Office of Science Final Report

Project Title: Scientific Discovery with the Blue Gene/L
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This project succeeded in developing key software optimization tools to bring fundamental QCD calculations of nucleon structure from the Terascale era through the Petascale era and prepare for the Exascale era. It also enabled fundamental QCD physics calculations and demonstrated the power of placing small versions of frontier emerging architectures at MIT to attract outstanding students to computational science.

The work of computer scientist Joy Khoriaty, postdoctoral researcher Meifeng Lin, graduate student Sergey Syritsyn and postdoctoral researcher Stefan Krieg has been described in previous reports, and they have all moved on to the next stages in their careers.

At the suggestion of Dmitri Kusnezof of NNSA, MIT hosted a workshop September 19 2008 to brainstorm ways to promote computational science at top tier research universities and attract gifted students into the field, some of whom would provide the next generation of talent at our defense laboratories. Resources were added to the budget designated to support this workshop, and the unexpended workshop funds of \$21,279.70 were returned to the DOE. Sid Yip of MIT wrote a report summarizing this successful workshop.

Principal Research Scientist Andrew Pochinsky, who was supported by ASCR under SciDAC1 and SciDAC2, oversaw the software development carried out under this project. When the one year extension of SciDAC2 was not funded, subsequent to the original end date of this present project, we requested and were granted a no-cost extension to use the remaining funds to partially fill the the gap in funding his salary. In the next section, we describe his software development work.

Software Development

The MIT BG/L has been instrumental in developing an approach to QCD software that successfully scaled to ANL's BG/P, as well as SciDAC USQCD clusters at FNAL and JLab. Subsections below start from low level and build to application level software.

Compiler support for BG/L and BG/P hardware When the Blue Gene was first shipped, there were only two ways to access the machine's full potential: writing code in assembly or using IBM's XLC compiler extensions. The first approach is very time consuming and produces code that is hard to maintain; the second approach required careful programming around bugs in the compiler. We felt that complementing XLC with GCC would be advantageous. GCC has the advantage of being available in source form, also a large body of notes regarding its development is available on the Web. Our first task was designing and implementing a set of extensions mapping into BG/L hardware. The final design includes support for vector operations (very much like x86 SSE builtins) as well as building blocks for complex arithmetic. We did not implement complex arithmetic like XLC does, because, unfortunately, GCC takes complex data types apart too early in the compilation process, so making it use BG/L complex instructions would require too ambitious a redesign.

The completed set of patches to GCC is available on the net.

XLC and GCC serve as targets for the next layer: target independent QCD assembler, QA₀.

Middle layer — QA₀ Having a compiler to do instruction scheduling and feeding the floating point pipelines allowed us to address the next level problems. Blue Gene has a relatively narrow interface between the CPU and memory. The design tries to alleviate the problem by having a deep memory hierarchy. However, data caches are not a panacea; to utilize them efficiently, we exploit the spatial and temporal data locality. For LQCD, opportunities for data reuse are great, but require a lot of careful coding. To help with exploring possible QCD data layout and data flow, we need a tool that would provide natural lattice operations (spin projection, multiplying fermions by gauge fields, etc.) as building blocks, so that we can see how structuring the code in different ways would affect performance.

QA₀ is such a tool. It make it possible to write QCD leaf routings in a machine-independent way and then translates them into a form suitable for a particular target platform. The advantage is that target-specific tinkering is localized into internals of QA₀: once a new approach is devised and checked, all our code benefits from it.

We use QA₀ to unify supported backends and present a single interface to the next software layer.

Optimized level III routines USQCD software is organized in a layered fashion. The guiding philosophy of the design was to provide a full set of primitive data parallel QCD operations, and optimize the most time consuming routines (these routines are called Level III). We use QA₀ to write the Dirac operator inverters. The domain wall inverter was implemented first. It became the standard solver outside of HMC on ANL Intrepid. For a joint project with the Budapest Marseille Wuppertal (BMW) Collaboration, a Clover solver was written. The project pushed the pion mass to the physical point, which led to rethinking of the traditional wisdom on how the Dirac equation should be solved. Once confronted with slow CG convergence on light quark masses, we implemented and tuned the EigCG algorithm, which uses low eigenmodes of the Dirac operator to accelerate convergence. This led to a ten-fold speedup of the inverter and gave us an opportunity to address several questions that were considered too computationally demanding even for BG/P.

Parallel scripting with QLUA On the application level, we found that scripting is invaluable if done properly. Starting with the LUA programming language, we extended it with QCD data parallel data types and operations and Level III routines. Originally envisioned as a test bed for Level III, it quickly became our main production tool. Its salient features include: (i) full-fledged programming language (with variables, control flow structures and routines), (ii) automatic memory management (the user does not need to worry about remembering to free memory), and (iii) seamless integration of data parallel operations into the LUA core. This combination of features led to an unprecedented increase in productivity: new projects go from the drawing board to working code in a matter of hours, instead of weeks. The resulting environment, QLUA, is our LQCD programming tool of choice now. It used for all tasks, starting with quick prototyping, algorithm development, and ending with production scripting. The system runs on any Unix machine, so scripts developed on a laptop are used for production on Blue Gene after changing the lattice size and setting configuration file locations.

Building on the development of QLUA, the following extensions have been added:

1. EigCG solvers for Clover and MDWF are now intergrated with QLUA. The Clover EigCG solver is used in USQCD production; it allowed us to speed up the Dirac equation solver more than fourfold in BMW calculations.
2. Improved I/O performance. While scaling up on ANL's BG/P, several bottlenecks were identified in the I/O. We implemented modifications to QIO to address the GPFS metadata scalability issues.
3. Support for multiple colors. Full support for arbitrary number of colors is integrated with QLUA.
4. Support for multiple lattices. In collaboration with James Osborn, we have implemented support for multiple lattices in QDP and QLUA. Together with multicolor support, this extension enables using QLUA for multigrid algorithm development as well as increases its utility for lattice investigations of physics beyond the Standard Model of particle physics.

Software status All software we developed is being actively used by USQCD community and is freely available for download.

SciDAC USQCD tutorial 2007

Andrew Pochinsky and James Osborn of ANL hosted an LQCD tutorial at SciDAC 2007. The workshop introduced USQCD data parallel libraries and used MIT BG/L in an intensive one-day tutorial. It was attended by 27 participants.

Collaboration with IBM

We actively interact with IBM on programming of BG/L and BG/P. Several visits to Watson Research Center were invaluable in forging better understanding of hardware capabilities and limitations. At a meeting presenting information about the BG/Q at ANL earlier this year, IBM approached us with a suggestion of developing a GCC back end for the BG/Q.

Physics

As expected in the proposal, the Blue Gene/L enabled scientific discovery addressing a broad range of fundamental questions in understanding the structure of the nucleon and other hadrons and the observable properties of the quark-gluon plasma. Two particularly important features were the ability to try out innovative new ideas without having to wait to write proposals on a yearly proposal cycle and to simultaneously maintain full machine production by increasing statistics for large ongoing projects. Eleven major papers in refereed journals facilitated by the Blue Gene/L are listed in the references.

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