems. MDWF has been interfaced with Chroma for production use by Jefferson Lab (JLab) staff.
Figure 1. Performance on the Blue Gene/P for MDWF [7] (left) and AsqTAD (right) inverters. The MDWF measurements were made with Chroma interfaced to MDWF 1.1.4 on Surveyor. The AsqTAD numbers are from the MILC Code on Intrepid. Both machines are at the Argonne Leadership Computing Facility.

The MILC researchers have optimized their AsqTAD conjugate gradients solver for the Blue Gene/P and the Cray XT series and their gauge force for a variety of platforms. We show the performance of their AsqTAD inverter on the Argonne Blue Gene/P in the right-hand plot of figure 1. One can see that the weak scaling is excellent all the way out to 32K cores.

Figure 2. Production history of an AsqTAD staggered fermion run through late 2006, 2007, and early 2008 (left) and for some domain wall fermion production runs (right).

To emphasize the impact the leadership machines have had on our data production, we show in figure 2 the production history of both an AsqTAD run and some DWF runs over the past year. The AsqTAD production was performed by using the MILC code, while the domain wall fermion production was carried out by colleagues based at Columbia University and Brookhaven National Laboratory using the CPS code. The dramatic increases in production brought about by the Blue Gene/P for both sets of data production (red lines) are clearly evident.

In summary, USQCD has completed successful ports of its applications to leadership hardware
and is now reaping the benefits in terms of science production.

3. Threading investigations

In preparation for the arrival of multicore hardware, JLab staff, in collaboration with EPCC in Edinburgh, UK, have added threading support to one of our key computational kernels, called Wilson Dslash [8]. This kernel is a four-dimensional nearest-neighbor operator. We show a 2D schematic picture of the communications patterns in this operator in figure 3 for a pure MPI implementation on the left, versus a hybrid-threaded one on the right. Two potential efficiency gains are immediate. First, one can see that threading on-node eliminates on-node messaging (green arrows in the figure). Second, the threading effectively coalesces multiple messages that would have been sent by individual cores into fewer, larger messages sent by the node (red arrows, ellipses in figure), strategy that may be advantageous in some networks.

![Figure 3.](image)

Multithreading on a node is typically realized by using OpenMP or some custom thread library. We have developed a lightweight thread library called QCD Multi-Thread (QMT) [9], which enables a data-parallel programming technique similar in spirit to OpenMP: Work is supplied to QMT by calling the `qmt_call()` library function, with a callback procedure that can perform part of the desired work. QMT then invokes this function, with different parts of the problem from different threads. When `qmt_call()` completes, it calls a barrier among the threads to synchronize them. In the work described here, we used QMT with a queue-based barrier, optimized for the MOESI cache coherence protocol on AMD Barcelona cores.

Our numerical experiments consisted of running the Wilson Dslash operator on several nodes of the Jaguar Cray XT4 system at ORNL, either as a pure MPI or as a hybrid MPI-threaded application, using alternately both OpenMP and QMT for the threading. We performed our tests on a single node and then repeated them on 16 nodes that could be mapped as a $2^4 \times 2^4$ processor grid communicating in four directions. The tests were repeated using several local volumes: $2^4$, $4^4$, $6^4$, and $8^4$. In particular, the $2^4$ volume is our hard scaling limit with all sites on the surface, and the $8^4$ volume is typically too large to be cache resident. We have found the $6^4$ volume most efficient, with $4^4$ volume case less so because of a worse surface-to-volume ratio.

Our results are shown in figure 4. Figure 4(a) shows that on a single node the QMT and MPI performances are essentially identical. Looking at results for 16 nodes, we see that the threaded performances are much improved for the $4^4$ and $6^4$ volumes over the pure MPI case. In the cases of the smallest and largest volumes, there seems to be no difference between the pure MPI and
Figure 4. (a) Effects of threading the Wilson Dslash operator on a single node (left) and a partition of 16 nodes (right) of Jaguar. (b) Weak scaling of the performance of the Wilson Dslash operator on Jaguar for two fixed local volumes: $4^4$ sites (left) and $6^4$ sites (right), to 4096 cores.

hybrid threaded versions. In the situations where threading results in a gain, using QMT for on-node threading results in a higher performance than when using OpenMP.

We then performed a weak scaling benchmark for the $4^4$ and $6^4$ local volumes in an attempt to scale the gains from the hybrid-threaded approach up to a large partition. Our results are shown in figure 4(b). One can see that for both local volumes, a performance advantage is maintained over pure MPI for as far out as 4096 cores when using QMT. When using OpenMP, the weak scaling appears quite erratic, but typically performance is less than the QMT case except for the 4096 core partition size.

Our interpretation of these results is as follows. Since single node tests suggest no gain from eliminating on-node messages, we surmise that in our application, threading gains performance over pure MPI as a result of the collation of off-node messages. This gain is likely to be network and OpenMP implementation dependent. Our limiting $2^4$ volume is completely communications bound with very few flops to overlap with communication, hence the low performance in that case for all the approaches tried. In the cases of the $4^4$ and $6^4$ volumes, message collation reduces the number of messages and increases their size, thus taking better advantage of the Cray network. In the $8^4$ volume case we fall out of cache, and all approaches appear to perform equally.

In this investigation, we have neglected issues that arise in multisocket NUMA architectures such as thread, process, and memory affinity. We have also not explored general multicore aspects such as the abundance of floating point power versus the comparative lack of memory bandwidth. Partitioned Global Address Space languages such as UPC provide a natural programming model for NUMA based architectures, and aggressive prefetching and double buffering may alleviate the memory bandwidth issue to some degree. Some of these concerns are investigated in [10], and we intend to explore these issues more fully in future work.

4. Data sharing and Grid-related efforts
Our data-sharing efforts have continued in the past year by publishing many of our gauge configurations on the International Lattice Data Grid (ILDG) [11] and some through other
channels [12, 13]. Our ILDG infrastructure is based jointly at Fermi National Accelerator Laboratory, where the storage element is hosted and managed, and at JLab, where one can find the Metadata and File Catalog Web Services. Some 11,000 configurations are now published in 16 ensembles through the ILDG. Conversely, in the past year several U.S. researchers have joined the ILDG virtual organization, in order to use published data shared through ILDG.

Within USQCD data sharing has moved forward through the definition of file formats for quark propagators and the implementation of software to read and write the standard within the QIO library. Application codes have also been modified to read and write these files. European collaborators have defined propagator formats that are compatible with the USQCD format, and there is some hope that worldwide propagator sharing will eventually be formalized in the ILDG.

5. Other activities
The USQCD software program continues its work and collaboration in many other areas not discussed here for lack of space, including the application of workflows to QCD, algorithmic developments, improvements to data analysis, code optimization, visualization and the use of Grid technologies.

6. Summary
In this contribution, we presented an overview of software progress in lattice QCD in the U.S. over the past year, with emphasis on performance achieved on leadership computers, and our work on multicore architectures. Much of this work was carried out in international collaboration, in particular with colleagues in the UK. We intend to continue progress in the software area in the future in order to carry on with our highly successful exploitation of available resources and to continue producing high quality scientific results and discoveries from lattice QCD.

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